

Electronic Supplementary Information (ESI†)

Unravelling the Potential of Low-Valent Tunable Vanadium

Complexes in Nitrogen Reduction Reaction (NRR)

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Table S1: Calculated (M06-L-D3(heptane)/6-311+G*) important geometrical parameters, natural charges and pyramidalization angle (in degree) at the metal (θ_V) and apical (θ_X , X = B, C and Si) center for the Schrock complex ($\{[\text{HIPTN}_3\text{N}]\text{-V}\}$) and model vanadium complexes considered in this study. Also, given are the energies (in eV) of the donor (E_{HOMO}), acceptor (E_{LUMO}) orbitals (centered at the transition metal center) of the parent vanadium complexes $[\mathbf{1a}'_{\text{PC}}]\text{-}[\mathbf{1f}'_{\text{SB}}]$, $[\mathbf{1a}''_{\text{PC}}]\text{-}[\mathbf{1f}''_{\text{SB}}]$ and $\{[\text{HIPTN}_3\text{N}]\text{-V}\}$. Bond lengths are given in Å and WBI values are given within parenthesis.

Molecules	V-E	V-X	q_V	q_X	θ_V/θ_X	E_{HOMO}	E_{LUMO}
$\{[\text{HIPTN}_3\text{N}]\text{-V}\}$	1.955 (0.662)	2.113 (0.350)	1.179	-0.567	3.7/20.7	-4.09	-1.90
$[\mathbf{1a}'_{\text{PC}}]$	2.484 (0.501)	2.259 (0.556)	-0.094	-0.384	3.9/35.2	-2.41	-1.12
$[\mathbf{1b}'_{\text{PSi}}]$	2.494 (0.509)	2.489 (0.792)	-0.375	1.142	8.1/34.6	-2.47	-1.39
$[\mathbf{1c}'_{\text{PB}}]$	2.464 (0.445)	2.664 (0.233)	-0.139	0.726	6.7/10.7	-2.56	-1.37
$[\mathbf{1d}'_{\text{SC}}]$	2.491 (0.472)	2.201 (0.571)	0.042	-0.403	1.9/31.0	-2.02	-0.91
$[\mathbf{1e}'_{\text{SSi}}]$	2.492 (0.493)	2.465 (0.849)	-0.260	1.129	6.2/30.5	-2.32	-1.04
$[\mathbf{1f}'_{\text{SB}}]$	2.484 (0.437)	2.496 (0.260)	0.024	0.640	2.5/9.6	-2.16	-1.10
$[\mathbf{1a}''_{\text{PC}}]$	2.473 (0.484)	2.259 (0.435)	0.044	-0.404	8.0/24.1	-2.69	-1.38
$[\mathbf{1b}''_{\text{PSi}}]$	2.477 (0.492)	2.432 (0.742)	-0.383	1.166	11.0/34.0	-2.78	-1.41
$[\mathbf{1c}''_{\text{PB}}]$	2.486 (0.447)	2.490 (0.225)	-0.027	0.614	6.6/13.7	-2.84	-1.49
$[\mathbf{1d}''_{\text{SC}}]$	2.456 (0.497)	2.185 (0.514)	0.168	-0.432	1.8/26.7	-2.58	-1.39
$[\mathbf{1e}''_{\text{SSi}}]$	2.510 (0.452)	2.392 (0.843)	-0.120	1.102	5.9/32.6	-2.51	-1.38
$[\mathbf{1f}''_{\text{SB}}]$	2.463 (0.449)	2.409 (0.252)	0.156	0.541	2.3/13.4	-2.68	-1.29

Table S2: Calculated total energies (in hartree) of the model vanadium complexes ($[1a'_{PC}]$ - $[1f'_{SB}]$ and $[1a''_{PC}]$ - $[1f''_{SB}]$) and Schrock's vanadium complex ($\{[HIPTN_3N]-V\}$) in different spin states at M06-L-D3(heptane)/6-311+G* level of theory. The relative energy values are given in kcal mol⁻¹.

Molecules	Singlet	Triplet	Quintet
$[1a'_{PC}]$	-2952.464596	-2952.496129	-2952.517639
	33.3	13.5	0.0
$[1b'_{PSi}]$	-3203.913569	-3203.928098	-3203.94156
	17.6	8.4	0.0
$[1d'_{SC}]$	-2767.618285	-2767.650911	-2767.668511
	31.5	11.0	0.0
$[1e'_{SSi}]$	-3019.058286	-3019.075126	-3019.083593
	15.9	5.3	0.0
$[1a''_{PC}]$	-3409.749209	-3409.788918	-3409.796611
	29.7	4.8	0.0
$[1b''_{PSi}]$	-3661.170581	-3661.168336	-3661.210176
	24.8	26.3	0.0
$[1d''_{SC}]$	-3224.890452	-3224.933073	-3224.941794
	32.2	5.4	0.0
$[1e''_{SSi}]$	-3476.322323	-3476.330035	-3476.343678
	13.4	8.5	0.0
$\{[HIPTN_3N]-V\}$	-2093.430155	-2093.484933	-
	34.4	0.0	-
	Doublet	Quartet	Sextet
$[1c'_{PB}]$	-2939.250047	-2939.269191	-2939.287303
	23.4	11.4	0.0
$[1f'_{SB}]$	-2754.40212	-2754.432067	-2754.429904
	18.8	0.0	1.3
$[1c''_{PB}]$	-3396.539453	-3396.561486	-3396.550338
	13.8	0.0	7.0
$[1f''_{SB}]$	-3211.691152	-3211.719426	-3211.700927
	17.74	0.0	11.61

Table S3: Difference between the ideal spin and calculated spin (spin contamination) of the parent complexes in their different spin states at M06-L-D3(heptane)/6-311+G* level of theory.

Molecules	S	Ideal spin S(S+1)	Calculated Value <S ² >	Difference between <S ² > and S(S+1)
[1a' _{PC}]	1	2	2.006	0.006
	2	6	6.001	0.001
[1b' _{PSi}]	1	2	2.010	0.10
	2	6	6.001	0.001
[1c' _{PB}]	1/2	0.75	1.279	0.529
	3/2	3.75	3.757	0.003
	5/2	8.75	8.750	0.0
[1d' _{SC}]	1	2	2.028	0.028
	2	6	6.000	0.0
[1e' _{SSi}]	1	2	2.003	0.003
	2	6	6.000	0.0
[1f' _{SB}]	1/2	0.75	1.612	0.862
	3/2	3.75	3.755	0.005
	5/2	8.75	8.750	0.0
[1a'' _{PC}]	1	2	2.010	0.010
	2	6	6.001	0.001
[1b'' _{PSi}]	1	2	2.018	0.018
	2	6	6.001	0.001
[1c'' _{PB}]	1/2	0.75	0.824	0.074
	3/2	3.75	3.753	0.003
	5/2	8.75	8.750	0.0
[1d'' _{SC}]	1	2	2.012	0.012
	2	6	6.000	0.0
[1e'' _{SSi}]	1	2	2.002	0.002
	2	6	6.000	0.0
[1f'' _{SB}]	1/2	0.75	0.782	0.032
	3/2	3.75	3.751	0.001
	5/2	8.75	8.750	0.0

Table S4: Calculated total energies (in hartree) of the dinitrogen-vanadium complexes ($[2a'_{PC}]$ - $[2f'_{SB}]$, $[2a''_{PC}]$ - $[2f''_{SB}]$ and $\{[HIPTN_3N]-V-N_2\}$ in different spin states at M06-L-D3(heptane)/6-311+G* level of theory. The relative energy values are given in kcal mol⁻¹.

Molecules	Singlet	Triplet	Quintet
$[2a'_{PC}]$	-3062.061055	-3062.091439	-3062.105256
	27.7	8.7	0.0
$[2b'_{PSi}]$	-3313.505749	-3313.505749	-3313.533523
	17.4	7.2	0.0
$[2d'_{SC}]$	-2877.217256	-2877.247403	-2877.257312
	18.9	6.2	0.0
$[2e'_{SSi}]$	-3128.659431	-3128.668457	-3128.672737
	8.3	2.7	0.0
$[2a''_{PC}]$	-3519.347311	-3519.364609	-3519.383039
	22.4	11.6	0.0
$[2b''_{PSi}]$	-3770.757952	-3770.766436	-3770.793091
	22.1	16.7	0.0
$[2d''_{SC}]$	-3334.481208	-3334.512618	-3334.525177
	27.6	7.9	0.0
$[2e''_{SSi}]$	-3585.908719	-3585.921087	-3585.931978
	14.6	6.8	0.0
$\{[HIPTN_3N]-V-N_2\}$	-2202.998308	-2203.040594	-
	26.5	0.0	-
	Doublet	Quartet	Sextet
$[2c'_{PB}]$	-3048.847491	-3048.857882	-3048.877617
	18.9	12.4	0.0
$[2f'_{SB}]$	-2863.994574	-2864.006510	-2864.018742
	15.2	7.7	0.0
$[2c''_{PB}]$	-3506.108057	-3506.127517	-3506.135445
	17.2	5.0	0.0
$[2f''_{SB}]$	-3321.274745	-3321.271703	-3321.285024
	6.4	8.3	0.0

Table S5: Calculated (M06-L-D3(heptane)/6-311+G*) important geometrical parameters and natural charge at the metal (V) and α ($q_{N\alpha}$) and β ($q_{N\beta}$) nitrogen atoms of the dinitrogen complexes of Schrock complex and model vanadium complexes considered in this study. Bond lengths are given in Å and WBI values are given within parenthesis.

Molecule	V-E	V-X	V-N	N≡N	$\nu(N\equiv N)$	q_V	$q_{N\alpha}$	$q_{N\beta}$	θ_M/θ_X
{[HIPTN ₃ N]-V-N ₂ }	1.960 (0.774)	2.182 (0.360)	2.081 (0.598)	1.114 (2.773)	2229.66	0.887	-0.008	0.086	5.9/22.8
[2a' _{PC}]	2.492 (0.602)	2.332 (0.543)	2.019 (0.697)	1.135 (2.529)	2029.86	-0.394	-0.099	-0.061	8.1/36.9
[2b' _{PSi}]	2.509 (0.628)	2.563 (0.772)	2.006 (0.712)	1.139 (2.499)	2003.09	-0.811	-0.118	-0.070	13.8/36.8
[2c' _{PB}]	2.488 (0.510)	2.967 (0.164)	2.001 (0.623)	1.138 (2.491)	2009.86	-0.285	-0.180	-0.059	20.0/9.3
[2d' _{SC}]	2.519 (0.542)	2.262 (0.544)	2.016 (0.712)	1.136 (2.511)	2025.25	-0.159	-0.127	-0.066	4.9/33.6
[2e' _{SSi}]	2.534 (0.546)	2.543 (0.833)	2.010 (0.733)	1.139 (2.495)	2004.15	-0.523	-0.138	-0.073	11.4/32.2
[2f' _{SB}]	2.501 (0.508)	2.658 (0.226)	2.008 (0.670)	1.136 (2.512)	2027.92	-0.159	-0.153	-0.057	9.1/11.0
[2a'' _{PC}]	2.491 (0.581)	2.331 (0.420)	2.013 (0.683)	1.134 (2.537)	2037.3	-0.261	-0.104	-0.044	13.0/26.0
[2b'' _{PSi}]	2.537 (0.576)	2.503 (0.726)	2.023 (0.641)	1.133 (2.549)	2043.4	-0.679	-0.115	-0.044	15.9/38.0
[2c'' _{PB}]	2.521 (0.507)	2.612 (0.194)	2.009 (0.619)	1.134 (2.535)	2041.6	-0.220	-0.142	-0.037	13.7/15.5
[2d'' _{SC}]	2.476 (0.577)	2.251 (0.488)	2.023 (0.712)	1.132 (2.559)	2058.4	-0.119	-0.100	-0.039	4.6/29.3
[2e'' _{SSi}]	2.523 (0.554)	2.473 (0.840)	2.021 (0.714)	1.135 (2.534)	2033.7	-0.507	-0.124	-0.051	10.1/35.3
[2f'' _{SB}]	2.480 (0.528)	2.532 (0.237)	2.015 (0.670)	1.132 (2.558)	2060.7	-0.111	-0.125	-0.029	7.0/15.8

Table S6: Difference between the ideal spin and calculated spin (spin contamination) of the dinitrogen vanadium complexes in their different spin states at M06-L-D3(heptane)/6-311+G* level of theory.

Molecules	S	Ideal spin S(S+1)	Calculated Value <S ² >	Difference between <S ² > and S(S+1)
[2a' _{PC}]	1	2	2.002	0.002
	2	6	6.001	0.001
[2b' _{PSi}]	1	2	2.031	0.031
	2	6	6.001	0.001
[2c' _{PB}]	1/2	0.75	0.973	0.223
	3/2	3.75	3.753	0.003
	5/2	8.75	8.751	0.001
[2d' _{SC}]	1	2	2.008	0.008
	2	6	6.000	0.0
[2e' _{SSi}]	1	2	2.002	0.002
	2	6	6.001	0.001
[2f' _{SB}]	1/2	0.75	1.009	0.259
	3/2	3.75	3.756	0.006
	5/2	8.75	8.750	0.0
[2a'' _{PC}]	1	2	2.002	0.002
	2	6	6.001	0.001
[2b'' _{PSi}]	1	2	2.008	0.008
	2	6	6.001	0.001
[2c'' _{PB}]	1/2	0.75	0.974	0.224
	3/2	3.75	3.753	0.003
	5/2	8.75	8.751	0.001
[2d'' _{SC}]	1	2	2.005	0.005
	2	6	6.001	0.001
[2e'' _{SSi}]	1	2	2.002	0.002
	2	6	6.001	0.001
[2f'' _{SB}]	1/2	0.75	0.895	0.145
	3/2	3.75	3.751	0.001
	5/2	8.75	8.750	0.0

Table S7: Calculated relative energy difference (in kcal mol⁻¹) between the possible spin states of the complexes [1d'_{SC}]-[1f'_{SB}] and [2d'_{SC}]-[2f'_{SB}] at B3PW91-D3(heptane), PBE0-D3(heptane) and M06-L-D3(heptane) level of theory. The total energies (TE) are in hartrees and relative energy difference values are given in kcal mol⁻¹.

	B3PW91			PBE0			M06-L		
	Spin States	T.E.	Relative Energy	Spin States	T.E.	Relative Energy	Spin States	T.E.	Relative Energy
[1d' _{SC}]	Singlet	-2767.480814	30.8	Singlet	-2766.395144	31.5	Singlet	-2767.618285	31.52
	Triplet	-2767.507422	14.1	Triplet	-2766.425991	11.0	Triplet	-2767.650911	11.04
	Quintet	-2767.529825	0.0	Quintet	-2766.448601	0.0	Quintet	-2767.668511	0.0
[1e' _{SSI}]	Singlet	-3018.900104	17.3	Singlet	-3017.756243	19.4	Singlet	-3019.058286	15.9
	Triplet	-3018.91722	6.6	Triplet	-3017.776773	6.5	Triplet	-3019.075126	5.3
	Quintet	-3018.927702	0.0	Quintet	-3017.787211	0.0	Quintet	-3019.083593	0.0
[1f' _{SB}]	Doublet	-2754.265879	18.9	Doublet	-2753.187921	19.3	Doublet	-2754.40212	18.8
	Quartet	-2754.296035	0.0	Quartet	-2753.21870	0.0	Quartet	-2754.432067	0.0
	Sextet	-2754.291194	3.0	Sextet	-2753.213139	3.5	Sextet	-2754.429904	1.3
[2d' _{SC}]	Singlet	-2877.039376	22.1	Singlet	-2875.874093	25.1	Singlet	-2877.217256	18.9
	Triplet	-2877.068603	3.8	Triplet	-2875.907662	4.1	Triplet	-2877.247403	6.2
	Quintet	-2877.074657	0.0	Quintet	-2875.914153	0.0	Quintet	-2877.257312	0.0
[2e' _{SSI}]	Singlet	-3128.46092	7.2	Singlet	-3127.238553	8.9	Singlet	-3128.659431	8.3
	Triplet	-3128.472305	0.04	Triplet	-3127.252833	-0.1	Triplet	-3128.668457	2.7
	Quintet	-3128.472376	0.0	Quintet	-3127.252722	0.0	Quintet	-3128.672737	0.0
[2f' _{SB}]	Doublet	-2863.814039	13.0	Doublet	-2862.659204	11.8	Doublet	-2863.994574	15.2
	Quartet	-2863.82657	5.1	Quartet	-2862.669785	5.1	Quartet	-2864.00651	7.7
	Sextet	-2863.834679	0.0	Sextet	-2862.677976	0.0	Sextet	-2864.018742	0.0

Table S8: Calculated reaction free energies (ΔG , in kcal mol⁻¹) associated with the formation of the diazenido complex via the PCET pathway for our proposed complexes

Molecule	ΔG	Molecule	ΔG
[2a' _{PC}]	-1.9	[2a'' _{PC}]	0.8
[2b' _{PSi}]	-5.9	[2b'' _{PSi}]	1.4
[2c' _{PB}]	0.8	[2c'' _{PB}]	-0.8
[2d' _{SC}]	1.0	[2d'' _{SC}]	3.5
[2e' _{SSi}]	0.3	[2e'' _{SSi}]	1.3
[2f' _{SB}]	1.9	[2f'' _{SB}]	3.5

Table S9: Calculated total energies (in hartree) of the complex [3] in different spin states at M06-L-D3(heptane)/6-311+G* level of theory. The relative energy values are given in kcal mol⁻¹.

Molecule	Singlet	Triplet	Molecule	Singlet	Triplet
[3a' _{PC}]	-3062.485948	-3062.515879	[3a'' _{PC}]	-3519.762496	-3519.781959
	18.8	0.0		12.2	0.0
[3b' _{PSi}]	-3313.916134	-3313.941683	[3b'' _{PSi}]	-3771.160945	-3771.188296
	16.0	0.0		17.2	0.0
[3d' _{SC}]	-2877.633713	-2877.659059	[3d'' _{SC}]	-3334.888116	-3334.916108
	15.9	0.0		17.5	0.0
[3e' _{SSi}]	-3129.065253	-3129.076381	[3e'' _{SSi}]	-3586.306388	-3586.318558
	7.0	0.0		7.6	0.0
	Doublet	Quartet		Doublet	Quartet
[3c' _{PB}]	-3049.274818	-3049.279552	[3f' _{SB}]	-2864.408992	-2864.418883
	2.0	0.0		6.2	0.0
[3c'' _{PB}]	-3506.527884	-3506.526313	[3f'' _{SB}]	-3321.658404	-3321.670568
	0.0	1.0		7.6	0.0

Table S10: Calculated reaction free energies for the protonation of the equatorial sulphur and nitrogen atom, metal center and distal nitrogen atom of the dinitrogen complexes $[2a'_{PC}]-[2f'_{SB}]$ and $[2a''_{PC}]-[2f''_{SB}]$ and $\{[HIPTN_3N]-V\}$.

Molecules	S/N	V	N_β
$\{[HIPTN_3N]-V-N_2\}$	-7.0	29.7	38.4
$[2a'_{PC}]$	-	-18.8	-6.0
$[2b'_{PSi}]$	-	-17.8	-3.9
$[2c'_{PB}]$	-	-21.3	-0.7
$[2d'_{SC}]$	19.3	-17.4	0.4
$[2e'_{SSi}]$	16.9	-19.6	-1.6
$[2f'_{SB}]$	19.7	-25.3	0.2
$[2a''_{PC}]$	-	-12.2	0.7
$[2b''_{PSi}]$	-	-13.5	3.2
$[2c''_{PB}]$	-	-12.2	5.5
$[2d''_{SC}]$	19.7	-14.5	6.7
$[2e''_{SSi}]$	16.9	-11.3	8.3
$[2f''_{SB}]$	22.2	-15.2	8.7

Table S11: Calculated activation energy barrier (in kcal mol⁻¹) for the transition states **TS1** and **TS2** and reaction free energy (in kcal mol⁻¹) for the formation of the intermediate involved in the formation of the **[3]** from the metal protonated vanadium complexes **[3-V-H]⁺**. The reaction free energies were evaluated with respect to the metal protonated species.

Molecules	$\Delta G^{\ddagger}_{\text{TS1}}$	ΔG_{Int}	$\Delta G^{\ddagger}_{\text{TS2}}$
a' _{PC}	40.7	19.8	36.5
b' _{PSi}	40.9	17.5	33.6
c' _{PB}	40.0	16.0	25.9
d' _{SC}	40.0	22.0	25.8
e' _{SSi}	43.1	22.9	30.2
f' _{SB}	47.5	22.8	35.4
a'' _{PC}	41.7	17.7	34.8
b'' _{PSi}	41.3	14.1	28.7
c'' _{PB}	40.0	21.6	29.2
d'' _{SC}	38.5	18.1	31.8
e'' _{SSi}	41.9	17.6	36.7
f'' _{SB}	41.9	21.1	30.4

Table S12: Calculated (M06-L-D3(heptane)/6-311+G*) important geometrical parameters and natural charge at the metal (V) and α ($q_{N\alpha}$) and β ($q_{N\beta}$) nitrogen atoms of for the diazenido complex (**[4]**) of the Schrock complex and model vanadium complexes considered in this study. Bond lengths are given in Å and WBI values are given within parenthesis.

Molecule	V-E	V-X	V-N	N≡N	$\nu(\text{N}\equiv\text{N})$	q_V	$q_{N\alpha}$	$q_{N\beta}$
{[HIPTN ₃ N]-V}	1.946 (0.867)	2.220 (0.349)	1.783 (1.414)	1.218 (1.842)	1648.8	0.818	-0.132	-0.293
[4a' _{PC}]	2.486 (0.632)	2.388 (0.485)	1.838 (1.471)	1.239 (1.620)	1543.1	-0.184	-0.257	-0.543
[4b' _{PSi}]	2.472 (0.658)	2.604 (0.717)	1.818 (1.270)	1.244 (1.707)	1527.7	-0.774	-0.268	-0.405
[4c' _{PB}]	2.490 (0.543)	3.197 (0.124)	1.811 (1.198)	1.249 (1.672)	1519.7	-0.189	-0.369	-0.404
[4d' _{SC}]	2.544 (0.556)	2.258 (0.546)	1.847 (1.174)	1.240 (1.798)	1549.3	-0.022	-0.334	-0.379
[4e' _{SSi}]	2.509 (0.606)	2.571 (0.787)	1.841 (1.261)	1.238 (1.791)	1554.0	-0.485	-0.277	-0.382
[4f' _{SB}]	2.511 (0.534)	2.712 (0.214)	1.843 (1.166)	1.237 (1.800)	1557.7	-0.027	-0.341	-0.375
[4a'' _{PC}]	2.489 (0.606)	2.375 (0.407)	1.823 (1.254)	1.240 (1.745)	1536.4	-0.177	-0.270	-0.381
[4b'' _{PSi}]	2.531 (0.615)	2.529 (0.712)	1.828 (1.222)	1.237 (1.757)	1544.5	-0.649	-0.267	-0.373
[4c'' _{PB}]	2.524 (0.530)	2.657 (0.185)	1.828 (1.125)	1.238 (1.776)	1544.9	-0.115	-0.328	-0.373
[4d'' _{SC}]	2.478 (0.595)	2.294 (0.484)	1.833 (1.303)	1.235 (1.774)	1556.8	-0.024	-0.257	-0.374
[4e'' _{SSi}]	2.528 (0.575)	2.488 (0.831)	1.849 (1.235)	1.240 (1.782)	1542.9	-0.412	-0.296	-0.393
[4f'' _{SB}]	2.477 (0.555)	2.617 (0.226)	1.825 (1.257)	1.236 (1.769)	1553.8	-0.018	-0.290	-0.367

Table S13: Calculated total energies (in hartree) of the diazenido-vanadium complexes in different spin states at M06-L-D3/6-311+G*(heptane) level of theory. The relative energy values are given in kcal mol⁻¹.

	Doublet	Quartet	
[4a'_{PC}]	-3062.654015	-3062.653876	
	0.0	0.09	
[4b'_{PSi}]	-3314.086338	-3314.088377	
	1.3	0.0	
[4d'_{SC}]	-2877.803983	-2877.804475	
	0.31	0.00	
[4e'_{SSi}]	-3129.227147	-3129.217811	
	0.0	5.8	
[4a''_{PC}]	-3519.913382	-3519.92604	
	7.9	0.0	
[4b''_{PSi}]	-3771.333483	-3771.336353	
	1.8	0.0	
[4d''_{SC}]	-3335.061649	-3335.065002	
	2.1	0.0	
[4e''_{SSi}]	-3586.473019	-3586.475151	
	1.3	0.0	
	Singlet	Triplet	Quintet
[4c'_{PB}]	-3049.397483	-3049.418366	-3049.421541
	15.10	1.99	0.00
[4f'_{SB}]	-2864.543189	-2864.562611	-2864.561466
	12.2	0.0	0.7
[4c''_{PB}]	-3506.648425	-3506.671905	-3506.679846
	19.7	5.0	0.0
[4f''_{SB}]	-3321.806314	-3321.821651	-3321.825433
	12.0	2.4	0.0

Table S14: Reaction free energies (ΔG , in kcal mol⁻¹) obtained for the formation of the vanadium nitride complexes from the diazenido complexes [4].

Molecules	ΔG	Molecules	ΔG
[4a' _{PC}]	-77.3	[4a'' _{PC}]	-75.4
[4b' _{PSi}]	-73.2	[4b'' _{PSi}]	-70.8
[4c' _{PB}]	-80.9	[4c'' _{PB}]	-75.3
[4d' _{SC}]	-82.5	[4d'' _{SC}]	-76.1
[4e' _{SSi}]	-81.3	[4e'' _{SSi}]	-74.1
[4f' _{SB}]	-84.6	[4f'' _{SB}]	-81.1

Table S15: Calculated (M06-L-D3(heptane)/6-311+G*) important geometrical parameters for the vanadium-nitride complex ([8]_{dis}) of [1a'_{PC}]-[1f'_{SB}] and [1a''_{PC}]-[1f''_{SB}]. Bond lengths are given in Å and WBI values are given within parenthesis.

Molecules	V≡N	V-X	ΔE_{H-L}
a' _{PC}	1.592 (2.774)	2.307 (0.568)	1.82
b' _{PSi}	1.593 (2.768)	2.551 (0.727)	1.76
c' _{PB}	1.587 (2.722)	3.022 (0.140)	1.13
d' _{SC}	1.583 (2.837)	2.179 (0.602)	1.79
e' _{SSi}	1.583 (2.870)	2.488 (0.816)	1.74
f' _{SB}	1.580 (2.838)	2.568 (0.236)	1.57
a'' _{PC}	1.593 (2.670)	2.610 (0.183)	1.56
b'' _{PSi}	1.591 (2.759)	2.493 (0.717)	1.52
c'' _{PB}	1.580 (2.713)	2.644 (0.199)	1.15
d'' _{SC}	1.584 (2.850)	2.240 (0.475)	1.71
e'' _{SSi}	1.579 (2.876)	2.467 (0.789)	1.57
f'' _{SB}	1.575 (2.871)	2.570 (0.232)	1.40

Table S16: Reaction free energies (ΔG , in kcal mol⁻¹) obtained for the release of hydrazine from the vanadium-hydrazine complex of the proposed vanadium complexes and Schrock's vanadium complex ($\{[\text{HIPTN}_3\text{N}]\text{-V}\}$).

Molecules	ΔG	Molecules	ΔG
[1a' _{PC}]	14.8	[1a'' _{PC}]	15.7
[1b' _{PSi}]	17.2	[1b'' _{PSi}]	11.2
[1c' _{PB}]	14.8	[1c'' _{PB}]	14.8
[1d' _{SC}]	15.9	[1d'' _{SC}]	16.0
[1e' _{SSi}]	15.4	[1e'' _{SSi}]	17.7
[1f' _{SB}]	15.4	[1f'' _{SB}]	16.8
$\{[\text{HIPTN}_3\text{N}]\text{-V}\}$	9.7		

Table S17: Calculated (M06-L-D3(heptane)/6-311+G*) important geometrical parameters and pyramidalization angle (in degree) around the vanadium center of [5c''_{PB}]-[14c''_{PB}]. Bond lengths are given in Å and WBI values are given within parenthesis.

Molecules	V-N	N-N	V-B	θ_V
[5c'' _{PB}] _{alt}	2.062 (0.500)	1.278 (1.665)	2.621 (0.201)	17.3
[6c'' _{PB}] _{alt}	2.032 (0.557)	1.305 (1.509)	2.646 (0.182)	16.2
[7c'' _{PB}] _{alt}	1.920 (0.888)	1.404 (1.078)	2.672 (0.186)	19.8
[8c'' _{PB}] _{alt}	1.932 (0.865)	1.435 (1.040)	2.671 (0.176)	18.2
[9c'' _{PB}] _{alt}	2.273 (0.255)	1.443 (1.031)	2.570 (0.202)	13.9
[10c'' _{PB}] _{alt}	2.278 (0.191)	1.445 (1.029)	2.563 (0.262)	11.1
[11c'' _{PB}] _{alt}	2.288 (0.242)	1.469 (0.772)	2.549 (0.207)	10.9
[5c'' _{PB}] _{dis}	1.712 (1.646)	1.327 (1.204)	3.133 (0.091)	36.7
[6c'' _{PB}] _{dis}	1.708 (1.705)	1.359 (1.133)	2.715 (0.172)	20.2
[7c'' _{PB}] _{dis}	1.744 (1.504)	1.407 (1.018)	2.830 (0.162)	26.5
[8c'' _{PB}] _{dis}	1.580 (2.713)	-	2.644 (0.199)	16.1
[9c'' _{PB}] _{dis}	1.667 (2.003)	-	2.592 (0.185)	12.0
[10c'' _{PB}] _{dis}	1.693 (1.882)	-	2.760 (0.164)	22.7
[11c'' _{PB}] _{dis}	1.904 (0.972)	-	2.518 (0.210)	8.3
[12c'' _{PB}]	1.944 (0.822)	-	2.649 (0.182)	17.2
[13c'' _{PB}]	2.279 (0.270)	-	2.528 (0.191)	12.4
[14c'' _{PB}]	2.280 (0.273)	-	2.562 (0.191)	10.9

Table S18: Calculated (M06-L-D3(heptane)/6-311+G*) reaction free energies (in kcal mol⁻¹) for the protonation at the equatorial sulphur atom of the vanadium complex [**1f''**_{SB}] at different stages of dinitrogen reduction process. The numbering are given as per Fig. S20.

Reaction	Equatorial group
[4f'' _{SB}] + H ⁺	22.1
[6f'' _{SB}] _{alt} + H ⁺	23.3
[6f'' _{SB}] _{dis} + H ⁺	16.4
[8f'' _{SB}] _{alt} + H ⁺	22.5
[8f''] _{dis} + H ⁺	27.0
[10f'' _{SB}] _{alt} + H ⁺	11.1
[10f'' _{SB}] _{dis} + H ⁺	23.2
[12f'' _{SB}] + H ⁺	21.8

Table S19: Calculated (M06-L-D3(heptane)/6-311+G*) important geometrical parameters and pyramidalization angle (in degree) around the vanadium center of $[5f''_{SB}]-[14f''_{SB}]$. Bond lengths are in Å. Bond lengths are given in Å and WBI values are given within parenthesis.

Molecules	V-N	N-N	V-B	θ_V
$[5f''_{SB}]_{alt}$	2.031 (0.558)	1.280 (1.640)	2.659 (0.218)	14.7
$[6f''_{SB}]_{alt}$	2.027 (0.605)	1.314 (1.451)	2.546 (0.222)	8.4
$[7f''_{SB}]_{alt}$	1.922 (0.933)	1.396 (1.092)	2.594 (0.230)	11.8
$[8f''_{SB}]_{alt}$	1.937 (0.878)	1.443 (1.030)	2.565 (0.222)	10.0
$[9f''_{SB}]_{alt}$	2.267 (0.298)	1.443 (1.032)	2.443 (0.258)	5.0
$[10f''_{SB}]_{alt}$	2.255 (0.284)	1.446 (1.028)	2.466 (0.228)	4.3
$[11f''_{SB}]_{alt}$	2.294 (0.260)	1.467 (0.984)	2.453 (0.245)	4.5
$[5f''_{SB}]_{dis}$	1.713 (1.751)	1.323 (1.221)	3.252 (0.072)	40.4
$[6f''_{SB}]_{dis}$	1.705 (1.850)	1.359 (1.128)	2.667 (0.212)	14.5
$[7f''_{SB}]_{dis}$	1.743 (1.665)	1.410 (1.011)	2.823 (0.193)	20.5
$[8f''_{SB}]_{dis}$	1.575 (2.871)	-	2.570 (0.232)	12.0
$[9f''_{SB}]_{dis}$	1.670 (2.125)	-	2.590 (0.194)	10.3
$[10f''_{SB}]_{dis}$	1.692 (2.027)	-	2.710 (0.208)	15.2
$[11f''_{SB}]_{dis}$	1.876 (1.080)	-	2.461 (0.261)	5.9
$[12f''_{SB}]$	1.948 (0.898)	-	2.541 (0.226)	10.7
$[13f''_{SB}]$	2.259 (0.322)	-	2.444 (0.258)	5.1
$[14f''_{SB}]$	1.900 (0.424)	-	2.409 (0.229)	4.3

Table S20: Energies (in hartree) of the complexes $[5c''_{PB}]$ – $[14c''_{PB}]$ and $[5f''_{SB}]$ – $[14f''_{SB}]$ in their different multiplicities at (M06-L-D3(heptane)/6-311+G*) level of theory.

Molecules	Possible multiplicities	Energies	Molecules	Possible multiplicities	Energies
$[5c''_{PB}]_{alt}$	Quintet	-3507.096581	$[5f''_{SB}]_{alt}$	Quintet	-3322.249460
	Triplet	-3507.084563		Triplet	-3322.234034
	Singlet	-3507.064827		Singlet	-3322.226199
$[5c''_{PB}]_{dis}$	Quintet	-3507.096581	$[5f''_{SB}]_{dis}$	Quintet	-3322.243435
	Triplet	-3507.115363		Triplet	-3322.260350
	Singlet	-3507.092500		Singlet	-3322.238202
$[6c''_{PB}]_{alt}$	Sextet	-3507.237814	$[6f''_{SB}]_{alt}$	Sextet	-3322.393810
	Quartet	-3507.233562		Quartet	-3322.389916
	Doublet	-3507.230831		Doublet	*
$[6c''_{PB}]_{dis}$	Quartet	-3507.269012	$[6f''_{SB}]_{dis}$	Quartet	-3322.418409
	Doublet	-3507.259937		Doublet	*
$[7c''_{PB}]_{alt}$	Sextet	-3507.667447	$[7f''_{SB}]_{alt}$	Sextet	-3322.825538
	Quartet	-3507.697773		Quartet	-3322.850322
	Doublet	-3507.684093		Doublet	-3322.837823
$[7c''_{PB}]_{dis}$	Quartet	-3507.669748	$[7f''_{SB}]_{dis}$	Quartet	-3322.818914
	Doublet	-3507.656451		Doublet	*
$[8c''_{PB}]_{alt}$	Quintet	-3507.842418	$[8f''_{SB}]_{alt}$	Quintet	-3322.999688
	Triplet	-3507.833559		Triplet	-3322.996170
	Singlet	-3507.801856		Singlet	-3322.964305
$[8c''_{PB}]_{dis}$	Triplet	-3451.334767	$[8f''_{SB}]_{dis}$	Triplet	-3266.488000
	Singlet	-3451.323430		Singlet	-3266.472184
$[9c''_{PB}]_{alt}$	Quintet	-3508.283230	$[9f''_{SB}]_{alt}$	Quintet	-3323.442488
	Triplet	-3508.270490		Triplet	-3323.435223
	Singlet	-3508.225090		Singlet	-3323.390517
$[9c''_{PB}]_{dis}$	Triplet	-3451.783734	$[9f''_{SB}]_{dis}$	Triplet	-3266.933760
	Singlet	-3451.764701		Singlet	-3266.907792
$[10c''_{PB}]_{alt}$	Sextet	-3508.414634	$[10f''_{SB}]_{alt}$	Sextet	-3323.566068
	Quartet	-3508.402604		Quartet	-3323.553859
	Doublet	-3508.376446		Doublet	-3323.534133
$[10c''_{PB}]_{dis}$	Quartet	-3451.944309	$[10f''_{SB}]_{dis}$	Quartet	-3267.093000

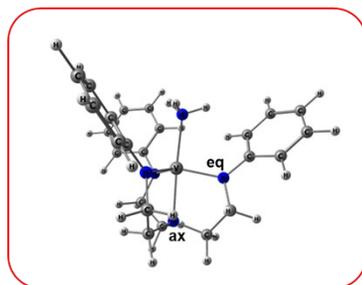
	Doublet	-3451.934595		Doublet	-3267.084615
[11c''_{PB}]_{alt}	Sextet	-3508.790101	[11f''_{SB}]_{alt}	Sextet	-3323.941554
	Quartet	-3508.775507		Quartet	*
	Doublet	*		Doublet	*
[11c''_{PB}]_{dis}	Quartet	-3452.390430	[11f''_{SB}]_{dis}	Quartet	-3267.535660
	Doublet	-3452.373403		Doublet	-3267.531863
[12c''_{PB}]	Quintet	-3452.541427	[12f''_{SB}]	Quintet	-3267.691925
	Triplet	-3452.530414		Triplet	*
	Singlet	-3452.503971		Singlet	-3267.655291
[13c''_{PB}]	Quintet	-3452.987807	[13f''_{SB}]	Quintet	-3268.143326
	Triplet	-3452.974157		Triplet	-3268.138992
	Singlet	-3452.935250		Singlet	-3268.092015
[14c''_{PB}]	Sextet	-3453.112714	[14f''_{SB}]	Sextet	-3268.265203
	Quartet	-3453.099904		Quartet	-3268.253042
	Doublet	-3453.075856		Doublet	-3268.233216
* Broken geometry					

Table S21: Difference between the ideal spin and calculated spin (spin contamination) of the parent complexes in their different spin states at (M06-L-D3(heptane)/6-311+G*) level of theory.

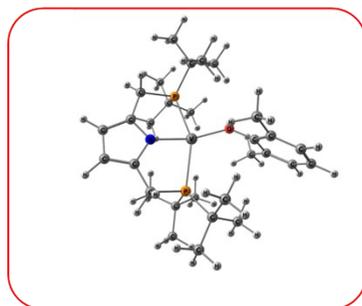
Molecules	S	Ideal spin S(S+1)	Calculated Value <S ² >	Difference between <S ² > and S(S+1)
[1c'' _{PB}]	5/2	8.75	8.750	0.0
	3/2	3.75	3.753	0.003
	1/2	0.75	0.824	0.074
[2c'' _{PB}]	5/2	8.75	8.751	0.001
	3/2	3.75	3.753	0.003
	1/2	0.75	0.974	0.224
[3c'' _{PB}]	3/2	3.75	3.7569	0.0069
	1/2	0.75	0.8448	0.0948
[4c'' _{PB}]	2	6	6.0041	0.0041
	1	2	2.0472	0.0472
[5c'' _{PB}] _{sym}	2	6	6.0011	0.0011
	1	2	2.0392	0.0392
[5c'' _{PB}] _{asym}	2	6	6.0011	0.0011
	1	2	2.0095	0.0095
[6c'' _{PB}] _{sym}	5/2	8.75	8.7510	0.010
	3/2	3.75	3.7662	0.016
	1/2	0.75	0.975	0.225
[6c'' _{PB}] _{asym}	3/2	3.75	3.7562	0.0062
	1/2	0.75	0.9397	0.1897
[7c'' _{PB}] _{sym}	5/2	8.75	8.7505	0.0005
	3/2	3.75	3.7570	0.0070
	1/2	0.75	1.2772	0.5272
[7c'' _{PB}] _{asym}	3/2	3.75	3.7529	0.0029
	1/2	0.75	0.8132	0.0632
[8c'' _{PB}] _{sym}	2	6	6.0036	0.0036
	1	2	2.0418	0.0418
[8c'' _{PB}] _{asym}	1	2	2.0025	0.0025
[9c'' _{PB}] _{sym}	2	6	6.0006	0.0006
	1	2	2.0401	0.0401
[9c'' _{PB}] _{asym}	1	2	2.0053	0.0053
[10c'' _{PB}] _{sym}	5/2	8.75	8.7507	0.0007
	3/2	3.75	3.8176	0.0676
	1/2	0.75	3.1638	2.41
[10c'' _{PB}] _{asym}	3/2	3.75	3.7543	0.0043
	1/2	0.75	1.0078	0.2578
[11c'' _{PB}] _{sym}	5/2	8.75	8.7507	0.0007
	3/2	3.75	3.8193	0.0693

	1/2	0.75	*	*
[11c'' _{PB}] _{asym}	3/2	3.75	3.7521	0.0021
	1/2	0.75	0.9091	0.1591
[12c'' _{PB}]	2	6	6.0013	0.0013
	1	2	2.0862	0.0862
[13c'' _{PB}]	2	6	6.0004	0.004
	1	2	2.0219	0.0219
[14c'' _{PB}]	5/2	8.75	8.7506	0.0006
	3/2	3.75	3.8118	0.0618
	1/2	0.75	1.9649	1.2149
[1f'' _{SB}]	5/2	8.75	8.750	0.0
	3/2	3.75	3.751	0.001
	1/2	0.75	0.782	0.032
[2f'' _{SB}]	5/2	8.75	8.750	0.0
	3/2	3.75	3.751	0.001
	1/2	0.75	0.895	0.145
[3f'' _{SB}]	3/2	3.75	3.7576	0.0076
	1/2	0.75	0.9802	0.2302
[4f'' _{SB}]	2	6	6.0041	0.0041
	1	2	2.0376	0.0376
[5f'' _{SB}] _{sym}	2	6	6.0009	0.0009
	1	2	2.0175	0.0175
[5f'' _{SB}] _{asym}	2	6	6.0008	0.008
	1	2	2.0095	0.0095
[6f'' _{SB}] _{sym}	5/2	8.75	8.7500	0.0
	3/2	3.75	3.7660	0.016
	1/2	0.75	*	*
[6f'' _{SB}] _{asym}	3/2	3.75	3.7556	0.0056
	1/2	0.75	*	*
[7f'' _{SB}] _{sym}	5/2	8.75	8.7503	0.0003
	3/2	3.75	3.7564	0.0064
	1/2	0.75	1.3219	0.5719
[7f'' _{SB}] _{asym}	3/2	3.75	3.7521	0.0021
	1/2	0.75	0.7538	0.0038
[8f'' _{SB}] _{sym}	2	6	6.0009	0.0009
	1	2	2.0089	0.0089
[8f'' _{SB}] _{asym}	1	2	2.0022	0.0022
[9f'' _{SB}] _{sym}	2	6	6.0003	0.0003
	1	2	2.0133	0.0133

$[9f''_{SB}]_{\text{asym}}$	1	2	2.0047	0.0047
$[10f''_{SB}]_{\text{sym}}$	5/2	8.75	8.7504	0.0004
	3/2	3.75	3.7977	0.0477
	1/2	0.75	0.9837	0.2337
$[10f''_{SB}]_{\text{asym}}$	3/2	3.75	3.7535	0.0035
	1/2	0.75	0.9988	0.2488
$[11f''_{SB}]_{\text{sym}}$	5/2	8.75	8.7504	0.0004
	3/2	3.75	*	*
	1/2	0.75	*	*
$[11f''_{SB}]_{\text{asym}}$	3/2	3.75	3.7509	0.0009
	1/2	0.75	0.8241	0.0741
$[12f''_{SB}]$	2	6	6.0006	0.0006
	1	2	*	*
$[13f''_{SB}]$	2	6	6.0003	0.0003
	1	2	2.0110	0.0110
$[14f''_{SB}]$	5/2	8.75	8.7503	0.0003
	3/2	3.75	3.7954	0.0454
	1/2	0.75	0.9518	0.2018
* Broken geometry				

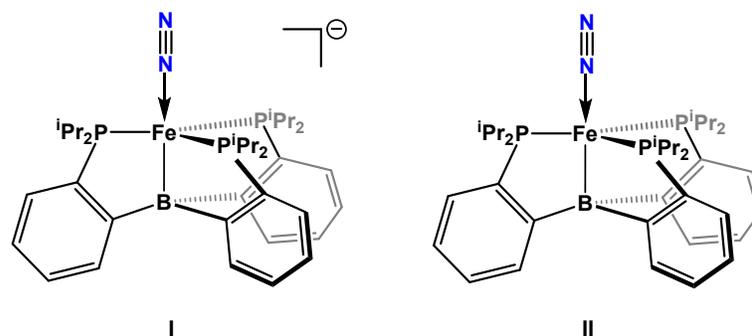


Geometrical parameters	Calculated values	Experimental values	difference
V-N _{eq}	1.955	1.972	0.017
V-N _{eq}	1.957	1.989	0.032
V-N _{eq}	1.952	1.975	0.023
V-N _{ax}	2.148	2.200	0.052
V-NH ₃	2.162	2.215	0.053



Geometrical parameters	Calculated values	Experimental value	difference
V-N	2.055	2.038	0.017
V-P	2.561	2.587	0.026
V-P	2.529	2.538	0.009
V-O	1.926	1.905	0.021

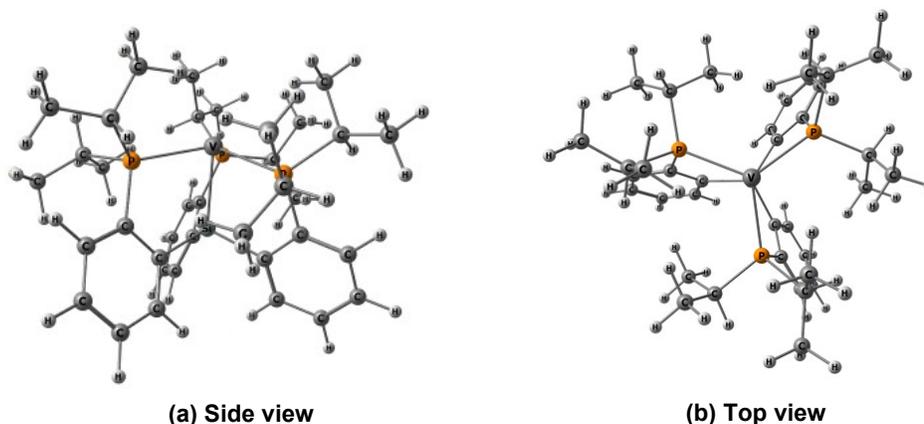
(a)



	$\nu(\text{N-N})$	$\nu(\text{N-N})$
Experimental	1918.0	2011.0
Computed	2005.5	2093.9

(b)

Fig. S1. Comparison of (a) the available X-ray data and our calculated (M06-L-D3(heptane)/6-311+G*) values of the important geometrical parameters (Bond lengths are given in Å) and (b) the available IR frequencies (in cm^{-1}) of some of the important bonds for the experimentally known complexes.



(a) Side view

(b) Top view

Fig. S2. Optimized geometry of a representative vanadium complex ($\text{E} = \text{P}^i\text{Pr}_2$ and $\text{X} = \text{Si}$) in two different orientations: (a) side view and (b) top view.

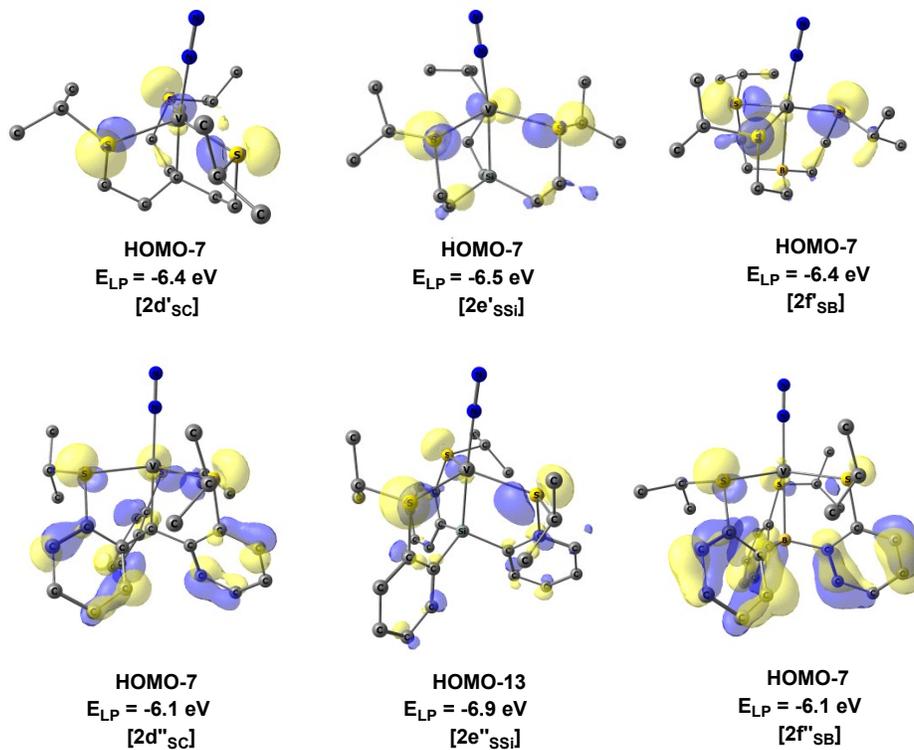


Fig. S3. Pictorial representation of the molecular orbital showing the lone pairs situated at the sulphur atoms of the dinitrogen vanadium complexes [2d'sc]-[2f'sb] and [2d''sc]-[2f''sb]. The hydrogen atoms of the methyl groups are omitted for the sake of clarity.

The reaction free energies obtained for protonation at the equatorial sulfur atom of [2d'sc]-[2f'sb] and [2d''sc]-[2f''sb] were substantially endergonic (16.9-22.2 kcal mol⁻¹, Table S10†). This may be attributed to the higher stability of the lone pair at the sulfur atoms (Fig. S3†).

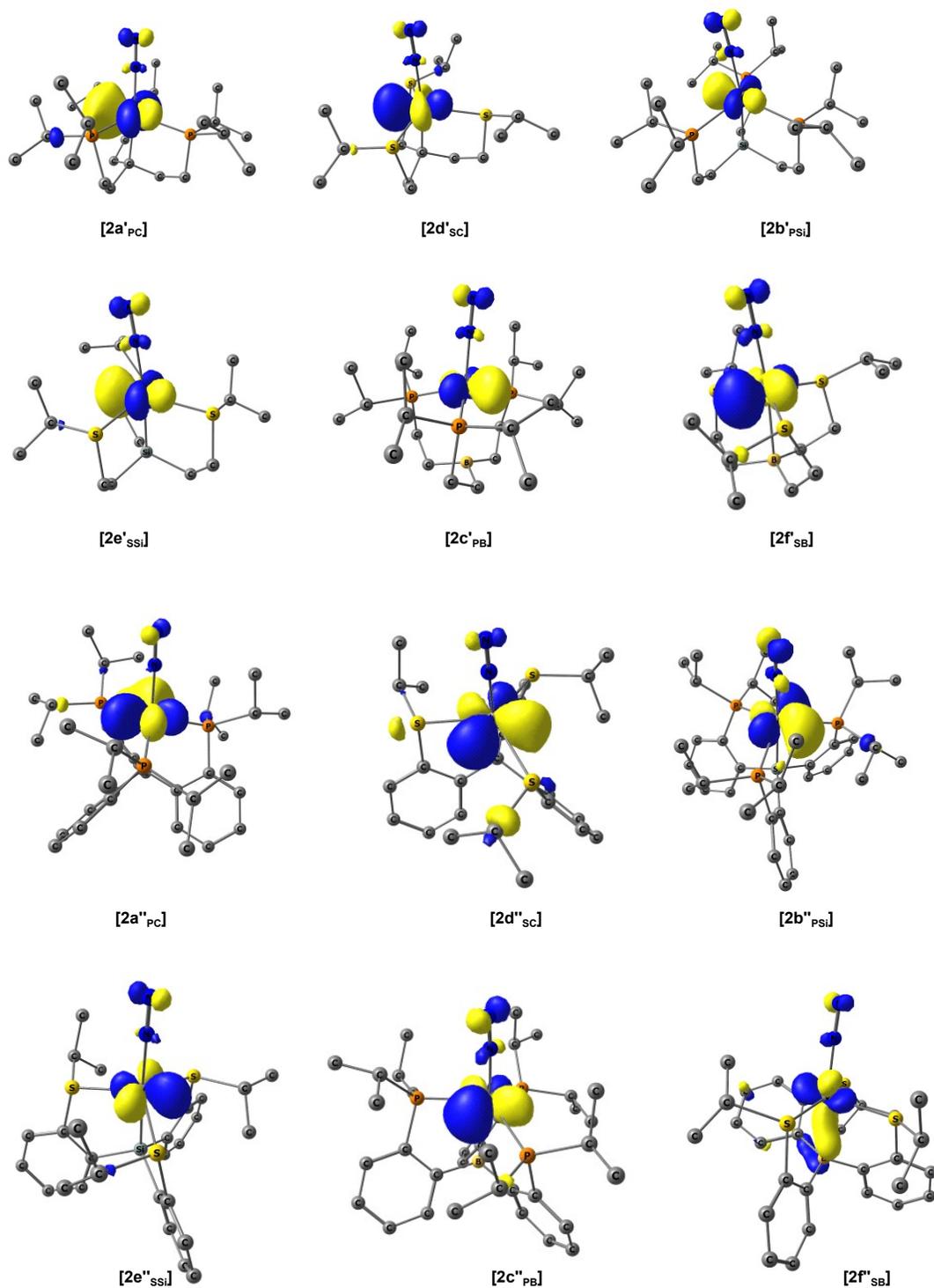


Fig. S4. Pictorial representation of the HOMO for the dinitrogen vanadium complexes $[2a'_{PC}]$ - $[2f'_{SB}]$ and $[2a''_{PC}]$ - $[2f''_{SB}]$. Hydrogen atoms of the methyl groups are omitted for clarity.

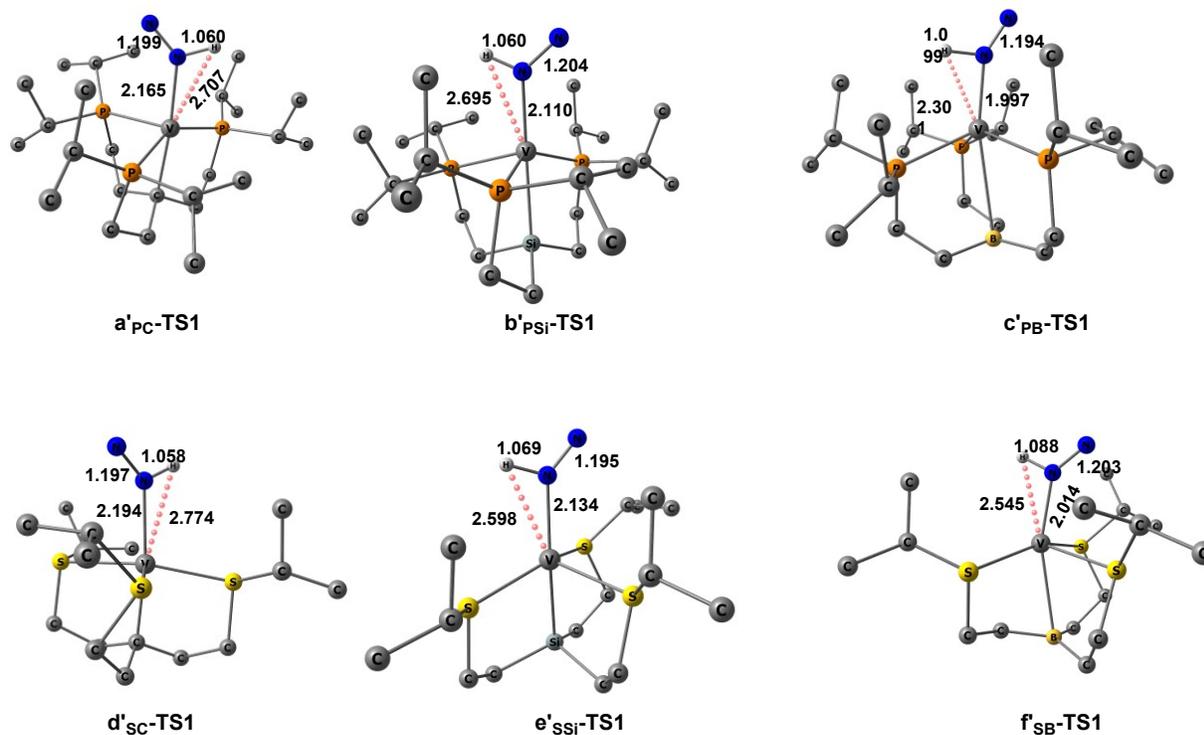


Fig. S5. Optimized geometries of the transition state (TS1) involved in the formation of the η^2 -intermediate from the metal protonated species $[3\text{-V-H}]^+$ for $[1\mathbf{a}'_{\text{PC}}]$ - $[1\mathbf{f}'_{\text{SB}}]$ at M06-L-D3(heptane)/6-311+G* level of theory. Hydrogen atoms of the methyl groups are omitted for clarity. Bond lengths are given in Å.

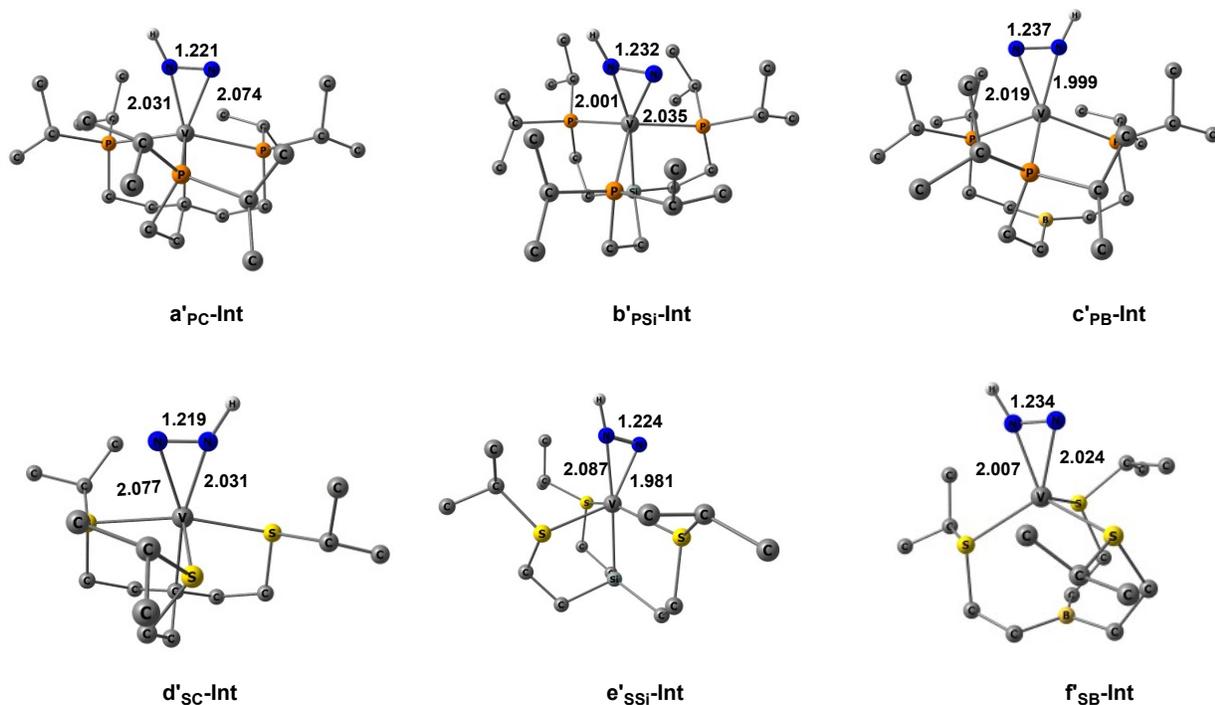


Fig. S6. Optimized geometries of the η^2 -intermediate involved in the formation of **[3]** from the metal protonated species **[3-V-H]⁺** for **[1a'PC]-[1f'SB]** at M06-L-D3(heptane)/6-311+G* level of theory. Hydrogen atoms of the methyl groups are omitted for clarity. Bond lengths are given in Å.

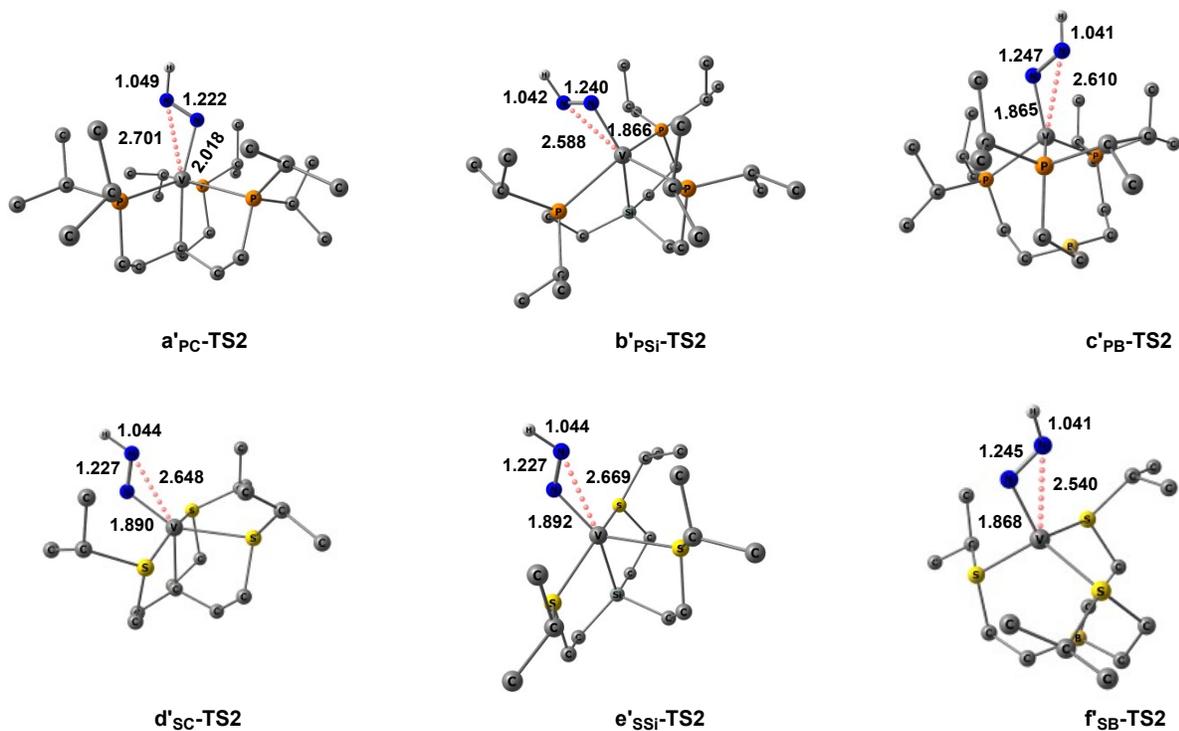


Fig. S7. Optimized geometries of the transition state (TS2) involved in the formation of **[3]** from the η^2 -intermediate of **[1a'_{PC}]-[1f'_{sB}]** at M06-L-D3(heptane)/6-311+G* level of theory. Hydrogen atoms of the methyl groups are omitted for clarity. Bond lengths are given in Å.

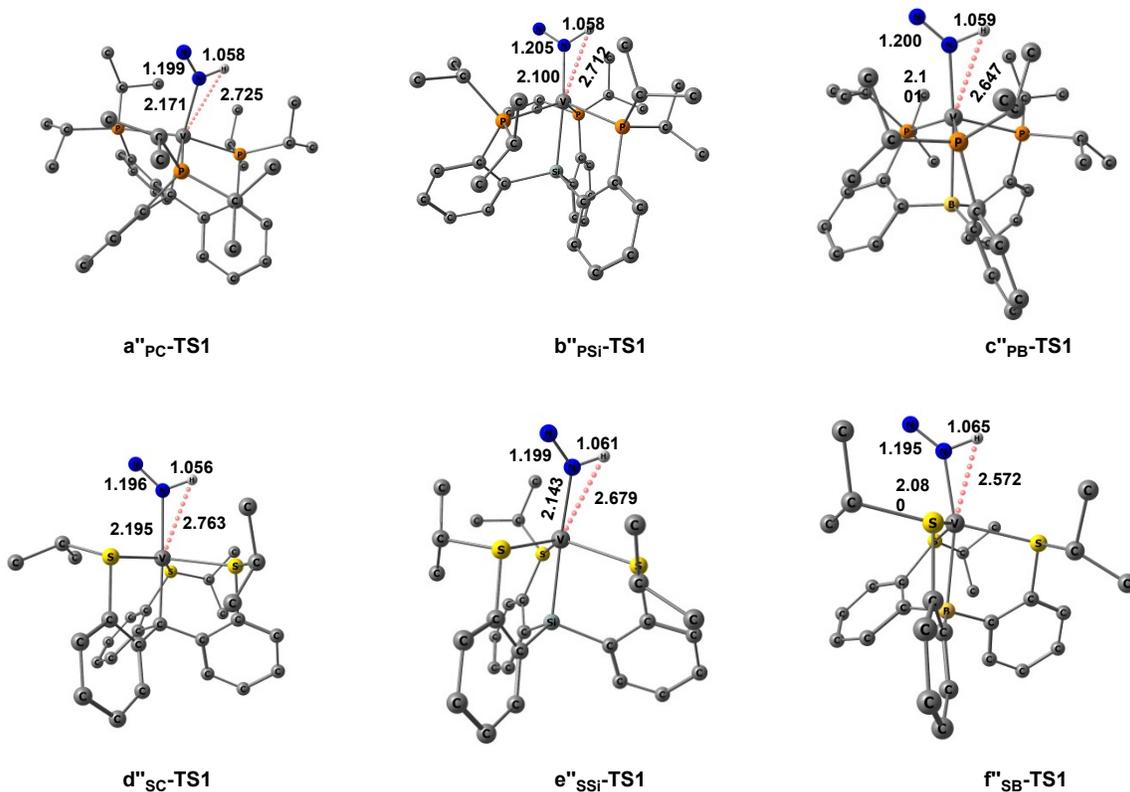


Fig. S8. Optimized geometries of the transition state (TS1) involved in the formation of the η^2 -intermediate from the metal protonated species $[3-V-H]^+$ of $[1a''_{PC}]$ - $[1f''_{SB}]$ at M06-L-D3(heptane)/6-311+G* level of theory. Hydrogen atoms of the methyl groups are omitted for clarity. Bond lengths are given in Å.

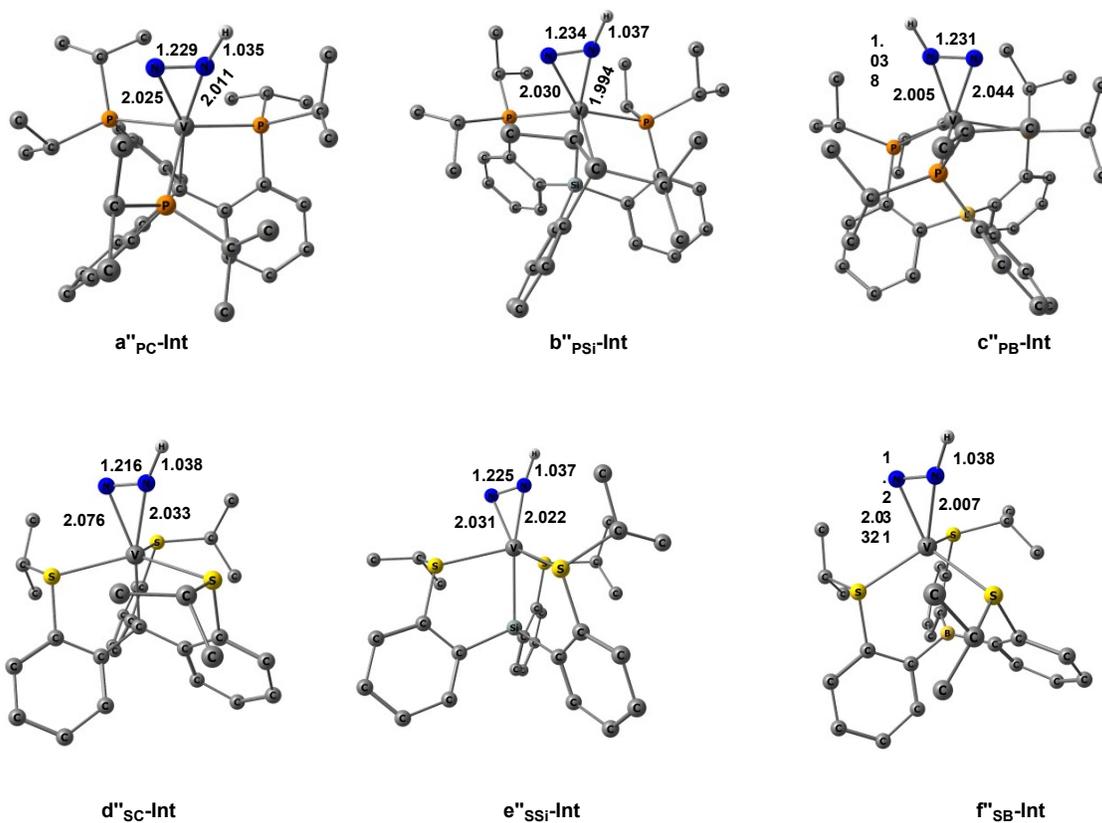


Fig. S9. Optimized geometries of the η^2 -intermediate involved in the formation of **[3]** from the metal protonated species **[3-V-H]⁺** of **[1a''_{PC}]-[1f''_{SB}]** at M06-L-D3(heptane)/6-311+G* level of theory. Hydrogen atoms of the methyl groups are omitted for clarity. Bond lengths are given in Å.

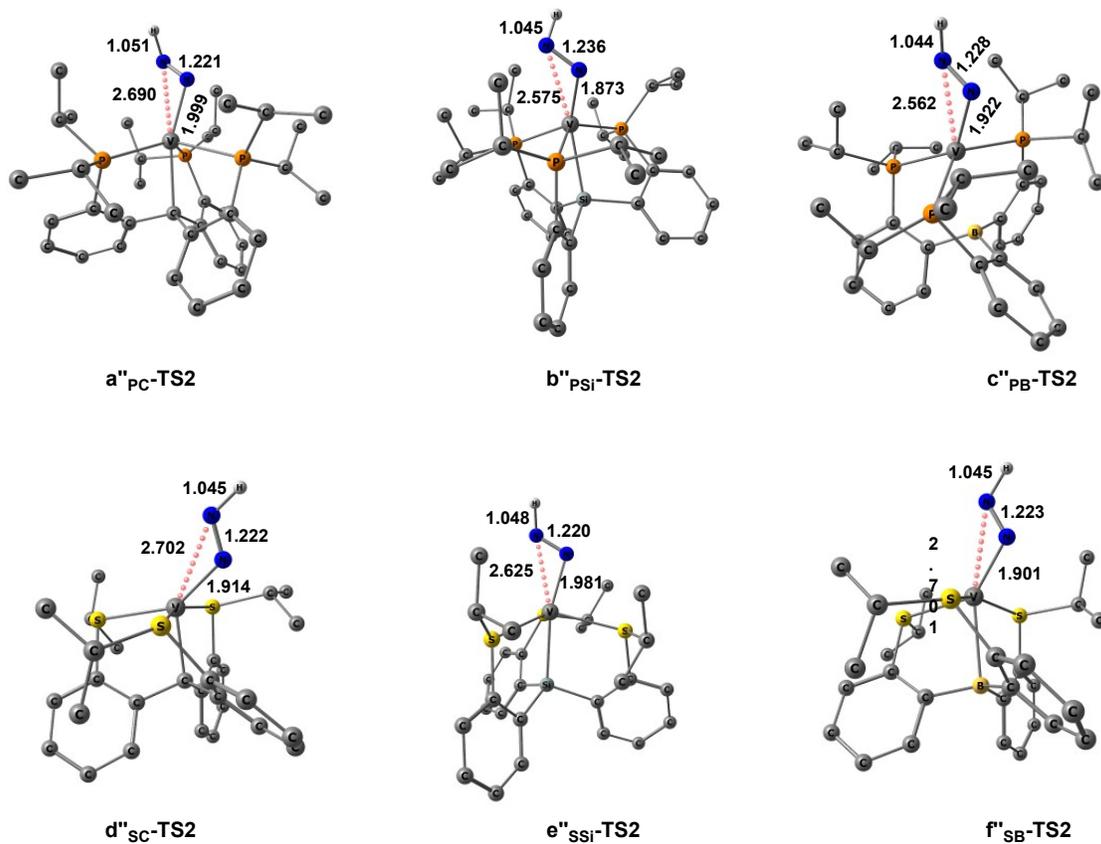


Fig. S10. Optimized geometries of the transition state (TS2) involved in the formation of the η^2 -intermediate from the metal protonated species $[3-V-H]^+$ of $[1a''_{PC}]-[1f''_{SB}]$ at M06-L-D3(heptane)/6-311+G* level of theory. Hydrogen atoms of the methyl groups are omitted for clarity. Bond lengths are given in Å.

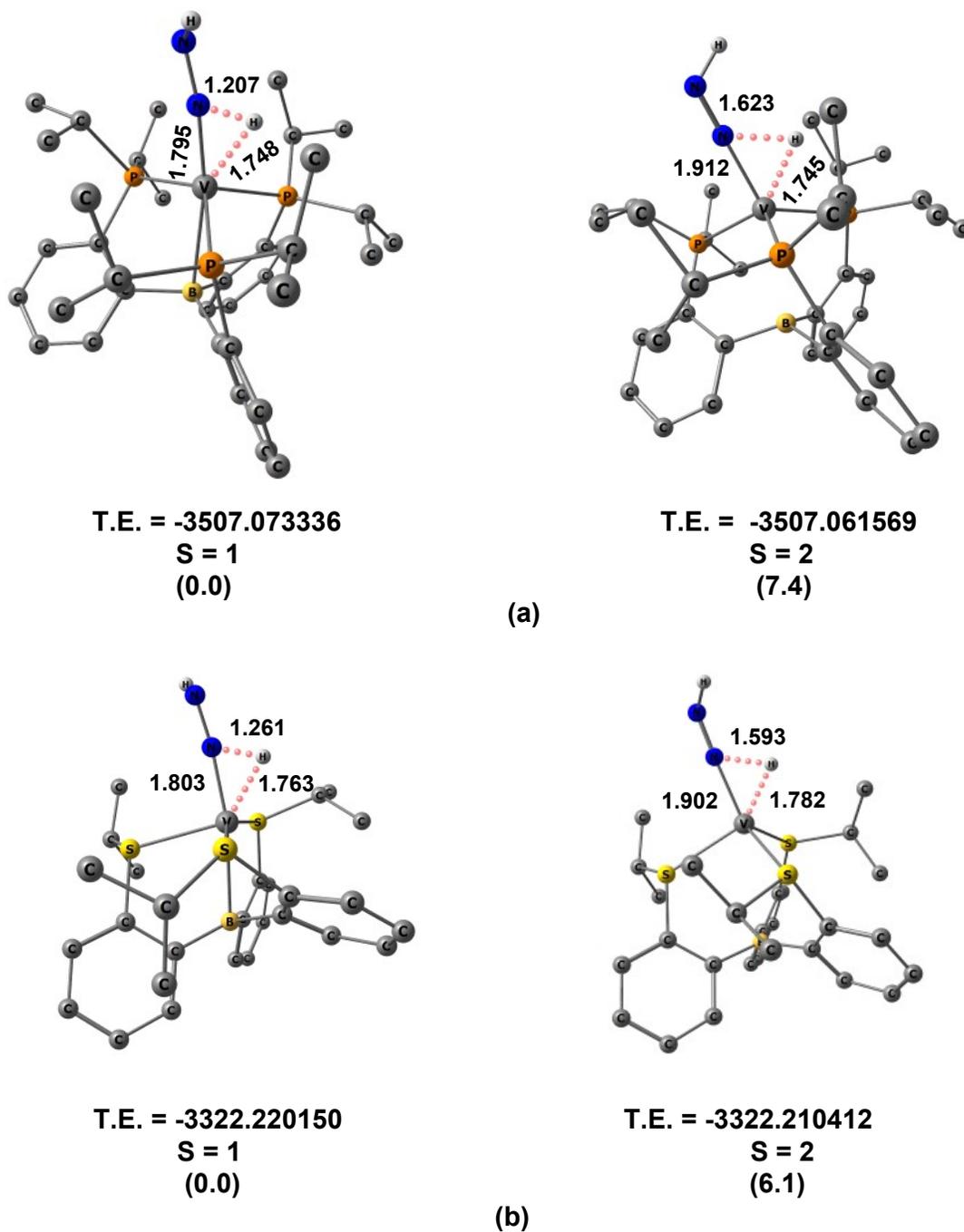


Fig. S11. Optimized geometries of the TS (TS3) involved during conversion of [4]→[5]_{alt} in all possible spin states for the molecules (a) [1c''_{PB}] and (b) [1f''_{SB}] at M06-L-D3(heptane)/6-311+G* level of theory. Total energy (T.E) values are given in hartree. The values given within parenthesis correspond to the relative energy difference (in kcal mol⁻¹) between the TSs. Hydrogen atoms of the methyl groups are omitted for clarity. Bond lengths are given in Å.

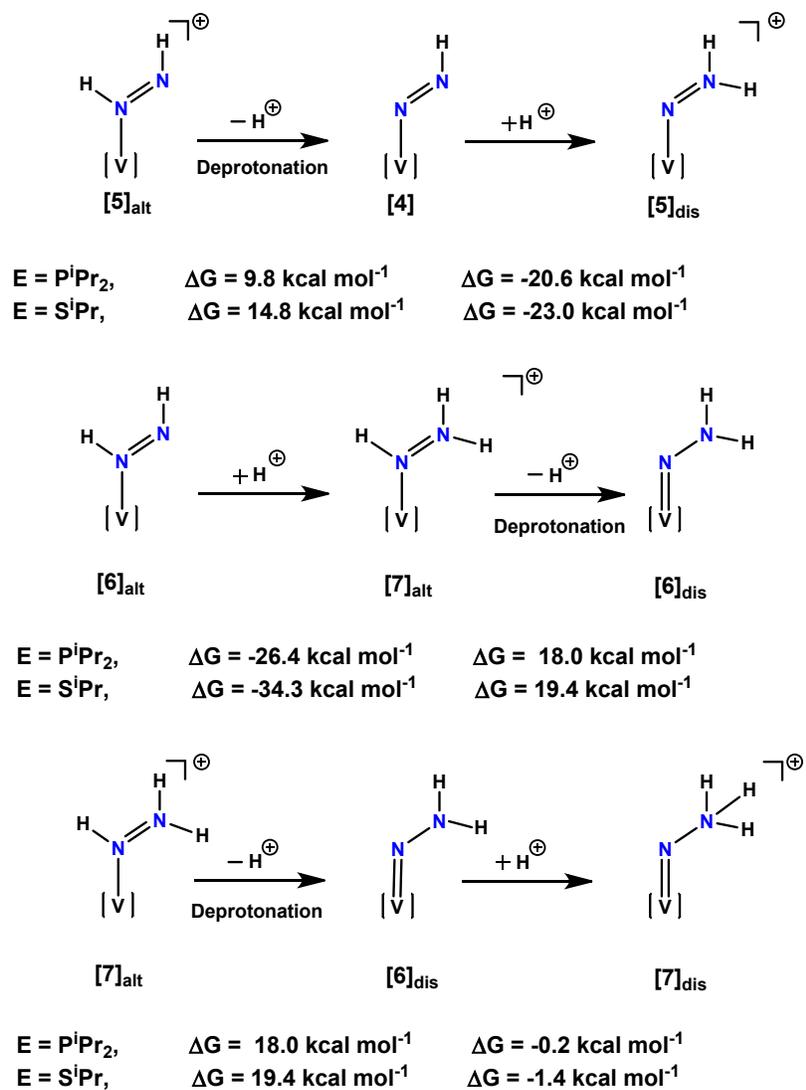


Fig. S12. Schematic representation of the possible proton-catalyzed pathway involved in the conversion of [5]_{alt}, [6]_{alt} and [7]_{alt} to [5]_{dis}, [6]_{dis} and [7]_{dis}, respectively.

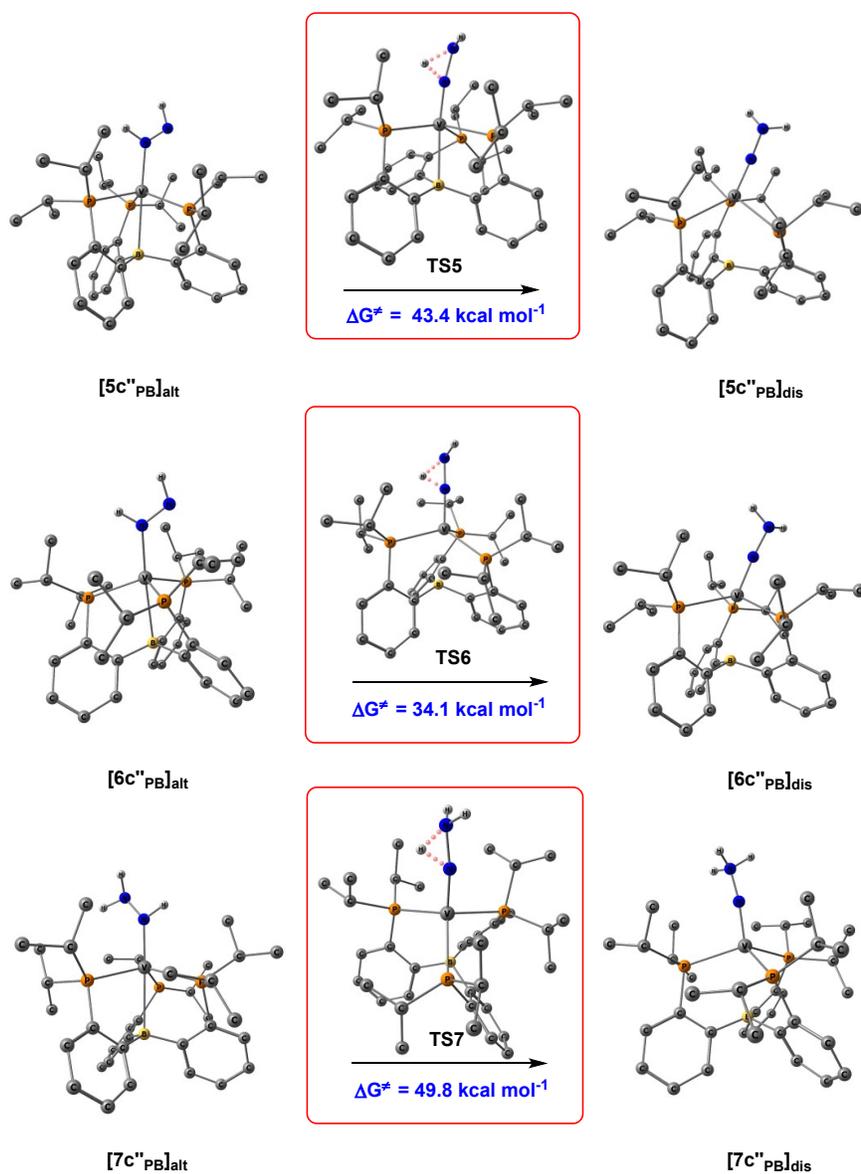


Fig. S13. Optimized geometries of the TSs involved in the conversion of $[5c''_{PB}]_{alt}$, $[6c''_{PB}]_{alt}$ and $[7c''_{PB}]_{alt}$ to $[5c''_{PB}]_{dis}$, $[6c''_{PB}]_{dis}$ and $[7c''_{PB}]_{dis}$ respectively via proton transfer pathway at M06-L-D3(heptane)/6-311+G* level of theory. The hydrogen atoms of the methyl groups are omitted for clarity.

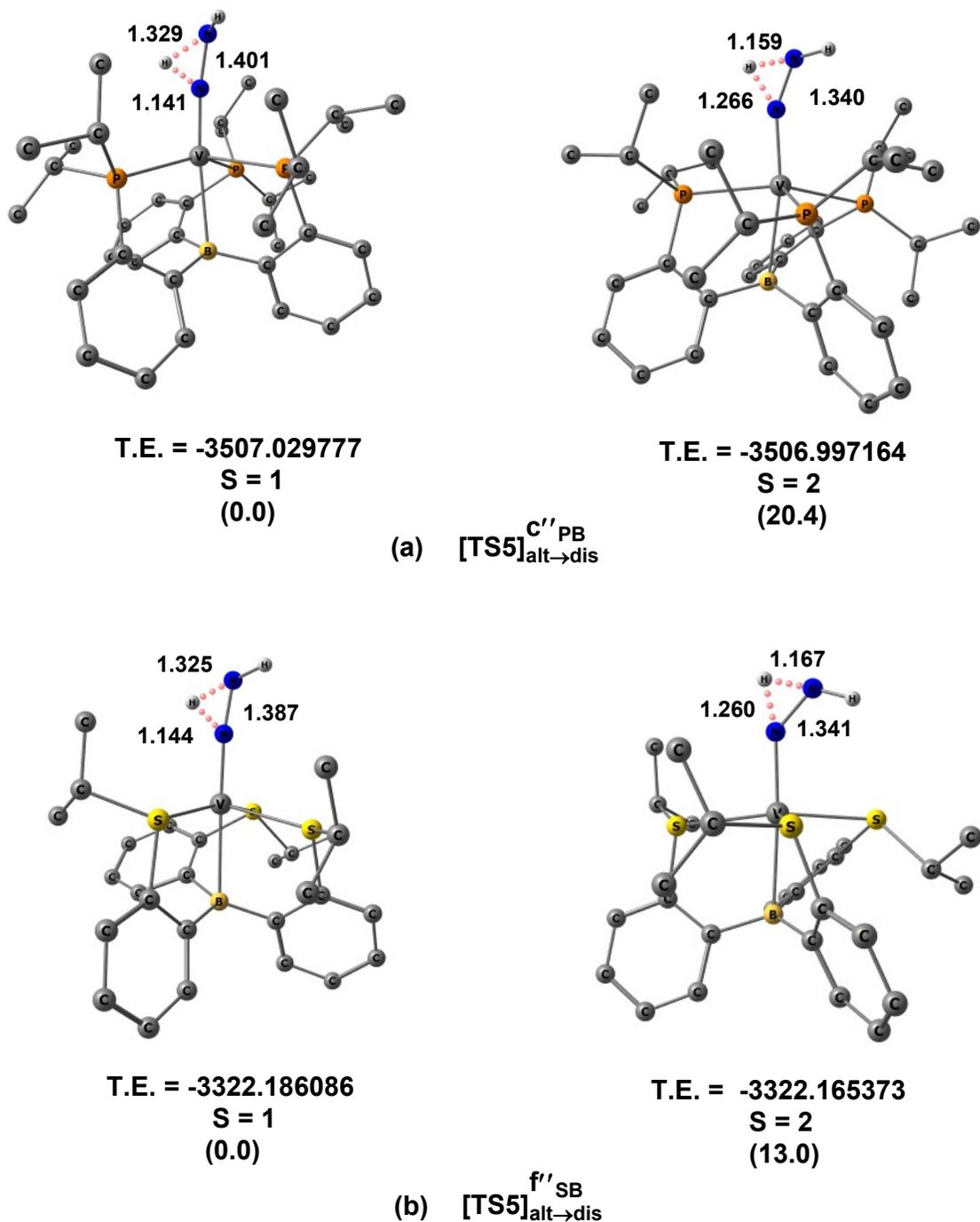
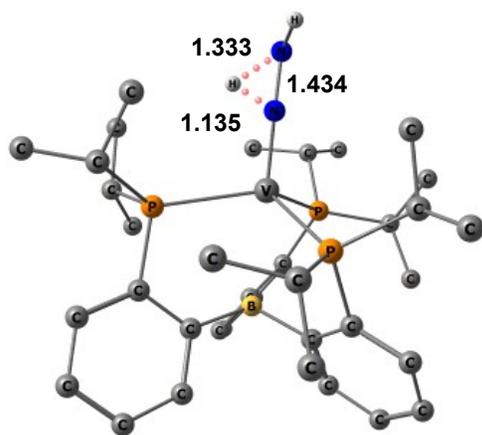
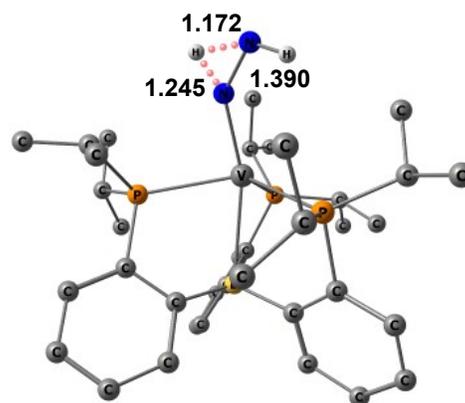


Fig. S14. Optimized geometries of the TS (TS5) involved during conversion of $[5]_{alt} \rightarrow [5]_{dis}$ in all possible spin states for the molecules (a) $[1c''_{PB}]$ and (b) $[1f''_{SB}]$ at M06-L-D3(heptane)/6-311+G* level of theory. Total energy (T.E) values are given in hartree. The values given within parenthesis correspond to the relative energy difference (in kcal mol⁻¹) between the TSs. Hydrogen atoms of the methyl groups are omitted for clarity. Bond lengths are given in Å.

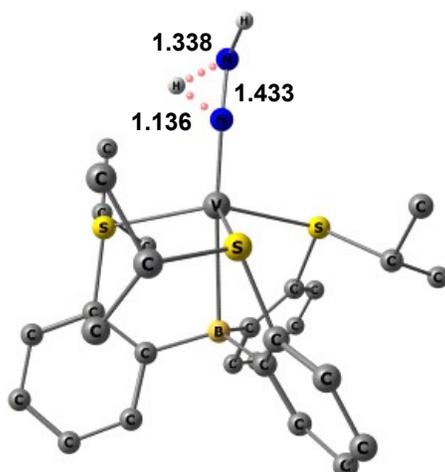


T.E. = -3507.183455
 S = 3/2
 (0.0)

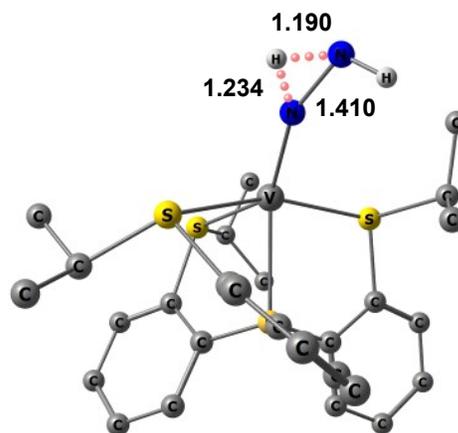


T.E. = -3507.149524
 S = 5/2
 (21.3)

(a) $[\text{TS6}]_{\text{alt} \rightarrow \text{dis}}^{\text{C}''_{\text{PB}}}$



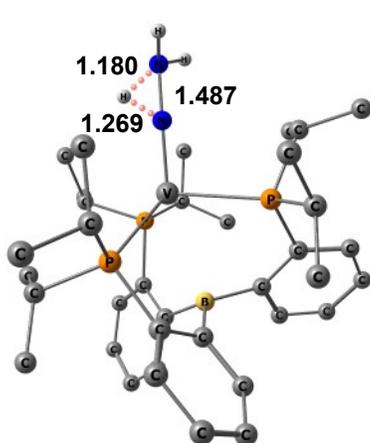
T.E. = -3322.331928
 S = 3/2
 (0.0)



T.E. = -3322.304097
 S = 5/2
 (17.4)

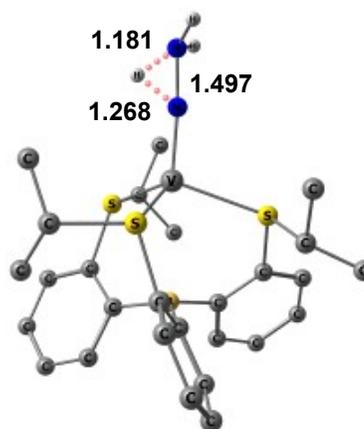
(b) $[\text{TS6}]_{\text{alt} \rightarrow \text{dis}}^{\text{f}''_{\text{SB}}}$

Fig. S15. Optimized geometries of the TS (TS6) involved during conversion of $[\mathbf{6}]_{\text{alt}} \rightarrow [\mathbf{6}]_{\text{dis}}$ in all possible spin states for the molecules (a) $[\mathbf{1c}''_{\text{PB}}]$ and (b) $[\mathbf{1f}''_{\text{SB}}]$ at M06-L-D3(heptane)/6-311+G* level of theory. Total energy (T.E) values are given in hartree. The values given within parenthesis correspond to the relative energy difference (in kcal mol⁻¹) between the TSs. Hydrogen atoms of the methyl groups are omitted for clarity. Bond lengths are given in Å.



T.E. = -3507.617766
S = 3/2

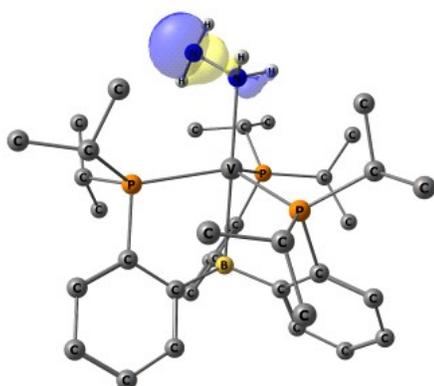
(a) $[\text{TS7}]_{\text{alt} \rightarrow \text{dis}}^{\text{c}''_{\text{PB}}}$



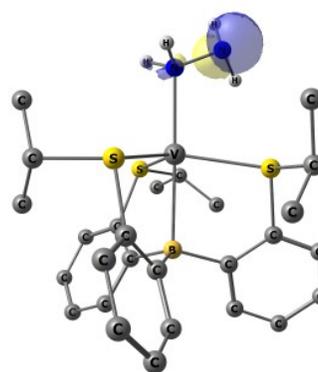
T.E. = -3322.770321
S = 3/2

(b) $[\text{TS7}]_{\text{alt} \rightarrow \text{dis}}^{\text{f}''_{\text{SB}}}$

Fig. S16. Optimized geometries of the TS (TS7) involved during conversion of $[7]_{\text{alt}} \rightarrow [7]_{\text{dis}}$ in all possible spin states for the molecules (a) $[1\text{c}''_{\text{PB}}]$ and (b) $[1\text{f}''_{\text{SB}}]$ at M06-L-D3(heptane)/6-311+G* level of theory. Total energy (T.E) values are given in hartree. Hydrogen atoms of the methyl groups are omitted for clarity. Bond lengths are given in Å.

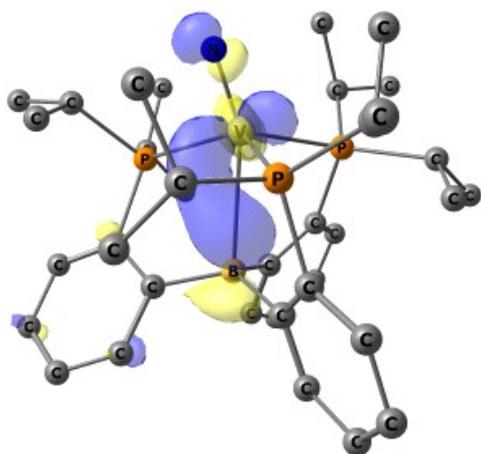


HOMO-13
 $E_{\text{LP}} = -6.7 \text{ eV}$
 $[10\text{c}''_{\text{PB}}]_{\text{alt}}$



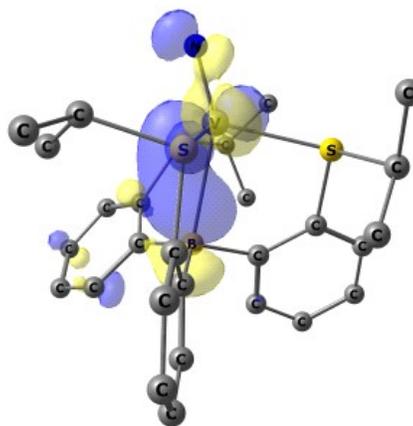
HOMO-14
 $E_{\text{LP}} = -6.7 \text{ eV}$
 $[10\text{f}''_{\text{SB}}]_{\text{alt}}$

Fig. S17. Molecular orbital showing the presence of amino lone pair on the β -nitrogen atom of the complexes $[10\text{c}''_{\text{PB}}]_{\text{alt}}$ and $[10\text{f}''_{\text{SB}}]_{\text{alt}}$. The hydrogen atoms of the methyl groups are omitted for the sake of clarity.



HOMO
 $E_{LP} = -3.5 \text{ eV}$

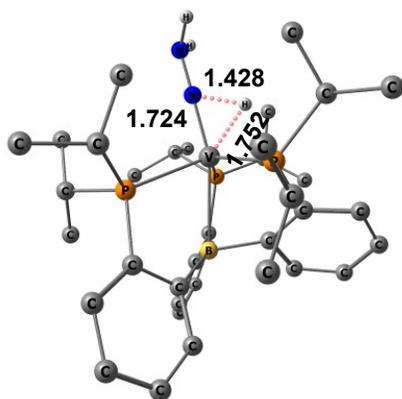
[8c''_{PB}]_{dis}



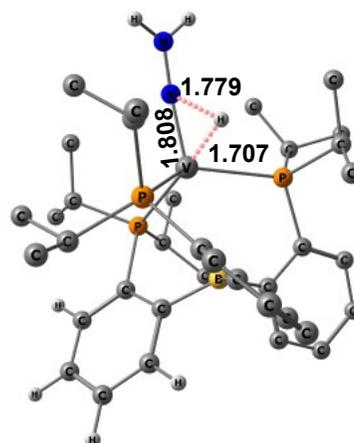
HOMO
 $E_{LP} = -3.6 \text{ eV}$

[8f''_{SB}]_{dis}

Fig. S18. Molecular orbital showing the presence of lone pair on the nitrogen atom of the complexes [8c''_{PB}]_{dis} and [8f''_{SB}]_{dis}. The hydrogen atoms of the methyl groups are omitted for the sake of clarity.

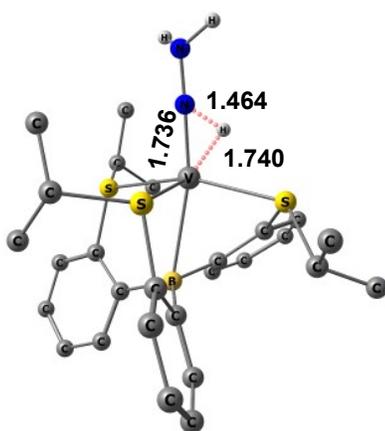


T.E. = -3507.662111
 S=1/2
 (4.0)

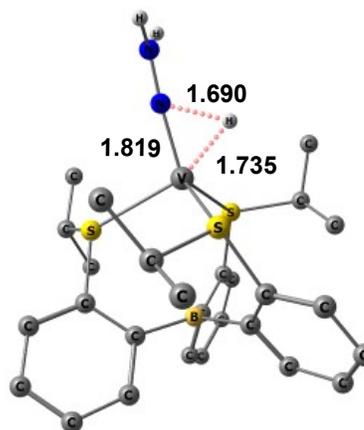


T.E. = -3507.668505
 S=3/2
 (0.0)

(a)



T.E. = -3322.822926
 S=1/2
 (0.0)



T.E. = -3322.822176
 S=3/2
 (0.5)

(b)

Fig. S19. Optimized geometries of the TS (TS_{hyb}) involved during conversion of [6]_{dis}→[7]_{alt} in all possible spin states for the molecules (a) [1c''_{PB}] and (b) [1f''_{SB}] at M06-L-D3(heptane)/6-311+G* level of theory. Total energy (T.E) values are given in hartree. The values given within parenthesis correspond to the relative energy difference (in kcal mol⁻¹) between the TSs. Hydrogen atoms of the methyl groups are omitted for clarity. Bond lengths are given in Å.

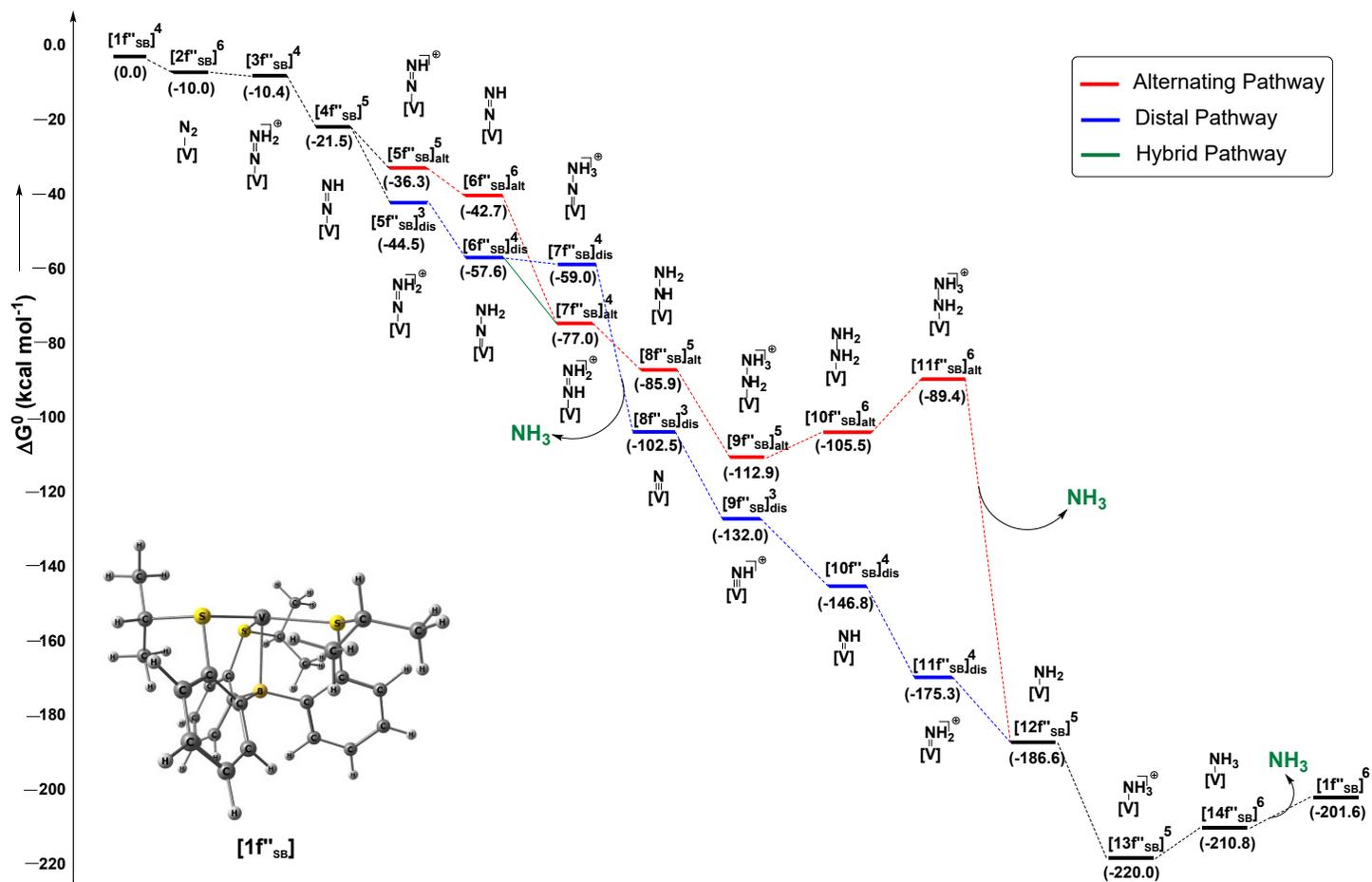


Fig. S20. Energy profile diagram for the reduction process of N₂ to NH₃ mediated by the catalyst [1f''_{SB}]. The energy values are given in kcal mol⁻¹ and calculated at M06-L-D3(heptane)/6-311+G* level of theory. The superscript outside the bracket indicate the spin state of the species.

Generation of $[5f''_{SB}]_{alt}$ and $[5f''_{SB}]_{dis}$ for the catalyst $[1f''_{SB}]$

Protonation at the N_α or N_β atoms of the diazenido complex $[4f''_{SB}]$, yielded the cationic complexes $[5f''_{SB}]_{alt}$ (in a quintet ground state) and $[5f''_{SB}]_{dis}$ (in a triplet ground state) respectively (Fig. S20†). Both of these complexes exhibit a TBP geometry around the vanadium center. The calculated reaction free energies obtained for the formation of $[5f''_{SB}]_{alt}$ and $[5f''_{SB}]_{dis}$ from the neutral diazenido complex $[4f''_{SB}]$ are considerably exergonic and found to be relatively more exergonic for the distal pathway (Fig. S21 and Fig. S22†). In addition, we have also calculated the reaction free energy for protonation at the metal center of the diazenido complex $[4f''_{SB}]$. This reaction is found to be exergonic in nature ($-13.8 \text{ kcal mol}^{-1}$) indicating its possibility during the nitrogen reduction process. However, protonation at the sulphur atom of $[4f''_{SB}]$ is computed to be considerably endergonic ($22.1 \text{ kcal mol}^{-1}$, Table S18†) which may be attributed to the higher stability of the sulphur lone pair (HOMO-13, $E_{LP} = -6.9 \text{ eV}$, Fig. S23†). Furthermore, we have also investigated the activation energy barrier associated with the formation of the cationic species $[5f''_{SB}]_{alt}$ and $[5f''_{SB}]_{dis}$, from the diazenido complex $[4f''_{SB}]$ by locating the probable TSs. The reaction profile diagram for the conversion of $[4f''_{SB}]$ to $[5f''_{SB}]_{alt}$ via the alternating pathway is shown in Fig. S21†. The first step involves the formation of a metal protonated species $[4f''_{SB} -V-H]^+$ which lie $-13.8 \text{ kcal mol}^{-1}$ lower in energy than the starting diazenido complex. Thereafter, the metal protonated species passes through a TS ($TS3_{alt}$) with an activation barrier of $17.5 \text{ kcal mol}^{-1}$ to generate $[5f''_{SB}]_{alt}$. However, unlike the alternating pathway, two intermediates and two TSs are possible for the transformation of $[4f''_{SB}]$

to $[5f''_{SB}]_{dis}$ via the distal pathway (Fig. S22[†]). The first intermediate, i.e., the metal protonated species $[4f''_{SB}-V-H]^+$ is common for both the pathways that rearranges via a TS ($TS4'_{dis}$) with

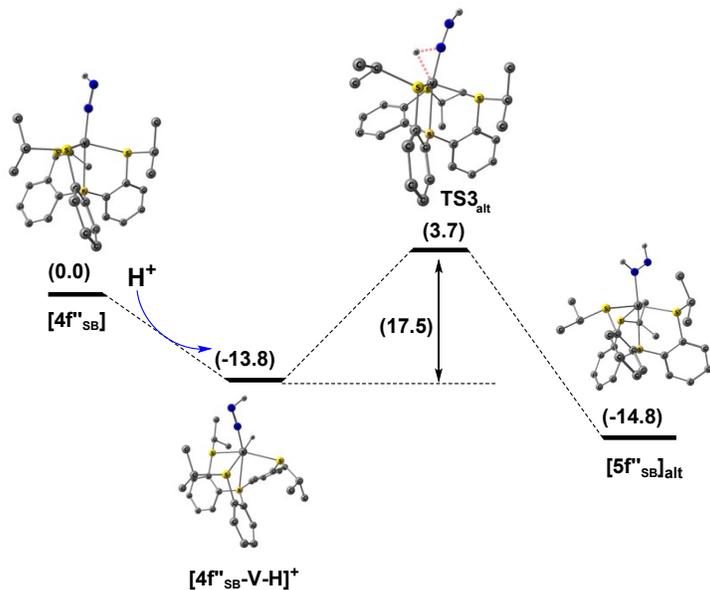


Fig. S21. Reaction profile diagram for the conversion of $[4f''_{SB}]$ to $[5f''_{SB}]_{alt}$ via alternating pathway at M06-L-D3(heptane)/6-311+G* level of theory. Hydrogen atoms of the methyl groups are omitted for clarity. The energy values are in kcal mol⁻¹.

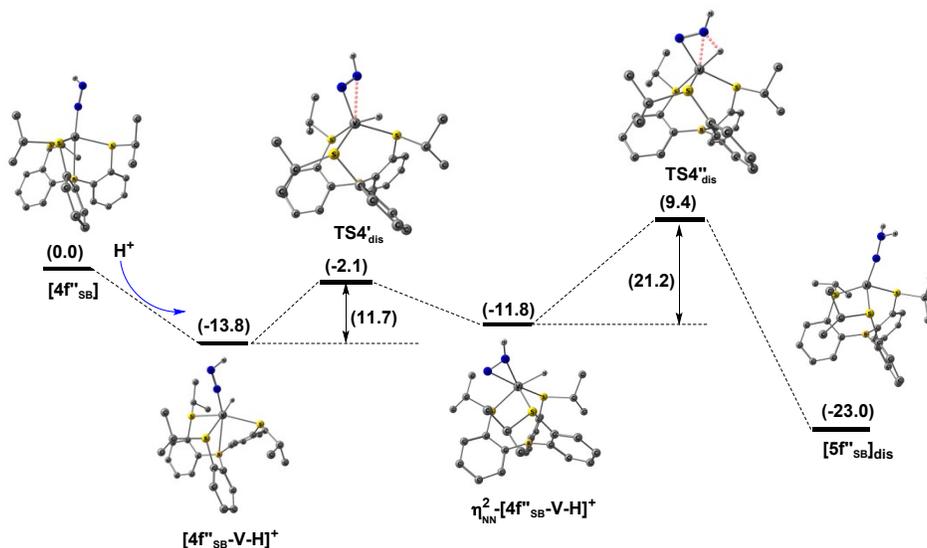
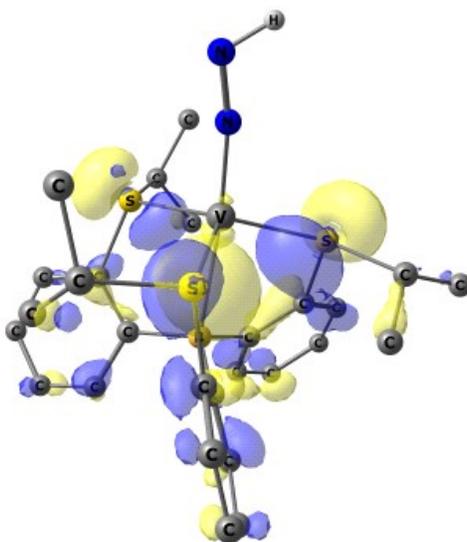


Fig. S22. Reaction profile diagram for the conversion of $[4f''_{SB}]$ to $[5f''_{SB}]_{dis}$ via distal pathway at M06-L-D3(heptane)/6-311+G* level of theory. Hydrogen atoms of the methyl groups are omitted for clarity. The energy values are in kcal mol⁻¹.

an activation barrier 11.7 kcal mol⁻¹ to generate an intermediate in which the metal center is bounded to the two N atoms in η^2 fashion ($\eta^2_{\text{NN}}\text{-[4f''}_{\text{SB}}\text{-V-H}]^+$). Finally, $\eta^2_{\text{NN}}\text{-[4f''}_{\text{SB}}\text{-V-H}]^+$ proceeds through another TS (TS4''_{dis}) in which the metal bound proton migrates to the β -nitrogen atom to yield [5f''_{SB}]_{dis}. The barrier height associated with this transformation is computed to be 21.2 kcal mol⁻¹. Since the transformations [4f''_{SB}] \rightarrow [5f''_{SB}]_{dis} and [4f''_{SB}] \rightarrow [5f''_{SB}]_{alt} involves comparable barriers therefore, both pathways may be viable.



HOMO-13
 $E_{\text{LP}} = -6.9 \text{ eV}$
[4f''_{SB}]

Fig. S23. Pictorial representation of the molecular orbital showing the lone pairs situated at the sulphur atoms of the complex [4f''_{SB}]. The hydrogen atoms of the methyl groups are omitted for the sake of clarity.

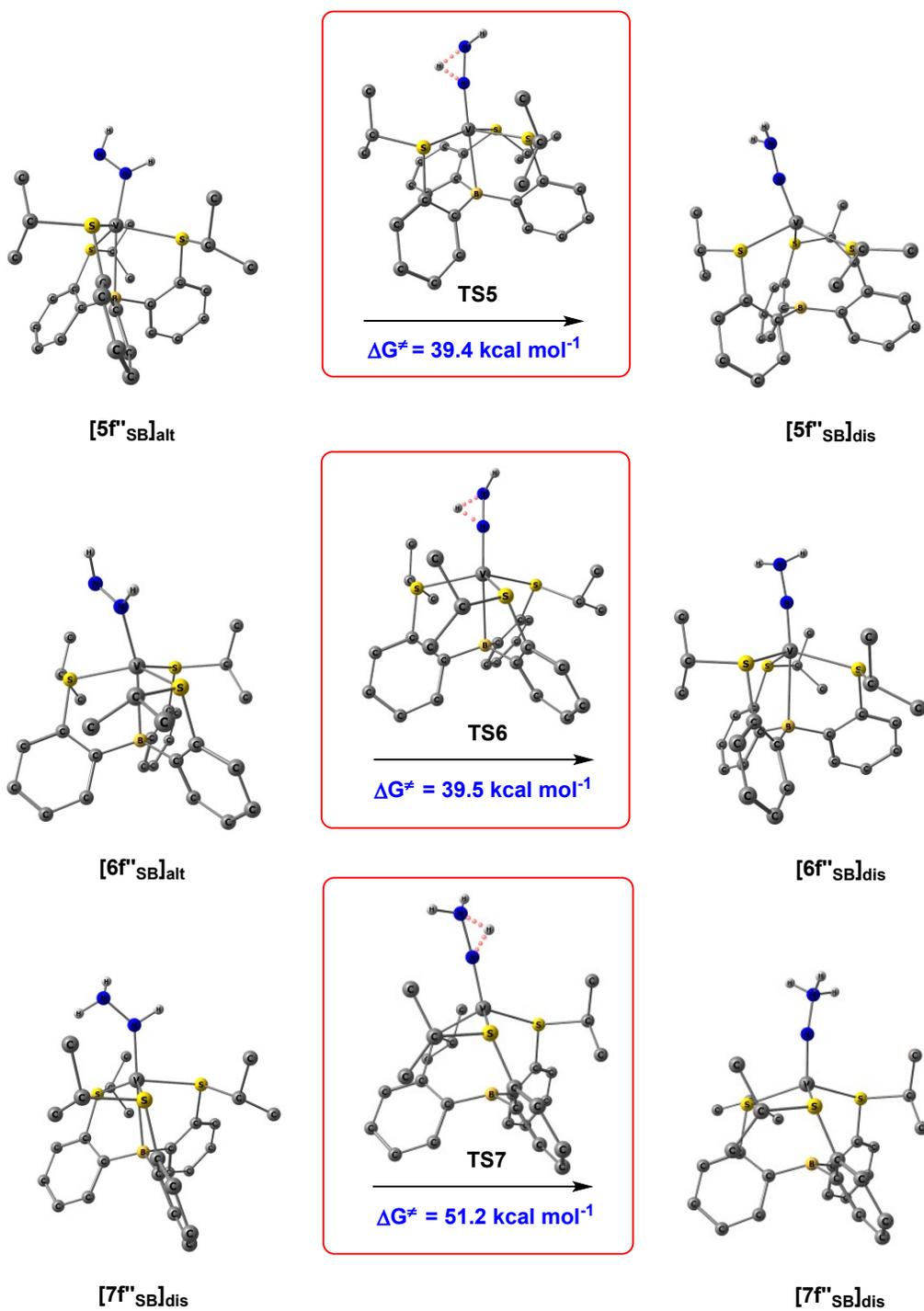


Fig. S24. Optimized geometries of the TSs involved in the conversion of $[5f''_{SB}]_{alt}$, $[6f''_{SB}]_{alt}$ and $[7f''_{SB}]_{alt}$ to $[5f''_{SB}]_{dis}$, $[6f''_{SB}]_{dis}$ and $[7f''_{SB}]_{dis}$ respectively via proton transfer pathway at M06-L-D3(heptane)/6-311+G* level of theory. The hydrogen atoms of the methyl groups are omitted for clarity.

Hybrid pathway for the catalyst $[1f''_{SB}]$

We have studied the kinetics of the transformation $[6f''_{SB}]_{dis} \rightarrow [7f''_{SB}]_{alt}$ by locating the probable intermediate and TS (Fig. S25[†]). The first step involves the formation of a metal protonated species $[6f''_{SB}-V-H]^+_{dis}$ which is computed to be exergonic in nature ($-20.0 \text{ kcal mol}^{-1}$). Thereafter, $[6f''_{SB}-V-H]^+_{dis}$ passes through a TS (TS_{hyb}) with an activation barrier $17.1 \text{ kcal mol}^{-1}$.

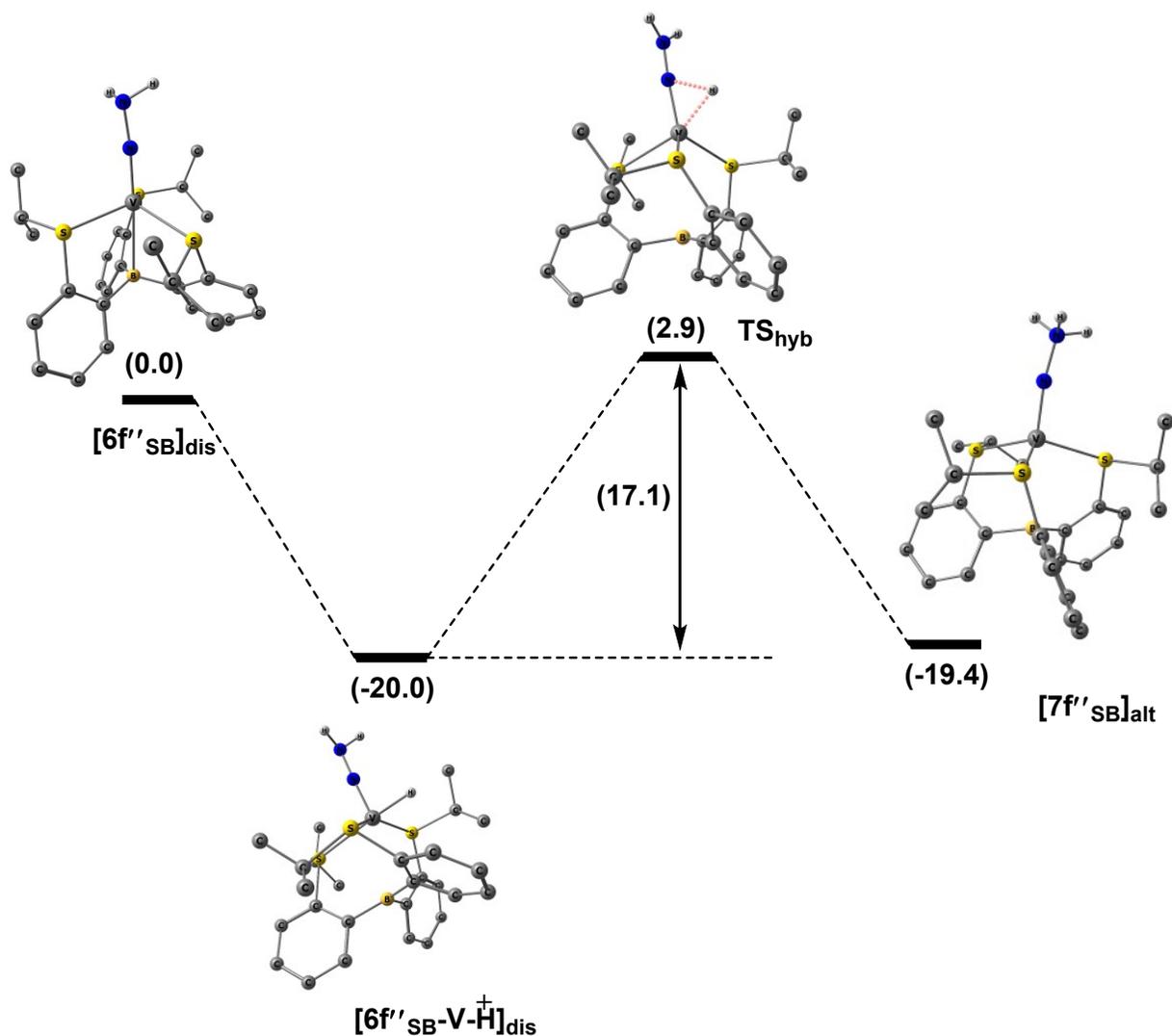


Fig. S25. Reaction profile diagram for the conversion of $[6f''_{SB}]_{dis} \rightarrow [7f''_{SB}]_{alt}$ via hybrid pathway at M06-L-D3(heptane)/6-311+G* level of theory. Hydrogen atoms of the methyl groups are omitted for clarity. The energy values are in kcal mol⁻¹.

mol⁻¹ to give $[7\mathbf{f}''_{\text{SB}}]_{\text{alt}}$. Since, the metal protonated species $[6\mathbf{f}''_{\text{SB}} - \mathbf{V}-\mathbf{H}]_{\text{dis}}^+$ (doublet) and $[7\mathbf{f}''_{\text{SB}}]_{\text{alt}}$ (quartet) exhibits different multiplicities, therefore, we attempted to locate the TS in both the spin states (doublet and quartet, Fig. S19†). However, the doublet and quartet states of TS_{hyb} are isoenergetic (the energy difference between these states is only 0.5 kcal mol⁻¹, Fig. S19†). Therefore, the activation barrier was computed by considering the quartet state TS. Thus, thermodynamic as well as kinetic studies suggest the viability of the hybrid pathway for the catalyst $[1\mathbf{f}''_{\text{SB}}]$.

Cartesian coordinates of $[1a'_{PC}]-[1f'_{SB}]$, $[1a''_{PC}]-[1f''_{SB}]$ and $\{[HIPTN_3N]-V\}$, along with their total energies (in hartree) including zero point vibrational correction at M06-L-D3(heptane)/6-311+G* level of theory.

$[1a'_{PC}]$ (TE = -2952.517639)

6	-0.031077000	2.443589000	1.770467000
6	0.562960000	1.186032000	2.395471000
6	-2.608327000	-0.016897000	1.500415000
6	-1.427776000	-0.353541000	2.414211000
6	2.255718000	-1.351094000	1.684650000
6	0.878598000	-1.274720000	2.343317000
1	-2.690505000	1.065448000	1.332953000
1	-1.568358000	0.187262000	3.370187000
1	2.839175000	-2.208753000	2.048662000
1	1.022617000	-1.231404000	3.444376000
1	0.362578000	3.362154000	2.225648000
1	1.652688000	1.215816000	2.239590000
6	-0.764490000	3.819536000	-0.734047000
1	-0.140768000	4.262790000	-1.525723000
6	-2.654513000	-2.586122000	0.154725000
1	-1.904803000	-2.759820000	0.943987000
6	3.694839000	-0.579468000	-0.731991000
1	3.478213000	0.474138000	-0.496890000
23	0.010750000	-0.053884000	-0.415394000
6	-0.009170000	-0.125853000	1.842083000
1	-1.117374000	2.468234000	1.924807000
1	0.433759000	1.244516000	3.496871000
1	0.357644000	-2.225543000	2.164477000
1	2.848415000	-0.461129000	1.932756000
1	-1.534405000	-1.413964000	2.691110000
1	-3.560733000	-0.329960000	1.951125000
6	4.993801000	-0.932691000	-0.014746000
1	5.766444000	-0.191667000	-0.252730000
1	4.884223000	-0.940270000	1.073418000
1	5.393004000	-1.904753000	-0.309045000
6	3.829802000	-0.688709000	-2.244824000
1	4.056244000	-1.713121000	-2.561098000
1	2.910075000	-0.387659000	-2.759901000
1	4.638838000	-0.052325000	-2.621369000
6	-4.017607000	-2.983136000	0.703996000
1	-4.013160000	-4.028529000	1.035318000
1	-4.322235000	-2.376119000	1.561657000
1	-4.801609000	-2.900071000	-0.056014000
6	-2.260590000	-3.457619000	-1.034062000
1	-3.024224000	-3.454675000	-1.816845000

1	-1.320251000	-3.124006000	-1.488666000
1	-2.125186000	-4.500680000	-0.725432000
6	-2.037794000	3.285443000	-1.376848000
1	-1.831812000	2.520603000	-2.132644000
1	-2.690459000	2.823392000	-0.625009000
1	-2.612606000	4.088836000	-1.852313000
6	-1.110595000	4.905358000	0.279019000
1	-0.239077000	5.314338000	0.793457000
1	-1.623590000	5.741516000	-0.210668000
1	-1.790997000	4.525616000	1.048276000
6	2.226069000	-3.197713000	-0.609490000
1	1.936510000	-3.225621000	-1.671305000
6	1.184886000	-3.980623000	0.183287000
1	1.488096000	-4.088012000	1.230868000
1	0.205377000	-3.494890000	0.174436000
1	1.063829000	-4.991649000	-0.221642000
6	3.589640000	-3.858340000	-0.461836000
1	3.513680000	-4.937840000	-0.640861000
1	4.328401000	-3.471416000	-1.166670000
1	3.997023000	-3.733314000	0.547856000
6	-3.825836000	-0.119077000	-1.150833000
1	-3.455315000	0.856229000	-1.494693000
6	-5.105298000	0.136633000	-0.363338000
1	-5.527051000	-0.777905000	0.062271000
1	-4.954082000	0.840099000	0.459588000
1	-5.873003000	0.568189000	-1.017032000
6	-4.096226000	-0.959766000	-2.392315000
1	-4.571448000	-1.913233000	-2.140519000
1	-4.778204000	-0.438255000	-3.073174000
1	-3.183056000	-1.186614000	-2.952708000
6	2.015726000	3.067230000	-0.201903000
1	2.584981000	2.363969000	0.426816000
6	2.265239000	4.479063000	0.305924000
1	3.334723000	4.719233000	0.275074000
1	1.758645000	5.226855000	-0.314145000
1	1.935392000	4.623821000	1.338887000
6	2.499612000	2.912729000	-1.638180000
1	3.570260000	3.131264000	-1.726951000
1	2.334537000	1.897694000	-2.015443000
1	1.979041000	3.602194000	-2.314006000
15	-2.356516000	-0.761739000	-0.174269000
15	0.267830000	2.398743000	-0.052804000
15	2.091825000	-1.373213000	-0.159316000

[1b' _{psi}] (TE = -3203.941560)

6	0.038342000	2.751433000	1.682851000
6	0.501329000	1.654749000	2.643103000
6	-2.826066000	-0.082332000	1.694883000
6	-1.728244000	-0.541260000	2.658476000
6	2.433928000	-1.506224000	1.600634000
6	1.294320000	-1.355138000	2.614081000
1	-2.908807000	1.014544000	1.704490000
1	-1.931257000	-0.147477000	3.664798000
1	3.085040000	-2.367397000	1.814942000
1	1.714628000	-1.099884000	3.597493000
1	0.385401000	3.752113000	1.973169000
1	1.598105000	1.690264000	2.733670000
6	-0.160640000	3.847065000	-1.023823000
1	0.563788000	4.012419000	-1.834873000
6	-2.891493000	-2.354580000	-0.092848000
1	-2.302831000	-2.713434000	0.766107000
6	3.469611000	-1.065971000	-1.051114000
1	3.479641000	0.009891000	-0.820654000
23	-0.049890000	-0.010795000	-0.521552000
1	-1.060074000	2.806665000	1.670282000
1	0.118880000	1.857805000	3.654006000
1	0.786430000	-2.317345000	2.752682000
1	3.088652000	-0.623387000	1.652868000
1	-1.772459000	-1.636045000	2.761025000
1	-3.819237000	-0.460733000	1.975950000
6	4.803705000	-1.625013000	-0.566794000
1	5.628084000	-1.031424000	-0.980652000
1	4.904010000	-1.591684000	0.521448000
1	4.975327000	-2.656100000	-0.879907000
6	3.307891000	-1.203221000	-2.558382000
1	3.284544000	-2.252825000	-2.873242000
1	2.377932000	-0.738615000	-2.909628000
1	4.135554000	-0.726597000	-3.096304000
6	-4.345943000	-2.730178000	0.151906000
1	-4.440321000	-3.807100000	0.336319000
1	-4.781471000	-2.216939000	1.014206000
1	-4.972049000	-2.507363000	-0.718217000
6	-2.348934000	-3.049642000	-1.335953000
1	-2.922003000	-2.788505000	-2.231746000
1	-1.302974000	-2.777941000	-1.523253000
1	-2.397219000	-4.139990000	-1.231416000
6	-1.496386000	3.472023000	-1.654983000
1	-1.431474000	2.562117000	-2.261598000
1	-2.252502000	3.284707000	-0.882454000

1	-1.878602000	4.279681000	-2.290352000
6	-0.311127000	5.141712000	-0.232565000
1	0.606066000	5.454966000	0.270007000
1	-0.618724000	5.962488000	-0.891374000
1	-1.084894000	5.048764000	0.536504000
6	1.640293000	-3.396110000	-0.519072000
1	1.171127000	-3.411923000	-1.514781000
6	0.638205000	-3.962975000	0.481701000
1	1.106727000	-4.113221000	1.460352000
1	-0.223911000	-3.304404000	0.627960000
1	0.264376000	-4.938715000	0.151344000
6	2.882964000	-4.274010000	-0.560310000
1	2.602012000	-5.331052000	-0.644972000
1	3.531883000	-4.049383000	-1.409354000
1	3.483836000	-4.178848000	0.351041000
6	-3.801878000	0.395332000	-0.989932000
1	-3.394898000	1.416772000	-0.967320000
6	-5.194687000	0.459764000	-0.373978000
1	-5.717016000	-0.498644000	-0.405553000
1	-5.178573000	0.791442000	0.667392000
1	-5.815722000	1.175551000	-0.926395000
6	-3.856487000	-0.036111000	-2.449391000
1	-4.317351000	-1.023560000	-2.561935000
1	-4.453401000	0.661557000	-3.047734000
1	-2.859347000	-0.088170000	-2.902580000
6	2.380961000	2.685468000	-0.064107000
1	2.747053000	1.815883000	0.505229000
6	2.889483000	3.947683000	0.616764000
1	3.983364000	3.929748000	0.692118000
1	2.632817000	4.847144000	0.048090000
1	2.501654000	4.071509000	1.631617000
6	2.931251000	2.578358000	-1.481663000
1	4.024371000	2.495993000	-1.480089000
1	2.533819000	1.706088000	-2.013125000
1	2.684277000	3.464886000	-2.076558000
15	-2.447185000	-0.526597000	-0.070307000
15	0.526044000	2.372817000	-0.070723000
15	1.877230000	-1.557014000	-0.180736000
14	0.010105000	-0.083501000	1.966160000

[1c'_{PB}] (TE = -2939.287303)

6	0.417016000	2.458497000	1.931098000
6	0.781518000	1.166921000	2.666338000
6	-2.617922000	0.490819000	1.649745000
6	-1.625817000	-0.163792000	2.619212000

6	2.037266000	-1.697745000	1.634367000
6	0.715773000	-1.553242000	2.392717000
1	-2.412361000	1.562903000	1.534512000
1	-1.761638000	0.313576000	3.605821000
1	2.619388000	-2.570388000	1.955501000
1	0.919874000	-1.716352000	3.469005000
1	0.892246000	3.353337000	2.356488000
1	1.868361000	1.007461000	2.583797000
6	0.221851000	3.823152000	-0.701726000
1	1.016287000	4.581368000	-0.638185000
6	-3.157254000	-1.948061000	0.172255000
1	-2.313578000	-2.472421000	0.648440000
6	3.455439000	-1.400071000	-0.880216000
1	3.698652000	-0.409819000	-0.464172000
23	-0.000990000	0.016683000	-0.405364000
1	-0.663051000	2.630427000	1.991685000
1	0.613981000	1.332033000	3.746674000
1	0.049236000	-2.386961000	2.115162000
1	2.679896000	-0.823475000	1.812084000
1	-1.950980000	-1.205774000	2.774161000
1	-3.657333000	0.414630000	2.001044000
6	4.530737000	-2.386523000	-0.448588000
1	5.517607000	-2.075336000	-0.811105000
1	4.600322000	-2.480567000	0.639272000
1	4.348659000	-3.387107000	-0.856345000
6	3.393402000	-1.269935000	-2.395921000
1	3.161192000	-2.227956000	-2.876276000
1	2.625304000	-0.554291000	-2.710988000
1	4.350593000	-0.932594000	-2.809302000
6	-4.360772000	-2.099328000	1.093835000
1	-4.622472000	-3.159055000	1.200315000
1	-4.165586000	-1.719116000	2.099862000
1	-5.250649000	-1.590653000	0.714838000
6	-3.399770000	-2.603605000	-1.180964000
1	-4.289522000	-2.195527000	-1.673172000
1	-2.553108000	-2.466810000	-1.862272000
1	-3.563188000	-3.681981000	-1.073764000
6	-0.059622000	3.523279000	-2.170660000
1	0.803638000	3.099106000	-2.692418000
1	-0.879132000	2.797980000	-2.258899000
1	-0.361514000	4.427533000	-2.711769000
6	-1.030754000	4.370790000	-0.032256000
1	-0.845760000	4.731895000	0.982613000
1	-1.447562000	5.204416000	-0.608501000
1	-1.812240000	3.601070000	0.028523000
6	1.499296000	-3.546181000	-0.650378000

1	2.161865000	-3.703134000	-1.515100000
6	0.069559000	-3.791012000	-1.111489000
1	-0.644375000	-3.621977000	-0.297039000
1	-0.219800000	-3.115525000	-1.923075000
1	-0.065277000	-4.821374000	-1.462122000
6	1.891630000	-4.537697000	0.436028000
1	1.754499000	-5.567666000	0.086123000
1	2.934186000	-4.438091000	0.749523000
1	1.269442000	-4.419620000	1.330033000
6	-3.593790000	0.794936000	-1.070906000
1	-3.268601000	1.811339000	-0.793491000
6	-5.080023000	0.674946000	-0.766951000
1	-5.482790000	-0.290467000	-1.090148000
1	-5.301809000	0.786025000	0.298500000
1	-5.648934000	1.446332000	-1.299567000
6	-3.310194000	0.623586000	-2.559031000
1	-3.634425000	-0.354094000	-2.928813000
1	-3.835557000	1.381039000	-3.152015000
1	-2.240063000	0.715824000	-2.779382000
6	2.699809000	2.499598000	0.153306000
1	3.052465000	1.575860000	0.638772000
6	3.214880000	3.687814000	0.951969000
1	4.305472000	3.766463000	0.871359000
1	2.804955000	4.638047000	0.590535000
1	2.978380000	3.611700000	2.016060000
6	3.238843000	2.514408000	-1.270660000
1	4.332653000	2.445066000	-1.282100000
1	2.849361000	1.679436000	-1.864056000
1	2.975415000	3.442707000	-1.791151000
15	-2.421162000	-0.231257000	-0.036614000
15	0.834799000	2.262062000	0.141344000
15	1.745931000	-1.724171000	-0.193072000
5	-0.049996000	-0.148393000	2.253256000

[1d'_{sc}] (TE = -2767.668511)

6	0.956324000	1.927594000	1.584134000
6	0.757260000	0.547469000	2.188438000
6	-2.473681000	1.074071000	0.908879000
6	-1.727493000	0.211264000	1.920395000
6	1.069058000	-2.444235000	1.413938000
6	-0.190822000	-1.754954000	1.909354000
1	-1.988174000	2.042441000	0.754563000
1	-1.695835000	0.786842000	2.866171000
1	1.065827000	-3.515127000	1.639450000
1	-0.221404000	-1.905339000	3.011155000

1	1.716238000	2.508392000	2.117991000
1	1.726495000	0.028144000	2.145186000
6	1.158760000	3.406307000	-0.873401000
1	1.564680000	3.296540000	-1.887138000
6	-3.492911000	-1.211972000	-0.463871000
1	-2.999556000	-1.698329000	0.386511000
6	3.117372000	-1.786899000	-0.429706000
1	3.212603000	-0.966787000	0.296009000
23	-0.082522000	-0.188459000	-0.679612000
16	-2.495028000	0.345533000	-0.779902000
16	1.496098000	1.714993000	-0.164110000
16	1.288967000	-2.228278000	-0.411175000
6	-0.328749000	-0.284811000	1.505441000
1	0.023696000	2.504222000	1.589697000
1	0.557684000	0.689063000	3.271629000
1	-1.057381000	-2.312429000	1.522586000
1	1.967850000	-2.020982000	1.874725000
1	-2.371777000	-0.648777000	2.156867000
1	-3.504977000	1.282544000	1.219900000
6	3.964222000	-2.971598000	-0.016530000
1	5.027418000	-2.704063000	0.000406000
1	3.706004000	-3.339929000	0.980373000
1	3.843987000	-3.804062000	-0.717617000
6	3.451653000	-1.281727000	-1.815972000
1	3.308923000	-2.062898000	-2.570980000
1	2.826824000	-0.425493000	-2.092303000
1	4.497460000	-0.961545000	-1.870708000
6	-4.933360000	-0.883951000	-0.133511000
1	-5.507457000	-1.800563000	0.044414000
1	-5.025806000	-0.268420000	0.765432000
1	-5.416983000	-0.347162000	-0.956149000
6	-3.349715000	-2.090727000	-1.687600000
1	-3.765078000	-1.611361000	-2.581381000
1	-2.295535000	-2.322005000	-1.881795000
1	-3.880949000	-3.037571000	-1.545995000
6	-0.318712000	3.727071000	-0.959605000
1	-0.880352000	2.933603000	-1.462697000
1	-0.759255000	3.871137000	0.032954000
1	-0.477210000	4.659505000	-1.512762000
6	1.945234000	4.468329000	-0.129678000
1	3.007611000	4.220470000	-0.062601000
1	1.857011000	5.437377000	-0.633240000
1	1.568194000	4.603761000	0.889186000

[1e' ssi] (TE = -3019.083593)

23	-0.011401000	-0.212553000	-1.017073000
16	2.063455000	-1.574640000	-1.041490000
16	-2.304978000	-1.207352000	-1.204824000
16	-0.379837000	1.913442000	0.218293000
14	-0.214694000	-1.005529000	1.308329000
6	-0.272646000	0.453361000	2.560032000
6	0.369284000	1.665349000	1.898976000
6	-2.284629000	-2.533028000	0.089131000
6	-1.810838000	-2.075020000	1.464142000
6	1.345875000	-2.079258000	1.659767000
6	1.837324000	-2.738371000	0.378469000
1	1.102132000	-3.452076000	-0.009801000
1	2.776406000	-3.292710000	0.493976000
1	2.134822000	-1.427443000	2.064248000
1	1.192910000	-2.860352000	2.419378000
1	-3.279721000	-2.994564000	0.096810000
1	-1.600050000	-3.271214000	-0.342466000
1	-2.599556000	-1.477724000	1.943211000
1	-1.692658000	-2.963566000	2.100827000
1	-1.317591000	0.686003000	2.807679000
1	0.235015000	0.260545000	3.515173000
1	1.446638000	1.509764000	1.759113000
1	0.232179000	2.596520000	2.463331000
6	3.476543000	-0.512957000	-0.406824000
1	3.034644000	0.109107000	0.384442000
6	-3.481979000	0.009481000	-0.419172000
1	-2.961221000	0.377903000	0.475663000
6	0.413392000	3.533214000	-0.266939000
1	0.139620000	3.590460000	-1.328459000
6	-4.799924000	-0.633100000	-0.040448000
1	-5.486424000	0.120830000	0.361614000
1	-5.286195000	-1.091028000	-0.908263000
1	-4.687422000	-1.403743000	0.726377000
6	-3.656128000	1.151683000	-1.399195000
1	-2.691521000	1.577845000	-1.695421000
1	-4.175446000	0.823905000	-2.306205000
1	-4.247098000	1.955344000	-0.948135000
6	-0.207667000	4.700679000	0.475527000
1	0.000184000	4.652839000	1.549385000
1	0.201105000	5.651942000	0.114960000
1	-1.292632000	4.732773000	0.349363000
6	1.923010000	3.492807000	-0.143364000
1	2.375332000	4.361279000	-0.635140000
1	2.242627000	3.517599000	0.903398000

1	2.340320000	2.590455000	-0.600830000
6	3.895673000	0.365927000	-1.567449000
1	4.615556000	1.123764000	-1.240823000
1	4.367080000	-0.222965000	-2.361403000
1	3.036243000	0.889142000	-2.004015000
6	4.626076000	-1.332562000	0.139472000
1	5.467471000	-0.679644000	0.398602000
1	4.358013000	-1.882612000	1.044878000
1	4.988745000	-2.054691000	-0.599823000

[$\mathbf{1f}_{SB}$] (TE = -2754.429904)

6	-1.088334000	-1.909816000	1.608422000
6	-0.841994000	-0.560484000	2.268320000
6	2.498242000	-1.244668000	0.854186000
6	1.894041000	-0.403586000	1.972875000
6	-0.873173000	2.562475000	1.382335000
6	0.385239000	1.868382000	1.873278000
1	1.928303000	-2.163744000	0.684873000
1	1.869781000	-1.060253000	2.860879000
1	-0.857719000	3.646221000	1.539132000
1	0.501545000	2.148884000	2.939270000
1	-1.878428000	-2.488769000	2.099923000
1	-1.774291000	0.022995000	2.211771000
6	-1.366502000	-3.341971000	-0.871548000
1	-1.763201000	-3.196296000	-1.884425000
6	3.521132000	1.070067000	-0.457707000
1	3.076446000	1.529680000	0.432582000
6	-3.014862000	1.950783000	-0.375209000
1	-3.142994000	1.158610000	0.376043000
23	0.075271000	0.144828000	-0.714955000
16	2.461659000	-0.438142000	-0.805697000
16	-1.604674000	-1.642893000	-0.142762000
16	-1.166295000	2.267180000	-0.425267000
1	-0.176804000	-2.520229000	1.601030000
1	-0.711626000	-0.761944000	3.348299000
1	1.257505000	2.327476000	1.382722000
1	-1.763034000	2.173139000	1.889704000
1	2.622606000	0.378222000	2.239911000
1	3.532747000	-1.549682000	1.056838000
6	-3.765861000	3.201063000	0.031470000
1	-4.843385000	3.006309000	0.085323000
1	-3.453815000	3.574055000	1.010808000
1	-3.611160000	4.006255000	-0.694250000
6	-3.431468000	1.435810000	-1.735797000

1	-3.260827000	2.185920000	-2.515940000
1	-2.880903000	0.529705000	-2.010088000
1	-4.498631000	1.190543000	-1.745751000
6	4.958574000	0.676550000	-0.191574000
1	5.570917000	1.563929000	0.005870000
1	5.056781000	0.019509000	0.676801000
1	5.395628000	0.159896000	-1.052323000
6	3.371167000	2.010522000	-1.633652000
1	3.746088000	1.561877000	-2.560609000
1	2.320709000	2.283798000	-1.788318000
1	3.936577000	2.932580000	-1.463459000
6	0.089821000	-3.747471000	-0.959404000
1	0.695776000	-2.984362000	-1.458246000
1	0.521056000	-3.921620000	0.032405000
1	0.193819000	-4.684318000	-1.517998000
6	-2.215834000	-4.365365000	-0.142555000
1	-3.261005000	-4.054264000	-0.068856000
1	-2.187820000	-5.328922000	-0.663106000
1	-1.846251000	-4.541567000	0.872587000
5	0.436441000	0.266650000	1.751909000

[1a''_{pc}] (TE = -3409.796611)

6	-1.168455000	0.729630000	1.595096000
6	-1.791861000	0.251621000	2.759043000
1	-1.338023000	-0.585577000	3.286754000
6	-2.962134000	0.812370000	3.260224000
1	-3.414193000	0.404287000	4.162768000
6	-3.540403000	1.900322000	2.618194000
1	-4.450602000	2.354921000	3.003565000
6	-2.948622000	2.394039000	1.458530000
1	-3.428523000	3.222390000	0.940544000
6	-1.791091000	1.818621000	0.920350000
6	0.314724000	-1.301633000	1.570780000
6	1.201743000	-1.607048000	2.616577000
1	1.737535000	-0.796195000	3.106172000
6	1.431486000	-2.912996000	3.036224000
1	2.137976000	-3.104929000	3.842107000
6	0.757564000	-3.966119000	2.430084000
1	0.928322000	-4.992761000	2.747189000
6	-0.140271000	-3.690941000	1.402965000
1	-0.657636000	-4.519306000	0.926226000
6	-0.361539000	-2.384272000	0.955590000
6	1.327928000	0.938377000	1.408335000
6	1.380515000	1.787583000	2.521537000
1	0.485557000	1.906722000	3.131056000

6	2.539745000	2.473202000	2.868550000
1	2.542142000	3.129027000	3.737671000
6	3.696431000	2.307457000	2.115885000
1	4.611745000	2.831490000	2.382703000
6	3.673772000	1.459812000	1.011105000
1	4.582159000	1.334373000	0.427863000
6	2.507408000	0.787891000	0.633676000
6	0.109187000	0.115624000	1.091034000
23	-0.105389000	0.058260000	-1.157584000
6	-2.809796000	2.635954000	-1.688520000
1	-3.355404000	3.397845000	-1.117939000
6	-1.090509000	-3.535506000	-1.632515000
1	-0.049591000	-3.807439000	-1.396143000
6	3.508306000	0.553579000	-2.192008000
1	3.163186000	0.035659000	-3.101278000
6	5.011397000	0.314318000	-2.096013000
1	5.511455000	0.749093000	-2.969852000
1	5.464416000	0.778462000	-1.216520000
1	5.272448000	-0.745041000	-2.077411000
6	3.201381000	2.036790000	-2.372956000
1	3.530893000	2.623182000	-1.508582000
1	3.718497000	2.435259000	-3.252727000
1	2.128797000	2.223503000	-2.498133000
6	-2.498078000	3.198324000	-3.070532000
1	-1.994832000	4.168244000	-3.035281000
1	-1.856033000	2.516749000	-3.642794000
1	-3.417346000	3.332946000	-3.651221000
6	-3.686571000	1.401604000	-1.801734000
1	-3.888975000	0.942161000	-0.829220000
1	-4.650007000	1.644274000	-2.264997000
1	-3.203054000	0.640583000	-2.424421000
6	-1.963899000	-4.766914000	-1.415567000
1	-1.612615000	-5.591208000	-2.047578000
1	-1.961947000	-5.132266000	-0.387239000
1	-3.005895000	-4.586880000	-1.691585000
6	-1.134293000	-3.112432000	-3.099053000
1	-2.135509000	-2.780851000	-3.396938000
1	-0.440495000	-2.287969000	-3.302937000
1	-0.861651000	-3.944206000	-3.758860000
15	2.340285000	-0.180359000	-0.914209000
15	-1.323070000	-2.007563000	-0.556923000
15	-1.215823000	2.238764000	-0.776968000
6	-3.114266000	-1.945801000	0.018793000
1	-3.152719000	-0.931421000	0.444915000
6	-4.090293000	-1.994271000	-1.151411000
1	-4.235329000	-3.012648000	-1.521760000

1	-5.076691000	-1.626098000	-0.847792000
1	-3.765226000	-1.381470000	-1.995963000
6	-3.502685000	-2.920311000	1.120867000
1	-4.520193000	-2.710393000	1.471996000
1	-3.492329000	-3.960076000	0.779525000
1	-2.838223000	-2.848859000	1.985801000
6	-0.450264000	3.960688000	-0.736381000
1	-0.193549000	4.128995000	-1.793651000
6	0.838067000	3.998346000	0.066754000
1	0.637059000	3.911064000	1.137819000
1	1.525754000	3.191884000	-0.198732000
1	1.358268000	4.950478000	-0.088912000
6	-1.386770000	5.068468000	-0.272879000
1	-0.869537000	6.034980000	-0.285882000
1	-2.278931000	5.177436000	-0.895074000
1	-1.716256000	4.901325000	0.758367000
6	3.003603000	-1.892661000	-0.526901000
1	2.172732000	-2.317493000	0.051301000
6	4.242250000	-1.963705000	0.354842000
1	4.446846000	-3.003484000	0.636791000
1	5.142163000	-1.581151000	-0.133876000
1	4.106657000	-1.399685000	1.282009000
6	3.121375000	-2.715997000	-1.803486000
1	3.304727000	-3.770499000	-1.569074000
1	2.201026000	-2.670610000	-2.398492000
1	3.943542000	-2.385508000	-2.446799000

[1b''_{psi}]-Quintet (TE = -3661.210176)

6	-0.793846000	1.725225000	1.799357000
6	-0.548215000	2.360355000	3.023000000
1	0.111979000	1.884840000	3.750156000
6	-1.099551000	3.602854000	3.324950000
1	-0.881623000	4.083289000	4.277352000
6	-1.923810000	4.233956000	2.398897000
1	-2.354161000	5.208413000	2.622297000
6	-2.192759000	3.619617000	1.178643000
1	-2.835744000	4.130132000	0.463941000
6	-1.629724000	2.378975000	0.865518000
6	-0.881722000	-1.368405000	1.990725000
6	-1.395821000	-1.397505000	3.292400000
1	-1.226119000	-0.545618000	3.953108000
6	-2.151133000	-2.470599000	3.757584000
1	-2.553571000	-2.461603000	4.769185000
6	-2.396610000	-3.552540000	2.918823000
1	-2.989778000	-4.395167000	3.269215000

6	-1.887566000	-3.554396000	1.622809000
1	-2.093886000	-4.408272000	0.981857000
6	-1.144588000	-2.470559000	1.144660000
6	1.841446000	0.059161000	1.789948000
6	2.257226000	-0.345829000	3.064574000
1	1.508436000	-0.537395000	3.834830000
6	3.599897000	-0.557517000	3.364277000
1	3.894641000	-0.890516000	4.358065000
6	4.564058000	-0.359085000	2.381024000
1	5.615553000	-0.535434000	2.599617000
6	4.181155000	0.061836000	1.111285000
1	4.947789000	0.213803000	0.354914000
6	2.832388000	0.270699000	0.803055000
23	-0.069811000	-0.041483000	-1.224729000
6	-3.679711000	0.943248000	-0.561692000
1	-4.300923000	1.839829000	-0.424226000
6	0.890346000	-3.656153000	-0.508483000
1	0.423892000	-4.617403000	-0.246092000
6	2.676069000	2.597346000	-0.963489000
1	2.790407000	2.787691000	-2.043284000
6	3.947724000	3.020356000	-0.239398000
1	4.147481000	4.084256000	-0.413996000
1	3.842206000	2.886886000	0.841819000
1	4.837061000	2.469587000	-0.548023000
6	1.503879000	3.423628000	-0.451965000
1	1.313397000	3.233342000	0.610783000
1	1.707956000	4.495397000	-0.557481000
1	0.577889000	3.197686000	-0.985477000
6	-4.132966000	0.195309000	-1.808089000
1	-3.989438000	0.759965000	-2.734654000
1	-3.572913000	-0.740756000	-1.912154000
1	-5.195649000	-0.065802000	-1.745559000
6	-3.829861000	0.053736000	0.663076000
1	-3.502234000	0.541261000	1.585854000
1	-4.877208000	-0.240542000	0.796260000
1	-3.245339000	-0.866462000	0.557050000
6	1.584562000	-3.779803000	-1.857640000
1	2.379194000	-4.533883000	-1.822256000
1	0.908966000	-4.058556000	-2.671539000
1	2.052141000	-2.827582000	-2.136321000
6	1.900898000	-3.290756000	0.568364000
1	2.397846000	-2.342381000	0.336886000
1	1.447393000	-3.184520000	1.558117000
1	2.680258000	-4.057967000	0.640375000
14	0.026270000	0.111805000	1.200622000
15	-0.499864000	-2.391085000	-0.589168000

15	2.255153000	0.756687000	-0.882974000
15	-1.910157000	1.550151000	-0.765727000
6	-2.104375000	2.998355000	-1.974650000
1	-1.459465000	3.774483000	-1.537686000
6	-3.493071000	3.595943000	-2.165546000
1	-3.441180000	4.474378000	-2.819370000
1	-4.184540000	2.893397000	-2.640360000
1	-3.958807000	3.921091000	-1.231912000
6	-1.504203000	2.594564000	-3.318422000
1	-0.472583000	2.235022000	-3.203894000
1	-2.078782000	1.788608000	-3.791785000
1	-1.488083000	3.435119000	-4.021844000
6	3.452695000	-0.037693000	-2.108158000
1	3.624234000	-1.036119000	-1.675803000
6	2.687103000	-0.210625000	-3.419733000
1	2.449813000	0.758601000	-3.875604000
1	3.271544000	-0.777160000	-4.153749000
1	1.739836000	-0.747585000	-3.271155000
6	4.799679000	0.614277000	-2.393208000
1	4.686917000	1.636764000	-2.768878000
1	5.459463000	0.654672000	-1.524587000
1	5.333736000	0.052642000	-3.168855000
6	-1.804544000	-3.270872000	-1.639488000
1	-2.747712000	-2.954670000	-1.166162000
6	-1.779191000	-4.793612000	-1.707089000
1	-2.640239000	-5.164187000	-2.275481000
1	-0.885132000	-5.163246000	-2.218684000
1	-1.810371000	-5.279329000	-0.729642000
6	-1.767633000	-2.690078000	-3.052134000
1	-1.800636000	-1.592514000	-3.043940000
1	-0.855881000	-2.983966000	-3.584986000
1	-2.616471000	-3.040449000	-3.650872000

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6	1.482139000	-0.420617000	2.071463000
6	1.620743000	-1.093442000	3.299667000
1	0.720009000	-1.383639000	3.840624000
6	2.857312000	-1.375910000	3.867032000
1	2.911025000	-1.882097000	4.830062000
6	4.028881000	-0.986098000	3.220751000
1	5.001184000	-1.174538000	3.671419000
6	3.938274000	-0.369274000	1.978525000
1	4.854389000	-0.078604000	1.465466000
6	2.693524000	-0.122470000	1.387159000
6	-0.134048000	1.592536000	1.490224000

6	0.774620000	2.427872000	2.227107000
1	1.494827000	1.928263000	2.873947000
6	0.737813000	3.797188000	2.242724000
1	1.419860000	4.348580000	2.888905000
6	-0.188763000	4.495969000	1.434800000
1	-0.230543000	5.583242000	1.448759000
6	-1.048562000	3.777792000	0.647120000
1	-1.778505000	4.313319000	0.044758000
6	-1.054529000	2.348208000	0.622396000
6	-1.138244000	-1.000972000	1.715242000
6	-1.757592000	-1.153179000	2.968242000
1	-1.489008000	-0.464042000	3.770040000
6	-2.710443000	-2.135463000	3.214917000
1	-3.174029000	-2.213997000	4.197396000
6	-3.070297000	-3.020806000	2.202978000
1	-3.806267000	-3.801077000	2.387148000
6	-2.479316000	-2.903112000	0.948934000
1	-2.757034000	-3.609604000	0.171757000
6	-1.537171000	-1.897116000	0.696333000
23	0.107042000	0.722419000	-0.663974000
6	3.821832000	1.811323000	-0.535614000
1	4.796942000	1.381934000	-0.261989000
6	-3.964519000	1.486399000	0.152522000
1	-4.233044000	2.551400000	0.226354000
6	0.395121000	-3.232377000	-1.031352000
1	1.135011000	-2.988286000	-1.808016000
6	-0.325396000	-4.507497000	-1.449697000
1	0.381655000	-5.345524000	-1.462970000
1	-1.116436000	-4.777529000	-0.743206000
1	-0.768851000	-4.449439000	-2.445476000
6	1.129263000	-3.469545000	0.285464000
1	0.435831000	-3.803113000	1.064787000
1	1.888824000	-4.250171000	0.165225000
1	1.624369000	-2.576608000	0.672642000
6	3.883702000	2.291269000	-1.980778000
1	4.244938000	1.526325000	-2.672102000
1	2.895637000	2.613175000	-2.334419000
1	4.554445000	3.152500000	-2.073799000
6	3.518787000	2.971447000	0.397425000
1	3.474625000	2.663106000	1.445290000
1	4.286903000	3.748034000	0.306897000
1	2.553796000	3.432201000	0.158839000
6	-4.876137000	0.803098000	-0.858426000
1	-5.916023000	0.819014000	-0.514182000
1	-4.856250000	1.275473000	-1.845255000
1	-4.597885000	-0.249148000	-0.988452000

6	-4.086559000	0.850673000	1.526277000
1	-3.896092000	-0.225598000	1.483055000
1	-3.382686000	1.277494000	2.246261000
1	-5.098371000	0.991098000	1.922399000
5	0.052614000	0.052959000	1.526167000
15	2.551760000	0.457227000	-0.346829000
15	-2.199294000	1.466584000	-0.448181000
15	-0.643109000	-1.669516000	-0.892380000
6	-2.282129000	2.392043000	-2.080887000
1	-2.757878000	1.639346000	-2.729490000
6	-0.853843000	2.574337000	-2.592931000
1	-0.835453000	3.004710000	-3.600237000
1	-0.266257000	3.237023000	-1.947612000
1	-0.315025000	1.607167000	-2.697078000
6	-3.103533000	3.669251000	-2.200167000
1	-3.228854000	3.944836000	-3.253780000
1	-4.106607000	3.562808000	-1.777335000
1	-2.629249000	4.521833000	-1.708705000
6	3.286571000	-0.959390000	-1.352788000
1	2.856675000	-1.836676000	-0.853091000
6	4.801251000	-1.102965000	-1.319999000
1	5.108720000	-2.006125000	-1.859758000
1	5.307282000	-0.261781000	-1.805089000
1	5.195614000	-1.189848000	-0.305279000
6	2.767390000	-0.949354000	-2.787352000
1	3.011743000	-1.889478000	-3.296350000
1	1.679813000	-0.823916000	-2.820677000
1	3.205193000	-0.143428000	-3.384167000
6	-1.880525000	-1.732248000	-2.314544000
1	-2.305477000	-0.720276000	-2.253910000
6	-1.115735000	-1.810127000	-3.633062000
1	-0.600756000	-2.766894000	-3.768104000
1	-1.797171000	-1.693375000	-4.482812000
1	-0.359049000	-1.022002000	-3.711238000
6	-3.062042000	-2.693104000	-2.278538000
1	-2.773133000	-3.746345000	-2.265480000
1	-3.706059000	-2.516082000	-1.414924000
1	-3.680932000	-2.545176000	-3.172086000

[1d''_{sc}] (TE = -3224.941794)

6	-0.136847000	1.532528000	0.983608000
6	0.453186000	2.054050000	2.147715000
1	1.048309000	1.387298000	2.769498000
6	0.303497000	3.381546000	2.532972000
1	0.782671000	3.736768000	3.443498000

6	-0.458573000	4.250992000	1.760199000
1	-0.581491000	5.292016000	2.050179000
6	-1.033832000	3.780313000	0.585443000
1	-1.586779000	4.457861000	-0.062782000
6	-0.868590000	2.449659000	0.197242000
6	-1.157673000	-0.739291000	1.178179000
6	-1.753144000	-0.419881000	2.410560000
1	-1.399197000	0.460877000	2.943675000
6	-2.768899000	-1.183437000	2.974508000
1	-3.195390000	-0.890620000	3.932240000
6	-3.234081000	-2.318954000	2.320537000
1	-4.028330000	-2.924381000	2.751301000
6	-2.694244000	-2.650598000	1.083595000
1	-3.083165000	-3.501740000	0.527550000
6	-1.684808000	-1.871055000	0.515087000
6	1.325081000	-0.499170000	1.037815000
6	1.490264000	-1.123893000	2.285873000
1	0.626467000	-1.199469000	2.943798000
6	2.702816000	-1.656075000	2.708167000
1	2.772836000	-2.131913000	3.684697000
6	3.817999000	-1.587253000	1.881784000
1	4.769752000	-2.012984000	2.191339000
6	3.692353000	-0.995300000	0.630759000
1	4.536560000	-0.986420000	-0.054472000
6	2.473290000	-0.453491000	0.211691000
16	2.354240000	0.053895000	-1.511300000
16	-1.412993000	1.989374000	-1.450633000
16	-1.234934000	-2.223168000	-1.187095000
23	-0.107948000	-0.085278000	-1.572166000
6	-3.294807000	1.912102000	-1.289220000
1	-3.589008000	2.958179000	-1.137272000
6	-0.226512000	-3.818136000	-1.052817000
1	-0.963711000	-4.571880000	-0.748924000
6	3.195623000	1.748842000	-1.588307000
1	3.154565000	1.920034000	-2.672310000
6	4.638091000	1.656570000	-1.140740000
1	5.155809000	2.601460000	-1.340959000
1	4.708750000	1.474617000	-0.063895000
1	5.184529000	0.861716000	-1.655846000
6	2.424937000	2.824311000	-0.863805000
1	2.377206000	2.626694000	0.211648000
1	2.913647000	3.796611000	-0.997799000
1	1.400047000	2.910954000	-1.231562000
6	-3.804753000	1.409923000	-2.622460000
1	-3.479207000	2.035897000	-3.458368000
1	-3.454168000	0.386797000	-2.808039000

1	-4.899141000	1.386013000	-2.630060000
6	-3.748464000	1.058631000	-0.131848000
1	-3.327533000	1.391849000	0.820348000
1	-4.840748000	1.093863000	-0.044086000
1	-3.460206000	0.012833000	-0.275612000
6	0.277246000	-4.106753000	-2.450065000
1	0.833160000	-5.049561000	-2.470555000
1	-0.533437000	-4.181483000	-3.180697000
1	0.961828000	-3.316183000	-2.782838000
6	0.885811000	-3.721199000	-0.039996000
1	1.618317000	-2.961867000	-0.331134000
1	0.518623000	-3.464305000	0.956886000
1	1.412403000	-4.679928000	0.035564000
6	-0.010323000	0.071715000	0.605067000

[1e''_{ssi}] (TE = -3476.343678)

6	-0.848957000	1.714123000	1.200441000
6	-0.763924000	2.292652000	2.474550000
1	-0.194520000	1.783913000	3.253534000
6	-1.375503000	3.506048000	2.776380000
1	-1.285880000	3.930114000	3.774858000
6	-2.095548000	4.181384000	1.795553000
1	-2.571118000	5.133993000	2.019419000
6	-2.186878000	3.646293000	0.514367000
1	-2.722853000	4.182913000	-0.266792000
6	-1.568953000	2.429692000	0.225743000
6	-1.002861000	-1.372258000	1.387512000
6	-1.461849000	-1.469498000	2.708868000
1	-1.238404000	-0.664256000	3.410088000
6	-2.207662000	-2.556968000	3.154503000
1	-2.552358000	-2.597777000	4.186200000
6	-2.520244000	-3.588738000	2.274727000
1	-3.109755000	-4.439347000	2.610454000
6	-2.096354000	-3.519172000	0.951281000
1	-2.361126000	-4.307837000	0.248839000
6	-1.349940000	-2.423308000	0.518188000
6	1.772722000	-0.023188000	1.230831000
6	2.183248000	-0.368347000	2.525771000
1	1.431856000	-0.483037000	3.308105000
6	3.518949000	-0.601195000	2.842279000
1	3.800288000	-0.878233000	3.856690000
6	4.490887000	-0.499960000	1.852991000
1	5.535270000	-0.699327000	2.083727000
6	4.121269000	-0.164123000	0.553556000

1	4.871008000	-0.114338000	-0.233216000
6	2.780454000	0.078538000	0.250373000
16	2.378586000	0.435355000	-1.489393000
16	-1.683365000	1.827769000	-1.487393000
16	-0.887117000	-2.384663000	-1.240264000
23	-0.072562000	-0.076370000	-1.760388000
6	-3.486184000	1.274428000	-1.493154000
1	-4.051898000	2.194120000	-1.298906000
6	0.473105000	-3.691814000	-1.221308000
1	-0.038795000	-4.607479000	-0.900161000
6	2.775008000	2.279548000	-1.571418000
1	2.452270000	2.498526000	-2.597973000
6	4.261587000	2.530859000	-1.433047000
1	4.487518000	3.582626000	-1.642573000
1	4.605041000	2.327761000	-0.414013000
1	4.852534000	1.917745000	-2.118706000
6	1.952972000	3.080437000	-0.589192000
1	2.176147000	2.796961000	0.445404000
1	2.173728000	4.149155000	-0.689834000
1	0.881723000	2.941997000	-0.747506000
6	-3.772543000	0.761016000	-2.887300000
1	-3.591558000	1.517203000	-3.656407000
1	-3.142274000	-0.110187000	-3.111251000
1	-4.814912000	0.437522000	-2.971552000
6	-3.766338000	0.241210000	-0.426753000
1	-3.496624000	0.587237000	0.575236000
1	-4.833300000	-0.009327000	-0.416162000
1	-3.210822000	-0.681706000	-0.620602000
6	0.957844000	-3.828465000	-2.647998000
1	1.739177000	-4.592074000	-2.717205000
1	0.155178000	-4.104652000	-3.337598000
1	1.395334000	-2.883101000	-2.996209000
6	1.587234000	-3.339480000	-0.263680000
1	2.104500000	-2.430096000	-0.584779000
1	1.228614000	-3.175033000	0.756563000
1	2.326511000	-4.148057000	-0.230434000
14	-0.035036000	0.087637000	0.625723000

$[1f'_{SB}]$ (TE = -3211.719426)

6	0.248550000	1.494728000	0.860118000
6	1.428270000	1.911551000	1.581960000
1	1.842672000	1.198552000	2.294410000
6	1.993233000	3.156226000	1.510788000
1	2.840320000	3.398750000	2.151606000
6	1.473971000	4.138763000	0.629270000

1	1.923135000	5.127305000	0.568957000
6	0.395002000	3.816222000	-0.147513000
1	-0.029170000	4.548323000	-0.832574000
6	-0.213834000	2.524801000	-0.088449000
6	-1.622503000	-0.648911000	0.924114000
6	-2.398714000	-0.679369000	2.098415000
1	-2.048253000	-0.118855000	2.965936000
6	-3.583454000	-1.401448000	2.199390000
1	-4.148079000	-1.393459000	3.130101000
6	-4.047691000	-2.135778000	1.110588000
1	-4.974626000	-2.701075000	1.177990000
6	-3.326620000	-2.120017000	-0.076900000
1	-3.695580000	-2.656177000	-0.949886000
6	-2.138598000	-1.391226000	-0.153402000
6	0.963683000	-1.002171000	1.400314000
6	0.818189000	-1.751269000	2.583977000
1	-0.092290000	-1.619451000	3.168774000
6	1.780589000	-2.642395000	3.041164000
1	1.620798000	-3.185600000	3.971073000
6	2.944365000	-2.851916000	2.303845000
1	3.697373000	-3.560733000	2.641088000
6	3.113298000	-2.173624000	1.104472000
1	3.980029000	-2.380483000	0.478894000
6	2.149999000	-1.256294000	0.677799000
16	2.303409000	-0.614086000	-1.003097000
16	-1.644699000	2.303817000	-1.125625000
16	-1.294718000	-1.303159000	-1.740565000
23	0.162747000	0.638930000	-1.231559000
6	-3.248407000	2.546958000	-0.138713000
1	-3.631284000	3.470642000	-0.589771000
6	-0.718534000	-3.059571000	-2.011828000
1	-1.651405000	-3.613079000	-2.178022000
6	3.803293000	0.526374000	-1.094169000
1	4.462676000	0.007688000	-1.799786000
6	4.509271000	0.695860000	0.230236000
1	5.348670000	1.388437000	0.102633000
1	3.843690000	1.117163000	0.986293000
1	4.912545000	-0.240996000	0.617991000
6	3.348427000	1.841093000	-1.695377000
1	2.695532000	2.388352000	-1.008617000
1	4.213676000	2.478345000	-1.911705000
1	2.809721000	1.698286000	-2.639045000
6	-4.224748000	1.421885000	-0.395858000
1	-4.331172000	1.199080000	-1.461964000
1	-3.928390000	0.504444000	0.112852000
1	-5.216550000	1.702352000	-0.021918000

6	-2.943573000	2.783997000	1.320580000
1	-2.280294000	3.639994000	1.469211000
1	-3.875038000	2.982245000	1.863497000
1	-2.468829000	1.913321000	1.776758000
6	0.109638000	-3.056454000	-3.280479000
1	0.416004000	-4.076689000	-3.532072000
1	-0.439587000	-2.654004000	-4.136132000
1	1.021289000	-2.463773000	-3.149100000
6	0.020355000	-3.634062000	-0.825261000
1	0.992556000	-3.155763000	-0.689487000
1	-0.538611000	-3.526333000	0.108088000
1	0.196939000	-4.703815000	-0.985557000
5	-0.167249000	0.016549000	0.903890000

{[HIPTN₃N]-V} (TE = -2093.484933)

23	0.415341000	0.537039000	-0.265360000
7	-0.813317000	1.043539000	-1.698260000
7	2.377982000	0.410894000	-0.338327000
7	-0.489050000	0.843160000	1.425721000
6	-1.385287000	2.340613000	-1.379024000
1	-1.963074000	2.756484000	-2.220391000
1	-2.093125000	2.276385000	-0.534210000
6	-0.241262000	3.289940000	-1.042615000
1	0.256363000	3.599116000	-1.965295000
1	-0.603329000	4.201062000	-0.550356000
6	-0.536040000	2.233100000	1.844230000
1	-1.464482000	2.732472000	1.516119000
1	-0.518812000	2.332518000	2.940782000
6	0.667363000	2.941053000	1.253100000
1	1.577756000	2.577090000	1.739714000
1	0.621692000	4.029459000	1.402264000
6	3.072338000	1.677120000	-0.200182000
1	3.384332000	1.858704000	0.844436000
1	4.003122000	1.704773000	-0.789293000
6	2.168883000	2.789165000	-0.702098000
1	2.563337000	3.784579000	-0.448973000
1	2.101867000	2.725261000	-1.791970000
7	0.786026000	2.616516000	-0.189460000
6	3.094797000	-0.741918000	-0.070154000
6	2.459338000	-1.992130000	-0.235186000
6	4.430859000	-0.756091000	0.377017000
6	3.109393000	-3.180613000	0.045573000
1	1.433911000	-2.019231000	-0.612595000
6	5.079004000	-1.957119000	0.649324000
1	4.966882000	0.177839000	0.521760000

6	4.431755000	-3.177196000	0.493291000
1	2.582725000	-4.122709000	-0.094653000
1	6.111219000	-1.932017000	0.994985000
1	4.945181000	-4.110287000	0.709935000
6	-1.669541000	-0.022280000	-1.922348000
6	-1.080876000	-1.263445000	-2.258401000
6	-3.069932000	0.017036000	-1.766017000
6	-1.846638000	-2.414866000	-2.371952000
1	-0.011294000	-1.289491000	-2.474061000
6	-3.824865000	-1.141142000	-1.897383000
1	-3.564185000	0.953712000	-1.521545000
6	-3.226576000	-2.365422000	-2.187618000
1	-1.362435000	-3.355308000	-2.628710000
1	-4.903216000	-1.087072000	-1.758065000
1	-3.829374000	-3.264939000	-2.281975000
6	-1.511959000	-0.001384000	1.833802000
6	-1.403371000	-1.378255000	1.545528000
6	-2.682679000	0.437777000	2.479607000
6	-2.433943000	-2.256761000	1.831951000
1	-0.478417000	-1.762651000	1.108495000
6	-3.704250000	-0.457487000	2.780335000
1	-2.800612000	1.486341000	2.740106000
6	-3.598969000	-1.804373000	2.451635000
1	-2.321234000	-3.309706000	1.581500000
1	-4.600278000	-0.089048000	3.277061000
1	-4.404126000	-2.495926000	2.686003000

Cartesian coordinates of $[1a'_{PC}]-[1f'_{SB}]$ and $[1a''_{PC}]-[1f''_{SB}]$ along with their total energies (in hartree) including zero point vibrational correction at M06-D3(heptane)/def2-SVP level of theory.

$[1a'_{PC}]$ (TE = -2950.485167)

6	-0.057442000	2.458634000	1.778219000
6	0.505181000	1.212256000	2.453192000
6	-2.612267000	-0.074047000	1.618040000
6	-1.402352000	-0.440843000	2.477688000
6	2.292719000	-1.293180000	1.672674000
6	0.953696000	-1.221646000	2.402530000
1	-2.719009000	1.022004000	1.503653000
1	-1.543475000	0.015164000	3.486817000
1	2.927379000	-2.117849000	2.050743000
1	1.158683000	-1.121328000	3.498075000
1	0.319458000	3.389145000	2.242054000
1	1.610501000	1.254722000	2.359286000
6	-0.613935000	3.837571000	-0.783356000
1	0.032786000	4.164628000	-1.621972000

6	-2.710114000	-2.554327000	0.046900000
1	-1.964240000	-2.800706000	0.831704000
6	3.629967000	-0.699738000	-0.854853000
1	3.452573000	0.373565000	-0.641539000
23	-0.020628000	-0.052825000	-0.331807000
6	-0.003887000	-0.128445000	1.907217000
1	-1.160035000	2.486927000	1.869926000
1	0.317468000	1.291053000	3.552574000
1	0.457986000	-2.204770000	2.296433000
1	2.872883000	-0.363411000	1.830186000
1	-1.472831000	-1.531962000	2.664726000
1	-3.552526000	-0.434432000	2.078796000
6	4.953315000	-1.073621000	-0.204074000
1	5.752424000	-0.404866000	-0.570496000
1	4.925721000	-0.974114000	0.892744000
1	5.266027000	-2.102181000	-0.438374000
6	3.665527000	-0.863505000	-2.366135000
1	3.870932000	-1.908236000	-2.659355000
1	2.706071000	-0.572938000	-2.830371000
1	4.457188000	-0.238680000	-2.815704000
6	-4.073774000	-3.018239000	0.529965000
1	-4.039908000	-4.087284000	0.804599000
1	-4.425125000	-2.464019000	1.415786000
1	-4.838667000	-2.917800000	-0.258594000
6	-2.285006000	-3.276983000	-1.223721000
1	-3.014964000	-3.132433000	-2.038637000
1	-1.305213000	-2.907064000	-1.578132000
1	-2.197688000	-4.364188000	-1.051908000
6	-1.934050000	3.349761000	-1.358933000
1	-1.799008000	2.495752000	-2.044376000
1	-2.607001000	3.016241000	-0.546662000
1	-2.457038000	4.155455000	-1.903101000
6	-0.852798000	5.017503000	0.147676000
1	0.070722000	5.415674000	0.592592000
1	-1.342547000	5.844134000	-0.396545000
1	-1.526034000	4.736935000	0.975676000
6	2.063199000	-3.250187000	-0.559681000
1	1.780500000	-3.267344000	-1.632356000
6	0.955325000	-3.935964000	0.227775000
1	1.259991000	-4.096464000	1.277135000
1	0.035732000	-3.327285000	0.236281000
1	0.718204000	-4.925543000	-0.199628000
6	3.374977000	-3.998105000	-0.387726000
1	3.219185000	-5.080444000	-0.544181000
1	4.148591000	-3.677717000	-1.101590000
1	3.782650000	-3.877451000	0.631716000

6	-3.826145000	0.082567000	-1.015797000
1	-3.500769000	1.140036000	-0.970774000
6	-5.210223000	0.003297000	-0.390893000
1	-5.641694000	-1.007164000	-0.463980000
1	-5.213282000	0.294290000	0.671608000
1	-5.900701000	0.685708000	-0.917503000
6	-3.845537000	-0.325429000	-2.480887000
1	-4.216501000	-1.357505000	-2.609016000
1	-4.514787000	0.330453000	-3.064134000
1	-2.840710000	-0.272188000	-2.935566000
6	2.117734000	2.914391000	-0.145603000
1	2.602879000	2.120680000	0.459736000
6	2.507295000	4.266648000	0.423868000
1	3.605004000	4.386585000	0.411953000
1	2.091636000	5.094564000	-0.176531000
1	2.177779000	4.400913000	1.467100000
6	2.591008000	2.757079000	-1.582939000
1	3.689777000	2.841896000	-1.656040000
1	2.296441000	1.773902000	-1.990671000
1	2.161886000	3.535385000	-2.239170000
15	-2.388605000	-0.708956000	-0.107442000
15	0.317387000	2.381849000	-0.034559000
15	2.031527000	-1.405303000	-0.162019000

[1b'_{psi}] (TE = -3201.859420)

6	-0.106651000	2.744280000	1.722550000
6	0.414624000	1.672840000	2.677698000
6	-2.809897000	-0.290589000	1.717208000
6	-1.689602000	-0.667954000	2.686883000
6	2.531361000	-1.343504000	1.613478000
6	1.388408000	-1.290473000	2.629171000
1	-2.966764000	0.807080000	1.717597000
1	-1.918473000	-0.279510000	3.697688000
1	3.264087000	-2.147812000	1.824155000
1	1.788965000	-1.024561000	3.626017000
1	0.204112000	3.767346000	2.005858000
1	1.517804000	1.753460000	2.763495000
6	-0.467006000	3.824884000	-0.979332000
1	0.196937000	3.985304000	-1.851937000
6	-2.720295000	-2.538528000	-0.147267000
1	-2.083692000	-2.878943000	0.695495000
6	3.528200000	-0.834800000	-1.059806000
1	3.439430000	0.247479000	-0.837885000
23	-0.040602000	-0.022261000	-0.488790000
1	-1.215406000	2.750546000	1.721943000
1	0.019602000	1.846931000	3.697102000

1	0.929250000	-2.290112000	2.741011000
1	3.104503000	-0.394974000	1.654541000
1	-1.644889000	-1.770783000	2.791958000
1	-3.784790000	-0.738510000	1.991709000
6	4.902905000	-1.276550000	-0.580449000
1	5.681515000	-0.658522000	-1.062142000
1	5.027234000	-1.161783000	0.507766000
1	5.126013000	-2.323863000	-0.833671000
6	3.363218000	-1.002629000	-2.561618000
1	3.469878000	-2.057699000	-2.870324000
1	2.368384000	-0.657829000	-2.899001000
1	4.123193000	-0.423005000	-3.114604000
6	-4.132439000	-3.040889000	0.101081000
1	-4.131349000	-4.137565000	0.230912000
1	-4.590267000	-2.606091000	1.004479000
1	-4.794779000	-2.823249000	-0.753960000
6	-2.135341000	-3.121782000	-1.425213000
1	-2.754737000	-2.874713000	-2.304906000
1	-1.119166000	-2.723698000	-1.606195000
1	-2.068565000	-4.222531000	-1.368551000
6	-1.823559000	3.367284000	-1.494021000
1	-1.750681000	2.434601000	-2.078648000
1	-2.512529000	3.171988000	-0.650133000
1	-2.294883000	4.140095000	-2.126094000
6	-0.614552000	5.138736000	-0.224979000
1	0.331841000	5.515158000	0.190198000
1	-1.016406000	5.920113000	-0.893882000
1	-1.327984000	5.039060000	0.610702000
6	1.873295000	-3.292018000	-0.527672000
1	1.483323000	-3.315418000	-1.565952000
6	0.815807000	-3.898429000	0.384200000
1	1.210177000	-4.033089000	1.406865000
1	-0.074878000	-3.251543000	0.450069000
1	0.500673000	-4.891899000	0.020521000
6	3.153181000	-4.109274000	-0.469476000
1	2.922223000	-5.184210000	-0.576453000
1	3.862968000	-3.851273000	-1.269603000
1	3.672173000	-3.988548000	0.498003000
6	-3.797013000	0.195574000	-0.962829000
1	-3.460639000	1.241639000	-0.818106000
6	-5.215804000	0.091638000	-0.424987000
1	-5.651024000	-0.906996000	-0.585385000
1	-5.279945000	0.317208000	0.651090000
1	-5.868607000	0.813707000	-0.946976000
6	-3.739777000	-0.097632000	-2.454058000
1	-4.120198000	-1.109050000	-2.682164000

1	-4.359118000	0.616702000	-3.023856000
1	-2.708008000	-0.035090000	-2.844526000
6	2.187940000	2.808614000	-0.124826000
1	2.606859000	1.964141000	0.461087000
6	2.663433000	4.110824000	0.494716000
1	3.766952000	4.141091000	0.523179000
1	2.338439000	4.982863000	-0.098692000
1	2.307344000	4.248493000	1.528578000
6	2.679394000	2.666661000	-1.557713000
1	3.782588000	2.640666000	-1.602985000
1	2.297098000	1.737452000	-2.017694000
1	2.351070000	3.514168000	-2.185181000
15	-2.399949000	-0.684579000	-0.060625000
15	0.350645000	2.396135000	-0.053662000
15	1.979922000	-1.439419000	-0.174760000
14	0.019908000	-0.093014000	1.988493000

[1c'_{pb}] (TE = -2937.272954)

6	0.247604000	2.435721000	1.962589000
6	0.711184000	1.182979000	2.700839000
6	-2.605764000	0.251189000	1.701045000
6	-1.568259000	-0.368673000	2.637596000
6	2.196729000	-1.563759000	1.633696000
6	0.896502000	-1.530449000	2.430866000
1	-2.464925000	1.344906000	1.617596000
1	-1.730647000	0.054385000	3.652886000
1	2.865757000	-2.392101000	1.928271000
1	1.143106000	-1.640630000	3.511441000
1	0.656611000	3.375758000	2.380758000
1	1.815611000	1.107306000	2.629149000
6	-0.078096000	3.801713000	-0.659594000
1	0.649664000	4.631314000	-0.568286000
6	-3.022874000	-2.146462000	0.087848000
1	-2.143211000	-2.626746000	0.564136000
6	3.498433000	-1.112530000	-0.932006000
1	3.641397000	-0.101898000	-0.496738000
23	-0.002012000	0.000362000	-0.427266000
1	-0.850759000	2.523027000	2.024866000
1	0.510496000	1.324408000	3.785793000
1	0.292917000	-2.429142000	2.185118000
1	2.772873000	-0.630812000	1.791366000
1	-1.801529000	-1.448472000	2.742077000
1	-3.643502000	0.097527000	2.055796000
6	4.692276000	-1.976623000	-0.565010000
1	5.623196000	-1.548922000	-0.977344000
1	4.827914000	-2.066722000	0.525038000

1	4.598897000	-2.995132000	-0.980983000
6	3.357633000	-0.955065000	-2.437638000
1	3.226687000	-1.930822000	-2.938994000
1	2.483460000	-0.329799000	-2.695331000
1	4.253593000	-0.482543000	-2.876833000
6	-4.233947000	-2.418935000	0.965294000
1	-4.421110000	-3.506032000	1.020436000
1	-4.093868000	-2.063255000	1.998314000
1	-5.151145000	-1.954080000	0.569619000
6	-3.181306000	-2.750721000	-1.298687000
1	-4.098729000	-2.389104000	-1.795864000
1	-2.325423000	-2.503773000	-1.951231000
1	-3.254532000	-3.850924000	-1.244485000
6	-0.311909000	3.485609000	-2.130720000
1	0.612291000	3.199858000	-2.658889000
1	-1.015944000	2.635480000	-2.215588000
1	-0.752805000	4.346032000	-2.663321000
6	-1.385024000	4.214568000	-0.003028000
1	-1.251779000	4.578758000	1.027131000
1	-1.875354000	5.016355000	-0.581332000
1	-2.087221000	3.359632000	0.028758000
6	1.720022000	-3.434358000	-0.652020000
1	2.303341000	-3.508038000	-1.591596000
6	0.275730000	-3.784763000	-0.969075000
1	-0.356440000	-3.703384000	-0.065203000
1	-0.152060000	-3.097799000	-1.718712000
1	0.187320000	-4.818097000	-1.348782000
6	2.301514000	-4.410039000	0.358368000
1	2.219762000	-5.445169000	-0.017328000
1	3.364208000	-4.222922000	0.577897000
1	1.750070000	-4.370159000	1.313878000
6	-3.620320000	0.644111000	-1.000652000
1	-3.320553000	1.661624000	-0.672867000
6	-5.097284000	0.461413000	-0.695046000
1	-5.465206000	-0.518009000	-1.045885000
1	-5.321204000	0.541727000	0.381002000
1	-5.695848000	1.231090000	-1.213482000
6	-3.337341000	0.552617000	-2.493346000
1	-3.638264000	-0.424356000	-2.907894000
1	-3.889022000	1.329420000	-3.050771000
1	-2.260550000	0.684601000	-2.704312000
6	2.508648000	2.634461000	0.154877000
1	2.903430000	1.727207000	0.657192000
6	2.960353000	3.858161000	0.931776000
1	4.054904000	3.982248000	0.855113000
1	2.506031000	4.785258000	0.538646000

1	2.715672000	3.791593000	2.003585000
6	3.038668000	2.642607000	-1.269743000
1	4.142372000	2.612145000	-1.284206000
1	2.669107000	1.769641000	-1.836449000
1	2.733442000	3.555254000	-1.812307000
15	-2.385004000	-0.379169000	-0.025445000
15	0.658943000	2.276118000	0.161841000
15	1.845919000	-1.599564000	-0.187636000
5	0.001372000	-0.202687000	2.279101000

[1d'_{sc}] (TE = -2766.135508)

6	1.016393000	2.003803000	1.590402000
6	0.754570000	0.675167000	2.279475000
6	-2.448368000	1.179390000	0.904703000
6	-1.729800000	0.351446000	1.965338000
6	1.018009000	-2.368050000	1.556016000
6	-0.205407000	-1.630602000	2.072380000
1	-1.966144000	2.157712000	0.739821000
1	-1.726470000	0.969569000	2.894687000
1	1.035219000	-3.419459000	1.889360000
1	-0.197033000	-1.742932000	3.187212000
1	1.769913000	2.608009000	2.124888000
1	1.716875000	0.124555000	2.308604000
6	1.322076000	3.287668000	-0.974604000
1	1.745830000	3.067666000	-1.972215000
6	-3.517724000	-1.078621000	-0.468265000
1	-3.296348000	-1.390059000	0.568314000
6	2.897769000	-1.978481000	-0.543919000
1	3.115235000	-1.135338000	0.140310000
23	-0.043575000	-0.134165000	-0.546926000
16	-2.426532000	0.417708000	-0.771457000
16	1.632800000	1.664471000	-0.113255000
16	1.085472000	-2.332987000	-0.290228000
6	-0.328156000	-0.175666000	1.619496000
1	0.089384000	2.599821000	1.513057000
1	0.521577000	0.899669000	3.350447000
1	-1.100843000	-2.191308000	1.734663000
1	1.953774000	-1.896663000	1.904160000
1	-2.392000000	-0.499919000	2.220155000
1	-3.499671000	1.381581000	1.183684000
6	3.746250000	-3.185396000	-0.211856000
1	4.817996000	-2.959027000	-0.349232000
1	3.606325000	-3.515705000	0.829887000
1	3.489078000	-4.031128000	-0.872307000
6	3.066283000	-1.515539000	-1.974285000
1	2.764215000	-2.304326000	-2.685955000

1	2.454973000	-0.616138000	-2.167748000
1	4.119842000	-1.263114000	-2.180059000
6	-4.975270000	-0.701414000	-0.615553000
1	-5.627798000	-1.566942000	-0.405576000
1	-5.265474000	0.108208000	0.073342000
1	-5.185696000	-0.360429000	-1.643687000
6	-3.080202000	-2.165665000	-1.422248000
1	-3.221123000	-1.852601000	-2.472916000
1	-2.010387000	-2.399054000	-1.271935000
1	-3.668299000	-3.085562000	-1.265552000
6	-0.150511000	3.597710000	-1.119851000
1	-0.703336000	2.723455000	-1.506880000
1	-0.599731000	3.881252000	-0.151497000
1	-0.303520000	4.447267000	-1.806749000
6	2.109413000	4.409452000	-0.330947000
1	3.175876000	4.153352000	-0.232033000
1	2.031213000	5.331789000	-0.931789000
1	1.718976000	4.643325000	0.674210000

[1e'_{ssi}] (TE = -3017.497547)

23	-0.055569000	-0.147107000	-0.907639000
16	1.796221000	-1.819925000	-0.992077000
16	-2.359183000	-1.154509000	-1.141356000
16	-0.187769000	2.029271000	0.254475000
14	-0.304030000	-0.897854000	1.408304000
6	-0.222433000	0.592023000	2.633096000
6	0.540446000	1.708758000	1.935898000
6	-2.474607000	-2.350362000	0.269377000
6	-1.984399000	-1.836545000	1.616054000
6	1.162870000	-2.102257000	1.779633000
6	1.547279000	-2.860285000	0.519148000
1	0.738103000	-3.541475000	0.200045000
1	2.451993000	-3.485925000	0.623758000
1	2.019997000	-1.492463000	2.129616000
1	0.958675000	-2.833885000	2.585662000
1	-3.513649000	-2.726793000	0.285424000
1	-1.848086000	-3.184293000	-0.094099000
1	-2.724226000	-1.129850000	2.039871000
1	-1.943186000	-2.688473000	2.321738000
1	-1.254308000	0.929065000	2.852351000
1	0.258386000	0.379898000	3.606617000
1	1.597163000	1.419348000	1.783290000
1	0.521872000	2.666725000	2.487508000
6	3.327222000	-0.854319000	-0.549568000
1	3.020167000	-0.191326000	0.282753000
6	-3.465813000	0.220178000	-0.565806000

1	-3.000720000	0.609356000	0.359778000
6	0.829604000	3.500564000	-0.278936000
1	0.524987000	3.576139000	-1.339269000
6	-4.877574000	-0.253964000	-0.302321000
1	-5.516400000	0.597308000	-0.009957000
1	-5.312520000	-0.709694000	-1.208542000
1	-4.928368000	-0.993901000	0.512129000
6	-3.400069000	1.290698000	-1.634910000
1	-2.350585000	1.576797000	-1.829926000
1	-3.847414000	0.935502000	-2.579880000
1	-3.946466000	2.193039000	-1.314393000
6	0.419452000	4.761829000	0.452386000
1	0.666256000	4.702050000	1.526184000
1	0.954487000	5.637853000	0.045794000
1	-0.661876000	4.948202000	0.363472000
6	2.315243000	3.224655000	-0.209807000
1	2.884950000	4.004719000	-0.743058000
1	2.675174000	3.213097000	0.833080000
1	2.551443000	2.247484000	-0.664031000
6	3.642385000	-0.014279000	-1.768733000
1	4.453368000	0.701890000	-1.554921000
1	3.954880000	-0.648385000	-2.616585000
1	2.746122000	0.558263000	-2.075829000
6	4.480663000	-1.741959000	-0.140793000
1	5.387701000	-1.134994000	0.023466000
1	4.281675000	-2.289021000	0.794113000
1	4.704997000	-2.478652000	-0.931694000

[$\mathbf{1f}_{\text{SB}}$] (TE = -2752.915242)

6	1.187863000	1.937104000	1.629899000
6	0.827798000	0.659229000	2.369242000
6	-2.417257000	1.468647000	0.802781000
6	-1.897914000	0.652659000	1.976820000
6	0.664628000	-2.510968000	1.529946000
6	-0.532361000	-1.714204000	2.010957000
1	-1.789243000	2.357116000	0.615510000
1	-1.845619000	1.353612000	2.838005000
1	0.607158000	-3.582493000	1.787695000
1	-0.649527000	-1.933094000	3.097938000
1	1.989383000	2.514161000	2.124212000
1	1.725109000	0.008510000	2.400979000
6	1.660254000	3.144358000	-0.949509000
1	2.084810000	2.870929000	-1.933472000
6	-3.482652000	-0.846626000	-0.489030000
1	-3.170997000	-1.229682000	0.499129000
6	2.711664000	-2.226906000	-0.426201000

1	2.967906000	-1.426736000	0.295208000
23	-0.023488000	-0.103032000	-0.641836000
16	-2.354622000	0.605786000	-0.827854000
16	1.778150000	1.509245000	-0.065773000
16	0.859821000	-2.389818000	-0.306722000
1	0.304573000	2.594313000	1.526380000
1	0.642412000	0.943610000	3.429330000
1	-1.449503000	-2.131619000	1.547233000
1	1.603798000	-2.115608000	1.956519000
1	-2.679904000	-0.078877000	2.265464000
1	-3.450643000	1.835132000	0.949882000
6	3.402365000	-3.524285000	-0.070125000
1	4.498688000	-3.410845000	-0.131479000
1	3.159373000	-3.856695000	0.951569000
1	3.103143000	-4.325227000	-0.767644000
6	3.030222000	-1.757647000	-1.828550000
1	2.707988000	-2.500807000	-2.579327000
1	2.524035000	-0.799429000	-2.043777000
1	4.115460000	-1.604941000	-1.950439000
6	-4.928994000	-0.405506000	-0.459984000
1	-5.592530000	-1.262144000	-0.248990000
1	-5.115611000	0.354065000	0.316378000
1	-5.225842000	0.022431000	-1.432856000
6	-3.195970000	-1.892662000	-1.541793000
1	-3.423076000	-1.513422000	-2.554537000
1	-2.130943000	-2.185830000	-1.509746000
1	-3.810836000	-2.792627000	-1.373936000
6	0.231117000	3.601670000	-1.136275000
1	-0.394036000	2.790090000	-1.549055000
1	-0.217224000	3.921447000	-0.178959000
1	0.185735000	4.466919000	-1.819248000
6	2.541222000	4.189127000	-0.297136000
1	3.569824000	3.822801000	-0.153713000
1	2.584067000	5.099676000	-0.918987000
1	2.143161000	4.488352000	0.687295000
5	-0.475277000	-0.114141000	1.819800000

[1a''_{pc}] (TE = -3407.054006)

6	1.102277000	-0.868547000	1.596696000
6	1.782655000	-0.462513000	2.759578000
1	1.409249000	0.408940000	3.308387000
6	2.907556000	-1.129665000	3.238245000
1	3.405744000	-0.770988000	4.144653000
6	3.383969000	-2.256135000	2.574813000
1	4.262081000	-2.794703000	2.943086000
6	2.732902000	-2.683151000	1.418402000

1	3.133209000	-3.549386000	0.880290000
6	1.621102000	-2.002374000	0.905326000
6	-0.166521000	1.301423000	1.607333000
6	-0.995405000	1.684768000	2.678370000
1	-1.605632000	0.922556000	3.174363000
6	-1.076836000	3.002451000	3.120592000
1	-1.742899000	3.254741000	3.951846000
6	-0.309417000	3.990797000	2.511050000
1	-0.363398000	5.030292000	2.847554000
6	0.531153000	3.637616000	1.457755000
1	1.126665000	4.419504000	0.977076000
6	0.604796000	2.319445000	0.991265000
6	-1.412216000	-0.822706000	1.427133000
6	-1.550807000	-1.673427000	2.535328000
1	-0.666918000	-1.889323000	3.146661000
6	-2.777181000	-2.233449000	2.885090000
1	-2.845325000	-2.891647000	3.757240000
6	-3.915368000	-1.942607000	2.137937000
1	-4.885958000	-2.367544000	2.410065000
6	-3.805824000	-1.098407000	1.033393000
1	-4.703278000	-0.871276000	0.450665000
6	-2.574045000	-0.553792000	0.654193000
6	-0.115662000	-0.126213000	1.119063000
23	0.094395000	-0.078241000	-1.098345000
6	2.523848000	-2.826976000	-1.767094000
1	3.042257000	-3.658608000	-1.255235000
6	1.320047000	3.382486000	-1.648203000
1	0.305700000	3.721693000	-1.354086000
6	-3.510927000	-0.214314000	-2.203996000
1	-3.102444000	0.308105000	-3.093800000
6	-4.991349000	0.128277000	-2.127392000
1	-5.507736000	-0.257447000	-3.024117000
1	-5.491719000	-0.325424000	-1.256777000
1	-5.174615000	1.212674000	-2.092285000
6	-3.290196000	-1.705787000	-2.418341000
1	-3.694355000	-2.296406000	-1.577649000
1	-3.795181000	-2.047823000	-3.337618000
1	-2.215258000	-1.946843000	-2.501076000
6	2.120482000	-3.278054000	-3.164616000
1	1.553779000	-4.222458000	-3.170676000
1	1.496128000	-2.509769000	-3.658449000
1	3.012700000	-3.428472000	-3.796073000
6	3.455927000	-1.633436000	-1.847751000
1	3.794818000	-1.297690000	-0.853171000
1	4.350109000	-1.867125000	-2.451493000
1	2.932449000	-0.780465000	-2.318950000

6	2.280124000	4.555245000	-1.512494000
1	1.937103000	5.396560000	-2.139790000
1	2.370839000	4.934645000	-0.483317000
1	3.293769000	4.296615000	-1.858775000
6	1.241226000	2.913863000	-3.096858000
1	2.202595000	2.495202000	-3.444416000
1	0.470518000	2.130144000	-3.218503000
1	0.982653000	3.749068000	-3.771090000
15	-2.306203000	0.403749000	-0.896887000
15	1.508067000	1.861484000	-0.546343000
15	0.984010000	-2.358859000	-0.793851000
6	3.306934000	1.698576000	-0.002970000
1	3.277701000	0.676270000	0.427863000
6	4.260574000	1.678513000	-1.189420000
1	4.462821000	2.693354000	-1.569112000
1	5.233212000	1.248464000	-0.893733000
1	3.879133000	1.076215000	-2.029553000
6	3.781719000	2.644475000	1.086342000
1	4.805995000	2.374170000	1.398864000
1	3.814692000	3.692308000	0.742021000
1	3.139889000	2.600920000	1.980304000
6	0.090653000	-4.017390000	-0.742512000
1	-0.160827000	-4.175416000	-1.810812000
6	-1.208637000	-3.923659000	0.034727000
1	-1.011351000	-3.832284000	1.115864000
1	-1.809872000	-3.049194000	-0.261417000
1	-1.816036000	-4.832446000	-0.116456000
6	0.921935000	-5.187930000	-0.244289000
1	0.331061000	-6.119578000	-0.287226000
1	1.840221000	-5.358903000	-0.828759000
1	1.211455000	-5.039229000	0.810774000
6	-2.800841000	2.170712000	-0.497564000
1	-1.939913000	2.476335000	0.126576000
6	-4.057247000	2.377328000	0.330518000
1	-4.134234000	3.434971000	0.639653000
1	-4.978842000	2.131093000	-0.221628000
1	-4.041935000	1.768735000	1.249129000
6	-2.762440000	3.018536000	-1.759655000
1	-2.805874000	4.092420000	-1.508650000
1	-1.827855000	2.846009000	-2.324660000
1	-3.610041000	2.808501000	-2.435418000

[1b''_{psi}] (TE = -3658.414947)

6	0.897001000	-1.698350000	1.817454000
6	0.691133000	-2.354540000	3.038361000
1	0.000277000	-1.920140000	3.772688000

6	1.323018000	-3.562168000	3.333464000
1	1.136533000	-4.062423000	4.289134000
6	2.189793000	-4.132459000	2.403939000
1	2.690074000	-5.080428000	2.624871000
6	2.415262000	-3.496210000	1.183701000
1	3.096954000	-3.961424000	0.463626000
6	1.767913000	-2.294506000	0.875855000
6	0.845258000	1.408856000	2.001914000
6	1.391195000	1.462846000	3.290940000
1	1.274990000	0.600789000	3.960782000
6	2.108384000	2.572764000	3.735543000
1	2.538436000	2.583862000	4.742148000
6	2.279219000	3.666712000	2.890430000
1	2.839978000	4.543675000	3.228319000
6	1.738019000	3.641790000	1.605783000
1	1.883233000	4.510672000	0.956357000
6	1.038349000	2.519626000	1.146545000
6	-1.833562000	-0.141218000	1.829641000
6	-2.260671000	0.260881000	3.102515000
1	-1.513527000	0.476641000	3.877165000
6	-3.610943000	0.439603000	3.398444000
1	-3.917012000	0.772807000	4.395230000
6	-4.569253000	0.208424000	2.413913000
1	-5.631420000	0.357946000	2.630711000
6	-4.172893000	-0.211648000	1.145785000
1	-4.939366000	-0.389491000	0.385301000
6	-2.816759000	-0.385091000	0.840871000
23	0.057017000	0.037273000	-1.184576000
6	3.733492000	-0.792915000	-0.623845000
1	4.398984000	-1.671080000	-0.517656000
6	-1.055223000	3.626374000	-0.524324000
1	-0.620309000	4.620172000	-0.301921000
6	-2.577548000	-2.710986000	-0.942075000
1	-2.636651000	-2.895710000	-2.035599000
6	-3.855822000	-3.187776000	-0.271057000
1	-3.983329000	-4.272975000	-0.430021000
1	-3.805166000	-3.022789000	0.818852000
1	-4.764791000	-2.693019000	-0.641501000
6	-1.389701000	-3.481031000	-0.387698000
1	-1.272502000	-3.305681000	0.698022000
1	-1.522023000	-4.566591000	-0.535450000
1	-0.447744000	-3.169993000	-0.864603000
6	4.098830000	-0.009573000	-1.873641000
1	4.016006000	-0.598137000	-2.802244000
1	3.425464000	0.860311000	-1.972215000
1	5.132472000	0.372352000	-1.812274000

6	3.878656000	0.090453000	0.604530000
1	3.666200000	-0.446858000	1.542775000
1	4.904457000	0.492288000	0.667756000
1	3.185462000	0.950261000	0.551504000
6	-1.765282000	3.657123000	-1.867878000
1	-2.638273000	4.331642000	-1.838267000
1	-1.118959000	3.987816000	-2.697226000
1	-2.131983000	2.643868000	-2.115998000
6	-2.032495000	3.251873000	0.577657000
1	-2.439451000	2.237653000	0.409871000
1	-1.568083000	3.258183000	1.576926000
1	-2.882401000	3.955509000	0.593535000
14	-0.012912000	-0.121557000	1.230395000
15	0.373265000	2.401132000	-0.586520000
15	-2.221556000	-0.856309000	-0.854086000
15	1.975267000	-1.453945000	-0.772190000
6	2.134688000	-2.882503000	-2.012189000
1	1.500065000	-3.667248000	-1.556595000
6	3.513796000	-3.469531000	-2.269221000
1	3.438217000	-4.328726000	-2.958318000
1	4.189411000	-2.738784000	-2.744436000
1	4.011722000	-3.830980000	-1.355885000
6	1.476070000	-2.447887000	-3.316941000
1	0.444863000	-2.083674000	-3.139214000
1	2.040696000	-1.631301000	-3.803898000
1	1.419702000	-3.282604000	-4.037253000
6	-3.426060000	-0.082762000	-2.089414000
1	-3.598747000	0.921896000	-1.650918000
6	-2.646345000	0.088615000	-3.389884000
1	-2.397777000	-0.891392000	-3.838153000
1	-3.228691000	0.654508000	-4.137937000
1	-1.697199000	0.636491000	-3.224052000
6	-4.768648000	-0.734863000	-2.381446000
1	-4.644948000	-1.748182000	-2.800938000
1	-5.423630000	-0.812459000	-1.500654000
1	-5.316346000	-0.144066000	-3.136397000
6	1.654794000	3.265308000	-1.680822000
1	2.608776000	2.952858000	-1.208026000
6	1.630818000	4.782201000	-1.789951000
1	2.468644000	5.130671000	-2.418879000
1	0.704333000	5.141310000	-2.268943000
1	1.720377000	5.296736000	-0.821345000
6	1.586152000	2.633985000	-3.068062000
1	1.594377000	1.527743000	-3.004016000
1	0.666492000	2.930704000	-3.603616000
1	2.444045000	2.939648000	-3.692500000

[1c''_{PB}] (TE = -3393.825304)

6	1.120257000	-1.136340000	1.738734000
6	0.969903000	-1.836762000	2.950438000
1	0.086376000	-1.635856000	3.568740000
6	1.892479000	-2.782264000	3.391569000
1	1.729973000	-3.304907000	4.339656000
6	3.017814000	-3.060954000	2.620846000
1	3.752324000	-3.801661000	2.951282000
6	3.194930000	-2.390308000	1.413078000
1	4.075645000	-2.624842000	0.805532000
6	2.261514000	-1.448264000	0.961150000
6	0.357796000	1.489569000	1.723081000
6	1.008605000	1.738279000	2.945778000
1	1.340651000	0.882526000	3.547156000
6	1.247462000	3.025170000	3.421381000
1	1.763321000	3.169180000	4.376171000
6	0.816228000	4.124797000	2.684487000
1	0.979809000	5.142642000	3.051199000
6	0.179874000	3.915082000	1.463328000
1	-0.149473000	4.783463000	0.884566000
6	-0.026111000	2.623140000	0.961484000
6	-1.509050000	-0.460748000	1.705270000
6	-2.059600000	-0.045164000	2.931565000
1	-1.445795000	0.567157000	3.604409000
6	-3.362094000	-0.357758000	3.311461000
1	-3.751206000	-0.005595000	4.272226000
6	-4.171727000	-1.106132000	2.460201000
1	-5.201379000	-1.348836000	2.739522000
6	-3.657455000	-1.537918000	1.240990000
1	-4.302100000	-2.114779000	0.570492000
6	-2.345242000	-1.226680000	0.857872000
23	0.096921000	0.026876000	-1.114592000
6	3.984952000	0.342367000	-0.540838000
1	4.795158000	-0.354935000	-0.251924000
6	-2.450494000	2.952660000	-0.673313000
1	-2.406802000	4.031026000	-0.426475000
6	-1.478680000	-3.518200000	-0.819011000
1	-1.465948000	-3.759703000	-1.903020000
6	-2.556445000	-4.334255000	-0.123030000
1	-2.328054000	-5.410615000	-0.213392000
1	-2.583519000	-4.098109000	0.954453000
1	-3.566582000	-4.179086000	-0.527330000
6	-0.120517000	-3.859296000	-0.228341000
1	-0.086482000	-3.614774000	0.849287000
1	0.097898000	-4.935496000	-0.334879000

1	0.683408000	-3.283475000	-0.709135000
6	4.354584000	1.015964000	-1.853901000
1	4.551818000	0.301145000	-2.667641000
1	3.552590000	1.688716000	-2.198831000
1	5.263128000	1.630276000	-1.730003000
6	3.799938000	1.362462000	0.572458000
1	3.653044000	0.882093000	1.553022000
1	4.683512000	2.019658000	0.644670000
1	2.916765000	2.002651000	0.392729000
6	-3.104044000	2.762717000	-2.033545000
1	-4.150281000	3.113356000	-2.020459000
1	-2.585428000	3.297664000	-2.846247000
1	-3.117835000	1.690584000	-2.301208000
6	-3.237288000	2.238382000	0.409011000
1	-3.254890000	1.149187000	0.230383000
1	-2.807671000	2.394201000	1.411474000
1	-4.281323000	2.595529000	0.425144000
5	0.008030000	-0.037718000	1.382567000
15	2.426682000	-0.692846000	-0.717592000
15	-0.672799000	2.356223000	-0.747413000
15	-1.691415000	-1.645940000	-0.809387000
6	0.111898000	3.684158000	-1.850377000
1	-0.089172000	3.251633000	-2.852061000
6	1.616824000	3.682955000	-1.651131000
1	2.130703000	4.205578000	-2.475833000
1	1.900949000	4.180435000	-0.707761000
1	1.993985000	2.648958000	-1.600965000
6	-0.447093000	5.099100000	-1.847631000
1	0.067214000	5.697602000	-2.619888000
1	-1.523920000	5.144975000	-2.071422000
1	-0.280435000	5.617500000	-0.889502000
6	2.955110000	-2.143953000	-1.819182000
1	2.502494000	-3.005475000	-1.294650000
6	4.437563000	-2.439615000	-1.990366000
1	4.567847000	-3.374379000	-2.562928000
1	4.961013000	-1.649487000	-2.552344000
1	4.968698000	-2.572184000	-1.035026000
6	2.259441000	-2.004738000	-3.167767000
1	2.429072000	-2.893246000	-3.800648000
1	1.165929000	-1.887824000	-3.035284000
1	2.625979000	-1.125749000	-3.728512000
6	-3.078189000	-1.298819000	-2.041555000
1	-3.547005000	-0.388454000	-1.616337000
6	-2.403210000	-0.920474000	-3.355906000
1	-1.853884000	-1.778334000	-3.786360000
1	-3.141145000	-0.590476000	-4.108083000

1	-1.682300000	-0.092054000	-3.210073000
6	-4.160418000	-2.336665000	-2.290049000
1	-3.740799000	-3.276543000	-2.688468000
1	-4.746567000	-2.579570000	-1.390909000
1	-4.872765000	-1.961390000	-3.045282000

[1d''_{sc}] (TE = -3222.697317)

6	0.055657000	-1.552241000	0.993890000
6	-0.571792000	-2.070630000	2.142120000
1	-1.143395000	-1.385342000	2.777659000
6	-0.485090000	-3.413114000	2.502130000
1	-0.989241000	-3.763980000	3.408079000
6	0.243866000	-4.304472000	1.718134000
1	0.318930000	-5.360487000	1.992702000
6	0.847537000	-3.837049000	0.554137000
1	1.374570000	-4.528991000	-0.111905000
6	0.747831000	-2.491223000	0.191887000
6	1.199659000	0.661308000	1.205142000
6	1.797298000	0.298446000	2.426650000
1	1.401895000	-0.572304000	2.961188000
6	2.861976000	1.002647000	2.982275000
1	3.286278000	0.677064000	3.937224000
6	3.380808000	2.119041000	2.330587000
1	4.215897000	2.680864000	2.758560000
6	2.842413000	2.488407000	1.101573000
1	3.271332000	3.324717000	0.538823000
6	1.781871000	1.769811000	0.541872000
6	-1.294389000	0.559999000	1.073686000
6	-1.425438000	1.196369000	2.322505000
1	-0.555059000	1.219592000	2.986992000
6	-2.606421000	1.800872000	2.742728000
1	-2.649587000	2.280446000	3.725622000
6	-3.723825000	1.800181000	1.912864000
1	-4.654750000	2.283473000	2.222604000
6	-3.628734000	1.201766000	0.660210000
1	-4.474761000	1.246461000	-0.032078000
6	-2.443458000	0.584047000	0.243334000
16	-2.357883000	0.098240000	-1.492234000
16	1.293599000	-2.040904000	-1.460220000
16	1.363377000	2.141742000	-1.167003000
23	0.099548000	0.094390000	-1.511764000
6	3.170347000	-1.997055000	-1.359816000
1	3.465138000	-3.060350000	-1.291152000
6	0.406019000	3.761530000	-1.084037000
1	1.167538000	4.516649000	-0.815729000
6	-3.258749000	-1.554869000	-1.608936000

1	-3.250749000	-1.674398000	-2.709178000
6	-4.684735000	-1.441305000	-1.121350000
1	-5.227671000	-2.379816000	-1.326826000
1	-4.717444000	-1.276653000	-0.030841000
1	-5.228175000	-0.619431000	-1.613888000
6	-2.500763000	-2.686810000	-0.965260000
1	-2.442449000	-2.556235000	0.129294000
1	-3.007045000	-3.647252000	-1.164056000
1	-1.472075000	-2.750411000	-1.353231000
6	3.614552000	-1.405542000	-2.679714000
1	3.253404000	-1.989931000	-3.541599000
1	3.223504000	-0.374540000	-2.771482000
1	4.714528000	-1.358435000	-2.733859000
6	3.689353000	-1.221171000	-0.177618000
1	3.328531000	-1.626151000	0.780949000
1	4.792591000	-1.249330000	-0.165981000
1	3.374112000	-0.165644000	-0.241495000
6	-0.095357000	3.983741000	-2.493898000
1	-0.660924000	4.927469000	-2.561839000
1	0.725426000	4.020964000	-3.228488000
1	-0.775487000	3.157514000	-2.776292000
6	-0.710840000	3.738040000	-0.074479000
1	-1.441458000	2.951563000	-0.332236000
1	-0.349409000	3.543824000	0.947630000
1	-1.237455000	4.708024000	-0.071434000
6	0.005131000	-0.083249000	0.650742000

[1e''_{ssi}] (TE = -3474.046310)

6	0.873813000	-1.702548000	1.272089000
6	0.855323000	-2.230700000	2.571260000
1	0.327612000	-1.685344000	3.364007000
6	1.483090000	-3.434538000	2.887482000
1	1.450976000	-3.817559000	3.912273000
6	2.144311000	-4.154916000	1.894110000
1	2.633320000	-5.104522000	2.131296000
6	2.160588000	-3.672911000	0.587338000
1	2.648178000	-4.247204000	-0.208024000
6	1.536951000	-2.459326000	0.286204000
6	1.011936000	1.405084000	1.426031000
6	1.412550000	1.557882000	2.761573000
1	1.157784000	0.777614000	3.490002000
6	2.133992000	2.669306000	3.194755000
1	2.429431000	2.756326000	4.245048000
6	2.487203000	3.664963000	2.285791000
1	3.060728000	4.536908000	2.614317000
6	2.126938000	3.534765000	0.946634000

1	2.426948000	4.294841000	0.216953000
6	1.394713000	2.420611000	0.527731000
6	-1.759913000	0.027235000	1.300189000
6	-2.163452000	0.313559000	2.612233000
1	-1.404284000	0.384513000	3.401361000
6	-3.499010000	0.536783000	2.944552000
1	-3.777078000	0.762255000	3.978865000
6	-4.475270000	0.495971000	1.952086000
1	-5.523319000	0.693189000	2.196545000
6	-4.109316000	0.224968000	0.635137000
1	-4.864280000	0.228999000	-0.157275000
6	-2.770277000	-0.024159000	0.317040000
16	-2.391997000	-0.312348000	-1.444776000
16	1.566064000	-1.935533000	-1.457418000
16	1.012878000	2.319175000	-1.249822000
23	0.075627000	0.060277000	-1.706460000
6	3.356816000	-1.406091000	-1.635131000
1	3.943051000	-2.336322000	-1.523052000
6	-0.324037000	3.632101000	-1.384972000
1	0.188460000	4.584400000	-1.157006000
6	-2.844778000	-2.127918000	-1.634164000
1	-2.528881000	-2.282255000	-2.683477000
6	-4.335443000	-2.352145000	-1.510853000
1	-4.583880000	-3.391619000	-1.786009000
1	-4.672823000	-2.201005000	-0.471479000
1	-4.910435000	-1.677232000	-2.164253000
6	-2.039380000	-3.021482000	-0.722715000
1	-2.259538000	-2.813823000	0.339182000
1	-2.282082000	-4.080390000	-0.915093000
1	-0.959050000	-2.880836000	-0.878922000
6	3.478544000	-0.865608000	-3.043073000
1	3.201187000	-1.613441000	-3.803488000
1	2.813754000	0.013486000	-3.156642000
1	4.510556000	-0.534525000	-3.244349000
6	3.760235000	-0.387235000	-0.598100000
1	3.638960000	-0.761168000	0.431063000
1	4.817425000	-0.103755000	-0.737019000
1	3.142857000	0.521420000	-0.705355000
6	-0.773737000	3.600258000	-2.828834000
1	-1.562186000	4.349573000	-3.007901000
1	0.054672000	3.795698000	-3.528801000
1	-1.197090000	2.602514000	-3.058427000
6	-1.465345000	3.391354000	-0.428121000
1	-1.939668000	2.418874000	-0.646710000
1	-1.140496000	3.380389000	0.624757000
1	-2.228736000	4.179834000	-0.542236000

14 0.051080000 -0.077748000 0.672361000

[$\mathbf{1f''}_{SB}$] (TE = -3209.473694)

6	0.352700000	-1.658846000	1.073807000
6	-0.042029000	-2.245178000	2.290949000
1	-0.595852000	-1.632254000	3.013348000
6	0.228831000	-3.573911000	2.609101000
1	-0.100708000	-3.982937000	3.569375000
6	0.910355000	-4.383026000	1.702109000
1	1.123046000	-5.429938000	1.937488000
6	1.292704000	-3.849907000	0.474811000
1	1.789389000	-4.478778000	-0.272169000
6	1.016904000	-2.513230000	0.171829000
6	1.204911000	0.911389000	1.261929000
6	1.808842000	0.738637000	2.521889000
1	1.494669000	-0.111035000	3.141082000
6	2.797870000	1.589977000	3.008948000
1	3.234987000	1.408940000	3.995964000
6	3.234887000	2.664427000	2.237162000
1	4.015309000	3.336828000	2.605169000
6	2.684982000	2.854680000	0.973343000
1	3.043362000	3.665526000	0.329767000
6	1.690842000	1.992927000	0.498946000
6	-1.453049000	0.383731000	1.166279000
6	-1.697610000	0.900615000	2.452855000
1	-0.863050000	0.951148000	3.163226000
6	-2.942769000	1.378058000	2.853459000
1	-3.076007000	1.773085000	3.865468000
6	-4.009218000	1.371920000	1.957902000
1	-4.988022000	1.763661000	2.249488000
6	-3.806714000	0.885874000	0.670036000
1	-4.618334000	0.920122000	-0.063253000
6	-2.556137000	0.386278000	0.285985000
16	-2.377328000	-0.054991000	-1.458352000
16	1.390311000	-1.971166000	-1.506283000
16	1.182755000	2.228484000	-1.214386000
23	0.072228000	0.092462000	-1.591640000
6	3.253871000	-1.727565000	-1.469336000
1	3.660027000	-2.754938000	-1.426189000
6	0.051854000	3.729813000	-1.118067000
1	0.739743000	4.575894000	-0.935721000
6	-3.117450000	-1.782821000	-1.558582000
1	-2.928996000	-1.996835000	-2.627705000
6	-4.606762000	-1.754927000	-1.297554000

1	-5.044551000	-2.744996000	-1.511674000
1	-4.817593000	-1.527644000	-0.238733000
1	-5.123547000	-1.009817000	-1.922856000
6	-2.386232000	-2.780410000	-0.696526000
1	-2.472364000	-2.520064000	0.373246000
1	-2.812327000	-3.788860000	-0.834579000
1	-1.315613000	-2.818045000	-0.947775000
6	3.597446000	-1.074345000	-2.789572000
1	3.274015000	-1.679991000	-3.651759000
1	3.102309000	-0.086629000	-2.852269000
1	4.684961000	-0.913902000	-2.871585000
6	3.721032000	-0.918509000	-0.286468000
1	3.430424000	-1.372875000	0.673901000
1	4.820766000	-0.829545000	-0.304481000
1	3.293415000	0.098029000	-0.322881000
6	-0.577731000	3.840361000	-2.488746000
1	-1.245057000	4.716257000	-2.540518000
1	0.175581000	3.935158000	-3.287810000
1	-1.185034000	2.936947000	-2.689113000
6	-0.974120000	3.626845000	-0.018997000
1	-1.638949000	2.763603000	-0.194001000
1	-0.514872000	3.503429000	0.974570000
1	-1.594503000	4.539269000	0.001585000
5	0.038211000	-0.105960000	0.829696000

Cartesian coordinates of $[\mathbf{1a}'_{PC}]^-$ - $[\mathbf{1f}'_{SB}]^-$ and $[\mathbf{1a}''_{PC}]^-$ - $[\mathbf{1f}''_{SB}]^-$, along with their total energies (in hartree) including zero point vibrational correction at M06-D3(heptane)/def2-SVP level of theory.

$[\mathbf{1a}'_{PC}]^-$ (TE = -2950.495590)

23	0.007550000	-0.001928000	-0.385515000
15	-1.811775000	1.570141000	-0.259353000
15	2.352746000	0.487580000	-0.081360000
15	-0.553748000	-2.344467000	-0.163406000
6	-0.015457000	0.030544000	1.888922000
6	-0.861909000	1.225808000	2.350456000
6	1.402346000	0.164659000	2.479921000
6	-0.682011000	-1.251491000	2.401385000
6	2.559120000	-0.304404000	1.591553000
6	-0.303850000	-2.547875000	1.684016000
6	-2.167760000	1.459546000	1.580788000
1	-0.250649000	2.145239000	2.258459000
1	-1.120403000	1.162083000	3.442660000
1	-2.718545000	2.339372000	1.973478000
1	-2.845353000	0.595323000	1.714686000
1	-1.780136000	-1.136884000	2.332907000

1	-0.485010000	-1.393655000	3.497487000
1	0.776120000	-2.750571000	1.822152000
1	-0.840163000	-3.425138000	2.101552000
1	1.595773000	1.233115000	2.714669000
1	1.489342000	-0.351870000	3.469483000
1	3.545040000	-0.125016000	2.067937000
1	2.488431000	-1.390940000	1.391013000
6	3.765565000	-0.275215000	-1.072361000
1	3.569941000	-1.346585000	-0.875331000
6	2.834089000	2.283642000	0.271071000
1	1.947557000	2.575095000	0.868156000
6	-1.733123000	3.440524000	-0.573115000
1	-1.511750000	3.483658000	-1.659023000
6	-3.429986000	1.067523000	-1.109448000
1	-3.276074000	-0.028226000	-1.154852000
6	-2.327438000	-2.987696000	-0.453862000
1	-2.484404000	-2.662364000	-1.503606000
6	0.446728000	-3.785126000	-0.893299000
1	-0.140974000	-4.071769000	-1.788955000
6	1.793640000	-3.267189000	-1.360980000
1	2.419128000	-2.996771000	-0.488925000
1	2.345415000	-4.030317000	-1.940663000
1	1.674627000	-2.354375000	-1.973045000
6	0.643612000	-5.003097000	-0.001792000
1	-0.294906000	-5.423631000	0.387610000
1	1.166955000	-5.808688000	-0.549866000
1	1.275069000	-4.750837000	0.867892000
6	-3.309750000	-2.231352000	0.426028000
1	-4.339728000	-2.290403000	0.028465000
1	-3.327562000	-2.649036000	1.449163000
1	-3.024994000	-1.170980000	0.503886000
6	-2.605132000	-4.479148000	-0.364283000
1	-3.667104000	-4.682557000	-0.598019000
1	-2.001371000	-5.078975000	-1.063485000
1	-2.429138000	-4.863033000	0.657326000
6	-4.745314000	1.331002000	-0.393769000
1	-4.973933000	2.405738000	-0.303841000
1	-5.583732000	0.866883000	-0.946597000
1	-4.755942000	0.906495000	0.623779000
6	-3.435284000	1.545290000	-2.552940000
1	-4.242046000	1.053319000	-3.125961000
1	-3.591745000	2.635510000	-2.638632000
1	-2.472283000	1.295368000	-3.039319000
6	-0.530521000	4.004445000	0.163246000
1	-0.251338000	5.003778000	-0.216801000
1	-0.737149000	4.107806000	1.244372000

1	0.330904000	3.327117000	0.052468000
6	-2.974318000	4.267697000	-0.282005000
1	-2.763440000	5.345418000	-0.415119000
1	-3.820967000	4.021211000	-0.941613000
1	-3.312897000	4.136435000	0.762026000
6	5.195877000	0.022509000	-0.655158000
1	5.901382000	-0.648177000	-1.180106000
1	5.486616000	1.054177000	-0.919157000
1	5.361701000	-0.108377000	0.427512000
6	3.554904000	-0.044330000	-2.561480000
1	3.806427000	0.992909000	-2.847955000
1	4.189278000	-0.717810000	-3.167062000
1	2.493724000	-0.208005000	-2.834185000
6	4.061020000	2.593104000	1.114599000
1	5.002936000	2.408002000	0.574063000
1	4.062874000	3.660718000	1.403490000
1	4.089673000	2.006670000	2.047885000
6	2.805829000	3.095364000	-1.014698000
1	2.772137000	4.180689000	-0.805186000
1	3.704887000	2.908093000	-1.630121000
1	1.920527000	2.831887000	-1.625324000

[1b'_{psi}]' (TE = -3201.883971)

6	-0.304680000	2.718874000	1.704127000
6	0.252765000	1.699654000	2.697639000
6	-2.749569000	-0.547771000	1.769441000
6	-1.582193000	-0.869765000	2.702794000
6	2.652446000	-1.171348000	1.581533000
6	1.542749000	-1.158115000	2.636976000
1	-2.994405000	0.532504000	1.833019000
1	-1.828409000	-0.566814000	3.740647000
1	3.435939000	-1.930630000	1.785357000
1	1.954640000	-0.819594000	3.608732000
1	-0.080973000	3.767399000	1.982199000
1	1.341241000	1.871392000	2.834517000
6	-0.599281000	3.760351000	-1.025111000
1	0.117864000	3.940046000	-1.850628000
6	-2.663416000	-2.661052000	-0.232743000
1	-2.038953000	-3.053594000	0.597035000
6	3.560093000	-0.701294000	-1.129250000
1	3.422928000	0.387126000	-0.973980000
23	-0.041520000	-0.046441000	-0.483526000
1	-1.410704000	2.637345000	1.660879000
1	-0.205465000	1.846021000	3.696604000
1	1.167219000	-2.185537000	2.805359000
1	3.172720000	-0.190952000	1.590088000

1	-1.425459000	-1.968171000	2.734583000
1	-3.679031000	-1.090102000	2.038282000
6	4.954506000	-1.053896000	-0.631699000
1	5.711612000	-0.464785000	-1.182346000
1	5.090124000	-0.832171000	0.439039000
1	5.205463000	-2.115311000	-0.785350000
6	3.397966000	-0.961787000	-2.617550000
1	3.578390000	-2.023405000	-2.869559000
1	2.369108000	-0.707657000	-2.942244000
1	4.109654000	-0.358208000	-3.210741000
6	-4.083183000	-3.161958000	-0.026188000
1	-4.101613000	-4.266466000	0.026912000
1	-4.543404000	-2.782961000	0.901553000
1	-4.736722000	-2.875388000	-0.868651000
6	-2.078140000	-3.180134000	-1.537229000
1	-2.700582000	-2.881005000	-2.400006000
1	-1.070357000	-2.754242000	-1.709617000
1	-2.011811000	-4.284415000	-1.539849000
6	-1.894828000	3.259388000	-1.641522000
1	-1.738175000	2.295074000	-2.161320000
1	-2.660437000	3.094244000	-0.858916000
1	-2.312564000	3.991498000	-2.356877000
6	-0.840533000	5.066418000	-0.282435000
1	0.066195000	5.478873000	0.186796000
1	-1.237024000	5.836987000	-0.969533000
1	-1.593542000	4.935964000	0.514567000
6	1.992253000	-3.182266000	-0.500245000
1	1.617572000	-3.226757000	-1.543853000
6	0.930233000	-3.794630000	0.399975000
1	1.302542000	-3.898082000	1.435775000
1	0.035669000	-3.148872000	0.427833000
1	0.635108000	-4.801175000	0.051662000
6	3.290363000	-3.965740000	-0.403974000
1	3.094388000	-5.050756000	-0.493706000
1	4.008070000	-3.702212000	-1.196466000
1	3.790346000	-3.811377000	0.569743000
6	-3.756582000	0.126926000	-0.847011000
1	-3.399632000	1.153139000	-0.625247000
6	-5.164424000	-0.010010000	-0.287916000
1	-5.614344000	-0.986683000	-0.529048000
1	-5.203288000	0.114676000	0.806357000
1	-5.824746000	0.761238000	-0.726572000
6	-3.728177000	-0.041976000	-2.356675000
1	-4.131865000	-1.025815000	-2.661035000
1	-4.336699000	0.732181000	-2.859987000
1	-2.688291000	0.026363000	-2.733433000

6	2.046130000	2.847539000	-0.065487000
1	2.480977000	1.987960000	0.484622000
6	2.451002000	4.131346000	0.637685000
1	3.552405000	4.211648000	0.695243000
1	2.099198000	5.021671000	0.086706000
1	2.064298000	4.194913000	1.668438000
6	2.586330000	2.803320000	-1.487349000
1	3.692227000	2.790835000	-1.498473000
1	2.215159000	1.904438000	-2.016155000
1	2.267181000	3.688460000	-2.067695000
15	-2.317217000	-0.806152000	-0.045481000
15	0.219514000	2.339866000	-0.061927000
15	2.026468000	-1.307507000	-0.196478000
14	0.051626000	-0.102590000	1.982956000

[1c'_{PB}] (TE = -2937.277050)

6	-0.226152000	2.596447000	1.726398000
6	0.333761000	1.396725000	2.492032000
6	-2.785221000	-0.309930000	1.564044000
6	-1.625342000	-0.515435000	2.543059000
6	2.336447000	-1.119422000	1.616477000
6	1.016567000	-1.203711000	2.396273000
1	-2.942371000	0.770187000	1.374248000
1	-1.869145000	0.035172000	3.483861000
1	3.101180000	-1.858025000	1.940433000
1	1.271180000	-1.116710000	3.484369000
1	0.117999000	3.582767000	2.106495000
1	1.440247000	1.467759000	2.491636000
6	-1.100143000	3.671213000	-0.878562000
1	-0.570603000	4.024420000	-1.786943000
6	-2.235540000	-2.856132000	0.303289000
1	-1.372857000	-2.929448000	0.993092000
6	3.495599000	-0.371898000	-1.043696000
1	3.128191000	0.670011000	-0.989710000
23	-0.070175000	0.001998000	-0.430458000
1	-1.332123000	2.600533000	1.806806000
1	0.048213000	1.518726000	3.567383000
1	0.603718000	-2.227942000	2.287121000
1	2.792980000	-0.122818000	1.773055000
1	-1.618813000	-1.587663000	2.840375000
1	-3.758151000	-0.721887000	1.909098000
6	4.863809000	-0.406769000	-0.381855000
1	5.545382000	0.313443000	-0.873269000
1	4.812678000	-0.127622000	0.683639000
1	5.344565000	-1.396379000	-0.440958000
6	3.541900000	-0.728109000	-2.521623000

1	3.890989000	-1.761333000	-2.695498000
1	2.539743000	-0.631736000	-2.978324000
1	4.226326000	-0.057085000	-3.071763000
6	-3.455583000	-3.417258000	1.011939000
1	-3.345763000	-4.504664000	1.182802000
1	-3.613345000	-2.947087000	1.996111000
1	-4.381803000	-3.280798000	0.423689000
6	-1.901425000	-3.623648000	-0.964512000
1	-2.748233000	-3.625417000	-1.675627000
1	-1.033681000	-3.157373000	-1.470858000
1	-1.652375000	-4.679357000	-0.750750000
6	-2.346914000	2.923643000	-1.313312000
1	-2.096483000	2.057726000	-1.948868000
1	-2.867672000	2.514197000	-0.427379000
1	-3.055333000	3.580896000	-1.851627000
6	-1.494446000	4.868863000	-0.025740000
1	-0.637308000	5.449129000	0.345132000
1	-2.142370000	5.559654000	-0.597016000
1	-2.074857000	4.543430000	0.854639000
5	-0.126487000	-0.097321000	1.984159000
15	2.027042000	-1.239848000	-0.214764000
15	-2.248931000	-0.999971000	-0.074115000
15	0.106907000	2.428325000	-0.095052000
6	2.361428000	-3.075631000	-0.588160000
1	2.061006000	-3.167850000	-1.652403000
6	3.784750000	-3.587064000	-0.431018000
1	3.820247000	-4.683544000	-0.574353000
1	4.487045000	-3.144271000	-1.153804000
1	4.173374000	-3.384807000	0.583610000
6	1.415763000	-3.928316000	0.242196000
1	1.368565000	-4.964353000	-0.140060000
1	1.751493000	-3.976607000	1.293238000
1	0.399274000	-3.507956000	0.244090000
6	-3.790870000	-0.944562000	-1.196809000
1	-4.286940000	-1.931800000	-1.121502000
6	-4.806487000	0.114389000	-0.803326000
1	-5.654798000	0.129113000	-1.512909000
1	-5.217575000	-0.053713000	0.205143000
1	-4.359308000	1.122947000	-0.815100000
6	-3.331061000	-0.750581000	-2.635110000
1	-2.631503000	-1.540483000	-2.956717000
1	-4.184104000	-0.741330000	-3.339496000
1	-2.789871000	0.207048000	-2.742214000
6	1.759776000	3.341087000	-0.383487000
1	2.009560000	2.991881000	-1.408252000
6	1.791079000	4.861048000	-0.381533000

1	2.810953000	5.220931000	-0.614983000
1	1.111813000	5.314197000	-1.120833000
1	1.533984000	5.266833000	0.613473000
6	2.820661000	2.810694000	0.568615000
1	2.723148000	1.722854000	0.706765000
1	3.840602000	3.029145000	0.200985000
1	2.719970000	3.276248000	1.565165000

[1d'_{sc}] (TE = -2766.144111)

6	0.379368000	2.202958000	1.577905000
6	0.356436000	0.941860000	2.432796000
6	-2.700725000	0.445647000	1.302204000
6	-1.767004000	-0.407480000	2.144902000
6	1.785747000	-1.809872000	1.612590000
6	0.443306000	-1.560180000	2.280388000
1	-2.500262000	1.524624000	1.428746000
1	-1.978641000	-0.167276000	3.222341000
1	2.292122000	-2.703564000	2.024264000
1	0.627518000	-1.573986000	3.389468000
1	0.873663000	3.042470000	2.104830000
1	1.413892000	0.722417000	2.694987000
6	0.796695000	3.270041000	-1.054475000
1	1.520768000	3.156639000	-1.884732000
6	-3.439981000	-1.496214000	-0.635662000
1	-3.699412000	-1.742241000	0.410291000
6	3.202295000	-1.342305000	-0.784385000
1	3.326879000	-0.407406000	-0.204249000
23	-0.056588000	-0.188655000	-0.404960000
16	-2.433990000	0.143898000	-0.523047000
16	1.293977000	1.799157000	0.006092000
16	1.528442000	-2.009081000	-0.230182000
6	-0.283468000	-0.302366000	1.807457000
1	-0.639699000	2.518924000	1.292815000
1	-0.127117000	1.215281000	3.407178000
1	-0.194652000	-2.445553000	2.080337000
1	2.460312000	-0.941426000	1.736543000
1	-2.088730000	-1.462407000	2.017572000
1	-3.769576000	0.282270000	1.546735000
6	4.310038000	-2.326981000	-0.482125000
1	5.292303000	-1.937758000	-0.807754000
1	4.381927000	-2.551949000	0.595053000
1	4.131108000	-3.278846000	-1.013546000
6	3.094640000	-1.001264000	-2.252721000
1	2.885529000	-1.905032000	-2.855759000
1	2.258662000	-0.287904000	-2.411716000
1	4.034059000	-0.550411000	-2.621753000

6	-4.687371000	-1.231711000	-1.446853000
1	-5.306077000	-2.141513000	-1.561814000
1	-5.312575000	-0.448897000	-0.984769000
1	-4.415404000	-0.882058000	-2.459606000
6	-2.555461000	-2.571908000	-1.212551000
1	-2.225220000	-2.299274000	-2.234101000
1	-1.631927000	-2.670224000	-0.609257000
1	-3.074559000	-3.547734000	-1.256676000
6	-0.597478000	3.088967000	-1.601561000
1	-0.664025000	2.104864000	-2.113166000
1	-1.358812000	3.086287000	-0.800365000
1	-0.852910000	3.893167000	-2.315545000
6	1.026584000	4.593327000	-0.357483000
1	2.036510000	4.649833000	0.083399000
1	0.915974000	5.434428000	-1.065399000
1	0.293322000	4.754619000	0.451353000

[1e'_{ssi}] (TE = -3017.507099)

23	-0.048757000	-0.076876000	-0.885172000
16	1.697605000	-1.843011000	-0.965866000
16	-2.310708000	-1.099007000	-1.170016000
16	-0.257088000	2.061406000	0.291018000
14	-0.294870000	-0.838327000	1.421425000
6	-0.264648000	0.634505000	2.687094000
6	0.444528000	1.807353000	2.025214000
6	-2.460799000	-2.297714000	0.263271000
6	-1.983680000	-1.793957000	1.618997000
6	1.152077000	-2.056818000	1.859665000
6	1.536079000	-2.846119000	0.620574000
1	0.730750000	-3.550187000	0.340027000
1	2.455885000	-3.451863000	0.721731000
1	2.007885000	-1.436024000	2.197069000
1	0.929601000	-2.762619000	2.686019000
1	-3.499140000	-2.681128000	0.264037000
1	-1.820432000	-3.122488000	-0.099306000
1	-2.730795000	-1.093236000	2.043138000
1	-1.939430000	-2.653248000	2.318282000
1	-1.313694000	0.921113000	2.904996000
1	0.216864000	0.418180000	3.661355000
1	1.525676000	1.595630000	1.906827000
1	0.331532000	2.754885000	2.585746000
6	3.260883000	-0.875698000	-0.620515000
1	2.926013000	-0.084154000	0.079093000
6	-3.445768000	0.259973000	-0.599233000
1	-2.977181000	0.661175000	0.320098000
6	0.854870000	3.460587000	-0.285405000

1	0.336136000	3.723776000	-1.227050000
6	-4.850294000	-0.231901000	-0.323979000
1	-5.509041000	0.612350000	-0.050751000
1	-5.273459000	-0.715511000	-1.222516000
1	-4.889024000	-0.958574000	0.503702000
6	-3.409909000	1.332456000	-1.668640000
1	-2.360322000	1.611858000	-1.885027000
1	-3.867890000	0.967870000	-2.606245000
1	-3.961078000	2.231204000	-1.338764000
6	0.856617000	4.653265000	0.646157000
1	1.417842000	4.441244000	1.572756000
1	1.342044000	5.523734000	0.168631000
1	-0.168457000	4.946910000	0.929652000
6	2.231899000	2.943493000	-0.625210000
1	2.842016000	3.713290000	-1.132029000
1	2.780173000	2.621714000	0.279935000
1	2.125056000	2.063219000	-1.290964000
6	3.658058000	-0.241668000	-1.937190000
1	4.458090000	0.506265000	-1.789317000
1	4.019346000	-1.007096000	-2.647652000
1	2.774911000	0.255349000	-2.386315000
6	4.376220000	-1.706852000	-0.026833000
1	5.300692000	-1.106198000	0.049126000
1	4.139532000	-2.074574000	0.984425000
1	4.594636000	-2.579545000	-0.668752000

[$\mathbf{1f}_{SB}$] (TE = -2752.932711)

6	1.161427000	2.000131000	1.671488000
6	0.777998000	0.779256000	2.489903000
6	-2.544666000	1.317993000	0.966992000
6	-1.902471000	0.4444465000	2.037885000
6	0.970718000	-2.403883000	1.581009000
6	-0.262513000	-1.726675000	2.154646000
1	-2.023222000	2.286938000	0.863890000
1	-1.950436000	1.036262000	2.987537000
1	1.079204000	-3.472232000	1.852187000
1	-0.241541000	-1.916088000	3.259712000
1	1.973069000	2.619992000	2.103556000
1	1.704095000	0.191321000	2.675935000
6	1.740116000	2.920596000	-1.010633000
1	1.995852000	2.488202000	-1.997905000
6	-3.751387000	-0.783271000	-0.519309000
1	-3.688530000	-1.050645000	0.550405000
6	2.777146000	-2.061491000	-0.592189000
1	3.082954000	-1.229585000	0.070694000
23	-0.168988000	-0.092930000	-0.540303000

16	-2.436115000	0.618506000	-0.745567000
16	1.705764000	1.365641000	0.022195000
16	0.957775000	-2.282499000	-0.268158000
1	0.278474000	2.645274000	1.502905000
1	0.453292000	1.146144000	3.495719000
1	-1.162202000	-2.269018000	1.789856000
1	1.888306000	-1.878733000	1.907502000
1	-2.584629000	-0.414838000	2.219462000
1	-3.614853000	1.544345000	1.159813000
6	3.559200000	-3.318016000	-0.277547000
1	4.638517000	-3.172453000	-0.468552000
1	3.445130000	-3.620227000	0.776279000
1	3.211593000	-4.155966000	-0.907494000
6	2.924191000	-1.624485000	-2.033777000
1	2.561704000	-2.408085000	-2.724009000
1	2.330869000	-0.709440000	-2.215954000
1	3.981114000	-1.417750000	-2.278408000
6	-5.118819000	-0.250009000	-0.876542000
1	-5.905967000	-1.016715000	-0.745044000
1	-5.395652000	0.620316000	-0.257670000
1	-5.141221000	0.073756000	-1.933088000
6	-3.313456000	-1.946091000	-1.371286000
1	-3.289616000	-1.661591000	-2.441494000
1	-2.286951000	-2.254814000	-1.094979000
1	-3.994172000	-2.810114000	-1.264238000
6	0.379343000	3.575800000	-1.105633000
1	-0.399784000	2.807441000	-1.277384000
1	0.126055000	4.110665000	-0.172934000
1	0.348851000	4.314436000	-1.926342000
6	2.833359000	3.872817000	-0.572656000
1	3.811590000	3.368274000	-0.517520000
1	2.922301000	4.725573000	-1.270737000
1	2.613562000	4.291056000	0.425357000
5	-0.380188000	-0.136701000	1.778060000

[1a''_{PC}]⁻ (TE = -3407.080623)

6	0.970803000	-1.005151000	1.626079000
6	1.717624000	-0.696272000	2.781043000
1	1.462869000	0.213899000	3.336435000
6	2.759600000	-1.502904000	3.238852000
1	3.318891000	-1.209891000	4.134469000
6	3.070275000	-2.684120000	2.572557000
1	3.882192000	-3.330174000	2.922307000
6	2.340455000	-3.024455000	1.430098000
1	2.612922000	-3.936535000	0.886530000
6	1.326676000	-2.201685000	0.925133000

6	-0.013519000	1.317280000	1.620994000
6	-0.806395000	1.825004000	2.670075000
1	-1.503058000	1.147666000	3.176384000
6	-0.750071000	3.157207000	3.074837000
1	-1.398983000	3.505868000	3.885820000
6	0.134065000	4.034101000	2.453901000
1	0.189631000	5.085062000	2.755816000
6	0.949318000	3.554066000	1.427308000
1	1.635122000	4.252333000	0.938838000
6	0.880852000	2.226443000	0.987065000
6	-1.517739000	-0.632780000	1.446391000
6	-1.782843000	-1.476380000	2.539858000
1	-0.938949000	-1.815554000	3.152755000
6	-3.076698000	-1.875279000	2.870232000
1	-3.239668000	-2.534762000	3.730026000
6	-4.159820000	-1.418628000	2.123443000
1	-5.181862000	-1.716063000	2.379547000
6	-3.925112000	-0.576017000	1.033364000
1	-4.778516000	-0.221016000	0.446809000
6	-2.629762000	-0.200872000	0.663388000
6	-0.141613000	-0.111198000	1.172944000
23	0.081407000	-0.097400000	-1.074134000
6	2.117705000	-3.116740000	-1.761637000
1	2.514855000	-4.014566000	-1.251153000
6	1.822720000	3.168960000	-1.643099000
1	0.840308000	3.635001000	-1.418208000
6	-3.480487000	0.238383000	-2.217907000
1	-2.985685000	0.708660000	-3.094007000
6	-4.903508000	0.771166000	-2.150598000
1	-5.462660000	0.464924000	-3.053889000
1	-5.466280000	0.380997000	-1.286162000
1	-4.942630000	1.870818000	-2.106583000
6	-3.448862000	-1.263410000	-2.455163000
1	-3.896365000	-1.816434000	-1.609502000
1	-4.012678000	-1.530111000	-3.366633000
1	-2.405268000	-1.612843000	-2.572736000
6	1.656940000	-3.488327000	-3.163970000
1	0.982197000	-4.359952000	-3.184141000
1	1.117690000	-2.630859000	-3.616335000
1	2.520240000	-3.722654000	-3.812063000
6	3.194922000	-2.053789000	-1.838318000
1	3.575728000	-1.773280000	-0.840870000
1	4.050067000	-2.389291000	-2.453213000
1	2.761154000	-1.140215000	-2.294696000
6	2.917581000	4.204883000	-1.425892000
1	2.738394000	5.086253000	-2.068602000

1	2.992806000	4.569872000	-0.389769000
1	3.908602000	3.810752000	-1.705430000
6	1.798073000	2.726770000	-3.100762000
1	2.748090000	2.239689000	-3.388543000
1	0.993502000	1.983520000	-3.272003000
1	1.645005000	3.588517000	-3.776612000
15	-2.193524000	0.680235000	-0.905346000
15	1.711322000	1.617773000	-0.552619000
15	0.648052000	-2.421665000	-0.791440000
6	3.470855000	1.209810000	0.029968000
1	3.285858000	0.203849000	0.459141000
6	4.439437000	1.051365000	-1.133503000
1	4.811546000	2.026600000	-1.490216000
1	5.324074000	0.463798000	-0.827334000
1	3.979596000	0.534766000	-1.991348000
6	4.057257000	2.078562000	1.129414000
1	5.019682000	1.658400000	1.476147000
1	4.259223000	3.106959000	0.781958000
1	3.389646000	2.145608000	2.002970000
6	-0.452129000	-3.964314000	-0.759207000
1	-0.700737000	-4.087052000	-1.832699000
6	-1.741990000	-3.695852000	-0.009445000
1	-1.560520000	-3.647845000	1.077612000
1	-2.188591000	-2.732403000	-0.302647000
1	-2.479621000	-4.498360000	-0.189923000
6	0.204437000	-5.235100000	-0.246963000
1	-0.503883000	-6.082815000	-0.291210000
1	1.099422000	-5.528559000	-0.819917000
1	0.502768000	-5.118806000	0.810343000
6	-2.460123000	2.509645000	-0.532829000
1	-1.566860000	2.699752000	0.091447000
6	-3.677297000	2.900452000	0.287606000
1	-3.618066000	3.967273000	0.572857000
1	-4.625497000	2.761437000	-0.258437000
1	-3.738510000	2.315190000	1.219976000
6	-2.294397000	3.329100000	-1.802590000
1	-2.171531000	4.401686000	-1.565932000
1	-1.396478000	2.996259000	-2.356960000
1	-3.162666000	3.240133000	-2.480290000

[1b''_{psi}] (TE = -3658.442058)

6	0.949934000	-1.668698000	1.826277000
6	0.763968000	-2.330209000	3.048102000
1	0.062504000	-1.912447000	3.782905000
6	1.425085000	-3.522821000	3.346691000
1	1.248111000	-4.029104000	4.302102000

6	2.309403000	-4.066724000	2.419014000
1	2.835502000	-5.002160000	2.638412000
6	2.517189000	-3.421685000	1.198117000
1	3.214561000	-3.869024000	0.481791000
6	1.835001000	-2.241846000	0.879783000
6	0.775454000	1.434521000	2.010162000
6	1.306858000	1.502151000	3.305027000
1	1.199183000	0.637829000	3.974434000
6	2.001938000	2.624012000	3.758887000
1	2.425030000	2.641661000	4.769381000
6	2.157602000	3.719485000	2.914272000
1	2.701345000	4.607773000	3.253653000
6	1.626434000	3.681316000	1.623759000
1	1.764325000	4.553218000	0.977507000
6	0.956262000	2.546892000	1.149461000
6	-1.842780000	-0.213128000	1.827977000
6	-2.283949000	0.161760000	3.104948000
1	-1.543227000	0.367866000	3.889272000
6	-3.637421000	0.331756000	3.396451000
1	-3.952663000	0.648616000	4.396731000
6	-4.584244000	0.112522000	2.399212000
1	-5.650118000	0.256295000	2.606636000
6	-4.172536000	-0.285925000	1.126989000
1	-4.935085000	-0.452379000	0.360342000
6	-2.814194000	-0.446503000	0.822360000
23	0.062438000	0.042578000	-1.179999000
6	3.720512000	-0.673907000	-0.645344000
1	4.422442000	-1.521432000	-0.523985000
6	-1.143814000	3.564806000	-0.564228000
1	-0.753846000	4.572660000	-0.321129000
6	-2.479586000	-2.754263000	-0.951263000
1	-2.618622000	-2.941276000	-2.036819000
6	-3.678327000	-3.284355000	-0.180307000
1	-3.779786000	-4.374555000	-0.334204000
1	-3.544090000	-3.120178000	0.903082000
1	-4.633768000	-2.821451000	-0.467237000
6	-1.224424000	-3.479983000	-0.499449000
1	-1.040810000	-3.324844000	0.580505000
1	-1.311041000	-4.568140000	-0.671030000
1	-0.337569000	-3.100381000	-1.030059000
6	4.051684000	0.109347000	-1.903852000
1	3.993494000	-0.498738000	-2.822643000
1	3.318631000	0.927684000	-2.018452000
1	5.063147000	0.552212000	-1.848198000
6	3.824916000	0.230628000	0.570572000
1	3.646490000	-0.308333000	1.515629000

1	4.825460000	0.695749000	0.625150000
1	3.077241000	1.042132000	0.508598000
6	-1.829846000	3.579958000	-1.920099000
1	-2.735675000	4.213487000	-1.904525000
1	-1.177030000	3.941078000	-2.732417000
1	-2.129771000	2.549035000	-2.185709000
6	-2.126003000	3.139172000	0.512863000
1	-2.465489000	2.103064000	0.332575000
1	-1.683015000	3.164595000	1.522192000
1	-3.016357000	3.793082000	0.512800000
14	-0.020643000	-0.128124000	1.213579000
15	0.338911000	2.386150000	-0.623071000
15	-2.182222000	-0.872779000	-0.896837000
15	1.978955000	-1.405861000	-0.803493000
6	2.270916000	-2.901596000	-1.968328000
1	1.689243000	-3.704407000	-1.474199000
6	3.694762000	-3.397996000	-2.173206000
1	3.697775000	-4.296702000	-2.816875000
1	4.318041000	-2.643361000	-2.683132000
1	4.210783000	-3.669129000	-1.238003000
6	1.617692000	-2.606787000	-3.311431000
1	0.584577000	-2.226284000	-3.182561000
1	2.163889000	-1.812235000	-3.854062000
1	1.598040000	-3.507560000	-3.953470000
6	-3.521087000	-0.195710000	-2.077260000
1	-3.748905000	0.791976000	-1.623778000
6	-2.848171000	0.039882000	-3.424238000
1	-2.615709000	-0.922920000	-3.918982000
1	-3.502657000	0.619094000	-4.102641000
1	-1.877292000	0.564455000	-3.306594000
6	-4.821383000	-0.955552000	-2.299590000
1	-4.631538000	-1.961362000	-2.714138000
1	-5.434490000	-1.079756000	-1.393784000
1	-5.448143000	-0.424632000	-3.039230000
6	1.614604000	3.395638000	-1.628732000
1	2.563689000	3.127265000	-1.119163000
6	1.489823000	4.912132000	-1.680528000
1	2.331714000	5.345445000	-2.251052000
1	0.566963000	5.219600000	-2.202283000
1	1.483822000	5.401485000	-0.694297000
6	1.663483000	2.840547000	-3.047313000
1	1.612708000	1.731981000	-3.049468000
1	0.793468000	3.183685000	-3.637175000
1	2.578246000	3.168569000	-3.576042000

[1c''_{PB}] (TE = -3393.874450)

6	0.889783000	-1.252040000	1.704476000
6	0.568290000	-2.029044000	2.841407000
1	-0.347800000	-1.782547000	3.394979000
6	1.364743000	-3.076605000	3.298464000
1	1.067240000	-3.641147000	4.190455000
6	2.551150000	-3.395265000	2.635057000
1	3.195117000	-4.206650000	2.991177000
6	2.895408000	-2.668418000	1.495670000
1	3.814350000	-2.934498000	0.958939000
6	2.074789000	-1.640064000	1.014660000
6	0.536457000	1.425441000	1.683777000
6	1.302049000	1.601839000	2.857721000
1	1.597361000	0.706019000	3.421541000
6	1.663869000	2.853923000	3.346162000
1	2.248292000	2.933163000	4.270819000
6	1.252484000	4.011813000	2.680074000
1	1.503391000	5.003707000	3.071256000
6	0.525165000	3.883095000	1.497863000
1	0.218350000	4.789697000	0.962977000
6	0.211204000	2.620939000	0.973935000
6	-1.574620000	-0.192477000	1.648826000
6	-2.109331000	0.386555000	2.820271000
1	-1.440332000	0.984491000	3.454438000
6	-3.440689000	0.236548000	3.198604000
1	-3.806229000	0.708179000	4.118741000
6	-4.311477000	-0.517681000	2.409201000
1	-5.362265000	-0.640460000	2.693108000
6	-3.824370000	-1.107204000	1.243944000
1	-4.513013000	-1.685387000	0.617950000
6	-2.486335000	-0.943793000	0.857526000
23	0.103820000	0.015626000	-1.072395000
6	4.019376000	-0.045623000	-0.489526000
1	4.748874000	-0.825887000	-0.195591000
6	-2.142440000	3.171302000	-0.778969000
1	-2.016493000	4.248940000	-0.556918000
6	-1.807875000	-3.365844000	-0.765085000
1	-1.934855000	-3.622671000	-1.838331000
6	-2.897870000	-4.040748000	0.051403000
1	-2.806192000	-5.140311000	-0.019599000
1	-2.798323000	-3.771825000	1.117471000
1	-3.917803000	-3.774466000	-0.264014000
6	-0.447184000	-3.865115000	-0.313008000
1	-0.279325000	-3.642016000	0.756096000
1	-0.356511000	-4.957517000	-0.451270000

1	0.359792000	-3.362905000	-0.866451000
6	4.456101000	0.568404000	-1.811070000
1	4.535625000	-0.168182000	-2.626578000
1	3.740751000	1.339567000	-2.142112000
1	5.441298000	1.058851000	-1.710533000
6	3.966548000	1.004542000	0.607677000
1	3.746415000	0.560312000	1.591516000
1	4.928481000	1.543562000	0.679989000
1	3.173215000	1.749182000	0.414010000
6	-2.728547000	2.996345000	-2.171644000
1	-3.751120000	3.410208000	-2.232202000
1	-2.127037000	3.476117000	-2.962241000
1	-2.788669000	1.918184000	-2.413290000
6	-3.060222000	2.564116000	0.262987000
1	-3.151114000	1.474061000	0.113827000
1	-2.682554000	2.711747000	1.286974000
1	-4.070857000	3.006169000	0.198832000
5	-0.022944000	-0.012585000	1.242410000
15	2.343625000	-0.903122000	-0.654380000
15	-0.425548000	2.391002000	-0.736826000
15	-1.822335000	-1.467594000	-0.776328000
6	0.504142000	3.656303000	-1.831486000
1	0.282228000	3.245074000	-2.838221000
6	1.996905000	3.507372000	-1.604917000
1	2.581571000	3.978493000	-2.415442000
1	2.308181000	3.966591000	-0.649994000
1	2.259578000	2.438141000	-1.551710000
6	0.093143000	5.120759000	-1.835355000
1	0.695066000	5.678891000	-2.576308000
1	-0.965077000	5.275773000	-2.099364000
1	0.269052000	5.605213000	-0.860304000
6	2.788799000	-2.413070000	-1.738932000
1	2.232515000	-3.218758000	-1.225845000
6	4.235633000	-2.868733000	-1.855576000
1	4.290801000	-3.813278000	-2.427423000
1	4.866649000	-2.139466000	-2.390231000
1	4.707661000	-3.058473000	-0.878606000
6	2.160432000	-2.218716000	-3.113301000
1	2.251841000	-3.128277000	-3.735193000
1	1.083598000	-1.976153000	-3.015315000
1	2.639742000	-1.389728000	-3.666375000
6	-3.188521000	-1.091676000	-2.044301000
1	-3.567149000	-0.113208000	-1.685062000
6	-2.482512000	-0.867707000	-3.377105000
1	-2.029064000	-1.804836000	-3.752139000
1	-3.179823000	-0.503410000	-4.154051000

1	-1.667718000	-0.125190000	-3.269711000
6	-4.367654000	-2.033171000	-2.229543000
1	-4.041250000	-3.036577000	-2.555907000
1	-4.971821000	-2.155709000	-1.317217000
1	-5.044841000	-1.649400000	-3.014794000

[1d''_{sc}] (TE = -3222.720508)

6	1.028560000	1.073683000	1.002048000
6	2.003247000	0.928348000	1.996430000
1	2.069825000	-0.034630000	2.516748000
6	2.867526000	1.982737000	2.364038000
1	3.628511000	1.822623000	3.135398000
6	2.738233000	3.226713000	1.746128000
1	3.393501000	4.057988000	2.032179000
6	1.789347000	3.408726000	0.743553000
1	1.708245000	4.370006000	0.222078000
6	0.946752000	2.337978000	0.350143000
6	-1.281953000	0.149987000	1.267697000
6	-1.452792000	0.801564000	2.497779000
1	-0.562806000	1.218235000	2.984859000
6	-2.704982000	0.896247000	3.125818000
1	-2.797045000	1.418408000	4.084297000
6	-3.826964000	0.321580000	2.528856000
1	-4.806973000	0.380553000	3.015828000
6	-3.703781000	-0.301729000	1.289372000
1	-4.584714000	-0.713961000	0.783415000
6	-2.448209000	-0.373465000	0.651004000
6	0.640515000	-1.395137000	0.958096000
6	0.274723000	-2.107177000	2.111995000
1	-0.435809000	-1.640855000	2.803375000
6	0.791677000	-3.379095000	2.406104000
1	0.469448000	-3.900785000	3.313829000
6	1.704112000	-3.974189000	1.540280000
1	2.109194000	-4.969678000	1.753266000
6	2.085901000	-3.301571000	0.379645000
1	2.773116000	-3.770353000	-0.333504000
6	1.564604000	-2.025425000	0.085258000
16	1.826739000	-1.395707000	-1.576568000
16	0.174178000	2.442399000	-1.262365000
16	-2.423176000	-0.751989000	-1.105798000
23	-0.161982000	0.027955000	-1.487330000
6	-1.334477000	3.569674000	-1.065434000
1	-0.901625000	4.580549000	-0.942404000
6	-2.709959000	-2.622674000	-1.234010000
1	-3.766430000	-2.763996000	-0.938593000
6	3.553519000	-0.540471000	-1.577190000

1	4.037624000	-1.041635000	-2.435873000
6	4.332030000	-0.809673000	-0.313218000
1	5.330149000	-0.340862000	-0.385828000
1	3.818417000	-0.370299000	0.559271000
1	4.472350000	-1.884660000	-0.122459000
6	3.394741000	0.932768000	-1.862325000
1	2.987564000	1.461922000	-0.983832000
1	4.372058000	1.384735000	-2.111522000
1	2.707658000	1.116078000	-2.707080000
6	-2.070107000	3.466226000	-2.382416000
1	-1.435600000	3.760101000	-3.235612000
1	-2.390450000	2.418421000	-2.542155000
1	-2.971183000	4.103114000	-2.385785000
6	-2.200395000	3.218257000	0.114283000
1	-1.624227000	3.194800000	1.053005000
1	-3.017544000	3.953714000	0.224374000
1	-2.649904000	2.218938000	-0.019057000
6	-2.512297000	-2.934668000	-2.699739000
1	-2.644024000	-4.011777000	-2.898858000
1	-3.209396000	-2.373371000	-3.344403000
1	-1.479112000	-2.654336000	-2.988633000
6	-1.784880000	-3.415376000	-0.351305000
1	-0.734894000	-3.220214000	-0.635595000
1	-1.893437000	-3.146449000	0.711167000
1	-1.979656000	-4.497582000	-0.458475000
6	0.080370000	-0.037151000	0.658743000

[1e''_{ssi}]- (TE = -3474.066383)

6	1.455493000	-1.265124000	1.303224000
6	1.625253000	-1.751025000	2.607331000
1	0.935204000	-1.411824000	3.391835000
6	2.629368000	-2.664723000	2.933018000
1	2.739483000	-3.017488000	3.964268000
6	3.486160000	-3.138014000	1.938814000
1	4.268324000	-3.865231000	2.181105000
6	3.322962000	-2.704218000	0.624787000
1	3.960706000	-3.100728000	-0.173943000
6	2.322415000	-1.775402000	0.318492000
6	0.578057000	1.702150000	1.269906000
6	1.065242000	2.067663000	2.541702000
1	1.185996000	1.289858000	3.307337000
6	1.404955000	3.381786000	2.858369000
1	1.779506000	3.622076000	3.859998000
6	1.277670000	4.391105000	1.903653000
1	1.549022000	5.424327000	2.142830000
6	0.822768000	4.061436000	0.621552000

1	0.749737000	4.830789000	-0.156191000
6	0.483877000	2.743329000	0.318536000
6	-1.630890000	-0.471830000	1.356860000
6	-2.145380000	-0.085969000	2.607301000
1	-1.441031000	0.306939000	3.356942000
6	-3.496425000	-0.135931000	2.937710000
1	-3.838367000	0.178812000	3.929899000
6	-4.435612000	-0.563397000	1.947917000
1	-5.508200000	-0.585311000	2.172511000
6	-3.986679000	-0.937984000	0.698432000
1	-4.706791000	-1.235385000	-0.075840000
6	-2.606094000	-0.938136000	0.372207000
16	-2.166712000	-1.246751000	-1.323071000
16	2.130353000	-1.314954000	-1.437816000
16	-0.016100000	2.402418000	-1.399347000
23	0.029248000	-0.059024000	-1.692447000
6	3.640648000	-0.190901000	-1.645231000
1	4.512665000	-0.852027000	-1.486508000
6	-1.766805000	3.104570000	-1.390073000
1	-1.629685000	4.198125000	-1.293927000
6	-1.841273000	-3.119749000	-1.403617000
1	-1.397115000	-3.213852000	-2.415685000
6	-3.159977000	-3.854699000	-1.323530000
1	-3.017397000	-4.946376000	-1.423196000
1	-3.631699000	-3.668486000	-0.342196000
1	-3.862413000	-3.522671000	-2.105811000
6	-0.861108000	-3.575019000	-0.352339000
1	-1.242022000	-3.339350000	0.657525000
1	-0.696875000	-4.666220000	-0.411340000
1	0.110857000	-3.070604000	-0.468131000
6	3.582516000	0.294941000	-3.075562000
1	3.627155000	-0.535318000	-3.799920000
1	2.627040000	0.836454000	-3.229466000
1	4.409508000	0.992497000	-3.291915000
6	3.631702000	0.948202000	-0.657478000
1	3.652225000	0.597319000	0.386975000
1	4.502195000	1.608218000	-0.818869000
1	2.711219000	1.544526000	-0.788634000
6	-2.340520000	2.758083000	-2.746232000
1	-3.376854000	3.124596000	-2.839237000
1	-1.745815000	3.185174000	-3.571309000
1	-2.355424000	1.656492000	-2.864079000
6	-2.604818000	2.561947000	-0.258620000
1	-2.691368000	1.463740000	-0.334076000
1	-2.179318000	2.796364000	0.730031000
1	-3.622357000	2.989681000	-0.303775000

14	0.076249000	-0.054821000	0.697145000
[1f'' _{SB}] (TE = -3209.519336)			
6	0.129041000	-1.676503000	1.045052000
6	-0.404568000	-2.253175000	2.218600000
1	-0.927085000	-1.592873000	2.924506000
6	-0.290031000	-3.608173000	2.521895000
1	-0.717619000	-3.998679000	3.452977000
6	0.374722000	-4.470555000	1.647036000
1	0.472501000	-5.536872000	1.876773000
6	0.886333000	-3.956158000	0.456998000
1	1.362799000	-4.619877000	-0.274798000
6	0.754396000	-2.594394000	0.166350000
6	1.320642000	0.716356000	1.246620000
6	1.993817000	0.374969000	2.441016000
1	1.607074000	-0.472699000	3.023161000
6	3.112207000	1.057831000	2.913617000
1	3.586066000	0.747587000	3.852499000
6	3.626019000	2.141883000	2.199155000
1	4.503038000	2.689250000	2.560558000
6	3.019355000	2.498065000	0.995585000
1	3.435084000	3.308983000	0.385048000
6	1.902960000	1.794491000	0.529059000
6	-1.366177000	0.580103000	1.152074000
6	-1.513152000	1.259961000	2.383678000
1	-0.647841000	1.281342000	3.060021000
6	-2.686869000	1.897621000	2.776367000
1	-2.738209000	2.397616000	3.750906000
6	-3.797315000	1.901749000	1.930098000
1	-4.724715000	2.407319000	2.219132000
6	-3.695169000	1.274613000	0.689635000
1	-4.529900000	1.322380000	-0.018724000
6	-2.512120000	0.625358000	0.311317000
16	-2.386527000	0.115687000	-1.418856000
16	1.155712000	-2.058422000	-1.508347000
16	1.391242000	2.115105000	-1.172525000
23	0.058183000	0.123782000	-1.495963000
6	3.046384000	-2.015612000	-1.527816000
1	3.352076000	-3.079032000	-1.532997000
6	0.442502000	3.761062000	-1.054424000
1	1.218170000	4.512170000	-0.813878000
6	-3.296416000	-1.547706000	-1.494742000
1	-3.067532000	-1.827760000	-2.541450000
6	-4.786335000	-1.350408000	-1.324884000
1	-5.329989000	-2.292726000	-1.519891000
1	-5.020783000	-1.045597000	-0.290055000
1	-5.179715000	-0.578111000	-2.006131000

6	-2.730033000	-2.575523000	-0.550338000
1	-2.873558000	-2.264473000	0.499314000
1	-3.230274000	-3.550974000	-0.688873000
1	-1.649005000	-2.708134000	-0.707647000
6	3.404614000	-1.346753000	-2.835758000
1	3.015458000	-1.901387000	-3.706174000
1	2.959498000	-0.332112000	-2.849968000
1	4.497900000	-1.247419000	-2.946713000
6	3.625691000	-1.294255000	-0.338443000
1	3.326497000	-1.759532000	0.614102000
1	4.729098000	-1.288102000	-0.392180000
1	3.270308000	-0.249392000	-0.321615000
6	-0.117717000	3.977795000	-2.441000000
1	-0.726371000	4.897024000	-2.488152000
1	0.674065000	4.043129000	-3.206120000
1	-0.769415000	3.117994000	-2.697394000
6	-0.635447000	3.725849000	-0.005254000
1	-1.344820000	2.910112000	-0.233240000
1	-0.230594000	3.537898000	1.001703000
1	-1.193377000	4.679459000	0.015097000
5	0.028427000	-0.100469000	0.738810000

Cartesian coordinates of $[2\mathbf{a}'_{\text{PC}}]-[2\mathbf{f}'_{\text{SB}}]$, $[2\mathbf{a}''_{\text{PC}}]-[2\mathbf{f}''_{\text{SB}}]$ and $\{[\text{HIPTN}_3\text{N}]-\text{V}-\text{N}_2\}$, along with their total energies (in hartree) including zero point vibrational correction at M06-L-D3(heptane)/6-311+G* level of theory.

$[2\mathbf{a}'_{\text{PC}}]$ (TE = -3062.105256)

6	-0.049391000	2.453084000	1.934138000
6	0.575066000	1.195316000	2.525208000
6	-2.613424000	-0.009144000	1.675972000
6	-1.422360000	-0.326223000	2.580136000
6	2.266203000	-1.329893000	1.885844000
6	0.869750000	-1.264575000	2.500405000
1	-2.699760000	1.070050000	1.488967000
1	-1.541766000	0.237510000	3.524550000
1	2.837697000	-2.197761000	2.242116000
1	0.976104000	-1.221729000	3.604949000
1	0.347911000	3.372597000	2.382914000
1	1.658498000	1.235671000	2.333746000
6	-0.855501000	3.774552000	-0.594482000
1	-0.234986000	4.227329000	-1.382670000
6	-2.586760000	-2.603193000	0.358670000
1	-1.833730000	-2.762953000	1.147747000
6	3.708748000	-0.473604000	-0.520482000
1	3.475244000	0.576222000	-0.284685000
23	0.010967000	-0.059470000	-0.352377000

6	-0.009749000	-0.115998000	1.978681000
1	-1.131075000	2.464865000	2.118251000
1	0.482848000	1.237691000	3.630253000
1	0.358788000	-2.217259000	2.303814000
1	2.854168000	-0.449152000	2.172588000
1	-1.526221000	-1.379069000	2.884968000
1	-3.563654000	-0.317905000	2.133075000
6	5.006612000	-0.812996000	0.204699000
1	5.780040000	-0.078208000	-0.048432000
1	4.896767000	-0.798234000	1.292762000
1	5.403344000	-1.791909000	-0.069882000
6	3.851706000	-0.577040000	-2.034115000
1	4.111068000	-1.593074000	-2.350267000
1	2.928687000	-0.302695000	-2.555006000
1	4.645009000	0.083290000	-2.401882000
6	-3.943626000	-3.018581000	0.909571000
1	-3.925385000	-4.064181000	1.238929000
1	-4.254980000	-2.416294000	1.768238000
1	-4.728700000	-2.943545000	0.149936000
6	-2.180500000	-3.468237000	-0.832563000
1	-2.962854000	-3.508567000	-1.594430000
1	-1.269133000	-3.099975000	-1.318022000
1	-1.991764000	-4.500278000	-0.516198000
6	-2.105718000	3.202405000	-1.248498000
1	-1.869188000	2.438398000	-1.995776000
1	-2.757745000	2.733998000	-0.500436000
1	-2.692768000	3.987740000	-1.738267000
6	-1.234124000	4.856860000	0.410279000
1	-0.374266000	5.292830000	0.922916000
1	-1.768143000	5.674718000	-0.087181000
1	-1.905870000	4.464408000	1.180912000
6	2.258979000	-3.104423000	-0.469351000
1	1.959811000	-3.092412000	-1.529070000
6	1.228517000	-3.919255000	0.305289000
1	1.541313000	-4.061444000	1.345876000
1	0.246261000	-3.441114000	0.320589000
1	1.109842000	-4.915773000	-0.134014000
6	3.626787000	-3.763091000	-0.353542000
1	3.554882000	-4.832618000	-0.584577000
1	4.364378000	-3.339510000	-1.037720000
1	4.031785000	-3.685404000	0.661839000
6	-3.771771000	-0.177082000	-1.011205000
1	-3.397721000	0.789209000	-1.374176000
6	-5.070172000	0.088032000	-0.258684000
1	-5.491611000	-0.819752000	0.182186000
1	-4.943759000	0.814450000	0.548552000

1	-5.827386000	0.493813000	-0.940072000
6	-4.004902000	-1.050697000	-2.237643000
1	-4.486354000	-1.998041000	-1.975422000
1	-4.669401000	-0.545607000	-2.947114000
1	-3.077571000	-1.286003000	-2.769233000
6	1.939944000	3.084381000	-0.092148000
1	2.539150000	2.409763000	0.539501000
6	2.163520000	4.512463000	0.381721000
1	3.224939000	4.779198000	0.318465000
1	1.622205000	5.233648000	-0.240294000
1	1.855535000	4.670121000	1.419529000
6	2.393662000	2.909565000	-1.536554000
1	3.455536000	3.155136000	-1.652747000
1	2.245436000	1.884993000	-1.891565000
1	1.840306000	3.570819000	-2.214138000
15	-2.333146000	-0.778647000	0.024800000
15	0.209575000	2.397245000	0.110051000
15	2.128390000	-1.304349000	0.044840000
7	-0.006055000	-0.250973000	-3.500892000
7	0.006737000	-0.171837000	-2.368207000

[2b'_{psi}] (TE = -3313.522070)

6	-0.165477000	2.761594000	1.797130000
6	0.401971000	1.702749000	2.740694000
6	-2.806620000	-0.202041000	1.879369000
6	-1.675740000	-0.600442000	2.827329000
6	2.569340000	-1.264050000	1.816222000
6	1.386237000	-1.224314000	2.785621000
1	-2.943880000	0.889350000	1.882204000
1	-1.865522000	-0.194651000	3.830809000
1	3.280181000	-2.074700000	2.033750000
1	1.738639000	-0.927209000	3.783436000
1	0.118415000	3.785511000	2.072629000
1	1.494450000	1.820731000	2.805885000
6	-0.493465000	3.767349000	-0.942863000
1	0.216435000	3.967304000	-1.758311000
6	-2.695709000	-2.498118000	0.124381000
1	-2.069733000	-2.806501000	0.976629000
6	3.629875000	-0.719638000	-0.811828000
1	3.559438000	0.359014000	-0.609176000
23	-0.042442000	-0.044931000	-0.470430000
1	-1.265099000	2.740249000	1.815139000
1	0.030309000	1.868458000	3.761972000
1	0.965072000	-2.228862000	2.909043000
1	3.149858000	-0.334037000	1.907479000
1	-1.672294000	-1.693399000	2.950737000

1	-3.777299000	-0.626135000	2.170053000
6	4.976917000	-1.176594000	-0.259971000
1	5.779638000	-0.571648000	-0.698443000
1	5.050706000	-1.062952000	0.824622000
1	5.205476000	-2.216908000	-0.496786000
6	3.542404000	-0.900759000	-2.321331000
1	3.601294000	-1.955251000	-2.612077000
1	2.608255000	-0.504998000	-2.729803000
1	4.367072000	-0.385270000	-2.826428000
6	-4.117002000	-2.969084000	0.399028000
1	-4.132896000	-4.049918000	0.582067000
1	-4.567007000	-2.488383000	1.272552000
1	-4.774910000	-2.787514000	-0.456753000
6	-2.126668000	-3.167100000	-1.121882000
1	-2.702628000	-2.921225000	-2.019253000
1	-1.091598000	-2.865683000	-1.308926000
1	-2.144121000	-4.258107000	-1.017296000
6	-1.796539000	3.280604000	-1.563822000
1	-1.666379000	2.359434000	-2.141389000
1	-2.542006000	3.074991000	-0.785888000
1	-2.227914000	4.040485000	-2.225354000
6	-0.736751000	5.062268000	-0.175164000
1	0.157489000	5.455561000	0.312271000
1	-1.111943000	5.842051000	-0.848070000
1	-1.495217000	4.925505000	0.602659000
6	1.919036000	-3.152564000	-0.364162000
1	1.461341000	-3.160482000	-1.365716000
6	0.942472000	-3.803244000	0.611337000
1	1.416721000	-3.968385000	1.584823000
1	0.049629000	-3.193307000	0.779186000
1	0.616966000	-4.781896000	0.241843000
6	3.207933000	-3.960988000	-0.414603000
1	2.982137000	-5.024407000	-0.558718000
1	3.866833000	-3.662443000	-1.232154000
1	3.777029000	-3.882745000	0.518527000
6	-3.819897000	0.157581000	-0.811753000
1	-3.472858000	1.199244000	-0.849853000
6	-5.195366000	0.172860000	-0.154038000
1	-5.648595000	-0.818930000	-0.095157000
1	-5.175068000	0.586418000	0.857364000
1	-5.879848000	0.798245000	-0.739723000
6	-3.892669000	-0.343593000	-2.248308000
1	-4.305884000	-1.356479000	-2.302789000
1	-4.547127000	0.295980000	-2.851009000
1	-2.912334000	-0.361204000	-2.734029000
6	2.135382000	2.820171000	-0.006702000

1	2.580606000	2.005898000	0.587144000
6	2.560985000	4.143877000	0.611251000
1	3.654339000	4.211070000	0.656166000
1	2.221999000	4.996886000	0.015035000
1	2.190362000	4.279330000	1.631164000
6	2.654203000	2.697934000	-1.435979000
1	3.749976000	2.691725000	-1.461012000
1	2.303768000	1.784357000	-1.928653000
1	2.332562000	3.544553000	-2.052230000
15	-2.404624000	-0.643836000	0.123935000
15	0.310385000	2.385386000	0.046271000
15	2.061875000	-1.320483000	0.026328000
14	0.020037000	-0.073816000	2.092016000
7	-0.147028000	-0.715161000	-3.540943000
7	-0.107660000	-0.444073000	-2.435670000

[2c'_{PB}] (TE = -3048.877617)

6	0.043551000	2.457295000	2.097692000
6	0.602625000	1.242386000	2.836579000
6	-2.637629000	0.127661000	1.860026000
6	-1.573112000	-0.435370000	2.803872000
6	2.269842000	-1.380611000	1.832457000
6	0.942959000	-1.454681000	2.583296000
1	-2.581342000	1.221742000	1.800045000
1	-1.768007000	-0.025623000	3.810490000
1	2.978006000	-2.158867000	2.140095000
1	1.163287000	-1.591012000	3.659481000
1	0.395476000	3.415478000	2.503596000
1	1.700002000	1.248123000	2.748666000
6	-0.351910000	3.774713000	-0.525145000
1	0.349462000	4.619182000	-0.453431000
6	-2.769267000	-2.303154000	0.281641000
1	-1.841311000	-2.686498000	0.734047000
6	3.647981000	-0.863559000	-0.659776000
1	3.751813000	0.155336000	-0.255991000
23	-0.002807000	-0.000054000	-0.502804000
1	-1.047777000	2.479943000	2.177654000
1	0.418919000	1.386628000	3.916738000
1	0.413283000	-2.378154000	2.297912000
1	2.771370000	-0.422478000	2.029985000
1	-1.754695000	-1.516643000	2.909748000
1	-3.658017000	-0.103443000	2.197125000
6	4.832967000	-1.693802000	-0.185594000
1	5.776639000	-1.257155000	-0.532399000
1	4.890885000	-1.765514000	0.904393000
1	4.795831000	-2.713670000	-0.583998000

6	3.613969000	-0.766516000	-2.178981000
1	3.494315000	-1.750840000	-2.646965000
1	2.792511000	-0.139151000	-2.534012000
1	4.547878000	-0.344791000	-2.566860000
6	-3.918110000	-2.708306000	1.196458000
1	-3.953581000	-3.800216000	1.289304000
1	-3.811211000	-2.308061000	2.208107000
1	-4.892410000	-2.392358000	0.816981000
6	-2.902573000	-2.929991000	-1.100665000
1	-3.858857000	-2.670137000	-1.567466000
1	-2.105277000	-2.608640000	-1.779786000
1	-2.864274000	-4.023536000	-1.042446000
6	-0.606772000	3.466326000	-1.997166000
1	0.288749000	3.130196000	-2.527517000
1	-1.351224000	2.667035000	-2.097158000
1	-0.994126000	4.347509000	-2.521033000
6	-1.653841000	4.167035000	0.160027000
1	-1.505472000	4.533899000	1.178763000
1	-2.164707000	4.955654000	-0.403216000
1	-2.345575000	3.315768000	0.212658000
6	1.988045000	-3.245091000	-0.478598000
1	2.693742000	-3.299023000	-1.320692000
6	0.621310000	-3.670912000	-0.995257000
1	-0.135727000	-3.617664000	-0.204889000
1	0.272904000	-3.030776000	-1.811150000
1	0.642699000	-4.704312000	-1.360934000
6	2.475684000	-4.193171000	0.608348000
1	2.476203000	-5.226151000	0.241835000
1	3.490697000	-3.969778000	0.946976000
1	1.824310000	-4.167757000	1.488768000
6	-3.722043000	0.375554000	-0.802607000
1	-3.566166000	1.420854000	-0.487338000
6	-5.147376000	-0.017042000	-0.437788000
1	-5.399354000	-1.011656000	-0.819428000
1	-5.329068000	-0.019207000	0.640668000
1	-5.863871000	0.680541000	-0.886856000
6	-3.507028000	0.323609000	-2.310494000
1	-3.610297000	-0.691042000	-2.707393000
1	-4.246958000	0.945363000	-2.827085000
1	-2.515541000	0.682406000	-2.595928000
6	2.276155000	2.748840000	0.284937000
1	2.747791000	1.868110000	0.747285000
6	2.660677000	3.977191000	1.096289000
1	3.730611000	4.190057000	0.990551000
1	2.127767000	4.875529000	0.764233000
1	2.463021000	3.853499000	2.164020000

6	2.776134000	2.849322000	-1.150319000
1	3.870460000	2.896695000	-1.185131000
1	2.461747000	1.991610000	-1.755187000
1	2.403964000	3.755136000	-1.642433000
15	-2.353336000	-0.480168000	0.145724000
15	0.455009000	2.300196000	0.306423000
15	1.989878000	-1.417183000	0.007235000
5	-0.021819000	-0.186645000	2.458158000
7	0.043226000	-0.224316000	-3.633516000
7	0.022127000	-0.123786000	-2.500173000

[2d'_{sc}]-Quintet (TE = -2877.257312)

6	-0.762178000	2.024044000	-1.787742000
6	-0.700964000	0.636564000	-2.405386000
6	2.561013000	0.859351000	-1.292390000
6	1.721734000	-0.015484000	-2.209859000
6	-1.378426000	-2.284928000	-1.693871000
6	-0.040304000	-1.758822000	-2.176992000
1	2.168261000	1.877970000	-1.211891000
1	1.731743000	0.459040000	-3.210849000
1	-1.518365000	-3.342766000	-1.936026000
1	-0.030013000	-1.881960000	-3.281800000
1	-1.449404000	2.687298000	-2.323795000
1	-1.721133000	0.225904000	-2.366069000
6	-0.843864000	3.395893000	0.759065000
1	-1.332512000	3.295239000	1.736557000
6	3.375940000	-1.390550000	0.268341000
1	2.829566000	-1.911182000	-0.527724000
6	-3.286596000	-1.419663000	0.218290000
1	-3.311205000	-0.578183000	-0.488645000
23	0.087570000	-0.217755000	0.511662000
16	2.542490000	0.265428000	0.438627000
16	-1.352290000	1.815110000	-0.065151000
16	-1.540380000	-2.071099000	0.129400000
6	0.289372000	-0.327067000	-1.739096000
1	0.221873000	2.505632000	-1.764968000
1	-0.489541000	0.762861000	-3.486963000
1	0.746646000	-2.434375000	-1.809199000
1	-2.216324000	-1.739604000	-2.140392000
1	2.272198000	-0.956157000	-2.356601000
1	3.600456000	0.952677000	-1.628852000
6	-4.275619000	-2.490224000	-0.194539000
1	-5.297752000	-2.095138000	-0.179996000
1	-4.086287000	-2.866465000	-1.203719000
1	-4.240410000	-3.343608000	0.490084000
6	-3.527704000	-0.910936000	1.624147000

1	-3.409676000	-1.708962000	2.365132000
1	-2.838972000	-0.104174000	1.889195000
1	-4.548062000	-0.525386000	1.718184000
6	4.835435000	-1.230385000	-0.103216000
1	5.312324000	-2.211153000	-0.208082000
1	4.970218000	-0.704775000	-1.052590000
1	5.383447000	-0.677131000	0.666030000
6	3.173254000	-2.135033000	1.572747000
1	3.605333000	-1.593868000	2.421601000
1	2.109381000	-2.292865000	1.777903000
1	3.657145000	-3.115848000	1.527379000
6	0.653968000	3.499976000	0.960318000
1	1.051452000	2.651705000	1.523856000
1	1.188610000	3.549611000	0.005263000
1	0.900974000	4.415434000	1.509118000
6	-1.422967000	4.590906000	0.025829000
1	-2.502165000	4.500555000	-0.120543000
1	-1.235570000	5.511846000	0.588037000
1	-0.960408000	4.717776000	-0.958362000
7	0.058015000	-0.432146000	3.657417000
7	0.055465000	-0.344203000	2.524097000

[2e'_{ssi}] (TE = -3128.668457)

23	-0.020789000	-0.010976000	0.816867000
16	-1.962810000	-1.647548000	0.946759000
16	2.202692000	-1.197089000	1.228960000
16	0.530859000	1.856396000	-0.759650000
14	0.279542000	-1.172565000	-1.425555000
6	0.416473000	0.096874000	-2.862173000
6	-0.195984000	1.412442000	-2.399715000
6	2.222086000	-2.626440000	0.063039000
6	1.854983000	-2.278990000	-1.373847000
6	-1.237312000	-2.316553000	-1.705662000
6	-1.687474000	-2.899342000	-0.375936000
1	-0.919284000	-3.551675000	0.055266000
1	-2.599282000	-3.504412000	-0.435321000
1	-2.055124000	-1.731295000	-2.150602000
1	-1.047196000	-3.142607000	-2.406410000
1	3.198930000	-3.113984000	0.164078000
1	1.491434000	-3.309693000	0.510260000
1	2.691592000	-1.745814000	-1.846587000
1	1.750532000	-3.215817000	-1.939541000
1	1.472917000	0.257464000	-3.116924000
1	-0.077635000	-0.215952000	-3.791469000
1	-1.279669000	1.313805000	-2.262257000
1	-0.011157000	2.246951000	-3.086810000

6	-3.393098000	-0.679184000	0.240139000
1	-2.966442000	-0.086898000	-0.582036000
6	3.444743000	-0.073912000	0.425034000
1	3.002055000	0.212492000	-0.539275000
6	-0.348417000	3.440686000	-0.354356000
1	0.034158000	3.637154000	0.655646000
6	4.774792000	-0.765738000	0.208948000
1	5.497289000	-0.064749000	-0.223425000
1	5.193635000	-1.131211000	1.152103000
1	4.701578000	-1.613475000	-0.477096000
6	3.570940000	1.157730000	1.300985000
1	2.602955000	1.639260000	1.471480000
1	3.999550000	0.910642000	2.277718000
1	4.227307000	1.893548000	0.825821000
6	0.074757000	4.565228000	-1.280122000
1	-0.272133000	4.397691000	-2.304674000
1	-0.359053000	5.515350000	-0.949453000
1	1.160270000	4.685424000	-1.309845000
6	-1.852353000	3.262791000	-0.289858000
1	-2.325840000	4.158916000	0.125553000
1	-2.284473000	3.104405000	-1.283562000
1	-2.129045000	2.410813000	0.337845000
6	-3.874788000	0.250086000	1.337719000
1	-4.635730000	0.934327000	0.948393000
1	-4.323547000	-0.311494000	2.163225000
1	-3.063441000	0.855974000	1.749827000
6	-4.500644000	-1.576646000	-0.271575000
1	-5.356492000	-0.969048000	-0.585311000
1	-4.198257000	-2.173297000	-1.135536000
1	-4.853504000	-2.261222000	0.506791000
7	-0.664828000	1.827135000	3.289233000
7	-0.427518000	1.120645000	2.427788000

[2f_{SB}] (TE = -2864.018742)

6	-0.906331000	1.979101000	-1.870671000
6	-0.752788000	0.612074000	-2.519237000
6	2.598438000	1.091562000	-1.170920000
6	1.953945000	0.222190000	-2.238890000
6	-1.063593000	-2.474457000	-1.674348000
6	0.259829000	-1.903565000	-2.142676000
1	2.083261000	2.051578000	-1.059982000
1	1.982611000	0.812996000	-3.171442000
1	-1.152073000	-3.555409000	-1.825116000
1	0.362950000	-2.172731000	-3.212064000
1	-1.642680000	2.615703000	-2.373954000
1	-1.729670000	0.105974000	-2.472302000

6	-1.131407000	3.341112000	0.677578000
1	-1.580175000	3.178913000	1.666116000
6	3.376511000	-1.236855000	0.287814000
1	2.861675000	-1.729157000	-0.545827000
6	-3.132618000	-1.696156000	0.110926000
1	-3.224516000	-0.893948000	-0.634973000
23	0.068304000	-0.134364000	0.631298000
16	2.493283000	0.384778000	0.520362000
16	-1.472295000	1.713968000	-0.143144000
16	-1.323032000	-2.139783000	0.123593000
1	0.045840000	2.522587000	-1.841352000
1	-0.591999000	0.789446000	-3.598574000
1	1.079537000	-2.451243000	-1.652647000
1	-1.906767000	-2.003706000	-2.191699000
1	2.627597000	-0.625413000	-2.439169000
1	3.650557000	1.327096000	-1.373573000
6	-3.970274000	-2.892488000	-0.292509000
1	-5.031132000	-2.620722000	-0.332230000
1	-3.697193000	-3.281052000	-1.277259000
1	-3.864219000	-3.709046000	0.428733000
6	-3.498182000	-1.164682000	1.481301000
1	-3.326939000	-1.915301000	2.260409000
1	-2.919531000	-0.274281000	1.741890000
1	-4.558936000	-0.895737000	1.512481000
6	4.836634000	-1.016615000	-0.048307000
1	5.345273000	-1.977582000	-0.182754000
1	4.970931000	-0.449676000	-0.973584000
1	5.353549000	-0.478673000	0.752722000
6	3.173431000	-2.050877000	1.549599000
1	3.594264000	-1.549644000	2.427995000
1	2.110337000	-2.231646000	1.741520000
1	3.668280000	-3.022812000	1.456583000
6	0.347981000	3.621447000	0.842951000
1	0.859476000	2.814851000	1.376004000
1	0.844435000	3.757614000	-0.124028000
1	0.497931000	4.547397000	1.408798000
6	-1.864621000	4.462578000	-0.033646000
1	-2.928709000	4.246211000	-0.156275000
1	-1.774082000	5.396226000	0.531454000
1	-1.442967000	4.648218000	-1.026704000
5	0.450529000	-0.317212000	-1.993008000
7	-0.088853000	-0.235840000	3.769994000
7	-0.042514000	-0.194190000	2.635607000

[2a''_{pc}] (TE = -3519.383039)

6	1.180147000	-0.669751000	1.748461000
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6	1.781388000	-0.156911000	2.909192000
1	1.310888000	0.684131000	3.415564000
6	2.954385000	-0.690034000	3.432940000
1	3.391069000	-0.255290000	4.330532000
6	3.558355000	-1.781890000	2.820704000
1	4.472990000	-2.210414000	3.224482000
6	2.987770000	-2.309466000	1.665950000
1	3.485569000	-3.139465000	1.167518000
6	1.827745000	-1.761593000	1.108290000
6	-0.358720000	1.312851000	1.691009000
6	-1.248895000	1.595351000	2.740963000
1	-1.764035000	0.773172000	3.233194000
6	-1.506817000	2.894520000	3.162748000
1	-2.214289000	3.068846000	3.971632000
6	-0.861790000	3.964266000	2.553881000
1	-1.057946000	4.986322000	2.870540000
6	0.036281000	3.711817000	1.522125000
1	0.525443000	4.553669000	1.040620000
6	0.287149000	2.410622000	1.075286000
6	-1.305474000	-0.949510000	1.554928000
6	-1.334889000	-1.785684000	2.678424000
1	-0.432034000	-1.892549000	3.278336000
6	-2.484915000	-2.475260000	3.047613000
1	-2.469719000	-3.122393000	3.923025000
6	-3.654546000	-2.327743000	2.310677000
1	-4.560190000	-2.858292000	2.596193000
6	-3.655217000	-1.491869000	1.196975000
1	-4.571385000	-1.379123000	0.622611000
6	-2.498023000	-0.817596000	0.799624000
6	-0.108039000	-0.100192000	1.213338000
23	0.095309000	-0.071962000	-1.109328000
6	2.838260000	-2.571239000	-1.504913000
1	3.423508000	-3.290402000	-0.917455000
6	1.044235000	3.588585000	-1.484152000
1	-0.000078000	3.858920000	-1.261081000
6	-3.437578000	-0.633453000	-2.051518000
1	-3.082128000	-0.114398000	-2.955965000
6	-4.948520000	-0.439706000	-1.987992000
1	-5.417127000	-0.902659000	-2.864410000
1	-5.401319000	-0.907321000	-1.109806000
1	-5.244539000	0.610654000	-1.989618000
6	-3.084051000	-2.109112000	-2.206675000
1	-3.421969000	-2.694145000	-1.344417000
1	-3.568348000	-2.528819000	-3.094830000
1	-2.005253000	-2.268196000	-2.306541000
6	2.532922000	-3.187599000	-2.865630000

1	2.081746000	-4.180681000	-2.794782000
1	1.852528000	-2.557020000	-3.448810000
1	3.451459000	-3.293239000	-3.453055000
6	3.657665000	-1.303048000	-1.665114000
1	3.858349000	-0.813675000	-0.707222000
1	4.622447000	-1.516582000	-2.139231000
1	3.131242000	-0.580105000	-2.297744000
6	1.918233000	4.809084000	-1.209267000
1	1.564466000	5.658908000	-1.804466000
1	1.921917000	5.129900000	-0.166500000
1	2.958582000	4.641127000	-1.497970000
6	1.117877000	3.216182000	-2.962382000
1	2.108137000	2.837503000	-3.239810000
1	0.390214000	2.445125000	-3.225702000
1	0.920859000	4.090809000	-3.592516000
15	-2.339820000	0.144380000	-0.746792000
15	1.258671000	2.044183000	-0.431293000
15	1.250587000	-2.215292000	-0.573048000
6	3.045645000	1.962668000	0.148351000
1	3.083490000	0.939298000	0.550764000
6	4.024397000	2.039336000	-1.018647000
1	4.172453000	3.066364000	-1.361747000
1	5.008703000	1.661415000	-0.720718000
1	3.701180000	1.449721000	-1.880072000
6	3.430760000	2.908416000	1.276479000
1	4.441147000	2.677022000	1.634078000
1	3.437164000	3.955383000	0.959234000
1	2.755636000	2.824800000	2.132209000
6	0.519665000	-3.946601000	-0.520734000
1	0.273208000	-4.127424000	-1.577965000
6	-0.770303000	-4.015361000	0.277665000
1	-0.575357000	-3.922930000	1.349200000
1	-1.478644000	-3.228330000	0.009050000
1	-1.263802000	-4.981070000	0.119970000
6	1.484427000	-5.025352000	-0.046037000
1	0.996455000	-6.006554000	-0.066937000
1	2.387713000	-5.106096000	-0.656054000
1	1.794474000	-4.849522000	0.989737000
6	-3.035939000	1.848365000	-0.409843000
1	-2.229114000	2.302848000	0.179091000
6	-4.298183000	1.913462000	0.437852000
1	-4.530930000	2.954657000	0.690491000
1	-5.176574000	1.501047000	-0.065406000
1	-4.174987000	1.373343000	1.381125000
6	-3.131681000	2.635006000	-1.711988000
1	-3.327592000	3.693935000	-1.511087000

1	-2.198409000	2.578269000	-2.286148000
1	-3.936838000	2.279745000	-2.363052000
7	0.027943000	-0.289469000	-4.246932000
7	0.089707000	-0.193894000	-3.118499000

[2b''_{psi}] (TE =-3770.793091)

6	0.811840000	-1.678102000	1.939382000
6	0.575797000	-2.270618000	3.186437000
1	-0.140558000	-1.813076000	3.870554000
6	1.210459000	-3.449862000	3.564046000
1	1.002069000	-3.899536000	4.533298000
6	2.106818000	-4.058903000	2.691102000
1	2.604930000	-4.984119000	2.974208000
6	2.358253000	-3.489585000	1.446528000
1	3.052600000	-3.988276000	0.774171000
6	1.712838000	-2.311058000	1.058587000
6	0.757735000	1.372777000	2.137231000
6	1.210878000	1.377784000	3.461969000
1	1.051445000	0.496398000	4.085343000
6	1.898275000	2.463860000	3.994502000
1	2.255095000	2.438070000	5.022665000
6	2.140765000	3.578680000	3.198857000
1	2.686775000	4.430563000	3.599489000
6	1.694282000	3.601473000	1.880903000
1	1.909068000	4.477701000	1.275718000
6	1.010102000	2.508499000	1.338424000
6	-1.873546000	-0.154559000	1.863231000
6	-2.295467000	0.194656000	3.152442000
1	-1.549650000	0.406272000	3.920253000
6	-3.643093000	0.330334000	3.467992000
1	-3.946020000	0.620015000	4.472680000
6	-4.602967000	0.116296000	2.483582000
1	-5.659994000	0.237451000	2.712212000
6	-4.210706000	-0.245888000	1.199444000
1	-4.977061000	-0.400650000	0.445255000
6	-2.856099000	-0.385821000	0.877015000
23	0.102441000	0.068233000	-1.208505000
6	3.674402000	-0.804965000	-0.435785000
1	4.354191000	-1.645653000	-0.240962000
6	-1.058493000	3.569912000	-0.381233000
1	-0.692958000	4.559358000	-0.074055000
6	-2.524890000	-2.676424000	-0.910145000
1	-2.719862000	-2.857828000	-1.978917000
6	-3.689334000	-3.210266000	-0.085394000
1	-3.824093000	-4.281647000	-0.274347000
1	-3.492116000	-3.094103000	0.985120000

1	-4.642081000	-2.722424000	-0.291987000
6	-1.255891000	-3.421332000	-0.525107000
1	-0.985942000	-3.241977000	0.521601000
1	-1.390898000	-4.502646000	-0.644087000
1	-0.404397000	-3.118413000	-1.136561000
6	4.076604000	-0.113101000	-1.731150000
1	3.958157000	-0.742337000	-2.618747000
1	3.464179000	0.780869000	-1.889574000
1	5.122717000	0.211068000	-1.695810000
6	3.758371000	0.164551000	0.732774000
1	3.469132000	-0.290968000	1.684541000
1	4.781186000	0.542475000	0.842196000
1	3.107111000	1.030554000	0.577102000
6	-1.681547000	3.666421000	-1.766945000
1	-2.536816000	4.351663000	-1.765177000
1	-0.984730000	4.016996000	-2.533716000
1	-2.049645000	2.685596000	-2.090491000
6	-2.090137000	3.101862000	0.631601000
1	-2.516940000	2.136489000	0.344983000
1	-1.677843000	2.988276000	1.638634000
1	-2.917841000	3.817748000	0.690603000
14	-0.060796000	-0.120163000	1.282724000
15	0.448648000	2.447256000	-0.424297000
15	-2.262411000	-0.805078000	-0.822505000
15	1.958406000	-1.545873000	-0.606277000
6	2.268584000	-3.062939000	-1.707886000
1	1.682152000	-3.847308000	-1.208262000
6	3.706565000	-3.558405000	-1.823475000
1	3.731686000	-4.494855000	-2.392213000
1	4.344548000	-2.850216000	-2.360368000
1	4.185793000	-3.756784000	-0.862135000
6	1.679943000	-2.851360000	-3.097618000
1	0.623555000	-2.565851000	-3.063476000
1	2.204670000	-2.061454000	-3.645630000
1	1.760224000	-3.766449000	-3.695148000
6	-3.595654000	-0.131960000	-1.985281000
1	-3.857210000	0.838278000	-1.533532000
6	-2.963818000	0.129106000	-3.349645000
1	-2.577585000	-0.794506000	-3.798719000
1	-3.702782000	0.540048000	-4.046217000
1	-2.129100000	0.829666000	-3.295184000
6	-4.874556000	-0.939133000	-2.187454000
1	-4.668170000	-1.934308000	-2.594390000
1	-5.470770000	-1.073132000	-1.284355000
1	-5.517175000	-0.432092000	-2.916142000
6	1.719050000	3.529440000	-1.323552000

1	2.653559000	3.297682000	-0.788716000
6	1.501084000	5.040087000	-1.287797000
1	2.371057000	5.550958000	-1.715574000
1	0.638198000	5.336393000	-1.892210000
1	1.346932000	5.452943000	-0.289292000
6	1.884497000	3.086245000	-2.772680000
1	2.145967000	2.031240000	-2.858741000
1	0.966405000	3.233755000	-3.352025000
1	2.672035000	3.667415000	-3.265499000
7	0.501730000	0.218150000	-4.336486000
7	0.350624000	0.169961000	-3.214104000
[2c'' _{PB}] (TE = -3506.135445)			
6	1.377609000	-0.760548000	1.886123000
6	1.415164000	-1.501338000	3.081954000
1	0.487786000	-1.650451000	3.635295000
6	2.587578000	-2.054932000	3.584616000
1	2.566797000	-2.624029000	4.512510000
6	3.783117000	-1.883237000	2.895840000
1	4.708760000	-2.311461000	3.274925000
6	3.779767000	-1.171384000	1.702110000
1	4.713654000	-1.063027000	1.155555000
6	2.599583000	-0.622248000	1.188706000
6	-0.241484000	1.430345000	1.904287000
6	0.259418000	1.842150000	3.151422000
1	0.887795000	1.152716000	3.716557000
6	-0.013235000	3.095364000	3.689926000
1	0.404940000	3.375661000	4.655377000
6	-0.825106000	3.985975000	2.996391000
1	-1.053131000	4.966305000	3.409591000
6	-1.334777000	3.613482000	1.756898000
1	-1.960335000	4.316555000	1.211139000
6	-1.037506000	2.366189000	1.198272000
6	-1.298543000	-1.019873000	1.710861000
6	-1.982324000	-0.870185000	2.931433000
1	-1.646887000	-0.100473000	3.627630000
6	-3.083317000	-1.645187000	3.273188000
1	-3.586612000	-1.488495000	4.225854000
6	-3.550419000	-2.607667000	2.384403000
1	-4.421802000	-3.212022000	2.627970000
6	-2.897606000	-2.783328000	1.171234000
1	-3.280936000	-3.525950000	0.477426000
6	-1.780807000	-2.010745000	0.827005000
23	0.128210000	0.133825000	-1.131010000
6	3.491743000	1.757305000	-0.262909000
1	4.507240000	1.486268000	0.060512000
6	-3.392560000	1.791128000	-0.483824000

1	-3.754814000	2.795265000	-0.222323000
6	-0.052891000	-3.750529000	-0.856619000
1	-0.164115000	-4.095526000	-1.895539000
6	-0.596692000	-4.817377000	0.082580000
1	-0.023896000	-5.745373000	-0.027672000
1	-0.507809000	-4.502849000	1.127614000
1	-1.645549000	-5.061639000	-0.094244000
6	1.428850000	-3.528704000	-0.600096000
1	1.614004000	-3.123594000	0.400200000
1	1.980914000	-4.472347000	-0.678508000
1	1.855109000	-2.830278000	-1.321799000
6	3.574859000	2.496179000	-1.593336000
1	4.117921000	1.938249000	-2.360217000
1	2.580842000	2.701191000	-2.000672000
1	4.081014000	3.460474000	-1.473731000
6	2.857777000	2.615216000	0.821471000
1	2.856183000	2.111911000	1.792475000
1	3.404003000	3.558472000	0.934640000
1	1.816731000	2.862787000	0.591347000
6	-3.890587000	1.419640000	-1.875037000
1	-4.985502000	1.416772000	-1.912771000
1	-3.539150000	2.097832000	-2.658997000
1	-3.553735000	0.412957000	-2.147725000
6	-3.913753000	0.818786000	0.558269000
1	-3.617985000	-0.210435000	0.335738000
1	-3.550809000	1.050661000	1.562910000
1	-5.009095000	0.844089000	0.585051000
5	-0.015056000	-0.093783000	1.467075000
15	2.556279000	0.150793000	-0.473318000
15	-1.526221000	1.920886000	-0.510444000
15	-0.995251000	-2.116475000	-0.827306000
6	-1.316328000	3.462175000	-1.583146000
1	-1.319762000	3.026927000	-2.593930000
6	0.052607000	4.086436000	-1.363882000
1	0.257859000	4.850546000	-2.121271000
1	0.126787000	4.567077000	-0.382549000
1	0.846739000	3.340297000	-1.419759000
6	-2.403792000	4.530923000	-1.549948000
1	-2.158184000	5.320617000	-2.269154000
1	-3.393057000	4.156476000	-1.821044000
1	-2.491136000	5.017899000	-0.574734000
6	3.766552000	-0.896211000	-1.486507000
1	3.678248000	-1.884735000	-1.016848000
6	5.241616000	-0.507151000	-1.452829000
1	5.835183000	-1.271419000	-1.967120000
1	5.437167000	0.436691000	-1.968550000

1	5.651440000	-0.413401000	-0.444971000
6	3.287614000	-1.010282000	-2.930297000
1	3.922860000	-1.699495000	-3.498013000
1	2.256191000	-1.372793000	-2.997472000
1	3.317937000	-0.044426000	-3.446713000
6	-2.420804000	-2.430820000	-2.024362000
1	-3.239302000	-1.827838000	-1.601590000
6	-2.049535000	-1.852809000	-3.387734000
1	-1.154658000	-2.335430000	-3.801106000
1	-2.859124000	-2.005795000	-4.110049000
1	-1.841486000	-0.781368000	-3.339639000
6	-2.916816000	-3.862180000	-2.200487000
1	-2.137141000	-4.522778000	-2.592699000
1	-3.299669000	-4.316669000	-1.285665000
1	-3.735666000	-3.882167000	-2.928407000
7	0.462330000	1.118354000	-4.095747000
7	0.336489000	0.714087000	-3.043798000

[2d''_{sc}] (TE = -3334.525177)

6	-0.007645000	-1.625328000	1.072893000
6	-0.681649000	-2.191235000	2.169061000
1	-1.294850000	-1.543967000	2.793352000
6	-0.585125000	-3.539879000	2.490675000
1	-1.126542000	-3.928508000	3.351204000
6	0.203480000	-4.389029000	1.721092000
1	0.284748000	-5.446010000	1.963320000
6	0.854945000	-3.874896000	0.606806000
1	1.425669000	-4.532780000	-0.046054000
6	0.742606000	-2.522171000	0.282967000
6	1.113131000	0.556639000	1.480020000
6	1.627945000	0.104378000	2.707315000
1	1.219153000	-0.807136000	3.139199000
6	2.629322000	0.779747000	3.394444000
1	2.991241000	0.386045000	4.342443000
6	3.163089000	1.955914000	2.878113000
1	3.947084000	2.492226000	3.407488000
6	2.709850000	2.414470000	1.647709000
1	3.157669000	3.295963000	1.192583000
6	1.714701000	1.721565000	0.956247000
6	-1.361234000	0.465451000	1.227593000
6	-1.536239000	1.002501000	2.514800000
1	-0.688032000	1.005303000	3.196297000
6	-2.744520000	1.532042000	2.950842000
1	-2.822850000	1.937301000	3.958012000
6	-3.845490000	1.551230000	2.102378000
1	-4.792379000	1.977387000	2.425316000

6	-3.706867000	1.054677000	0.812490000
1	-4.534406000	1.123013000	0.110605000
6	-2.491309000	0.516748000	0.380809000
16	-2.320999000	0.157177000	-1.369692000
16	1.364832000	-1.983046000	-1.306390000
16	1.385587000	2.202138000	-0.735798000
23	0.161170000	0.177399000	-1.440333000
6	3.232437000	-1.940059000	-1.119327000
1	3.521054000	-2.998352000	-1.092581000
6	0.410294000	3.802605000	-0.609407000
1	1.150892000	4.540929000	-0.277131000
6	-3.198392000	-1.483400000	-1.650403000
1	-3.123192000	-1.542157000	-2.744176000
6	-4.653837000	-1.393831000	-1.244078000
1	-5.185164000	-2.299782000	-1.555535000
1	-4.759290000	-1.317894000	-0.157369000
1	-5.161330000	-0.537577000	-1.696185000
6	-2.487959000	-2.657206000	-1.020711000
1	-2.471661000	-2.578203000	0.070578000
1	-3.004944000	-3.589706000	-1.275262000
1	-1.455303000	-2.743774000	-1.366024000
6	3.757483000	-1.286838000	-2.381759000
1	3.408897000	-1.787585000	-3.289643000
1	3.442800000	-0.237897000	-2.434927000
1	4.851835000	-1.304324000	-2.390214000
6	3.690412000	-1.237513000	0.134880000
1	3.251994000	-1.668945000	1.038578000
1	4.780210000	-1.311918000	0.225528000
1	3.431628000	-0.175067000	0.111835000
6	-0.047238000	4.117301000	-2.019142000
1	-0.553504000	5.087325000	-2.045872000
1	0.782043000	4.153786000	-2.731557000
1	-0.759978000	3.362402000	-2.372284000
6	-0.733853000	3.723342000	0.370610000
1	-1.486889000	3.001138000	0.041615000
1	-0.406137000	3.431998000	1.371918000
1	-1.223768000	4.700515000	0.451722000
6	-0.042766000	-0.137886000	0.779349000
7	0.518322000	0.628892000	-4.542419000
7	0.377712000	0.462498000	-3.431386000

[2e''_{ssi}] (TE = -3585.931978)

6	0.854225000	-1.796102000	1.325354000
6	0.791078000	-2.428067000	2.575102000
1	0.209598000	-1.970398000	3.376297000
6	1.444142000	-3.631091000	2.824815000

1	1.373973000	-4.097491000	3.805643000
6	2.181319000	-4.242806000	1.814709000
1	2.688440000	-5.187411000	1.998916000
6	2.248324000	-3.655690000	0.555867000
1	2.796496000	-4.143471000	-0.248331000
6	1.591167000	-2.447627000	0.321606000
6	0.962717000	1.257022000	1.707367000
6	1.366723000	1.278622000	3.049846000
1	1.139391000	0.424896000	3.689486000
6	2.060794000	2.355039000	3.593249000
1	2.361484000	2.339505000	4.639129000
6	2.379318000	3.449331000	2.793765000
1	2.929465000	4.291605000	3.207706000
6	2.015079000	3.452981000	1.451896000
1	2.288752000	4.289964000	0.811773000
6	1.315334000	2.368005000	0.922777000
6	-1.776475000	-0.117585000	1.466659000
6	-2.176070000	0.032848000	2.801694000
1	-1.417835000	0.069294000	3.584711000
6	-3.514288000	0.161122000	3.161583000
1	-3.789453000	0.281686000	4.207676000
6	-4.499080000	0.157876000	2.178821000
1	-5.545992000	0.279813000	2.447987000
6	-4.139641000	0.024107000	0.841622000
1	-4.899207000	0.059060000	0.063701000
6	-2.795109000	-0.124895000	0.496010000
16	-2.393224000	-0.238463000	-1.269080000
16	1.675594000	-1.760500000	-1.353524000
16	0.921332000	2.411211000	-0.845057000
23	0.076726000	0.169117000	-1.623108000
6	3.461651000	-1.182997000	-1.378558000
1	4.042800000	-2.108776000	-1.282797000
6	-0.436434000	3.705541000	-0.850565000
1	0.066584000	4.623197000	-0.520670000
6	-2.757763000	-2.046027000	-1.624032000
1	-2.362688000	-2.122961000	-2.645818000
6	-4.247410000	-2.318524000	-1.621401000
1	-4.443091000	-3.335251000	-1.979625000
1	-4.661325000	-2.251707000	-0.610477000
1	-4.798175000	-1.625162000	-2.261885000
6	-1.994644000	-2.970794000	-0.703161000
1	-2.304351000	-2.844158000	0.339947000
1	-2.183200000	-4.014903000	-0.975722000
1	-0.917269000	-2.800282000	-0.754095000
6	3.699886000	-0.550895000	-2.733783000
1	3.447510000	-1.222143000	-3.559465000

1	3.102548000	0.361350000	-2.846959000
1	4.752373000	-0.269467000	-2.839004000
6	3.773659000	-0.242595000	-0.236868000
1	3.552339000	-0.678722000	0.741291000
1	4.837027000	0.021633000	-0.249695000
1	3.202656000	0.686730000	-0.326229000
6	-0.899887000	3.847386000	-2.285284000
1	-1.642441000	4.647545000	-2.365147000
1	-0.079173000	4.081297000	-2.969096000
1	-1.374438000	2.922329000	-2.633303000
6	-1.565211000	3.354053000	0.091633000
1	-2.076185000	2.441853000	-0.231010000
1	-1.224351000	3.201018000	1.119462000
1	-2.307102000	4.160382000	0.104284000
14	0.022153000	-0.154355000	0.828318000
7	0.146863000	0.396808000	-4.770775000
7	0.116043000	0.322482000	-3.638567000

[2f'_{SB}] (TE = -3321.285024)

6	-0.222352000	1.773758000	1.121187000
6	0.257512000	2.435356000	2.266214000
1	0.862099000	1.872508000	2.978548000
6	-0.003008000	3.776874000	2.522081000
1	0.389973000	4.244292000	3.423091000
6	-0.756448000	4.524037000	1.621443000
1	-0.958706000	5.576646000	1.806118000
6	-1.220427000	3.918569000	0.460335000
1	-1.769009000	4.498575000	-0.279738000
6	-0.955675000	2.568654000	0.223135000
6	-1.131702000	-0.717179000	1.585945000
6	-1.642193000	-0.397223000	2.857631000
1	-1.285055000	0.508035000	3.349762000
6	-2.586356000	-1.182604000	3.508969000
1	-2.948976000	-0.891419000	4.493072000
6	-3.075328000	-2.333645000	2.898435000
1	-3.821442000	-2.951074000	3.393505000
6	-2.624592000	-2.668578000	1.628038000
1	-3.030604000	-3.537378000	1.112907000
6	-1.670956000	-1.871839000	0.991171000
6	1.516813000	-0.295932000	1.320658000
6	1.795954000	-0.691594000	2.641792000
1	0.984750000	-0.681439000	3.370421000
6	3.054728000	-1.114952000	3.052582000
1	3.216427000	-1.413614000	4.086723000
6	4.098772000	-1.179869000	2.135954000
1	5.082283000	-1.533393000	2.437168000

6	3.862741000	-0.819369000	0.815250000
1	4.651452000	-0.916249000	0.072725000
6	2.598610000	-0.369909000	0.422682000
16	2.335168000	-0.087459000	-1.335554000
16	-1.423566000	1.896900000	-1.375129000
16	-1.270338000	-2.268070000	-0.713536000
23	-0.138660000	-0.218456000	-1.518022000
6	-3.285773000	1.707751000	-1.240544000
1	-3.654299000	2.741212000	-1.227529000
6	-0.182916000	-3.789496000	-0.558576000
1	-0.869770000	-4.569934000	-0.207549000
6	3.093007000	1.604580000	-1.640812000
1	2.860722000	1.727693000	-2.706773000
6	4.593869000	1.564698000	-1.442605000
1	5.040135000	2.506390000	-1.780318000
1	4.851139000	1.450403000	-0.385135000
1	5.067175000	0.751340000	-1.998708000
6	2.428106000	2.693424000	-0.832728000
1	2.522111000	2.507618000	0.242574000
1	2.900362000	3.660030000	-1.041455000
1	1.365356000	2.784013000	-1.063054000
6	-3.733350000	1.007658000	-2.507180000
1	-3.410491000	1.530483000	-3.412050000
1	-3.334538000	-0.012956000	-2.547986000
1	-4.825127000	0.935415000	-2.533865000
6	-3.712630000	0.979168000	0.011034000
1	-3.317273000	1.440633000	0.920039000
1	-4.806004000	0.978382000	0.086006000
1	-3.381337000	-0.062894000	-0.004907000
6	0.301228000	-4.107341000	-1.958332000
1	0.883791000	-5.033900000	-1.956476000
1	-0.521139000	-4.230398000	-2.668877000
1	0.953167000	-3.309212000	-2.333462000
6	0.949908000	-3.600592000	0.421140000
1	1.655384000	-2.844070000	0.066255000
1	0.601423000	-3.292754000	1.410720000
1	1.501903000	-4.540017000	0.539085000
5	0.033047000	0.200641000	0.973052000
7	-0.427892000	-0.739540000	-4.608629000
7	-0.311737000	-0.549037000	-3.499012000

{[HIPTN₃N]-V-N₂} (TE= -2203.040594)

23	-0.170321000	-0.003856000	-0.522504000
7	-2.131179000	-0.029088000	-0.663498000

7	0.970655000	-1.476908000	-1.147411000
7	0.682478000	1.746878000	-0.557166000
6	-2.583952000	0.902152000	-1.687661000
1	-3.654322000	0.768656000	-1.900957000
1	-2.473214000	1.954712000	-1.375408000
6	-1.801802000	0.622669000	-2.960590000
1	-2.202297000	-0.280428000	-3.428061000
1	-1.902957000	1.437022000	-3.689326000
6	0.426814000	2.513928000	-1.774033000
1	-0.544045000	3.037295000	-1.750502000
1	1.184993000	3.297326000	-1.910490000
6	0.489392000	1.551678000	-2.939867000
1	1.519045000	1.198114000	-3.045302000
1	0.198775000	2.020218000	-3.891041000
6	1.340251000	-1.383580000	-2.552210000
1	2.225561000	-0.740712000	-2.704343000
1	1.617347000	-2.368422000	-2.958130000
6	0.154492000	-0.850981000	-3.324602000
1	0.398633000	-0.657300000	-4.379852000
1	-0.648404000	-1.592656000	-3.294996000
7	-0.363523000	0.371541000	-2.663440000
6	1.823242000	-2.224266000	-0.339799000
6	1.364072000	-2.700677000	0.904393000
6	3.148605000	-2.538233000	-0.700431000
6	2.193882000	-3.408204000	1.758783000
1	0.324602000	-2.531966000	1.177245000
6	3.971717000	-3.256993000	0.159482000
1	3.547391000	-2.200346000	-1.652973000
6	3.510984000	-3.690653000	1.397829000
1	1.801198000	-3.761745000	2.710308000
1	4.993728000	-3.474499000	-0.146139000
1	4.159970000	-4.251567000	2.065456000
6	-3.053784000	-0.419478000	0.298104000
6	-2.837337000	-1.622507000	0.998737000
6	-4.207246000	0.321347000	0.618736000
6	-3.709007000	-2.046427000	1.988277000
1	-1.974908000	-2.231169000	0.725981000
6	-5.083439000	-0.118050000	1.605032000
1	-4.403935000	1.263148000	0.112151000
6	-4.843393000	-1.297906000	2.301812000
1	-3.512906000	-2.982318000	2.508137000
1	-5.962461000	0.480483000	1.837928000
1	-5.532229000	-1.635052000	3.072169000
6	1.325514000	2.427215000	0.479002000
6	2.176633000	1.721196000	1.348238000
6	1.175379000	3.809608000	0.688187000

6	2.815469000	2.360232000	2.399766000
1	2.347182000	0.659854000	1.168212000
6	1.828126000	4.445185000	1.738055000
1	0.521759000	4.384799000	0.036072000
6	2.646464000	3.728496000	2.605549000
1	3.469699000	1.786826000	3.053435000
1	1.686522000	5.514675000	1.882945000
1	3.155076000	4.230023000	3.425073000
7	-0.362823000	-0.011718000	2.661187000
7	-0.231162000	-0.073678000	1.556795000

Cartesian coordinates of $[2a'_{PC}]^-$ - $[2f'_{SB}]^-$, $[2a''_{PC}]^-$ - $[2f''_{SB}]^-$ and $\{[HIPTN_3N]-V-N_2\}^-$, along with their total energies (in hartree) including zero point vibrational correction at M06-L-D3(heptane)/6-311+G* level of theory.

$[2a'_{PC}]^-$ (TE = -3062.130489)

6	-0.004952000	2.366729000	1.911036000
6	0.570428000	1.097484000	2.521841000
6	-2.638018000	0.037645000	1.732988000
6	-1.452165000	-0.376032000	2.603071000
6	2.222127000	-1.422361000	1.901842000
6	0.816379000	-1.358955000	2.498891000
1	-2.693565000	1.129953000	1.625152000
1	-1.526702000	0.141985000	3.582606000
1	2.758864000	-2.335193000	2.202485000
1	0.908304000	-1.337821000	3.610074000
1	0.432527000	3.276722000	2.345936000
1	1.655328000	1.102975000	2.334495000
6	-0.717743000	3.719331000	-0.624970000
1	-0.031240000	4.177430000	-1.353774000
6	-2.668628000	-2.453006000	0.293250000
1	-1.912494000	-2.671055000	1.064518000
6	3.720655000	-0.463970000	-0.448408000
1	3.514164000	0.593572000	-0.231981000
23	-0.009735000	-0.137744000	-0.440718000
6	-0.046179000	-0.197245000	1.983421000
1	-1.084169000	2.424011000	2.097996000
1	0.469683000	1.156206000	3.631132000
1	0.300652000	-2.304857000	2.276426000
1	2.830395000	-0.585526000	2.268153000
1	-1.598347000	-1.439592000	2.853312000
1	-3.596032000	-0.278801000	2.174353000
6	4.988921000	-0.824571000	0.318182000
1	5.795746000	-0.121187000	0.071327000
1	4.848364000	-0.779446000	1.402342000

1	5.362512000	-1.823194000	0.082386000
6	3.907973000	-0.580286000	-1.956359000
1	4.178192000	-1.598439000	-2.257733000
1	2.993596000	-0.318994000	-2.499416000
1	4.708354000	0.081274000	-2.311779000
6	-4.030379000	-2.849087000	0.847714000
1	-4.042937000	-3.908033000	1.139637000
1	-4.315599000	-2.269065000	1.731013000
1	-4.822652000	-2.723628000	0.101037000
6	-2.310887000	-3.294521000	-0.928921000
1	-3.112910000	-3.296447000	-1.672673000
1	-1.407386000	-2.926463000	-1.425035000
1	-2.138631000	-4.341202000	-0.646954000
6	-1.944788000	3.234751000	-1.380536000
1	-1.704578000	2.425192000	-2.078627000
1	-2.692903000	2.841947000	-0.681589000
1	-2.423030000	4.049077000	-1.940432000
6	-1.120088000	4.779658000	0.392922000
1	-0.278695000	5.165680000	0.973167000
1	-1.599863000	5.636156000	-0.099054000
1	-1.847769000	4.381146000	1.108799000
6	2.239238000	-3.039241000	-0.527225000
1	2.009924000	-2.973420000	-1.601584000
6	1.153881000	-3.879909000	0.134881000
1	1.395005000	-4.074289000	1.187462000
1	0.179939000	-3.384730000	0.108604000
1	1.053233000	-4.855377000	-0.357620000
6	3.583276000	-3.733446000	-0.352678000
1	3.509161000	-4.795224000	-0.625349000
1	4.372600000	-3.303476000	-0.972749000
1	3.926644000	-3.699980000	0.688720000
6	-3.797498000	0.043408000	-0.952626000
1	-3.422611000	1.017713000	-1.286452000
6	-5.084065000	0.297761000	-0.176235000
1	-5.513026000	-0.618946000	0.239387000
1	-4.934803000	0.990470000	0.657277000
1	-5.848629000	0.740191000	-0.829439000
6	-4.053364000	-0.773515000	-2.212049000
1	-4.544349000	-1.726345000	-1.986400000
1	-4.716490000	-0.232780000	-2.899166000
1	-3.127687000	-0.996133000	-2.752272000
6	2.006146000	2.962394000	-0.077126000
1	2.588233000	2.273354000	0.553607000
6	2.245692000	4.379858000	0.421922000
1	3.312652000	4.636705000	0.374111000
1	1.719900000	5.120566000	-0.191932000

1	1.929483000	4.525767000	1.459458000
6	2.485653000	2.813394000	-1.514811000
1	3.562089000	3.009825000	-1.606264000
1	2.289392000	1.810394000	-1.906911000
1	1.976534000	3.523473000	-2.179019000
15	-2.323714000	-0.610702000	0.024212000
15	0.258210000	2.252408000	0.082528000
15	2.078188000	-1.242216000	0.059084000
7	0.026531000	-1.154088000	-3.365911000
7	0.001502000	-0.744893000	-2.277230000

[2b'_{psi}]' (TE = -3313.578313)

6	-0.461970000	2.636554000	1.885835000
6	0.260736000	1.660393000	2.807436000
6	-2.743734000	-0.451113000	1.898751000
6	-1.592539000	-0.792036000	2.846387000
6	2.717557000	-1.003371000	1.832425000
6	1.530837000	-1.137333000	2.790774000
1	-2.958879000	0.627171000	1.940559000
1	-1.799822000	-0.409505000	3.857610000
1	3.514163000	-1.743315000	2.013643000
1	1.827917000	-0.827429000	3.804658000
1	-0.312662000	3.698465000	2.134544000
1	1.333958000	1.906313000	2.846387000
6	-0.973918000	3.524585000	-0.863683000
1	-0.385846000	4.454752000	-0.908665000
6	-2.512653000	-2.659313000	0.102224000
1	-1.897145000	-2.963095000	0.964556000
6	3.668721000	-0.187201000	-0.780866000
1	3.452494000	0.869062000	-0.563847000
23	-0.005890000	-0.088297000	-0.433488000
1	-1.543279000	2.459453000	1.940138000
1	-0.107608000	1.750300000	3.841469000
1	1.229875000	-2.189391000	2.875551000
1	3.189136000	-0.019275000	1.976311000
1	-1.517767000	-1.885449000	2.952548000
1	-3.686358000	-0.956650000	2.158485000
6	5.068544000	-0.461363000	-0.238995000
1	5.784360000	0.255652000	-0.663509000
1	5.125857000	-0.361081000	0.848609000
1	5.438072000	-1.457068000	-0.493251000
6	3.599051000	-0.354363000	-2.292685000
1	3.824834000	-1.381840000	-2.601165000
1	2.603207000	-0.117573000	-2.679310000
1	4.322866000	0.297226000	-2.799207000
6	-3.926886000	-3.169582000	0.343190000

1	-3.928493000	-4.257451000	0.496028000
1	-4.401437000	-2.722008000	1.221632000
1	-4.577455000	-2.976867000	-0.517044000
6	-1.905864000	-3.311919000	-1.133042000
1	-2.482243000	-3.092676000	-2.037816000
1	-0.887128000	-2.959119000	-1.312913000
1	-1.876472000	-4.404361000	-1.024420000
6	-1.184648000	3.015555000	-2.285656000
1	-0.247438000	2.750736000	-2.784384000
1	-1.794944000	2.104082000	-2.286561000
1	-1.697035000	3.764146000	-2.904326000
6	-2.314344000	3.843879000	-0.215761000
1	-2.208367000	4.379424000	0.732021000
1	-2.934249000	4.462660000	-0.876879000
1	-2.885818000	2.929642000	-0.008816000
6	2.319472000	-2.837300000	-0.422898000
1	1.888115000	-2.863639000	-1.435247000
6	1.423047000	-3.665906000	0.492735000
1	1.884454000	-3.794772000	1.479074000
1	0.443698000	-3.200751000	0.645756000
1	1.259848000	-4.669584000	0.079883000
6	3.706530000	-3.463128000	-0.469719000
1	3.637206000	-4.543916000	-0.655507000
1	4.334899000	-3.046200000	-1.259860000
1	4.243328000	-3.340520000	0.478817000
6	-3.688389000	-0.025601000	-0.819135000
1	-3.357663000	1.021748000	-0.884345000
6	-5.063275000	-0.015334000	-0.161372000
1	-5.488359000	-1.016966000	-0.055199000
1	-5.046248000	0.437987000	0.833884000
1	-5.772203000	0.566518000	-0.766285000
6	-3.747878000	-0.558032000	-2.244521000
1	-4.154658000	-1.575228000	-2.280028000
1	-4.398554000	0.063797000	-2.872781000
1	-2.757904000	-0.584329000	-2.711017000
6	1.736614000	3.077588000	0.066005000
1	2.364701000	2.345864000	0.596943000
6	1.877688000	4.422929000	0.762325000
1	2.882051000	4.841820000	0.612564000
1	1.168257000	5.164818000	0.374929000
1	1.718472000	4.352806000	1.841835000
6	2.217607000	3.153034000	-1.376901000
1	3.286895000	3.395332000	-1.433682000
1	2.059536000	2.206079000	-1.906102000
1	1.685535000	3.934034000	-1.934261000
15	-2.234241000	-0.780470000	0.126211000

15	0.028453000	2.253253000	0.132230000
15	2.173802000	-1.003432000	0.037641000
14	0.054641000	-0.123371000	2.072652000
7	0.047085000	-1.071425000	-3.371682000
7	0.008735000	-0.701687000	-2.273644000

[2c'_{PB}]' (TE = -3048.900287)

6	0.302355000	2.610383000	1.823457000
6	0.709303000	1.342040000	2.571016000
6	-2.635802000	0.366981000	1.771053000
6	-1.526299000	-0.149243000	2.685001000
6	2.226319000	-1.444512000	1.833225000
6	0.895291000	-1.327254000	2.569355000
1	-2.533209000	1.448698000	1.600934000
1	-1.596802000	0.383723000	3.655590000
1	2.864703000	-2.287096000	2.142945000
1	1.111889000	-1.271225000	3.658806000
1	0.828256000	3.524607000	2.150914000
1	1.804204000	1.258793000	2.546365000
6	-0.505260000	3.761302000	-0.758670000
1	0.049434000	4.024418000	-1.671880000
6	-2.755388000	-2.225787000	0.499956000
1	-1.806248000	-2.544934000	0.952844000
6	3.505460000	-0.955464000	-0.813922000
1	3.345100000	0.114840000	-0.999652000
23	-0.036637000	-0.017479000	-0.588070000
1	-0.767651000	2.808352000	1.986279000
1	0.474823000	1.499889000	3.645837000
1	0.329426000	-2.266674000	2.449527000
1	2.820092000	-0.540476000	2.022749000
1	-1.757856000	-1.199551000	2.933394000
1	-3.658790000	0.207684000	2.152657000
6	4.771993000	-1.083449000	0.024760000
1	5.637565000	-0.685335000	-0.522137000
1	4.707335000	-0.530216000	0.965514000
1	5.007299000	-2.121235000	0.280556000
6	3.679976000	-1.593851000	-2.186833000
1	3.929511000	-2.658707000	-2.124269000
1	2.779806000	-1.498431000	-2.801226000
1	4.499416000	-1.110132000	-2.733117000
6	-3.858587000	-2.538627000	1.504269000
1	-3.850360000	-3.609001000	1.749447000
1	-3.731393000	-1.996748000	2.444909000
1	-4.857190000	-2.311457000	1.122965000
6	-2.949810000	-3.013115000	-0.790146000
1	-3.938523000	-2.830680000	-1.227047000

1	-2.205757000	-2.749732000	-1.550939000
1	-2.874593000	-4.093486000	-0.613297000
6	-1.887096000	3.285068000	-1.179701000
1	-1.838721000	2.412550000	-1.838266000
1	-2.479367000	2.992722000	-0.303987000
1	-2.442922000	4.079324000	-1.694984000
6	-0.647174000	5.004615000	0.114024000
1	0.301129000	5.389021000	0.492166000
1	-1.132996000	5.818060000	-0.440973000
1	-1.277982000	4.798608000	0.985321000
5	0.002238000	-0.052232000	2.092416000
7	0.235699000	-0.621627000	-3.644888000
7	0.170079000	-0.413482000	-2.513923000
6	-3.818556000	0.229239000	-0.873845000
1	-3.732859000	1.308731000	-0.683554000
6	-5.217455000	-0.191897000	-0.443766000
1	-5.980563000	0.405425000	-0.960959000
1	-5.421931000	-1.238667000	-0.692192000
1	-5.383853000	-0.070247000	0.630830000
6	-3.621884000	0.020267000	-2.370759000
1	-4.368136000	0.579391000	-2.950049000
1	-2.630122000	0.343585000	-2.699949000
1	-3.722366000	-1.032961000	-2.653671000
6	2.256898000	2.907352000	-0.364747000
1	2.435695000	2.486785000	-1.366971000
6	2.535872000	4.403756000	-0.421597000
1	3.581187000	4.582597000	-0.706139000
1	1.912620000	4.940440000	-1.141443000
1	2.396147000	4.874533000	0.558281000
6	3.242175000	2.264612000	0.603122000
1	3.026349000	1.209030000	0.774622000
1	4.271991000	2.345406000	0.231427000
1	3.208751000	2.760159000	1.579970000
6	1.796949000	-3.290069000	-0.422855000
1	1.848680000	-3.279427000	-1.521112000
6	0.453713000	-3.897631000	-0.052762000
1	0.372499000	-4.928682000	-0.421278000
1	0.302215000	-3.926538000	1.032172000
1	-0.364504000	-3.318399000	-0.483288000
6	2.934433000	-4.153168000	0.104437000
1	2.842463000	-5.184519000	-0.261861000
1	3.921307000	-3.793988000	-0.197095000
1	2.927273000	-4.207599000	1.198362000
15	1.864750000	-1.449226000	0.014148000
15	0.486254000	2.335221000	0.000778000
15	-2.357741000	-0.421033000	0.132467000

[2d'_{sc}]' (TE = -2877.282658)

6	0.157755000	2.061535000	1.727182000
6	0.255183000	0.817215000	2.598976000
6	-2.655893000	0.053929000	1.733061000
6	-1.605410000	-0.848165000	2.348913000
6	2.124909000	-1.610616000	1.816133000
6	0.741305000	-1.625820000	2.441220000
1	-2.554505000	1.088207000	2.081763000
1	-1.743772000	-0.814114000	3.456169000
1	2.770928000	-2.409702000	2.203406000
1	0.879207000	-1.610159000	3.547872000
1	0.574371000	2.946566000	2.226814000
1	1.304024000	0.748288000	2.930677000
6	0.659214000	3.182646000	-0.861035000
1	1.333441000	3.041358000	-1.716181000
6	-3.623270000	-1.318352000	-0.496122000
1	-3.423620000	-2.061430000	0.289334000
6	3.504237000	-0.890664000	-0.526936000
1	3.503486000	0.047680000	0.043941000
23	-0.089170000	-0.430929000	-0.380766000
16	-2.429008000	0.106563000	-0.113236000
16	1.102288000	1.709338000	0.190402000
16	1.930119000	-1.765771000	-0.016158000
6	-0.174725000	-0.506932000	1.942321000
1	-0.875775000	2.281645000	1.436995000
1	-0.317376000	1.021182000	3.529385000
1	0.277098000	-2.599482000	2.222952000
1	2.630958000	-0.650715000	1.993311000
1	-1.825779000	-1.886407000	2.055921000
1	-3.682644000	-0.257558000	1.964937000
6	4.724438000	-1.717961000	-0.176677000
1	5.649317000	-1.196564000	-0.456378000
1	4.783201000	-1.933705000	0.894494000
1	4.713701000	-2.677121000	-0.706303000
6	3.402021000	-0.582146000	-2.005668000
1	3.296494000	-1.496904000	-2.600291000
1	2.526117000	0.037497000	-2.219336000
1	4.299949000	-0.058943000	-2.356586000
6	-5.058427000	-0.838221000	-0.431979000
1	-5.764168000	-1.664461000	-0.591000000
1	-5.305188000	-0.380741000	0.531587000
1	-5.251216000	-0.088919000	-1.207774000
6	-3.254270000	-1.893383000	-1.842582000
1	-3.354237000	-1.145499000	-2.638370000
1	-2.213225000	-2.229876000	-1.846082000

1	-3.904068000	-2.739919000	-2.096738000
6	-0.774744000	3.125764000	-1.346241000
1	-0.981647000	2.197419000	-1.884466000
1	-1.486758000	3.178604000	-0.515495000
1	-0.989509000	3.969948000	-2.013430000
6	0.994998000	4.489842000	-0.168332000
1	2.018133000	4.498513000	0.218576000
1	0.889128000	5.335412000	-0.858948000
1	0.319793000	4.679934000	0.672705000
7	-0.102773000	-0.895383000	-3.455556000
7	-0.115624000	-0.730820000	-2.302884000

[2e' ssi] (TE = -3128.706615)

23	0.052279000	0.011096000	-0.788815000
16	1.872036000	-1.636591000	-0.873141000
16	-2.088618000	-1.209767000	-1.257338000
16	-0.600259000	1.839475000	0.630933000
14	-0.302761000	-1.097982000	1.414586000
6	-0.564462000	0.175804000	2.846340000
6	-0.016117000	1.515537000	2.379700000
6	-2.165502000	-2.638633000	-0.080845000
6	-1.849783000	-2.267867000	1.361324000
6	1.204970000	-2.240915000	1.822911000
6	1.673615000	-2.868454000	0.521304000
1	0.912592000	-3.550680000	0.122758000
1	2.601005000	-3.450808000	0.595957000
1	2.016714000	-1.642970000	2.265134000
1	0.979946000	-3.037086000	2.549907000
1	-3.136479000	-3.134403000	-0.217337000
1	-1.407641000	-3.316117000	-0.489467000
1	-2.717089000	-1.759419000	1.808227000
1	-1.719530000	-3.195159000	1.940462000
1	-1.641732000	0.274147000	3.047318000
1	-0.093850000	-0.091817000	3.803760000
1	1.080747000	1.489616000	2.342585000
1	-0.319900000	2.363623000	3.008361000
6	3.398239000	-0.738319000	-0.232086000
1	3.019092000	-0.104464000	0.583977000
6	-3.449080000	-0.150057000	-0.537114000
1	-3.066862000	0.165735000	0.444091000
6	0.312078000	3.453212000	0.315650000
1	0.027197000	3.632912000	-0.728802000
6	-4.759386000	-0.895093000	-0.384301000
1	-5.545759000	-0.217447000	-0.028115000
1	-5.094873000	-1.312961000	-1.340309000
1	-4.694798000	-1.716152000	0.334804000

6	-3.583682000	1.066905000	-1.430564000
1	-2.623122000	1.574834000	-1.560032000
1	-3.957282000	0.791717000	-2.423657000
1	-4.287413000	1.785959000	-0.996119000
6	-0.196794000	4.589283000	1.180619000
1	0.071766000	4.448124000	2.233392000
1	0.238614000	5.548077000	0.868817000
1	-1.285468000	4.685544000	1.127837000
6	1.816641000	3.288572000	0.383154000
1	2.324507000	4.158939000	-0.051622000
1	2.169745000	3.193309000	1.416432000
1	2.138219000	2.398317000	-0.167626000
6	3.898283000	0.142315000	-1.359375000
1	4.710299000	0.790660000	-1.008490000
1	4.290314000	-0.462151000	-2.185479000
1	3.107356000	0.778510000	-1.761356000
6	4.483114000	-1.665279000	0.280553000
1	5.395357000	-1.095937000	0.500608000
1	4.200147000	-2.183236000	1.200526000
1	4.745967000	-2.423654000	-0.466155000
7	1.077897000	1.890924000	-3.034751000
7	0.701406000	1.143228000	-2.228495000

[2f_{SB}]⁻ (TE = -3128.706615)

6	-0.970819000	2.127480000	-1.834898000
6	-0.629475000	0.849984000	-2.575412000
6	2.617621000	1.353983000	-1.040856000
6	2.004145000	0.491534000	-2.127735000
6	-0.920804000	-2.311955000	-1.903664000
6	0.355964000	-1.634410000	-2.350952000
1	2.057635000	2.287186000	-0.900271000
1	2.023875000	1.103161000	-3.054047000
1	-1.006198000	-3.373716000	-2.174349000
1	0.373858000	-1.714835000	-3.462323000
1	-1.750246000	2.746116000	-2.304322000
1	-1.576597000	0.306888000	-2.744277000
6	-1.584925000	3.154050000	0.793019000
1	-2.079373000	2.837592000	1.721360000
6	3.365385000	-1.039975000	0.294200000
1	2.806766000	-1.512035000	-0.523273000
6	-2.913943000	-2.060543000	0.077882000
1	-3.196390000	-1.229942000	-0.584571000
23	0.069130000	-0.090106000	0.634955000
16	2.467787000	0.559542000	0.612821000
16	-1.565163000	1.569447000	-0.178676000
16	-1.056496000	-2.168659000	-0.058516000

1	-0.081400000	2.755003000	-1.682222000
1	-0.292712000	1.149290000	-3.591900000
1	1.212449000	-2.244999000	-2.016529000
1	-1.803903000	-1.796039000	-2.303951000
1	2.709132000	-0.332463000	-2.339455000
1	3.670484000	1.638644000	-1.197682000
6	-3.570885000	-3.344851000	-0.387606000
1	-4.664715000	-3.270465000	-0.330789000
1	-3.313383000	-3.588315000	-1.422169000
1	-3.263358000	-4.190776000	0.237195000
6	-3.273652000	-1.710273000	1.506723000
1	-2.928653000	-2.480522000	2.206464000
1	-2.820895000	-0.762759000	1.813207000
1	-4.360539000	-1.622797000	1.621166000
6	4.805318000	-0.800213000	-0.110570000
1	5.324189000	-1.752323000	-0.276748000
1	4.881890000	-0.225001000	-1.037715000
1	5.353198000	-0.256595000	0.667455000
6	3.239757000	-1.894094000	1.539559000
1	3.701748000	-1.412929000	2.409677000
1	2.189245000	-2.086953000	1.780277000
1	3.735863000	-2.860155000	1.391992000
6	-0.186117000	3.637870000	1.122484000
1	0.394744000	2.859789000	1.628472000
1	0.362698000	3.924449000	0.218187000
1	-0.219798000	4.520071000	1.773931000
6	-2.423374000	4.220498000	0.112965000
1	-3.420578000	3.853800000	-0.147150000
1	-2.545270000	5.095826000	0.763084000
1	-1.948362000	4.570679000	-0.809444000
5	0.493965000	-0.091485000	-1.841052000
7	-0.083268000	-0.507456000	3.752238000
7	-0.003651000	-0.350374000	2.615063000

[2a''_{pc}]- (TE = -3519.417033)

6	0.291437000	1.522399000	1.657832000
6	0.961190000	1.807488000	2.859168000
1	1.234391000	0.982411000	3.515113000
6	1.294015000	3.108748000	3.236957000
1	1.828276000	3.281259000	4.170876000
6	0.929767000	4.182210000	2.433064000
1	1.179364000	5.202446000	2.721233000
6	0.249049000	3.931861000	1.243070000
1	-0.026780000	4.767495000	0.597679000
6	-0.038002000	2.623557000	0.831650000
6	-1.486140000	-0.232846000	1.788309000

6	-2.034638000	0.367942000	2.934099000
1	-1.468773000	1.148954000	3.438840000
6	-3.279094000	-0.001532000	3.444303000
1	-3.675280000	0.508339000	4.322343000
6	-3.997018000	-1.034123000	2.855620000
1	-4.961264000	-1.342072000	3.257280000
6	-3.468431000	-1.664062000	1.727937000
1	-4.028078000	-2.472751000	1.262054000
6	-2.258016000	-1.248689000	1.162576000
6	0.917251000	-0.867372000	1.813420000
6	0.725818000	-1.535070000	3.036150000
1	-0.215581000	-1.395416000	3.565115000
6	1.698641000	-2.351567000	3.602490000
1	1.502244000	-2.848323000	4.552378000
6	2.925990000	-2.511699000	2.968669000
1	3.702754000	-3.136713000	3.406418000
6	3.139997000	-1.877888000	1.747801000
1	4.087536000	-2.033113000	1.240144000
6	2.149162000	-1.095756000	1.138725000
23	-0.072321000	-0.064554000	-1.093680000
6	-2.396327000	3.183479000	-0.626829000
1	-2.115765000	4.198018000	-0.299381000
6	-1.300831000	-3.581117000	-0.380113000
1	-2.218032000	-4.088315000	-0.044157000
6	3.780403000	0.732657000	-0.506815000
1	3.758677000	1.209232000	-1.499079000
6	5.158662000	0.112091000	-0.314259000
1	5.931599000	0.891124000	-0.355449000
1	5.252864000	-0.365884000	0.665763000
1	5.413741000	-0.629030000	-1.073900000
6	3.555619000	1.806130000	0.548359000
1	3.608705000	1.379867000	1.556681000
1	4.323658000	2.587123000	0.481075000
1	2.579385000	2.284680000	0.459720000
6	-3.175239000	3.309745000	-1.927248000
1	-2.666743000	3.943831000	-2.658956000
1	-3.346131000	2.337202000	-2.401594000
1	-4.161893000	3.755132000	-1.747043000
6	-3.226214000	2.542874000	0.473649000
1	-2.727642000	2.605272000	1.444609000
1	-4.203596000	3.033075000	0.567267000
1	-3.405455000	1.479218000	0.285036000
6	-0.899380000	-4.107597000	-1.752265000
1	-0.666335000	-5.178681000	-1.711453000
1	-1.670861000	-3.968343000	-2.515620000
1	-0.002116000	-3.590839000	-2.113062000

6	-0.205749000	-3.859725000	0.634486000
1	0.728802000	-3.356863000	0.359775000
1	-0.470196000	-3.514167000	1.637068000
1	0.003212000	-4.935349000	0.693667000
6	-0.104061000	0.109418000	1.273297000
7	0.005301000	-1.053732000	-4.027292000
7	0.000501000	-0.651482000	-2.941889000
6	0.074736000	3.481270000	-2.018694000
1	-0.421044000	4.459531000	-1.903825000
6	-0.141425000	2.964503000	-3.441525000
1	0.172593000	3.710741000	-4.182344000
1	0.457562000	2.061948000	-3.606280000
1	-1.177162000	2.692018000	-3.660383000
6	1.568813000	3.644645000	-1.789635000
1	1.813814000	4.087808000	-0.821819000
1	2.064365000	2.667617000	-1.838858000
1	2.012749000	4.274857000	-2.570716000
6	2.861780000	-1.827924000	-1.703207000
1	1.890177000	-2.290308000	-1.926835000
6	3.770546000	-2.948871000	-1.218463000
1	3.915917000	-3.682059000	-2.023411000
1	4.766326000	-2.608676000	-0.918357000
1	3.338117000	-3.487071000	-0.370965000
6	3.351802000	-1.207052000	-3.007898000
1	4.359150000	-0.786040000	-2.916502000
1	3.386280000	-1.957707000	-3.806218000
1	2.682681000	-0.409566000	-3.348278000
6	-3.218615000	-1.838027000	-1.624117000
1	-2.735005000	-1.932357000	-2.608900000
6	-3.957002000	-0.510385000	-1.611502000
1	-4.715214000	-0.468192000	-2.403187000
1	-4.469339000	-0.347040000	-0.655844000
1	-3.263542000	0.322425000	-1.758291000
6	-4.195458000	-2.998875000	-1.478926000
1	-4.940962000	-2.963531000	-2.283824000
1	-3.717153000	-3.979871000	-1.536446000
1	-4.754661000	-2.959030000	-0.539361000
15	2.283976000	-0.424200000	-0.562868000
15	-0.741806000	2.268612000	-0.812881000
15	-1.694557000	-1.744954000	-0.505698000

[2b''_{psi}] (TE = -3770.830125)

6	0.513745000	1.893861000	1.718901000
6	1.042772000	2.272359000	2.958391000

1	1.230981000	1.510440000	3.716825000
6	1.368245000	3.601189000	3.236577000
1	1.807090000	3.870083000	4.197227000
6	1.118665000	4.583837000	2.286368000
1	1.352972000	5.626006000	2.500099000
6	0.565194000	4.234407000	1.052507000
1	0.342159000	5.018853000	0.334325000
6	0.299370000	2.894853000	0.749297000
6	-1.505093000	-0.358788000	2.129215000
6	-1.820356000	0.003859000	3.444981000
1	-1.103098000	0.586661000	4.026104000
6	-3.043637000	-0.329519000	4.024016000
1	-3.278231000	-0.008627000	5.038852000
6	-3.963775000	-1.080790000	3.300510000
1	-4.918952000	-1.356633000	3.745865000
6	-3.662565000	-1.477936000	1.998304000
1	-4.381383000	-2.086499000	1.456163000
6	-2.460744000	-1.093766000	1.394571000
6	1.481046000	-0.975539000	1.848959000
6	1.626539000	-1.327300000	3.195846000
1	0.859529000	-1.020596000	3.909970000
6	2.716632000	-2.066160000	3.648572000
1	2.809549000	-2.329765000	4.701913000
6	3.693739000	-2.453267000	2.739272000
1	4.563913000	-3.017053000	3.073764000
6	3.562169000	-2.127227000	1.390562000
1	4.346218000	-2.444248000	0.714868000
6	2.450886000	-1.413172000	0.918445000
23	-0.168653000	-0.114167000	-1.256468000
6	-2.081343000	3.146146000	-0.722524000
1	-1.887928000	4.186619000	-0.420597000
6	-1.691437000	-3.347838000	-0.162387000
1	-2.542627000	-3.741223000	0.414273000
6	3.618547000	0.335879000	-1.071516000
1	3.405785000	0.786228000	-2.051034000
6	5.031786000	-0.228326000	-1.124131000
1	5.752144000	0.587197000	-1.271499000
1	5.311563000	-0.722861000	-0.188181000
1	5.186114000	-0.935723000	-1.942296000
6	3.538923000	1.425804000	-0.015242000
1	3.766206000	1.030015000	0.981920000
1	4.260813000	2.226490000	-0.221071000
1	2.544516000	1.870453000	0.037536000
6	-2.813822000	3.152927000	-2.058863000
1	-2.436865000	3.928869000	-2.732409000
1	-2.708872000	2.199073000	-2.588914000

1	-3.888352000	3.330306000	-1.927582000
6	-2.878884000	2.482328000	0.389654000
1	-2.393721000	2.603986000	1.363884000
1	-3.888100000	2.906810000	0.463065000
1	-2.977247000	1.405567000	0.225238000
6	-1.638982000	-4.037356000	-1.520207000
1	-1.223821000	-5.049320000	-1.434519000
1	-2.623805000	-4.129978000	-1.986344000
1	-1.003622000	-3.484904000	-2.219975000
6	-0.427635000	-3.603384000	0.642822000
1	0.459929000	-3.227785000	0.123655000
1	-0.449400000	-3.111139000	1.620679000
1	-0.285184000	-4.678083000	0.813137000
7	-0.996698000	-0.697173000	-4.196581000
7	-0.616993000	-0.488664000	-3.127534000
14	0.080770000	0.120236000	1.152556000
6	0.305079000	3.366844000	-2.278286000
1	-0.354572000	3.020223000	-3.089378000
6	2.834990000	-2.293677000	-2.011071000
1	3.313584000	-1.695537000	-2.803391000
6	-3.597893000	-1.600525000	-1.378877000
1	-3.164776000	-1.901539000	-2.344930000
6	-4.225025000	-0.232797000	-1.583794000
1	-3.491230000	0.494370000	-1.933933000
1	-5.034139000	-0.277960000	-2.323639000
1	-4.658138000	0.154801000	-0.653759000
6	-4.683016000	-2.616501000	-1.024747000
1	-5.295584000	-2.831960000	-1.909751000
1	-4.303746000	-3.574888000	-0.661512000
1	-5.370692000	-2.228023000	-0.267670000
6	3.840617000	-3.327756000	-1.516333000
1	3.418682000	-3.936567000	-0.709394000
1	4.091949000	-4.019571000	-2.331851000
1	4.781813000	-2.907788000	-1.158121000
6	1.678831000	-3.045387000	-2.654096000
1	1.201221000	-3.720405000	-1.936307000
1	0.908191000	-2.375920000	-3.037538000
1	2.037490000	-3.666837000	-3.484917000
6	1.716459000	2.946211000	-2.651835000
1	1.776642000	1.865373000	-2.808681000
1	2.042905000	3.441747000	-3.574988000
1	2.436681000	3.210301000	-1.869238000
6	0.205721000	4.887078000	-2.219638000
1	0.327058000	5.313438000	-3.223999000
1	-0.749081000	5.254394000	-1.832222000
1	1.000793000	5.318885000	-1.604300000

15	-0.387132000	2.303560000	-0.862761000
15	-1.998345000	-1.491299000	-0.363650000
15	2.173895000	-0.889978000	-0.862188000

[2c''_{PB}] (TE = -3506.200645)

6	1.328295000	-0.732256000	1.812405000
6	1.385192000	-1.604260000	2.920869000
1	0.447222000	-1.909119000	3.388658000
6	2.580653000	-2.078588000	3.449852000
1	2.568753000	-2.750705000	4.308807000
6	3.797044000	-1.677574000	2.898461000
1	4.740335000	-2.031029000	3.312463000
6	3.785607000	-0.839217000	1.786885000
1	4.734649000	-0.556635000	1.333710000
6	2.580216000	-0.402743000	1.227221000
6	-0.344089000	1.362555000	1.869792000
6	0.152912000	1.805599000	3.112698000
1	0.868577000	1.171008000	3.639995000
6	-0.244975000	3.001181000	3.700154000
1	0.167744000	3.299434000	4.664847000
6	-1.195112000	3.809105000	3.073888000
1	-1.526292000	4.738471000	3.534960000
6	-1.700154000	3.416561000	1.837022000
1	-2.426843000	4.054975000	1.334922000
6	-1.257915000	2.240006000	1.222821000
6	-1.297707000	-1.064016000	1.621917000
6	-2.070402000	-0.914505000	2.792665000
1	-1.831138000	-0.091519000	3.469216000
6	-3.130011000	-1.755504000	3.109797000
1	-3.702777000	-1.593789000	4.023894000
6	-3.466313000	-2.803931000	2.254320000
1	-4.305793000	-3.459873000	2.481164000
6	-2.722261000	-2.992283000	1.093945000
1	-3.006766000	-3.797938000	0.419633000
6	-1.658317000	-2.139860000	0.774984000
23	0.106691000	0.137358000	-1.150210000
6	3.298286000	2.090075000	-0.167605000
1	4.328630000	1.890412000	0.163046000
6	-3.496052000	1.497441000	-0.612890000
1	-3.968505000	2.458055000	-0.364058000
6	0.378453000	-3.720565000	-0.727085000
1	0.164314000	-4.272883000	-1.651878000
6	0.085792000	-4.628242000	0.458654000
1	0.742247000	-5.507751000	0.442442000
1	0.260023000	-4.106001000	1.405646000
1	-0.946559000	-4.986671000	0.480697000

6	1.849497000	-3.342024000	-0.757139000
1	2.135700000	-2.759260000	0.123862000
1	2.481564000	-4.239361000	-0.779760000
1	2.089072000	-2.741537000	-1.638545000
6	3.345870000	2.850746000	-1.487931000
1	3.984774000	2.368535000	-2.232566000
1	2.352811000	2.933483000	-1.939904000
1	3.725211000	3.870148000	-1.344722000
6	2.602346000	2.889162000	0.922213000
1	2.642237000	2.376815000	1.887365000
1	3.071827000	3.873743000	1.042480000
1	1.543295000	3.050991000	0.702176000
6	-3.848847000	1.116324000	-2.045659000
1	-4.932918000	1.007443000	-2.174250000
1	-3.500491000	1.843087000	-2.787077000
1	-3.388927000	0.154645000	-2.304513000
6	-4.018665000	0.458881000	0.360964000
1	-3.601123000	-0.532262000	0.161423000
1	-3.776080000	0.703041000	1.397766000
1	-5.110282000	0.377356000	0.281040000
5	-0.050011000	-0.103015000	1.281428000
15	2.477345000	0.416404000	-0.405978000
15	-1.640976000	1.780426000	-0.503329000
15	-0.745150000	-2.186121000	-0.813021000
6	-1.555269000	3.389538000	-1.518683000
1	-1.473565000	2.998240000	-2.543862000
6	-0.265659000	4.136228000	-1.219385000
1	-0.101841000	4.946004000	-1.940732000
1	-0.279531000	4.582112000	-0.218505000
1	0.597747000	3.470726000	-1.263282000
6	-2.737856000	4.352225000	-1.494442000
1	-2.528756000	5.213468000	-2.142007000
1	-3.668153000	3.907163000	-1.855926000
1	-2.932997000	4.755826000	-0.496024000
6	3.819794000	-0.483355000	-1.421206000
1	3.782418000	-1.496743000	-1.000939000
6	5.263727000	-0.002297000	-1.315781000
1	5.929849000	-0.695895000	-1.844785000
1	5.411866000	0.979515000	-1.775620000
1	5.630316000	0.065816000	-0.289028000
6	3.406878000	-0.566823000	-2.886787000
1	4.100671000	-1.197922000	-3.456761000
1	2.398705000	-0.977827000	-3.005550000
1	3.399373000	0.419031000	-3.366321000
6	-2.063698000	-2.781161000	-2.044818000
1	-2.976241000	-2.292270000	-1.669106000

6	-1.753391000	-2.221426000	-3.428730000
1	-0.779462000	-2.575798000	-3.792658000
1	-2.506183000	-2.535009000	-4.163210000
1	-1.710058000	-1.129403000	-3.430948000
6	-2.329884000	-4.280172000	-2.156176000
1	-1.531277000	-4.790044000	-2.705723000
1	-2.429761000	-4.789685000	-1.195160000
1	-3.254365000	-4.464240000	-2.717729000
7	0.260839000	1.181803000	-4.113701000
7	0.210693000	0.769321000	-3.047683000

[2d''_{sc}] (TE = -3334.561521)

6	-0.328528000	1.641678000	-0.996735000
6	-1.108499000	2.144396000	-2.052169000
1	-1.582014000	1.432772000	-2.727962000
6	-1.290846000	3.509086000	-2.269777000
1	-1.914135000	3.847309000	-3.096718000
6	-0.674181000	4.435072000	-1.434220000
1	-0.808527000	5.503891000	-1.592008000
6	0.086577000	3.976391000	-0.363255000
1	0.528701000	4.684066000	0.336930000
6	0.242784000	2.605079000	-0.134635000
6	1.180455000	-0.248767000	-1.555762000
6	1.575483000	0.353328000	-2.760343000
1	0.966917000	1.160794000	-3.164448000
6	2.720202000	-0.037661000	-3.459325000
1	2.994800000	0.476427000	-4.379554000
6	3.501236000	-1.084307000	-2.980218000
1	4.396885000	-1.398668000	-3.514508000
6	3.140718000	-1.708719000	-1.790132000
1	3.765159000	-2.500064000	-1.376260000
6	2.011979000	-1.287405000	-1.074568000
6	-1.259748000	-0.651193000	-1.281589000
6	-1.331447000	-1.184092000	-2.582454000
1	-0.499821000	-1.001974000	-3.260180000
6	-2.407061000	-1.945630000	-3.030767000
1	-2.400698000	-2.343103000	-4.045187000
6	-3.479921000	-2.201658000	-2.185938000
1	-4.319754000	-2.810609000	-2.515507000
6	-3.446743000	-1.697139000	-0.889083000
1	-4.245959000	-1.937876000	-0.191293000
6	-2.362925000	-0.936695000	-0.438730000
16	-2.237586000	-0.613100000	1.325756000
16	0.921204000	2.073536000	1.434653000
16	1.823170000	-1.794842000	0.638790000
23	0.194566000	-0.264622000	1.447908000

6	2.765705000	2.463911000	1.272224000
1	2.816865000	3.560844000	1.256852000
6	1.275719000	-3.609881000	0.449009000
1	2.149781000	-4.121129000	0.023686000
6	-3.434026000	0.821252000	1.656634000
1	-3.404814000	0.821060000	2.754288000
6	-4.833277000	0.492018000	1.183968000
1	-5.540227000	1.263544000	1.513834000
1	-4.883250000	0.455477000	0.090767000
1	-5.185669000	-0.469641000	1.568663000
6	-2.937743000	2.145568000	1.131686000
1	-2.889403000	2.151102000	0.038293000
1	-3.611284000	2.956895000	1.437086000
1	-1.938636000	2.378495000	1.507484000
6	3.410553000	1.922309000	2.530510000
1	2.964480000	2.338160000	3.439098000
1	3.302505000	0.831886000	2.579058000
1	4.482101000	2.150671000	2.545558000
6	3.363940000	1.883259000	0.015436000
1	2.864725000	2.246708000	-0.887180000
1	4.427544000	2.143126000	-0.059485000
1	3.285322000	0.791342000	0.016279000
6	0.994653000	-4.100628000	1.851839000
1	0.695020000	-5.155073000	1.844293000
1	1.861881000	-3.999174000	2.511655000
1	0.177151000	-3.520837000	2.297688000
6	0.080680000	-3.747403000	-0.462205000
1	-0.786095000	-3.218766000	-0.049200000
1	0.270644000	-3.337083000	-1.457935000
1	-0.198651000	-4.802402000	-0.580969000
6	-0.078664000	0.162969000	-0.807742000
7	0.427729000	-1.163826000	4.419646000
7	0.345467000	-0.812204000	3.322908000

[2e''_{ssi}]- (TE = -3585.974105)

6	0.303205000	2.204254000	0.834717000
6	0.726829000	3.008497000	1.905222000
1	0.992199000	2.538226000	2.853433000
6	0.829664000	4.394202000	1.791267000
1	1.173064000	4.988732000	2.637393000
6	0.500023000	5.018838000	0.592321000
1	0.585828000	6.099650000	0.492068000
6	0.079459000	4.249822000	-0.493281000
1	-0.161933000	4.725304000	-1.443242000
6	-0.009914000	2.864267000	-0.364297000
6	-1.288184000	-0.163276000	1.986012000

6	-1.475100000	0.246942000	3.314641000
1	-0.717495000	0.868134000	3.795748000
6	-2.611734000	-0.100841000	4.042980000
1	-2.738803000	0.253631000	5.065403000
6	-3.592689000	-0.893313000	3.452031000
1	-4.491001000	-1.161071000	4.007073000
6	-3.431341000	-1.328869000	2.139172000
1	-4.203057000	-1.937879000	1.668639000
6	-2.292509000	-0.962861000	1.418796000
6	1.751370000	-0.451809000	1.529794000
6	2.164859000	-0.427725000	2.870460000
1	1.564729000	0.113360000	3.603583000
6	3.309620000	-1.090323000	3.307188000
1	3.594736000	-1.056204000	4.358288000
6	4.075089000	-1.818835000	2.401220000
1	4.958976000	-2.359904000	2.735322000
6	3.691556000	-1.871842000	1.063312000
1	4.260580000	-2.470168000	0.353640000
6	2.556358000	-1.181362000	0.634898000
16	2.082210000	-1.313985000	-1.120623000
16	-0.488512000	1.893567000	-1.820009000
16	-2.182482000	-1.423323000	-0.355355000
23	-0.247367000	-0.533604000	-1.464231000
6	-2.286282000	2.491675000	-1.959703000
1	-2.213637000	3.558615000	-2.208335000
6	-2.146141000	-3.303117000	-0.079107000
1	-3.029457000	-3.524306000	0.533002000
6	3.326499000	-0.117792000	-1.888975000
1	2.902564000	-0.039848000	-2.898704000
6	4.719710000	-0.708530000	-1.956907000
1	5.376101000	-0.071971000	-2.563614000
1	5.170880000	-0.773626000	-0.961516000
1	4.723249000	-1.709895000	-2.396327000
6	3.303375000	1.235937000	-1.216097000
1	3.674342000	1.177386000	-0.186452000
1	3.943038000	1.944258000	-1.756504000
1	2.292744000	1.649211000	-1.178783000
6	-2.898011000	1.718585000	-3.107933000
1	-2.335833000	1.844363000	-4.038393000
1	-2.922522000	0.646405000	-2.879412000
1	-3.928462000	2.045307000	-3.288146000
6	-3.034617000	2.291141000	-0.662258000
1	-2.617918000	2.884014000	0.156908000
1	-4.088231000	2.573506000	-0.778740000
1	-3.002154000	1.238937000	-0.358706000
6	-2.263876000	-3.951560000	-1.439698000

1	-2.269390000	-5.044196000	-1.349776000
1	-3.175113000	-3.649508000	-1.964869000
1	-1.414177000	-3.673540000	-2.071691000
6	-0.882536000	-3.710355000	0.645854000
1	0.000506000	-3.470163000	0.041256000
1	-0.772349000	-3.196960000	1.606645000
1	-0.872946000	-4.790736000	0.838456000
7	-0.449785000	-2.024423000	-4.194013000
7	-0.393536000	-1.472456000	-3.182953000
14	0.143291000	0.298667000	0.789889000

$[2f''_{SB}]^{\cdot}$ (TE = -3321.343122)

6	-1.163412000	-0.481431000	1.880344000
6	-1.934155000	0.027983000	2.940760000
1	-1.655388000	0.997524000	3.357366000
6	-3.032302000	-0.648099000	3.465518000
1	-3.605337000	-0.209547000	4.282307000
6	-3.389398000	-1.895066000	2.957796000
1	-4.238742000	-2.440202000	3.366502000
6	-2.659165000	-2.439183000	1.900873000
1	-2.947286000	-3.406754000	1.494527000
6	-1.599014000	-1.716801000	1.359290000
6	1.512060000	-0.393768000	1.629796000
6	1.741981000	-1.255315000	2.724736000
1	0.882761000	-1.564552000	3.322231000
6	3.009713000	-1.702988000	3.079667000
1	3.130919000	-2.372265000	3.931675000
6	4.130779000	-1.266721000	2.374755000
1	5.131404000	-1.586417000	2.660386000
6	3.953047000	-0.423625000	1.276254000
1	4.818872000	-0.087676000	0.710560000
6	2.669306000	-0.062555000	0.882197000
6	0.053206000	1.823290000	1.261071000
6	0.932775000	2.683293000	1.945875000
1	1.740331000	2.235056000	2.527436000
6	0.815540000	4.070758000	1.900069000
1	1.527134000	4.695742000	2.439629000
6	-0.218701000	4.661557000	1.179322000
1	-0.323021000	5.744626000	1.139782000
6	-1.116724000	3.851548000	0.477548000
1	-1.909505000	4.316297000	-0.104385000
6	-0.946689000	2.471970000	0.495858000
23	0.075068000	-0.119083000	-1.160042000
5	0.114006000	0.239179000	1.268652000
6	3.479870000	0.100497000	-1.919259000
1	2.933367000	0.389566000	-2.825396000

6	3.531315000	-1.411898000	-1.850813000
1	4.019252000	-1.810767000	-2.747911000
1	4.094004000	-1.764227000	-0.982164000
1	2.526487000	-1.842283000	-1.791439000
6	4.852238000	0.748803000	-1.965979000
1	5.394302000	0.420914000	-2.861587000
1	4.786158000	1.839570000	-1.997665000
1	5.469584000	0.479836000	-1.104377000
6	-1.986580000	-3.226992000	-1.029324000
1	-2.942942000	-2.842196000	-0.654287000
6	-1.852065000	-4.709793000	-0.735701000
1	-2.636554000	-5.285096000	-1.243315000
1	-0.886922000	-5.089558000	-1.087501000
1	-1.912940000	-4.931835000	0.332948000
6	-1.863248000	-2.927739000	-2.509388000
1	-2.599578000	-3.506679000	-3.079403000
1	-2.021856000	-1.866344000	-2.723515000
1	-0.871522000	-3.190500000	-2.894246000
6	-2.582200000	2.392440000	-1.856031000
1	-1.835215000	3.182099000	-2.007278000
6	-2.699707000	1.552581000	-3.113511000
1	-3.358780000	0.690590000	-2.954999000
1	-3.128642000	2.142356000	-3.931797000
1	-1.728786000	1.170651000	-3.439717000
6	-3.920605000	2.984585000	-1.450467000
1	-4.663643000	2.193474000	-1.304060000
1	-3.866365000	3.548608000	-0.516040000
1	-4.304241000	3.658159000	-2.227103000
7	0.711045000	-0.682387000	-4.179912000
7	0.445190000	-0.462627000	-3.082903000
16	2.356632000	0.866676000	-0.636226000
16	-0.683386000	-2.254469000	-0.096295000
16	-1.905417000	1.313166000	-0.499810000

{[HIPTN₃N]-V-N₂}⁻ (TE = -2203.110409)

23	-0.165067000	0.438077000	0.114684000
7	1.592883000	1.601322000	0.007616000
7	0.622768000	-1.201759000	1.145182000
7	-2.144056000	0.806055000	0.525982000
6	1.619789000	2.721421000	0.916145000
1	2.540462000	2.711223000	1.532178000
1	1.639080000	3.706475000	0.410792000
6	0.395537000	2.680981000	1.822062000
1	0.568315000	3.243462000	2.756146000
1	-0.459833000	3.149171000	1.323008000
6	-2.404652000	1.525570000	1.759330000

1	-2.474645000	2.620295000	1.611852000
1	-3.374366000	1.237704000	2.199673000
6	-1.308970000	1.195608000	2.755070000
1	-1.429859000	0.159656000	3.087480000
1	-1.356092000	1.840219000	3.649898000
6	0.887176000	-0.964720000	2.545901000
1	0.080707000	-1.377148000	3.186702000
1	1.806020000	-1.469872000	2.895204000
6	1.055883000	0.520540000	2.803595000
1	1.055994000	0.747229000	3.883140000
1	2.014956000	0.842854000	2.394470000
7	0.006887000	1.289076000	2.107380000
6	0.561601000	-2.512711000	0.771755000
6	0.326593000	-2.854834000	-0.588810000
6	0.715352000	-3.609954000	1.663758000
6	0.249044000	-4.167478000	-1.013644000
1	0.215049000	-2.050707000	-1.313416000
6	0.632513000	-4.925214000	1.220585000
1	0.897574000	-3.429590000	2.719378000
6	0.397269000	-5.230696000	-0.116688000
1	0.070810000	-4.368810000	-2.069885000
1	0.754896000	-5.730449000	1.945980000
1	0.332598000	-6.262482000	-0.454491000
6	2.744413000	1.378416000	-0.686293000
6	2.932453000	0.154566000	-1.385985000
6	3.823239000	2.303383000	-0.754881000
6	4.084235000	-0.107236000	-2.102217000
1	2.156129000	-0.604912000	-1.316618000
6	4.975137000	2.024730000	-1.482911000
1	3.745476000	3.262734000	-0.249365000
6	5.127211000	0.824164000	-2.170031000
1	4.180102000	-1.067125000	-2.609514000
1	5.770644000	2.770523000	-1.513101000
1	6.031465000	0.612080000	-2.736286000
6	-3.227663000	0.689223000	-0.323828000
6	-3.237568000	-0.330025000	-1.304158000
6	-4.369729000	1.520638000	-0.265650000
6	-4.290573000	-0.477354000	-2.189058000
1	-2.400100000	-1.025726000	-1.331569000
6	-5.426568000	1.360832000	-1.156640000
1	-4.419385000	2.318585000	0.471529000
6	-5.400496000	0.369649000	-2.131871000
1	-4.256001000	-1.279781000	-2.924810000
1	-6.283932000	2.030224000	-1.085985000
1	-6.230198000	0.247494000	-2.824587000
7	-0.214187000	0.398706000	-3.014263000

7 -0.228107000 0.328587000 -1.884573000

Cartesian coordinates of $[2a'_{PC}]^-$ - $[2f'_{SB}]^-$ and $[2a''_{PC}]^-$ - $[2f''_{SB}]^-$, along with their total energies (in hartree) including zero point vibrational correction at M06-D3(heptane)/def2-SVP level of theory.

$[2a'_{PC}]^-$ (TE = -3059.919348)

6	-0.029129000	2.464059000	1.883050000
6	0.512071000	1.224765000	2.585757000
6	-2.614809000	-0.044454000	1.866034000
6	-1.380349000	-0.432828000	2.678234000
6	2.307097000	-1.289791000	1.858671000
6	0.968266000	-1.197923000	2.587252000
1	-2.729883000	1.055605000	1.793091000
1	-1.476556000	-0.002800000	3.708161000
1	2.929867000	-2.128851000	2.229978000
1	1.169483000	-1.067634000	3.684355000
1	0.346792000	3.401492000	2.336231000
1	1.619059000	1.257676000	2.499615000
6	-0.497880000	3.790853000	-0.717282000
1	0.186919000	4.087407000	-1.536298000
6	-2.746454000	-2.458400000	0.215271000
1	-2.056293000	-2.761260000	1.030475000
6	3.596653000	-0.711369000	-0.704382000
1	3.448956000	0.371852000	-0.528591000
23	-0.045191000	-0.093638000	-0.312935000
6	0.001020000	-0.124284000	2.063355000
1	-1.133326000	2.497971000	1.953138000
1	0.317397000	1.326582000	3.685721000
1	0.476293000	-2.185844000	2.507128000
1	2.902818000	-0.369728000	2.021734000
1	-1.452032000	-1.529410000	2.837626000
1	-3.545569000	-0.428235000	2.331486000
6	4.920735000	-1.088446000	-0.055846000
1	5.736527000	-0.466677000	-0.470176000
1	4.914349000	-0.928046000	1.034786000
1	5.199353000	-2.138534000	-0.235072000
6	3.609502000	-0.922026000	-2.211054000
1	3.819702000	-1.974886000	-2.472424000
1	2.639263000	-0.657254000	-2.665781000
1	4.392732000	-0.307361000	-2.691925000
6	-4.151507000	-2.878323000	0.612908000
1	-4.184579000	-3.959824000	0.841878000

1	-4.521156000	-2.343457000	1.504103000
1	-4.871079000	-2.706805000	-0.206454000
6	-2.288567000	-3.166657000	-1.052027000
1	-2.955523000	-2.946421000	-1.903203000
1	-1.273826000	-2.836774000	-1.338004000
1	-2.276436000	-4.263888000	-0.914365000
6	-1.808412000	3.335242000	-1.336863000
1	-1.675221000	2.442556000	-1.971561000
1	-2.529859000	3.068396000	-0.541554000
1	-2.271054000	4.137557000	-1.939965000
6	-0.736779000	4.990094000	0.188583000
1	0.181669000	5.373265000	0.658275000
1	-1.192885000	5.822426000	-0.378517000
1	-1.439914000	4.734896000	1.000524000
6	1.969645000	-3.199832000	-0.393439000
1	1.638914000	-3.185070000	-1.452910000
6	0.885088000	-3.890372000	0.420147000
1	1.221608000	-4.067509000	1.458022000
1	-0.025776000	-3.270235000	0.462271000
1	0.623767000	-4.872559000	-0.013570000
6	3.271395000	-3.976881000	-0.287712000
1	3.095687000	-5.053208000	-0.472539000
1	4.030483000	-3.645268000	-1.012791000
1	3.709918000	-3.893643000	0.723740000
6	-3.762212000	0.211512000	-0.796260000
1	-3.382587000	1.250582000	-0.788724000
6	-5.143288000	0.230646000	-0.157915000
1	-5.630516000	-0.757276000	-0.187600000
1	-5.119113000	0.558929000	0.894236000
1	-5.805700000	0.929244000	-0.702789000
6	-3.819497000	-0.236631000	-2.250065000
1	-4.264817000	-1.244322000	-2.338416000
1	-4.456516000	0.444129000	-2.844343000
1	-2.822013000	-0.270463000	-2.723401000
6	2.180969000	2.828477000	-0.012973000
1	2.653889000	2.009797000	0.566797000
6	2.597443000	4.153771000	0.599750000
1	3.698603000	4.253107000	0.597540000
1	2.202441000	5.008751000	0.022700000
1	2.263146000	4.264351000	1.644945000
6	2.654033000	2.711235000	-1.454976000
1	3.757527000	2.728594000	-1.521168000
1	2.290881000	1.775454000	-1.914518000
1	2.280389000	3.549776000	-2.070177000
15	-2.333922000	-0.614909000	0.116723000
15	0.366622000	2.307656000	0.077223000

15	1.975229000	-1.348866000	0.025451000
7	-0.242323000	-0.424960000	-3.366200000
7	-0.144239000	-0.293084000	-2.213013000

[2b'_{psi}]⁻ (TE = -3311.316125)

6	-0.420228000	2.638670000	1.938033000
6	0.293842000	1.645829000	2.846297000
6	-2.741818000	-0.498396000	1.906387000
6	-1.597120000	-0.809820000	2.868722000
6	2.714834000	-1.037829000	1.835265000
6	1.532605000	-1.186685000	2.792833000
1	-2.978180000	0.585255000	1.932669000
1	-1.812673000	-0.410192000	3.879646000
1	3.523354000	-1.778955000	2.004782000
1	1.832011000	-0.912154000	3.823943000
1	-0.246342000	3.705008000	2.186636000
1	1.381214000	1.865052000	2.880347000
6	-1.048729000	3.525065000	-0.804069000
1	-0.475070000	4.471292000	-0.867506000
6	-2.445983000	-2.694773000	0.067147000
1	-1.793604000	-2.988968000	0.916505000
6	3.662036000	-0.159218000	-0.774222000
1	3.412458000	0.895212000	-0.543351000
23	0.000134000	-0.082477000	-0.399522000
1	-1.511548000	2.477925000	2.007939000
1	-0.073251000	1.727042000	3.889018000
1	1.199748000	-2.241461000	2.835190000
1	3.178955000	-0.041464000	1.983497000
1	-1.495733000	-1.908190000	2.988165000
1	-3.684092000	-1.025021000	2.157911000
6	5.061346000	-0.410539000	-0.229941000
1	5.777844000	0.293072000	-0.693928000
1	5.124195000	-0.262549000	0.859911000
1	5.426503000	-1.426189000	-0.448874000
6	3.605718000	-0.312781000	-2.286252000
1	3.898816000	-1.329545000	-2.604066000
1	2.591181000	-0.128136000	-2.678548000
1	4.298047000	0.393037000	-2.781512000
6	-3.834859000	-3.255314000	0.327936000
1	-3.793797000	-4.354348000	0.445234000
1	-4.300343000	-2.848387000	1.240868000
1	-4.516963000	-3.054573000	-0.517140000
6	-1.841162000	-3.295774000	-1.192288000
1	-2.443015000	-3.062163000	-2.087303000
1	-0.828295000	-2.898485000	-1.371389000
1	-1.778177000	-4.397140000	-1.112229000

6	-1.286346000	2.993499000	-2.211128000
1	-0.351037000	2.740177000	-2.736381000
1	-1.873951000	2.058379000	-2.172327000
1	-1.841516000	3.724960000	-2.826669000
6	-2.376386000	3.817049000	-0.122278000
1	-2.258354000	4.369015000	0.823593000
1	-3.030168000	4.418067000	-0.779985000
1	-2.921503000	2.881554000	0.106100000
6	2.333400000	-2.832902000	-0.478024000
1	1.942057000	-2.812428000	-1.516338000
6	1.383261000	-3.669614000	0.368125000
1	1.800405000	-3.838418000	1.377779000
1	0.408482000	-3.166948000	0.487629000
1	1.211530000	-4.661936000	-0.087619000
6	3.712988000	-3.470638000	-0.483739000
1	3.638073000	-4.549319000	-0.718093000
1	4.389337000	-3.025555000	-1.229808000
1	4.200844000	-3.392696000	0.505267000
6	-3.674076000	-0.055234000	-0.820034000
1	-3.351743000	1.005981000	-0.820540000
6	-5.063272000	-0.106985000	-0.201973000
1	-5.459416000	-1.134504000	-0.151727000
1	-5.087399000	0.309487000	0.817830000
1	-5.774216000	0.482132000	-0.811315000
6	-3.689704000	-0.518709000	-2.269012000
1	-4.079175000	-1.549150000	-2.356496000
1	-4.348813000	0.125155000	-2.879914000
1	-2.684128000	-0.503952000	-2.723018000
6	1.715976000	3.101932000	0.025183000
1	2.348568000	2.376030000	0.574462000
6	1.873296000	4.466466000	0.672517000
1	2.889416000	4.866927000	0.498890000
1	1.164484000	5.205641000	0.255998000
1	1.718998000	4.434696000	1.763164000
6	2.171078000	3.109718000	-1.425569000
1	3.250395000	3.335415000	-1.509008000
1	1.986817000	2.127717000	-1.897668000
1	1.633095000	3.874900000	-2.014241000
15	-2.210114000	-0.808158000	0.124038000
15	0.013430000	2.269525000	0.156877000
15	2.168420000	-1.006499000	0.029493000
14	0.060103000	-0.137793000	2.093329000
7	-0.004849000	-0.853654000	-3.358345000
7	-0.009302000	-0.566540000	-2.238683000

[2c'_{PB}] (TE = -3046.708132)

6	0.359412000	2.590952000	1.858990000
6	0.729403000	1.304067000	2.587099000
6	-2.662994000	0.422633000	1.781256000
6	-1.576025000	-0.090307000	2.716753000
6	2.130074000	-1.560796000	1.852488000
6	0.799868000	-1.375671000	2.573569000
1	-2.535244000	1.506477000	1.586593000
1	-1.620026000	0.484649000	3.671735000
1	2.723223000	-2.445182000	2.165066000
1	1.008316000	-1.313457000	3.670738000
1	0.895476000	3.501106000	2.204421000
1	1.827606000	1.171684000	2.538185000
6	-0.401130000	3.743865000	-0.758411000
1	0.181346000	3.975844000	-1.672317000
6	-2.796709000	-2.182376000	0.480734000
1	-1.860983000	-2.533251000	0.955351000
6	3.474067000	-1.030742000	-0.759776000
1	3.342015000	0.065260000	-0.818367000
23	-0.028956000	-0.019477000	-0.548988000
1	-0.721503000	2.796880000	1.996170000
1	0.515480000	1.446214000	3.674272000
1	0.186423000	-2.293846000	2.452000000
1	2.774391000	-0.681861000	2.047043000
1	-1.830808000	-1.133363000	3.004790000
1	-3.705905000	0.284439000	2.138648000
6	4.742029000	-1.300134000	0.036662000
1	5.619211000	-0.870798000	-0.482836000
1	4.708978000	-0.851087000	1.042202000
1	4.937988000	-2.377548000	0.167184000
6	3.593667000	-1.517829000	-2.196512000
1	3.785724000	-2.603512000	-2.255470000
1	2.682584000	-1.302550000	-2.779615000
1	4.437169000	-1.015441000	-2.703222000
6	-3.930380000	-2.478609000	1.450619000
1	-3.984380000	-3.566283000	1.643401000
1	-3.784573000	-1.984879000	2.424452000
1	-4.914056000	-2.172989000	1.060094000
6	-2.970512000	-2.942291000	-0.826225000
1	-3.949038000	-2.728090000	-1.292369000
1	-2.187963000	-2.674974000	-1.559228000
1	-2.920341000	-4.034246000	-0.661486000
6	-1.775056000	3.267003000	-1.193919000
1	-1.713233000	2.345659000	-1.796255000
1	-2.401811000	3.041415000	-0.310836000
1	-2.301716000	4.042901000	-1.779006000
6	-0.544809000	5.002860000	0.085212000

1	0.412609000	5.413270000	0.436498000
1	-1.058477000	5.797610000	-0.486734000
1	-1.162484000	4.802570000	0.977703000
5	-0.048404000	-0.057631000	2.082071000
7	0.164670000	-0.471252000	-3.596803000
7	0.082050000	-0.285534000	-2.466306000
6	-3.774679000	0.317552000	-0.892121000
1	-3.634950000	1.397898000	-0.692661000
6	-5.199212000	-0.034621000	-0.493645000
1	-5.923880000	0.582915000	-1.057129000
1	-5.438171000	-1.087786000	-0.723382000
1	-5.393997000	0.128476000	0.579121000
6	-3.554222000	0.103908000	-2.382421000
1	-4.239732000	0.732570000	-2.980241000
1	-2.518903000	0.343523000	-2.677609000
1	-3.737412000	-0.944521000	-2.675182000
6	2.353406000	2.867922000	-0.325444000
1	2.516241000	2.417135000	-1.326388000
6	2.654187000	4.355788000	-0.421205000
1	3.714989000	4.506619000	-0.694048000
1	2.049100000	4.880214000	-1.176893000
1	2.503913000	4.858919000	0.550722000
6	3.334684000	2.233881000	0.649447000
1	3.105295000	1.176969000	0.844907000
1	4.368916000	2.296053000	0.262920000
1	3.313632000	2.756381000	1.621955000
6	1.702746000	-3.356019000	-0.473963000
1	1.685422000	-3.298144000	-1.580625000
6	0.366443000	-3.924724000	-0.034389000
1	0.198946000	-4.930385000	-0.460822000
1	0.306578000	-4.011981000	1.065829000
1	-0.448917000	-3.262873000	-0.361321000
6	2.842617000	-4.264523000	-0.043590000
1	2.643618000	-5.307305000	-0.353001000
1	3.812298000	-3.978078000	-0.479679000
1	2.957864000	-4.274873000	1.054815000
15	1.814617000	-1.531898000	0.020385000
15	0.565370000	2.313806000	0.033400000
15	-2.341796000	-0.378672000	0.148269000

[2d'_{sc}]⁻ (TE = -2875.565304)

6	0.377459000	2.184027000	1.697879000
6	0.380863000	0.933257000	2.567290000
6	-2.674418000	0.419551000	1.626783000
6	-1.698463000	-0.471674000	2.370905000
6	1.893051000	-1.759591000	1.840313000

6	0.518743000	-1.560765000	2.454725000
1	-2.473646000	1.490649000	1.810271000
1	-1.840648000	-0.292529000	3.471302000
1	2.400815000	-2.657898000	2.238548000
1	0.654067000	-1.566941000	3.570985000
1	0.888334000	3.030082000	2.195726000
1	1.443031000	0.740791000	2.829286000
6	0.825145000	3.196682000	-0.954133000
1	1.481655000	2.991742000	-1.820560000
6	-3.550940000	-1.352653000	-0.367675000
1	-3.582114000	-1.795689000	0.645527000
6	3.357931000	-1.185839000	-0.511029000
1	3.479038000	-0.256518000	0.078526000
23	-0.100309000	-0.263629000	-0.341022000
16	-2.451870000	0.186031000	-0.197388000
16	1.253011000	1.746836000	0.133648000
16	1.702585000	-1.880091000	0.006450000
6	-0.236748000	-0.330805000	1.952542000
1	-0.647780000	2.500836000	1.437955000
1	-0.103483000	1.203522000	3.540931000
1	-0.081804000	-2.465886000	2.228773000
1	2.546817000	-0.887228000	2.031725000
1	-2.018288000	-1.521557000	2.204470000
1	-3.730987000	0.238888000	1.903554000
6	4.474107000	-2.161922000	-0.209455000
1	5.454233000	-1.748245000	-0.509933000
1	4.531930000	-2.408588000	0.863555000
1	4.319440000	-3.104120000	-0.764366000
6	3.257801000	-0.834472000	-1.979120000
1	3.020414000	-1.727779000	-2.585164000
1	2.445656000	-0.105660000	-2.139057000
1	4.211453000	-0.415282000	-2.346088000
6	-4.936859000	-0.929946000	-0.802278000
1	-5.618598000	-1.796893000	-0.884744000
1	-5.387754000	-0.211971000	-0.096032000
1	-4.893696000	-0.440474000	-1.791109000
6	-2.886418000	-2.318349000	-1.317359000
1	-2.775316000	-1.884737000	-2.327382000
1	-1.864997000	-2.550030000	-0.958805000
1	-3.471155000	-3.252568000	-1.400852000
6	-0.616072000	3.154213000	-1.412151000
1	-0.846401000	2.192472000	-1.899008000
1	-1.315115000	3.268964000	-0.564176000
1	-0.820598000	3.974678000	-2.123343000
6	1.215867000	4.518984000	-0.326609000
1	2.255403000	4.502827000	0.039660000

1	1.120338000	5.342893000	-1.056235000
1	0.558536000	4.764068000	0.525691000
7	-0.279995000	-0.739704000	-3.382972000
7	-0.191090000	-0.537003000	-2.241781000

[2e'_{ssi}] (TE = -3126.941113)

23	-0.002845000	0.017007000	-0.717575000
16	1.657155000	-1.768423000	-0.902706000
16	-2.218948000	-1.108334000	-1.166792000
16	-0.369504000	1.889937000	0.698124000
14	-0.353733000	-1.064560000	1.479548000
6	-0.426221000	0.234221000	2.924897000
6	0.258894000	1.494987000	2.424493000
6	-2.420257000	-2.454548000	0.092182000
6	-2.019869000	-2.079533000	1.510111000
6	1.074609000	-2.335545000	1.843897000
6	1.472190000	-2.977559000	0.529760000
1	0.663597000	-3.632595000	0.154982000
1	2.383554000	-3.602143000	0.565515000
1	1.931943000	-1.783271000	2.280844000
1	0.796151000	-3.121462000	2.574426000
1	-3.450098000	-2.848204000	-0.004112000
1	-1.750277000	-3.233275000	-0.314763000
1	-2.808819000	-1.452558000	1.971259000
1	-1.965459000	-3.003144000	2.120387000
1	-1.492312000	0.452312000	3.137840000
1	0.035077000	-0.086152000	3.879319000
1	1.349638000	1.327217000	2.331517000
1	0.094654000	2.380371000	3.068478000
6	3.270233000	-0.954779000	-0.416673000
1	2.992528000	-0.270954000	0.411348000
6	-3.473990000	0.125368000	-0.572857000
1	-3.137198000	0.426565000	0.437283000
6	0.716837000	3.373492000	0.321973000
1	0.413594000	3.559190000	-0.725126000
6	-4.873614000	-0.448548000	-0.524514000
1	-5.598271000	0.329959000	-0.225321000
1	-5.172864000	-0.826812000	-1.518076000
1	-4.966557000	-1.275185000	0.198323000
6	-3.373119000	1.320770000	-1.498937000
1	-2.333907000	1.690102000	-1.540633000
1	-3.686578000	1.051001000	-2.523501000
1	-4.023628000	2.139095000	-1.145370000
6	0.379229000	4.579182000	1.172840000
1	0.660073000	4.417588000	2.228732000

1	0.926849000	5.475630000	0.827025000
1	-0.699075000	4.805556000	1.142264000
6	2.187692000	3.019822000	0.334984000
1	2.788433000	3.789612000	-0.181955000
1	2.576774000	2.934493000	1.365496000
1	2.342627000	2.051440000	-0.174644000
6	3.729881000	-0.138685000	-1.607241000
1	4.623670000	0.453383000	-1.341432000
1	3.998444000	-0.801697000	-2.449215000
1	2.948572000	0.553023000	-1.957398000
6	4.337283000	-1.932419000	0.028610000
1	5.296038000	-1.403701000	0.176986000
1	4.090460000	-2.433243000	0.977721000
1	4.498052000	-2.709445000	-0.740510000
7	0.933853000	1.783181000	-3.039904000
7	0.573876000	1.072787000	-2.196709000

[2f_{SB}]⁻ (TE = -2862.362338)

6	0.738222000	-2.367818000	-1.801717000
6	0.451577000	-1.149823000	-2.654226000
6	-2.745376000	-1.157149000	-1.053914000
6	-2.091419000	-0.343503000	-2.150013000
6	1.164646000	2.036834000	-2.096787000
6	-0.131582000	1.465208000	-2.620725000
1	-2.285201000	-2.158845000	-0.959408000
1	-2.259039000	-0.906837000	-3.100847000
1	1.427054000	3.044195000	-2.478352000
1	-0.034443000	1.407765000	-3.734365000
1	1.416914000	-3.114658000	-2.261233000
1	1.432002000	-0.722872000	-2.962722000
6	1.472046000	-3.163557000	0.880637000
1	1.954533000	-2.732367000	1.778369000
6	-3.206950000	1.225644000	0.448785000
1	-2.754092000	1.660836000	-0.460561000
6	2.827028000	2.267103000	0.166603000
1	3.328488000	1.492817000	-0.446815000
23	-0.006332000	0.044026000	0.532729000
16	-2.428035000	-0.449810000	0.617558000
16	1.518118000	-1.704601000	-0.266676000
16	1.019667000	2.109155000	-0.253487000
1	-0.197663000	-2.881453000	-1.509400000
1	-0.018491000	-1.512577000	-3.601268000
1	-0.941227000	2.203616000	-2.433708000
1	2.015117000	1.357733000	-2.305727000
1	-2.679343000	0.591253000	-2.278788000
1	-3.837718000	-1.320823000	-1.162782000

6	3.354241000	3.642596000	-0.187668000
1	4.432500000	3.726263000	0.041672000
1	3.221714000	3.875589000	-1.256229000
1	2.822502000	4.416097000	0.394027000
6	3.015008000	1.938505000	1.631367000
1	2.417717000	2.614957000	2.269737000
1	2.690443000	0.907978000	1.848261000
1	4.075080000	2.046110000	1.921127000
6	-4.710217000	1.119950000	0.305794000
1	-5.162968000	2.122479000	0.203990000
1	-5.001912000	0.535550000	-0.582158000
1	-5.152868000	0.635053000	1.193875000
6	-2.789363000	2.048855000	1.649543000
1	-3.091591000	1.562335000	2.595165000
1	-1.693670000	2.178421000	1.667261000
1	-3.260473000	3.046426000	1.612804000
6	0.056892000	-3.567187000	1.238316000
1	-0.523081000	-2.692338000	1.581693000
1	-0.467166000	-4.006533000	0.370983000
1	0.056222000	-4.326439000	2.040470000
6	2.300644000	-4.322088000	0.363211000
1	3.322244000	-4.004085000	0.100242000
1	2.372719000	-5.124015000	1.119949000
1	1.841083000	-4.765081000	-0.537589000
5	-0.492594000	0.009523000	-1.952101000
7	0.272139000	0.212348000	3.612436000
7	0.178554000	0.139925000	2.468492000

[2a''_{pc}] (TE = -3516.494223)

6	-0.117164000	1.602212000	1.638891000
6	0.527963000	2.121190000	2.779278000
1	1.136621000	1.446856000	3.391747000
6	0.413633000	3.456178000	3.160896000
1	0.938048000	3.809621000	4.055595000
6	-0.377189000	4.332231000	2.421170000
1	-0.483564000	5.380519000	2.718451000
6	-1.018850000	3.850788000	1.280368000
1	-1.619388000	4.541581000	0.674235000
6	-0.874177000	2.523182000	0.864380000
6	-1.264251000	-0.614783000	1.798741000
6	-1.971966000	-0.191097000	2.939502000
1	-1.683137000	0.752118000	3.417300000
6	-3.006428000	-0.939707000	3.496781000
1	-3.525668000	-0.567625000	4.386926000
6	-3.358129000	-2.168364000	2.943750000
1	-4.153152000	-2.776268000	3.387495000

6	-2.689284000	-2.606500000	1.800289000
1	-2.970076000	-3.566264000	1.353334000
6	-1.691001000	-1.833104000	1.197053000
6	1.221468000	-0.497000000	1.804382000
6	1.261020000	-1.138282000	3.057079000
1	0.330191000	-1.233465000	3.627472000
6	2.439398000	-1.640024000	3.604219000
1	2.418073000	-2.129782000	4.584039000
6	3.640786000	-1.498931000	2.915584000
1	4.577976000	-1.874780000	3.338909000
6	3.630445000	-0.884754000	1.663710000
1	4.571748000	-0.800679000	1.112886000
6	2.444443000	-0.417383000	1.081399000
23	-0.058246000	-0.012067000	-1.003369000
6	-3.360974000	2.293013000	-0.522971000
1	-3.407825000	3.354639000	-0.204465000
6	-0.104800000	-3.849718000	-0.276864000
1	-0.844872000	-4.585090000	0.096936000
6	3.413311000	1.731522000	-0.710847000
1	3.192291000	2.140425000	-1.717826000
6	4.917398000	1.544945000	-0.586418000
1	5.427089000	2.523895000	-0.654341000
1	5.189674000	1.114755000	0.393068000
1	5.342737000	0.902189000	-1.372162000
6	2.929634000	2.732466000	0.325493000
1	3.198038000	2.399892000	1.344049000
1	3.393651000	3.722210000	0.163531000
1	1.836038000	2.855323000	0.302958000
6	-4.180618000	2.137373000	-1.793865000
1	-3.900002000	2.862673000	-2.573755000
1	-4.072936000	1.125625000	-2.222126000
1	-5.253691000	2.288859000	-1.578599000
6	-3.914226000	1.429355000	0.596051000
1	-3.412822000	1.628974000	1.556097000
1	-4.995799000	1.608227000	0.732397000
1	-3.772829000	0.355799000	0.378709000
6	0.423355000	-4.299449000	-1.631771000
1	1.027847000	-5.218599000	-1.532962000
1	-0.373850000	-4.503755000	-2.364358000
1	1.073970000	-3.520017000	-2.070607000
6	1.025717000	-3.748834000	0.730065000
1	1.756833000	-2.978847000	0.423907000
1	0.666938000	-3.466328000	1.732603000
1	1.559661000	-4.712025000	0.814940000
6	-0.055807000	0.134053000	1.288145000
7	-0.118903000	-0.848064000	-3.970831000

7	-0.090086000	-0.461674000	-2.876574000
6	-1.114168000	3.339501000	-1.990180000
1	-1.871640000	4.139871000	-1.859366000
6	-1.203836000	2.761684000	-3.399606000
1	-1.105270000	3.559170000	-4.158008000
1	-0.382358000	2.040273000	-3.552406000
1	-2.139018000	2.214157000	-3.597201000
6	0.278307000	3.914762000	-1.797431000
1	0.408641000	4.434700000	-0.835774000
1	1.016375000	3.092452000	-1.839651000
1	0.518489000	4.625194000	-2.608551000
6	3.203908000	-1.052047000	-1.780866000
1	2.379318000	-1.781259000	-1.895053000
6	4.432020000	-1.829316000	-1.336417000
1	4.734335000	-2.531593000	-2.135564000
1	5.303318000	-1.185006000	-1.129618000
1	4.235268000	-2.430734000	-0.434815000
6	3.394853000	-0.392724000	-3.140862000
1	4.280357000	0.267419000	-3.158986000
1	3.535470000	-1.154411000	-3.927590000
1	2.509230000	0.205014000	-3.417667000
6	-2.415993000	-2.726748000	-1.597047000
1	-1.858470000	-2.820078000	-2.551341000
6	-3.391511000	-1.579564000	-1.777725000
1	-4.091453000	-1.781265000	-2.608305000
1	-3.995217000	-1.420824000	-0.864219000
1	-2.840047000	-0.646613000	-1.991306000
6	-3.151836000	-4.032152000	-1.339322000
1	-3.785101000	-4.287195000	-2.208730000
1	-2.484239000	-4.891767000	-1.165301000
1	-3.830468000	-3.949533000	-0.473226000
15	2.306894000	0.193383000	-0.662443000
15	-1.510077000	1.942489000	-0.769752000
15	-0.991181000	-2.196990000	-0.468109000

[2b''_{psi}]' (TE = -3767.864828)

6	0.358231000	1.942886000	1.822147000
6	0.867974000	2.326075000	3.070473000
1	0.980815000	1.573898000	3.862584000
6	1.272380000	3.638893000	3.320157000
1	1.691378000	3.910052000	4.295508000
6	1.142487000	4.605299000	2.324522000
1	1.453959000	5.638214000	2.513281000
6	0.616885000	4.250667000	1.080518000
1	0.510099000	5.021158000	0.306211000
6	0.254415000	2.925642000	0.815725000

6	-1.744350000	-0.359761000	2.045672000
6	-2.199844000	-0.027959000	3.328311000
1	-1.572714000	0.597569000	3.978168000
6	-3.443141000	-0.456913000	3.795747000
1	-3.787358000	-0.168253000	4.795146000
6	-4.240451000	-1.263903000	2.987506000
1	-5.211176000	-1.620238000	3.349076000
6	-3.801875000	-1.616832000	1.709870000
1	-4.432210000	-2.269676000	1.098562000
6	-2.579415000	-1.143732000	1.216786000
6	1.259495000	-0.985653000	2.006048000
6	1.283324000	-1.434704000	3.332722000
1	0.491776000	-1.111414000	4.022368000
6	2.271034000	-2.305192000	3.792724000
1	2.263427000	-2.652338000	4.831848000
6	3.268892000	-2.730066000	2.919087000
1	4.055082000	-3.409350000	3.265734000
6	3.264929000	-2.294425000	1.593107000
1	4.057159000	-2.646117000	0.927854000
6	2.259849000	-1.440416000	1.116404000
23	-0.112984000	-0.048457000	-1.180645000
6	-2.045609000	3.324108000	-0.697079000
1	-1.742128000	4.330642000	-0.345748000
6	-1.628681000	-3.347752000	-0.361019000
1	-2.581186000	-3.786993000	-0.002765000
6	3.694538000	0.304150000	-0.691311000
1	3.605796000	0.791105000	-1.682932000
6	5.049859000	-0.381296000	-0.616821000
1	5.855992000	0.370065000	-0.707404000
1	5.193527000	-0.883139000	0.355184000
1	5.207678000	-1.124835000	-1.413024000
6	3.603556000	1.377624000	0.382451000
1	3.740363000	0.941757000	1.388593000
1	4.391075000	2.139878000	0.239016000
1	2.628963000	1.888397000	0.380109000
6	-2.798680000	3.488783000	-2.005882000
1	-2.250370000	4.105651000	-2.735546000
1	-3.013376000	2.517713000	-2.482709000
1	-3.770459000	3.983574000	-1.826826000
6	-2.914220000	2.679677000	0.369865000
1	-2.428748000	2.686954000	1.359526000
1	-3.881289000	3.205421000	0.463071000
1	-3.120252000	1.622778000	0.126392000
6	-1.264992000	-3.948149000	-1.709579000
1	-0.991517000	-5.013104000	-1.602536000
1	-2.080102000	-3.888660000	-2.448355000

1	-0.396043000	-3.420875000	-2.143212000
6	-0.547185000	-3.652801000	0.660457000
1	0.416218000	-3.211321000	0.350094000
1	-0.779695000	-3.247101000	1.659013000
1	-0.404000000	-4.743449000	0.761447000
7	-0.390030000	-1.101218000	-4.043109000
7	-0.242940000	-0.677614000	-2.981946000
6	0.480733000	3.457544000	-2.109628000
1	0.067016000	4.484153000	-2.031851000
6	0.203522000	2.886417000	-3.496156000
1	0.636381000	3.532151000	-4.281485000
1	0.667038000	1.885888000	-3.575779000
1	-0.867546000	2.751932000	-3.714643000
6	1.984052000	3.485541000	-1.897410000
1	2.285242000	3.946481000	-0.944032000
1	2.365299000	2.448374000	-1.905652000
1	2.483789000	4.031515000	-2.717327000
6	2.571894000	-2.234509000	-1.818845000
1	1.549940000	-2.638238000	-1.949664000
6	3.458461000	-3.408189000	-1.434642000
1	3.484800000	-4.136243000	-2.267017000
1	4.503957000	-3.116471000	-1.234703000
1	3.078450000	-3.943680000	-0.550552000
6	2.977411000	-1.631935000	-3.157950000
1	4.048999000	-1.366012000	-3.181057000
1	2.795426000	-2.345255000	-3.980919000
1	2.391075000	-0.722720000	-3.377797000
6	-3.389942000	-1.510308000	-1.711880000
1	-2.853919000	-1.871160000	-2.613059000
6	-3.842292000	-0.096136000	-2.016995000
1	-4.538190000	-0.074068000	-2.875045000
1	-4.363884000	0.356813000	-1.152782000
1	-2.968426000	0.533930000	-2.253729000
6	-4.584285000	-2.421712000	-1.474308000
1	-5.169011000	-2.528951000	-2.406433000
1	-4.309940000	-3.438182000	-1.146468000
1	-5.271808000	-1.996974000	-0.723260000
15	2.138364000	-0.790790000	-0.643738000
15	-0.402195000	2.359550000	-0.837490000
15	-1.920802000	-1.479565000	-0.510749000
14	-0.073587000	0.164385000	1.229331000

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6	-1.227428000	0.848789000	1.836367000
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1	-0.199158000	1.881004000	3.436295000

6	-2.301533000	2.314955000	3.500115000
1	-2.203222000	2.969457000	4.374291000
6	-3.561066000	2.078424000	2.945518000
1	-4.457840000	2.540582000	3.371608000
6	-3.655027000	1.261418000	1.820349000
1	-4.638546000	1.100075000	1.364504000
6	-2.511111000	0.690112000	1.249130000
6	0.190803000	-1.439859000	1.850189000
6	-0.361517000	-1.847946000	3.083604000
1	-1.015267000	-1.146721000	3.620724000
6	-0.087669000	-3.087125000	3.655374000
1	-0.538774000	-3.356212000	4.617979000
6	0.785706000	-3.977996000	3.024994000
1	1.025353000	-4.944136000	3.481545000
6	1.333738000	-3.622948000	1.793429000
1	2.005567000	-4.325001000	1.285161000
6	1.007440000	-2.401136000	1.192123000
6	1.430682000	0.867229000	1.639143000
6	2.172870000	0.612021000	2.812979000
1	1.828284000	-0.182801000	3.488353000
6	3.324655000	1.317983000	3.145018000
1	3.866267000	1.081279000	4.068515000
6	3.794498000	2.324791000	2.299266000
1	4.708018000	2.878869000	2.539925000
6	3.088426000	2.608740000	1.133452000
1	3.473586000	3.385774000	0.465931000
6	1.928859000	1.894259000	0.800958000
23	-0.126993000	-0.120551000	-1.132827000
6	-3.578916000	-1.654442000	-0.176462000
1	-4.573809000	-1.295204000	0.151407000
6	3.289158000	-1.904536000	-0.699100000
1	3.654060000	-2.936321000	-0.534652000
6	0.104277000	3.744408000	-0.682175000
1	0.358470000	4.241876000	-1.637401000
6	0.550575000	4.630433000	0.468613000
1	0.009232000	5.593643000	0.442539000
1	0.330045000	4.150687000	1.438371000
1	1.629006000	4.852078000	0.453701000
6	-1.400938000	3.559629000	-0.656784000
1	-1.729584000	3.031791000	0.256082000
1	-1.913095000	4.538801000	-0.682498000
1	-1.742986000	2.973726000	-1.524299000
6	-3.735646000	-2.396426000	-1.496872000
1	-4.286992000	-1.812082000	-2.250573000
1	-2.757371000	-2.642913000	-1.942416000
1	-4.281738000	-3.345955000	-1.351921000

6	-3.022658000	-2.550082000	0.917415000
1	-3.009942000	-2.040136000	1.893964000
1	-3.632887000	-3.465807000	1.015691000
1	-1.982675000	-2.855286000	0.711973000
6	3.627901000	-1.459833000	-2.114731000
1	4.720454000	-1.419385000	-2.272795000
1	3.199106000	-2.116007000	-2.891318000
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6	3.951428000	-1.000652000	0.321269000
1	3.614577000	0.043511000	0.207225000
1	3.722373000	-1.302014000	1.355731000
1	5.048605000	-1.018546000	0.192332000
5	0.068971000	0.065716000	1.281226000
15	-2.512342000	-0.118331000	-0.403434000
15	1.415896000	-1.961973000	-0.540942000
15	1.011986000	2.072267000	-0.786433000
6	1.072341000	-3.521034000	-1.577704000
1	1.057870000	-3.093697000	-2.600194000
6	-0.330390000	-4.018051000	-1.282013000
1	-0.681454000	-4.719014000	-2.059852000
1	-0.379887000	-4.537031000	-0.308121000
1	-1.028508000	-3.168404000	-1.236782000
6	2.067910000	-4.670699000	-1.571336000
1	1.718549000	-5.468655000	-2.251736000
1	3.074176000	-4.379313000	-1.911713000
1	2.168935000	-5.129984000	-0.573357000
6	-3.688801000	0.993481000	-1.422588000
1	-3.500169000	1.982060000	-0.966702000
6	-5.188624000	0.741417000	-1.356144000
1	-5.725280000	1.535221000	-1.906969000
1	-5.475183000	-0.214544000	-1.825513000
1	-5.589168000	0.738600000	-0.330449000
6	-3.222086000	1.051249000	-2.870477000
1	-3.788971000	1.810973000	-3.438847000
1	-2.146399000	1.294391000	-2.936872000
1	-3.358494000	0.082847000	-3.385149000
6	2.372340000	2.498159000	-2.050382000
1	3.203092000	1.836369000	-1.730476000
6	1.897134000	2.053027000	-3.426493000
1	0.965638000	2.579688000	-3.712548000
1	2.652678000	2.272816000	-4.202431000
1	1.673103000	0.974668000	-3.453119000
6	2.891025000	3.928183000	-2.133124000
1	2.136816000	4.604091000	-2.572479000
1	3.188955000	4.358618000	-1.165260000
1	3.773297000	3.974065000	-2.796703000

7	-0.365551000	-1.089144000	-4.066725000
7	-0.285781000	-0.681373000	-3.002535000

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6	-0.905418000	1.272348000	-1.082902000
6	-1.972644000	1.328067000	-1.987260000
1	-2.311578000	0.393363000	-2.449365000
6	-2.586329000	2.543179000	-2.350428000
1	-3.424504000	2.542279000	-3.055233000
6	-2.106929000	3.747380000	-1.822385000
1	-2.562523000	4.700420000	-2.115139000
6	-1.066078000	3.732760000	-0.903255000
1	-0.710770000	4.664898000	-0.447701000
6	-0.478671000	2.504025000	-0.508100000
6	1.141978000	-0.061694000	-1.519558000
6	1.329492000	0.572648000	-2.756165000
1	0.518648000	1.200217000	-3.143987000
6	2.493462000	0.390257000	-3.517519000
1	2.600426000	0.900635000	-4.480509000
6	3.509162000	-0.449891000	-3.051716000
1	4.414826000	-0.609045000	-3.647495000
6	3.380437000	-1.058842000	-1.809230000
1	4.188289000	-1.679710000	-1.404386000
6	2.215459000	-0.852624000	-1.039019000
6	-0.999907000	-1.212622000	-1.086762000
6	-0.850046000	-1.941528000	-2.277118000
1	-0.071117000	-1.630972000	-2.981792000
6	-1.665058000	-3.036612000	-2.594428000
1	-1.507649000	-3.576988000	-3.533883000
6	-2.670884000	-3.435789000	-1.712001000
1	-3.310920000	-4.293284000	-1.946624000
6	-2.837775000	-2.751707000	-0.513608000
1	-3.588580000	-3.081222000	0.212971000
6	-2.013745000	-1.650169000	-0.197190000
16	-2.016136000	-1.066976000	1.494265000
16	0.402094000	2.449658000	1.040645000
16	2.263399000	-1.255616000	0.699835000
23	0.248073000	-0.008875000	1.414944000
6	2.135808000	3.132117000	0.778069000
1	1.998751000	4.228926000	0.829480000
6	2.114118000	-3.119780000	0.856964000
1	3.114122000	-3.500440000	0.575245000
6	-3.449158000	0.165011000	1.690525000
1	-3.907202000	-0.198715000	2.628760000
6	-4.444699000	0.062492000	0.560441000
1	-5.282370000	0.758092000	0.744544000

1	-3.973199000	0.348797000	-0.395101000
1	-4.859452000	-0.951162000	0.449771000
6	-2.940052000	1.573809000	1.888356000
1	-2.564132000	1.995226000	0.940652000
1	-3.757310000	2.223985000	2.249174000
1	-2.119366000	1.613964000	2.625355000
6	2.939725000	2.656933000	1.969652000
1	2.459598000	2.923097000	2.926834000
1	3.042059000	1.556091000	1.940310000
1	3.951338000	3.097947000	1.959318000
6	2.761074000	2.753288000	-0.538440000
1	2.112955000	3.012754000	-1.390782000
1	3.724766000	3.279110000	-0.660678000
1	2.952578000	1.668199000	-0.585925000
6	1.849945000	-3.373918000	2.326017000
1	1.848554000	-4.456178000	2.539996000
1	2.601318000	-2.893969000	2.975777000
1	0.858599000	-2.966530000	2.599759000
6	1.053012000	-3.718450000	-0.028490000
1	0.055265000	-3.341196000	0.256216000
1	1.209852000	-3.472755000	-1.090461000
1	1.049923000	-4.817846000	0.077160000
6	-0.169146000	-0.000371000	-0.782719000
7	0.878253000	-0.004927000	4.450597000
7	0.628978000	-0.007763000	3.341936000

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6	-1.285551000	-0.737729000	-1.997752000
6	-1.528740000	-0.588266000	-3.372638000
1	-0.989595000	0.185998000	-3.934632000
6	-2.436539000	-1.396182000	-4.055702000
1	-2.599057000	-1.255256000	-5.129814000
6	-3.129342000	-2.394876000	-3.368777000
1	-3.837470000	-3.041247000	-3.898189000
6	-2.903746000	-2.576393000	-2.006598000
1	-3.421075000	-3.376108000	-1.463147000
6	-2.005719000	-1.745097000	-1.330773000
6	-0.766125000	2.072214000	-0.855179000
6	-1.025886000	2.890217000	-1.967112000
1	-0.816082000	2.507304000	-2.974584000
6	-1.544448000	4.177869000	-1.834445000
1	-1.735147000	4.787627000	-2.724317000
6	-1.831145000	4.684333000	-0.566967000
1	-2.250806000	5.689215000	-0.453061000
6	-1.595400000	3.895115000	0.558124000
1	-1.837284000	4.272084000	1.558503000

6	-1.055794000	2.614827000	0.408708000
6	1.654117000	0.375035000	-1.709643000
6	1.971512000	0.905144000	-2.968663000
1	1.162818000	1.202120000	-3.649722000
6	3.292761000	1.090943000	-3.381094000
1	3.507504000	1.526689000	-4.362974000
6	4.336542000	0.746859000	-2.524694000
1	5.376627000	0.916430000	-2.823572000
6	4.053259000	0.195885000	-1.274721000
1	4.869332000	-0.054831000	-0.588976000
6	2.725422000	-0.011472000	-0.883501000
16	2.389410000	-0.647909000	0.815442000
16	-1.689354000	-2.060147000	0.444105000
16	-0.780781000	1.626101000	1.910991000
23	0.049881000	-0.640344000	1.369823000
6	-3.405081000	-1.680870000	1.115533000
1	-4.074444000	-2.446561000	0.681003000
6	0.541841000	2.674949000	2.735055000
1	0.046328000	3.628051000	2.998043000
6	2.902188000	-2.449179000	0.594877000
1	2.631281000	-2.819306000	1.600983000
6	4.384956000	-2.646207000	0.366414000
1	4.644557000	-3.716157000	0.463494000
1	4.679380000	-2.330955000	-0.649084000
1	4.991161000	-2.082171000	1.094165000
6	2.053084000	-3.143483000	-0.444522000
1	2.223093000	-2.715222000	-1.449015000
1	2.297520000	-4.219749000	-0.489572000
1	0.980405000	-3.038143000	-0.207870000
6	-3.308424000	-1.855253000	2.615710000
1	-2.934582000	-2.854026000	2.895038000
1	-2.600296000	-1.113671000	3.028627000
1	-4.294130000	-1.701956000	3.088088000
6	-3.866941000	-0.292672000	0.735249000
1	-3.912565000	-0.148357000	-0.356412000
1	-4.872403000	-0.094824000	1.148202000
1	-3.174800000	0.462314000	1.147722000
6	0.937423000	1.923151000	3.987932000
1	1.699762000	2.486163000	4.553146000
1	0.075253000	1.743373000	4.650887000
1	1.361812000	0.939461000	3.713181000
6	1.718396000	2.918780000	1.820059000
1	2.163740000	1.955745000	1.514751000
1	1.432861000	3.464073000	0.906012000
1	2.493049000	3.507284000	2.342750000
7	0.399002000	-2.674080000	3.646140000

7	0.270777000	-1.873770000	2.827259000
14	-0.080471000	0.265922000	-0.867663000

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6	0.764441000	-0.656022000	-1.991020000
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6	2.323887000	-1.335536000	-3.762877000
1	2.921068000	-1.067003000	-4.641703000
6	2.325355000	-2.650747000	-3.296299000
1	2.918382000	-3.421643000	-3.799570000
6	1.571836000	-2.979526000	-2.167287000
1	1.579265000	-4.009569000	-1.794754000
6	0.847119000	-1.982542000	-1.513957000
6	-1.736131000	0.168321000	-1.505155000
6	-2.250683000	-0.469842000	-2.657608000
1	-1.535174000	-0.911846000	-3.363319000
6	-3.609840000	-0.528245000	-2.945769000
1	-3.952796000	-1.032738000	-3.856513000
6	-4.536125000	0.095279000	-2.104295000
1	-5.604285000	0.095501000	-2.344408000
6	-4.077536000	0.713254000	-0.941160000
1	-4.785857000	1.211483000	-0.272212000
6	-2.719739000	0.670613000	-0.616787000
6	0.313476000	1.882931000	-1.154807000
6	-0.393170000	3.006924000	-1.636462000
1	-1.354717000	2.835960000	-2.138147000
6	0.079715000	4.311421000	-1.505301000
1	-0.513468000	5.147384000	-1.893754000
6	1.312023000	4.554856000	-0.900782000
1	1.696275000	5.574696000	-0.795928000
6	2.051778000	3.475919000	-0.402495000
1	3.008200000	3.670946000	0.091651000
6	1.539149000	2.185115000	-0.498930000
23	0.060408000	0.020773000	1.133479000
5	-0.186784000	0.380383000	-1.242610000
6	-3.164809000	0.351154000	2.231263000
1	-2.549670000	0.538446000	3.130813000
6	-3.211050000	-1.136594000	1.963465000
1	-3.793274000	-1.647178000	2.750483000
1	-3.685883000	-1.354163000	0.990702000
1	-2.195914000	-1.568305000	1.943667000
6	-4.538166000	0.953845000	2.455921000
1	-4.971689000	0.558153000	3.391432000
1	-4.495029000	2.051461000	2.537350000
1	-5.236267000	0.693271000	1.643915000

6	0.989586000	-3.554788000	0.865210000
1	1.977118000	-3.486265000	0.373934000
6	0.384693000	-4.931468000	0.676533000
1	0.998479000	-5.706887000	1.169372000
1	-0.625180000	-4.968291000	1.121199000
1	0.283329000	-5.199534000	-0.387355000
6	1.124074000	-3.182551000	2.326259000
1	1.720261000	-3.938289000	2.867155000
1	1.607892000	-2.198146000	2.440970000
1	0.135038000	-3.119628000	2.816784000
6	3.426441000	1.440857000	1.543732000
1	2.910439000	2.342292000	1.923171000
6	3.554719000	0.411578000	2.649568000
1	3.929920000	-0.546879000	2.245804000
1	4.276766000	0.754739000	3.410453000
1	2.592875000	0.218983000	3.147666000
6	4.785124000	1.785056000	0.961017000
1	5.279345000	0.868841000	0.594271000
1	4.720176000	2.481446000	0.111087000
1	5.438320000	2.238696000	1.727780000
7	0.049851000	0.041458000	4.221108000
7	0.082806000	0.031088000	3.072904000
16	-2.132266000	1.277870000	0.977776000
16	-0.056203000	-2.257976000	0.020781000
16	2.323479000	0.728157000	0.236881000

Cartesian coordinates of $[3a'_{PC}]-[3f'_{SB}]$, $[3a''_{PC}]-[3f''_{SB}]$ and $\{[HIPTN_3N]-V-N=NH\}^+$ along with their total energies (in hartree) including zero point vibrational correction at M06-L-D3(heptane)/6-311+G* level of theory.

$[3a'_{PC}]$ (TE = -3062.515879)

6	-0.654179000	1.912782000	2.008941000
6	0.163412000	0.808433000	2.677218000
6	-2.297817000	-1.060571000	2.045521000
6	-0.902085000	-1.473937000	2.487711000
6	2.812180000	-0.718647000	1.811750000
6	1.536499000	-1.239149000	2.465531000
1	-2.568051000	-0.084970000	2.460775000
1	-0.879696000	-1.537284000	3.591288000
1	3.695498000	-1.296672000	2.106048000
1	1.632240000	-1.142778000	3.561870000
1	-0.577043000	2.860039000	2.555240000
1	1.183785000	1.201248000	2.797785000
6	-1.081341000	3.425227000	-0.546637000
1	-0.384602000	4.272148000	-0.611522000
6	-2.689468000	-2.676949000	-0.329630000

1	-1.957125000	-3.262608000	0.250917000
6	4.009486000	0.006329000	-0.813582000
1	3.999505000	1.042470000	-0.441934000
23	0.091839000	-0.320562000	-0.351084000
6	0.235061000	-0.572391000	1.975238000
1	-1.723676000	1.676826000	1.968906000
1	-0.198988000	0.680621000	3.712762000
1	1.477948000	-2.322498000	2.294678000
1	3.017125000	0.321961000	2.096116000
1	-0.723198000	-2.508409000	2.151525000
1	-3.069058000	-1.757528000	2.392514000
6	5.336227000	-0.633316000	-0.424558000
1	6.169870000	-0.055426000	-0.835730000
1	5.483522000	-0.687774000	0.657221000
1	5.426844000	-1.645910000	-0.829348000
6	3.828954000	0.036561000	-2.326569000
1	3.878288000	-0.968066000	-2.759750000
1	2.872607000	0.475788000	-2.623175000
1	4.623551000	0.621518000	-2.799100000
6	-4.085230000	-3.153459000	0.053720000
1	-4.177918000	-4.229737000	-0.123907000
1	-4.331745000	-2.978691000	1.104075000
1	-4.853787000	-2.668042000	-0.554945000
6	-2.418152000	-2.924785000	-1.811326000
1	-3.196761000	-2.493585000	-2.444789000
1	-1.468261000	-2.505592000	-2.151673000
1	-2.400420000	-3.999437000	-2.018205000
6	-1.468772000	3.030791000	-1.966075000
1	-0.596225000	2.796452000	-2.582452000
1	-2.117099000	2.149610000	-1.983560000
1	-2.008376000	3.846369000	-2.457763000
6	-2.278261000	3.893457000	0.271213000
1	-1.995817000	4.252817000	1.263970000
1	-2.776711000	4.720385000	-0.243972000
1	-3.031583000	3.111103000	0.407599000
6	2.519991000	-2.560837000	-0.464848000
1	2.912006000	-2.576009000	-1.492137000
6	1.060671000	-3.017303000	-0.520515000
1	0.569229000	-2.954958000	0.457670000
1	0.477239000	-2.436714000	-1.255398000
1	0.960644000	-4.056332000	-0.852299000
6	3.365994000	-3.484633000	0.398832000
1	3.356425000	-4.500138000	-0.010100000
1	4.409545000	-3.169810000	0.460058000
1	2.983697000	-3.551797000	1.421289000
6	-3.628097000	0.225415000	-0.275597000

1	-3.139209000	1.199216000	-0.121377000
6	-4.873183000	0.192299000	0.601573000
1	-5.425967000	-0.744933000	0.504665000
1	-4.647792000	0.334334000	1.661687000
1	-5.555620000	0.997081000	0.308233000
6	-3.964156000	0.110099000	-1.757811000
1	-4.565437000	-0.780892000	-1.961777000
1	-4.557278000	0.970988000	-2.082397000
1	-3.074395000	0.062544000	-2.393615000
6	1.615178000	2.831348000	0.396284000
1	2.230776000	2.039400000	0.846983000
6	1.683348000	4.062034000	1.288175000
1	2.699691000	4.468444000	1.300150000
1	1.027899000	4.865461000	0.935390000
1	1.412212000	3.844808000	2.324436000
6	2.139262000	3.104737000	-1.008870000
1	3.193471000	3.398467000	-0.985155000
1	2.051567000	2.225670000	-1.656352000
1	1.597022000	3.923819000	-1.492947000
15	-2.271528000	-0.942811000	0.211929000
15	-0.081485000	2.074325000	0.277906000
15	2.530222000	-0.750206000	0.004380000
7	-0.296462000	-0.007161000	-3.357224000
7	-0.054570000	-0.099069000	-2.165375000
1	0.553297000	0.212704000	-3.922689000

[3b'_{psi}]-Triplet (TE = -3313.941683)

6	-0.360363000	2.264953000	2.068660000
6	0.226208000	1.139828000	2.915951000
6	-2.714140000	-0.591117000	2.036981000
6	-1.579206000	-1.332697000	2.738361000
6	2.748352000	-1.408896000	1.742826000
6	1.567943000	-1.614552000	2.693244000
1	-2.775837000	0.445542000	2.392439000
1	-1.689312000	-1.259923000	3.827605000
1	3.510427000	-2.193501000	1.828823000
1	1.866414000	-1.347407000	3.714649000
1	-0.179049000	3.264419000	2.486099000
1	1.292915000	1.331796000	3.099172000
6	-0.342276000	3.683745000	-0.510722000
1	0.332516000	4.494891000	-0.198192000
6	-2.656998000	-2.284395000	-0.338314000
1	-1.689760000	-2.758545000	-0.097704000
6	3.801904000	-0.636861000	-0.845596000
1	3.920753000	0.383240000	-0.454040000

23	-0.002884000	-0.164465000	-0.479348000
1	-1.449864000	2.165827000	1.987673000
1	-0.239190000	1.137183000	3.910882000
1	1.293721000	-2.672996000	2.737279000
1	3.268799000	-0.469051000	1.978447000
1	-1.623153000	-2.405252000	2.504009000
1	-3.702733000	-1.028444000	2.221758000
6	5.040581000	-1.436495000	-0.459996000
1	5.917291000	-1.044479000	-0.985350000
1	5.260196000	-1.389855000	0.608655000
1	4.956661000	-2.492337000	-0.737432000
6	3.638858000	-0.553135000	-2.356881000
1	3.625559000	-1.547345000	-2.816062000
1	2.715948000	-0.039301000	-2.644980000
1	4.476036000	-0.009984000	-2.805751000
6	-3.729639000	-3.068629000	0.407712000
1	-3.754664000	-4.099058000	0.038312000
1	-3.546735000	-3.121138000	1.483426000
1	-4.728636000	-2.652874000	0.260141000
6	-2.849244000	-2.362967000	-1.850389000
1	-3.848422000	-2.027408000	-2.143908000
1	-2.127889000	-1.757288000	-2.408994000
1	-2.749951000	-3.397131000	-2.194992000
6	-0.287412000	3.554865000	-2.029016000
1	0.680382000	3.216822000	-2.405300000
1	-1.038386000	2.848283000	-2.391423000
1	-0.501913000	4.521026000	-2.496429000
6	-1.755114000	4.039947000	-0.065388000
1	-1.826509000	4.270826000	0.999585000
1	-2.108841000	4.919298000	-0.612384000
1	-2.460168000	3.230556000	-0.284162000
6	1.992383000	-2.959861000	-0.700853000
1	2.984041000	-3.309790000	-1.020521000
6	1.075415000	-2.914044000	-1.920476000
1	0.051215000	-2.619410000	-1.643662000
1	1.414009000	-2.221727000	-2.694429000
1	0.982518000	-3.904478000	-2.378030000
6	1.448180000	-3.932542000	0.335297000
1	1.293310000	-4.917316000	-0.116692000
1	2.121622000	-4.068051000	1.184385000
1	0.478415000	-3.603118000	0.729062000
6	-3.765754000	0.567630000	-0.408707000
1	-3.660895000	1.442482000	0.254129000
6	-5.170120000	0.008310000	-0.216651000
1	-5.368125000	-0.826528000	-0.895103000
1	-5.362550000	-0.334455000	0.803252000

1	-5.913681000	0.779228000	-0.443419000
6	-3.538227000	1.036726000	-1.839441000
1	-3.681620000	0.232365000	-2.565544000
1	-4.246578000	1.830904000	-2.096350000
1	-2.528343000	1.424746000	-1.990309000
6	2.122068000	2.514997000	0.582496000
1	2.516238000	1.576391000	1.003628000
6	2.421866000	3.642599000	1.560790000
1	3.502075000	3.806587000	1.628922000
1	1.979897000	4.592407000	1.242066000
1	2.063810000	3.434188000	2.571773000
6	2.791511000	2.756485000	-0.765628000
1	3.881517000	2.765662000	-0.662365000
1	2.533118000	1.989757000	-1.504575000
1	2.508550000	3.728199000	-1.182029000
15	-2.388436000	-0.514865000	0.220548000
15	0.303242000	2.161380000	0.356703000
15	2.234924000	-1.227899000	-0.027182000
14	0.064316000	-0.599411000	2.112255000
7	-0.334694000	0.393511000	-3.452999000
7	-0.093881000	0.243739000	-2.266518000
1	0.534159000	0.436653000	-4.032560000

[3c'_{PB}]-Quartet (TE = -3049.279552)

6	-0.476204000	2.330554000	2.055904000
6	0.430885000	1.433746000	2.897763000
6	-2.161709000	-0.705609000	2.093429000
6	-0.787655000	-1.082643000	2.649556000
6	2.909308000	-0.411047000	1.726434000
6	1.882719000	-0.835484000	2.783968000
1	-2.427852000	0.330106000	2.324197000
1	-0.891200000	-1.274052000	3.736546000
1	3.893351000	-0.848561000	1.929530000
1	2.303617000	-0.571755000	3.767508000
1	-0.396091000	3.381804000	2.356431000
1	1.450888000	1.844545000	2.879802000
6	-1.176227000	3.359361000	-0.645397000
1	-0.553947000	4.254652000	-0.781981000
6	-2.537731000	-2.740316000	0.070239000
1	-1.751878000	-3.167865000	0.714862000
6	3.714313000	-0.077238000	-1.060637000
1	3.662858000	0.990666000	-0.801127000
23	-0.009825000	-0.205023000	-0.694053000
1	-1.530748000	2.069053000	2.179907000
1	0.131223000	1.539255000	3.955795000

1	1.798759000	-1.930469000	2.793494000
1	3.056415000	0.676330000	1.747064000
1	-0.499957000	-2.074517000	2.271030000
1	-2.954132000	-1.317073000	2.541641000
6	5.127872000	-0.569731000	-0.782080000
1	5.849008000	0.022063000	-1.354749000
1	5.412957000	-0.490710000	0.270360000
1	5.259876000	-1.610661000	-1.092101000
6	3.362427000	-0.231293000	-2.535750000
1	3.360585000	-1.283166000	-2.843400000
1	2.376291000	0.176890000	-2.775216000
1	4.098359000	0.281297000	-3.162754000
6	-3.888490000	-3.218412000	0.588556000
1	-3.905129000	-4.311877000	0.637654000
1	-4.129959000	-2.848763000	1.588566000
1	-4.700618000	-2.922836000	-0.082209000
6	-2.293443000	-3.242519000	-1.348756000
1	-3.051916000	-2.881843000	-2.048238000
1	-1.323601000	-2.935572000	-1.743966000
1	-2.331919000	-4.336231000	-1.371119000
6	-1.530749000	2.819298000	-2.027160000
1	-0.645934000	2.532264000	-2.603660000
1	-2.167411000	1.930498000	-1.968535000
1	-2.072331000	3.571652000	-2.609218000
6	-2.410930000	3.781209000	0.139503000
1	-2.161965000	4.290898000	1.073546000
1	-3.014093000	4.473554000	-0.456015000
1	-3.060951000	2.936456000	0.390869000
6	2.656024000	-2.687185000	-0.134739000
1	3.005513000	-2.815708000	-1.170393000
6	1.338750000	-3.441838000	0.011031000
1	0.906098000	-3.308414000	1.009813000
1	0.595108000	-3.116978000	-0.722654000
1	1.489357000	-4.517165000	-0.129025000
6	3.706508000	-3.257542000	0.811017000
1	3.881449000	-4.312981000	0.579573000
1	4.671241000	-2.751104000	0.752148000
1	3.375348000	-3.215255000	1.853248000
6	-3.708823000	0.053866000	-0.284742000
1	-3.311450000	1.079011000	-0.271025000
6	-4.915842000	0.023755000	0.644606000
1	-5.410655000	-0.949212000	0.657997000
1	-4.664100000	0.282097000	1.676744000
1	-5.659066000	0.752889000	0.305144000
6	-4.079800000	-0.274093000	-1.726281000
1	-4.577696000	-1.245682000	-1.799544000

1	-4.780711000	0.469533000	-2.118199000
1	-3.211577000	-0.295123000	-2.392965000
6	1.602195000	2.947690000	0.108488000
1	2.291278000	2.226673000	0.571292000
6	1.738752000	4.276134000	0.837531000
1	2.723572000	4.715498000	0.649122000
1	0.997782000	5.010841000	0.504197000
1	1.636135000	4.173707000	1.920888000
6	1.966575000	3.067340000	-1.367494000
1	3.011861000	3.369060000	-1.489206000
1	1.831971000	2.123167000	-1.908751000
1	1.359965000	3.823686000	-1.875881000
15	-2.217823000	-0.911271000	0.259215000
15	-0.077082000	2.145312000	0.269576000
15	2.391561000	-0.837025000	0.006467000
5	0.469040000	-0.131286000	2.667035000
7	-0.577874000	-0.664770000	-3.612651000
7	-0.254831000	-0.693469000	-2.425730000
1	0.203532000	-0.978190000	-4.229117000

[3d'_{SC}]-Triplet (TE = -2877.659059)

6	-0.195305000	1.417693000	-2.254750000
6	-0.155121000	-0.040766000	-2.688439000
6	2.762371000	-0.201691000	-1.636008000
6	1.841611000	-1.368736000	-1.903533000
6	-1.843596000	-2.293077000	-1.281753000
6	-0.418455000	-2.370012000	-1.786194000
1	2.524541000	0.667254000	-2.256541000
1	2.000867000	-1.699015000	-2.946914000
1	-2.376813000	-3.242946000	-1.372703000
1	-0.451879000	-2.713678000	-2.835907000
1	-0.703577000	2.053842000	-2.985371000
1	-1.174258000	-0.310159000	-2.995583000
6	-0.829181000	3.171770000	-0.012785000
1	-1.435884000	3.145509000	0.900989000
6	3.294855000	-1.015999000	1.081938000
1	2.567327000	-1.841255000	1.037439000
6	-3.436477000	-0.913112000	0.637960000
1	-3.446329000	-0.225160000	-0.216575000
23	0.162545000	-0.273815000	0.434458000
16	2.574893000	0.396165000	0.087432000
16	-1.124042000	1.464216000	-0.680223000
16	-1.811420000	-1.804503000	0.487485000
6	0.361766000	-1.056679000	-1.642526000
1	0.796854000	1.840835000	-2.070996000
1	0.436016000	-0.095531000	-3.618063000

1	0.101435000	-3.175379000	-1.246920000
1	-2.427993000	-1.526857000	-1.804704000
1	2.163949000	-2.223106000	-1.288702000
1	3.820343000	-0.416438000	-1.805704000
6	-4.568535000	-1.913185000	0.524001000
1	-5.527747000	-1.387522000	0.563114000
1	-4.543419000	-2.470959000	-0.415299000
1	-4.552530000	-2.633470000	1.346554000
6	-3.458795000	-0.127577000	1.930789000
1	-3.322622000	-0.772394000	2.804523000
1	-2.688641000	0.645515000	1.961178000
1	-4.430021000	0.363477000	2.041245000
6	4.617279000	-1.484371000	0.514429000
1	5.052017000	-2.230246000	1.186324000
1	4.521028000	-1.956985000	-0.464850000
1	5.333045000	-0.661262000	0.432000000
6	3.420501000	-0.520489000	2.510066000
1	4.148276000	0.292125000	2.584051000
1	2.469672000	-0.160861000	2.909402000
1	3.765338000	-1.333344000	3.155140000
6	0.618006000	3.432021000	0.344883000
1	0.993421000	2.734467000	1.095695000
1	1.276387000	3.381455000	-0.528159000
1	0.715633000	4.442200000	0.754360000
6	-1.397131000	4.194292000	-0.978325000
1	-2.435518000	3.985674000	-1.244622000
1	-1.363326000	5.188336000	-0.523214000
1	-0.811926000	4.246365000	-1.901295000
7	-0.364846000	0.940056000	3.183205000
7	-0.054904000	0.386285000	2.147359000
1	0.292412000	0.748352000	3.969980000

[3e'_{ssi}]-Triplet (TE = -3129.076381)

6	-0.682770000	-0.034513000	2.543607000
6	-0.142037000	-1.454400000	2.518668000
6	-2.548586000	-2.429440000	0.035773000
6	-1.327211000	-3.282066000	0.314388000
6	2.875052000	-1.847125000	0.496857000
6	1.831211000	-2.938530000	0.632483000
1	-2.962241000	-1.998568000	0.953166000
1	-1.555087000	-3.986374000	1.123264000
1	3.877580000	-2.229264000	0.283454000
1	2.069885000	-3.545794000	1.514326000
1	-0.690987000	0.411430000	3.543541000
1	0.807623000	-1.492737000	3.067761000
6	-0.354330000	2.690410000	1.590897000

1	0.216529000	3.227252000	0.822839000
6	-3.643192000	-0.216210000	-1.498572000
1	-4.165673000	-0.983527000	-2.083711000
6	3.730414000	0.600746000	-0.631330000
1	3.763575000	0.732447000	0.457735000
23	0.080875000	0.028715000	-0.744125000
16	-2.033355000	-1.037753000	-1.058977000
16	0.408982000	0.999004000	1.484374000
16	2.432059000	-0.710996000	-0.890731000
1	-1.696754000	0.024303000	2.132540000
1	-0.831714000	-2.102140000	3.074960000
1	1.878501000	-3.615652000	-0.228395000
1	2.936649000	-1.225658000	1.398716000
1	-1.079108000	-3.883476000	-0.567288000
1	-3.357429000	-2.952047000	-0.485469000
6	5.066609000	0.101124000	-1.145440000
1	5.845313000	0.839471000	-0.930059000
1	5.375993000	-0.837832000	-0.681454000
1	5.045075000	-0.050280000	-2.228119000
6	3.299940000	1.894351000	-1.287935000
1	3.100629000	1.762939000	-2.356821000
1	2.404211000	2.308907000	-0.820025000
1	4.100057000	2.634682000	-1.196599000
6	-4.449429000	0.140666000	-0.267904000
1	-5.381929000	0.627893000	-0.569593000
1	-4.724577000	-0.732279000	0.327850000
1	-3.909001000	0.839517000	0.376968000
6	-3.330355000	0.978220000	-2.372963000
1	-2.798178000	1.757266000	-1.820070000
1	-2.721976000	0.713329000	-3.241451000
1	-4.261992000	1.415480000	-2.743098000
6	-1.822457000	2.686283000	1.222342000
1	-2.004855000	2.179582000	0.270460000
1	-2.432339000	2.205814000	1.993464000
1	-2.184750000	3.714310000	1.125688000
6	-0.080072000	3.304885000	2.949647000
1	0.984242000	3.316463000	3.192927000
1	-0.437361000	4.339015000	2.966435000
1	-0.605253000	2.774978000	3.749644000
14	0.120200000	-2.123231000	0.735714000
7	-0.273282000	2.706452000	-2.158033000
7	-0.041562000	1.646976000	-1.608162000
1	0.596608000	3.230867000	-2.403123000

[3f_{SB}]-Quartet (TE = -2864.418883)

6	0.985577000	2.062001000	1.700690000
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6	0.972443000	0.766528000	2.502134000
6	-2.415314000	1.160935000	1.296393000
6	-1.731513000	0.355471000	2.393960000
6	1.296139000	-2.307647000	1.520048000
6	-0.086384000	-1.692402000	1.713759000
1	-1.877888000	2.085560000	1.070213000
1	-1.724085000	0.998826000	3.286729000
1	1.300203000	-3.387097000	1.686120000
1	-0.627203000	-2.231509000	2.509998000
1	1.831413000	2.712874000	1.941001000
1	1.951341000	0.280661000	2.399291000
6	0.764995000	3.063671000	-1.056272000
1	0.977982000	2.698291000	-2.068833000
6	-3.558348000	-1.164838000	0.042923000
1	-3.065405000	-1.693359000	0.868791000
6	3.456291000	-1.087742000	0.003988000
1	3.226301000	-0.241563000	0.662860000
23	-0.154898000	-0.529800000	-0.558798000
16	-2.497557000	0.321965000	-0.327810000
16	1.134258000	1.548257000	-0.056497000
16	1.859800000	-2.013341000	-0.204795000
1	0.064179000	2.638175000	1.834687000
1	0.893623000	1.035316000	3.566662000
1	-0.743007000	-2.020304000	0.858971000
1	2.037624000	-1.870963000	2.194030000
1	-2.386564000	-0.486088000	2.661633000
1	-3.434532000	1.456475000	1.563224000
6	4.502135000	-1.987167000	0.627604000
1	5.430554000	-1.427128000	0.777800000
1	4.198217000	-2.375325000	1.603289000
1	4.730882000	-2.840781000	-0.016290000
6	3.847005000	-0.580099000	-1.368856000
1	4.036821000	-1.404715000	-2.062391000
1	3.074992000	0.060417000	-1.804340000
1	4.767255000	0.006816000	-1.299928000
6	-4.944187000	-0.722838000	0.464300000
1	-5.564973000	-1.602330000	0.660655000
1	-4.941444000	-0.124151000	1.378231000
1	-5.435057000	-0.142468000	-0.322015000
6	-3.569136000	-2.041720000	-1.194046000
1	-3.979421000	-1.513063000	-2.059537000
1	-2.573080000	-2.400949000	-1.464573000
1	-4.201618000	-2.915929000	-1.016188000
6	-0.679497000	3.504373000	-0.966238000
1	-1.374806000	2.710000000	-1.248668000
1	-0.934265000	3.854965000	0.039247000

1	-0.852767000	4.347349000	-1.642474000
6	1.743134000	4.163687000	-0.691288000
1	2.782622000	3.834404000	-0.751765000
1	1.619543000	5.009211000	-1.374205000
1	1.562895000	4.542680000	0.319126000
5	-0.249672000	-0.162728000	2.113560000
7	-0.634929000	-1.209760000	-3.488761000
7	-0.382704000	-0.897335000	-2.339527000
1	-0.279931000	-0.508961000	-4.177763000

[3a''_{PC}]-Triplet (TE = -3519.781959)

6	0.377158000	1.460737000	1.626730000
6	-0.329959000	2.160751000	2.620463000
1	-1.156232000	1.666501000	3.127049000
6	0.007496000	3.456579000	2.985568000
1	-0.562102000	3.960396000	3.763641000
6	1.076817000	4.105863000	2.373810000
1	1.347130000	5.118716000	2.660453000
6	1.784794000	3.448154000	1.376916000
1	2.594301000	3.971271000	0.871491000
6	1.449019000	2.146452000	0.985763000
6	-1.285092000	-0.431056000	1.836404000
6	-1.342152000	-1.192882000	3.012918000
1	-0.419512000	-1.458212000	3.522045000
6	-2.547156000	-1.633719000	3.547327000
1	-2.544515000	-2.230498000	4.456730000
6	-3.748389000	-1.313866000	2.926139000
1	-4.694941000	-1.656968000	3.335626000
6	-3.724055000	-0.558257000	1.761314000
1	-4.662520000	-0.327066000	1.265917000
6	-2.514000000	-0.126049000	1.209049000
6	1.120545000	-0.933163000	1.643841000
6	1.879914000	-0.774885000	2.808833000
1	1.770349000	0.139097000	3.391711000
6	2.751253000	-1.766928000	3.241866000
1	3.327821000	-1.620334000	4.152656000
6	2.880742000	-2.950225000	2.520408000
1	3.556666000	-3.730975000	2.859620000
6	2.143254000	-3.126709000	1.355013000
1	2.251198000	-4.049772000	0.792034000
6	1.276572000	-2.125491000	0.906959000
6	0.036167000	0.044880000	1.253318000
23	-0.015519000	0.213990000	-1.032966000
6	2.170392000	2.800752000	-1.740441000
1	2.730182000	3.627682000	-1.284812000
6	-3.828816000	0.000206000	-1.431905000

1	-3.875207000	-1.048144000	-1.097806000
6	1.355095000	-3.002640000	-1.968443000
1	0.766947000	-2.782395000	-2.872312000
6	1.543561000	-4.513600000	-1.897914000
1	2.084620000	-4.853274000	-2.787252000
1	2.136678000	-4.826818000	-1.035524000
1	0.601942000	-5.064206000	-1.870599000
6	2.692143000	-2.280919000	-2.102956000
1	3.330963000	-2.454347000	-1.230296000
1	3.233706000	-2.645464000	-2.980870000
1	2.566547000	-1.199650000	-2.218134000
6	2.855435000	2.379065000	-3.034621000
1	3.917978000	2.160991000	-2.901659000
1	2.383138000	1.489976000	-3.467686000
1	2.783873000	3.176542000	-3.780706000
6	0.748338000	3.275549000	-2.005116000
1	0.207430000	3.527084000	-1.086588000
1	0.744450000	4.171904000	-2.633482000
1	0.173885000	2.520399000	-2.556741000
6	-5.200425000	0.633960000	-1.216629000
1	-5.955565000	0.065041000	-1.768531000
1	-5.519769000	0.661814000	-0.174261000
1	-5.241221000	1.657335000	-1.597102000
6	-3.472212000	0.007355000	-2.915973000
1	-3.367120000	1.024703000	-3.306522000
1	-2.534943000	-0.517653000	-3.111223000
1	-4.260020000	-0.480187000	-3.498561000
15	0.339064000	-2.174181000	-0.648175000
15	-2.405956000	0.664990000	-0.420479000
15	2.156690000	1.387929000	-0.519270000
6	-2.602569000	2.508584000	-0.173660000
1	-1.614042000	2.787043000	0.224110000
6	-2.790192000	3.235049000	-1.501752000
1	-3.792336000	3.090009000	-1.912786000
1	-2.658199000	4.312908000	-1.364291000
1	-2.074138000	2.917218000	-2.265422000
6	-3.639375000	2.909648000	0.865828000
1	-3.575862000	3.985862000	1.057891000
1	-4.660434000	2.702734000	0.535421000
1	-3.486444000	2.398687000	1.820078000
6	3.976288000	1.005750000	-0.342565000
1	4.227359000	0.609189000	-1.337156000
6	4.276202000	-0.065234000	0.690149000
1	4.083150000	0.296855000	1.703003000
1	3.691237000	-0.975300000	0.545933000
1	5.335146000	-0.338228000	0.640879000

6	4.816786000	2.248709000	-0.075906000
1	5.875232000	1.972720000	-0.035114000
1	4.719354000	3.020786000	-0.842062000
1	4.570939000	2.695739000	0.892446000
6	-1.205457000	-3.177349000	-0.377184000
1	-1.844099000	-2.477322000	0.179721000
6	-1.026603000	-4.415167000	0.491214000
1	-1.999447000	-4.881888000	0.677561000
1	-0.390946000	-5.172945000	0.026354000
1	-0.592880000	-4.169568000	1.464137000
6	-1.882542000	-3.464728000	-1.712975000
1	-2.885165000	-3.873759000	-1.553565000
1	-1.992768000	-2.560531000	-2.322691000
1	-1.332557000	-4.196423000	-2.311596000
7	0.228718000	-0.321208000	-4.009768000
7	0.039508000	-0.049125000	-2.834252000
1	-0.660729000	-0.498815000	-4.526687000

[3b''_{psi}]-Triplet (TE = -3771.188296)

6	0.733165000	-2.358887000	1.102098000
6	0.423900000	-3.479064000	1.884476000
1	-0.445819000	-3.450860000	2.541754000
6	1.189855000	-4.637863000	1.825005000
1	0.928262000	-5.498278000	2.436907000
6	2.290855000	-4.695283000	0.975999000
1	2.893953000	-5.598377000	0.920906000
6	2.616760000	-3.598123000	0.186608000
1	3.475769000	-3.668008000	-0.474971000
6	1.843472000	-2.433267000	0.233321000
6	0.505443000	0.397299000	2.398297000
6	0.866444000	-0.041214000	3.678782000
1	0.718895000	-1.086830000	3.952010000
6	1.446798000	0.820006000	4.602200000
1	1.729148000	0.455998000	5.587570000
6	1.676527000	2.149183000	4.257596000
1	2.133848000	2.829144000	4.972367000
6	1.331645000	2.607106000	2.991685000
1	1.535024000	3.643453000	2.736436000
6	0.752149000	1.740396000	2.058173000
6	-2.061328000	-1.016507000	1.626754000
6	-2.473268000	-1.284654000	2.937097000
1	-1.729113000	-1.472629000	3.710884000
6	-3.818481000	-1.266951000	3.290091000
1	-4.116635000	-1.465905000	4.316980000
6	-4.780151000	-0.959249000	2.333096000
1	-5.830790000	-0.912284000	2.609188000

6	-4.400513000	-0.698838000	1.020806000
1	-5.167129000	-0.436945000	0.297562000
6	-3.050537000	-0.743678000	0.659917000
23	-0.013155000	0.328325000	-1.198372000
6	3.841071000	-0.351388000	-0.044370000
1	4.519416000	-1.202177000	-0.197012000
6	-1.199556000	3.340384000	0.604486000
1	-0.857229000	4.201224000	1.194073000
6	-2.189555000	-2.048189000	-1.887687000
1	-2.950822000	-2.095655000	-2.674695000
6	-2.344259000	-3.252309000	-0.975105000
1	-2.205930000	-4.176823000	-1.545302000
1	-1.599686000	-3.253135000	-0.172066000
1	-3.330065000	-3.293930000	-0.505054000
6	-0.816409000	-2.013144000	-2.546326000
1	-0.027796000	-1.927696000	-1.774893000
1	-0.574141000	-2.940587000	-3.076286000
1	-0.721562000	-1.200181000	-3.275924000
6	4.392815000	0.861659000	-0.778593000
1	4.421021000	0.745126000	-1.865233000
1	3.798039000	1.752166000	-0.561986000
1	5.415267000	1.071821000	-0.448970000
6	3.750524000	-0.090759000	1.450104000
1	3.312703000	-0.926597000	2.002403000
1	4.754268000	0.079301000	1.852872000
1	3.160263000	0.801382000	1.673055000
6	-1.725191000	3.819724000	-0.741312000
1	-2.566709000	4.506685000	-0.606513000
1	-0.973128000	4.339716000	-1.342383000
1	-2.084377000	2.974348000	-1.338323000
6	-2.282376000	2.623256000	1.393333000
1	-2.698958000	1.784703000	0.830579000
1	-1.927838000	2.230875000	2.350907000
1	-3.109598000	3.308917000	1.602855000
14	-0.260853000	-0.747794000	1.095961000
15	0.319933000	2.285073000	0.360041000
15	-2.425797000	-0.388598000	-1.024202000
15	2.242051000	-0.958455000	-0.801309000
6	2.811679000	-1.697144000	-2.450677000
1	2.201141000	-2.608082000	-2.533233000
6	4.280502000	-2.101442000	-2.546582000
1	4.447657000	-2.628825000	-3.490986000
1	4.947006000	-1.234840000	-2.550548000
1	4.618260000	-2.766205000	-1.750366000
6	2.460527000	-0.779518000	-3.618010000
1	1.386724000	-0.610209000	-3.713880000

1	2.933878000	0.204592000	-3.523194000
1	2.807984000	-1.214168000	-4.560648000
6	-3.845298000	0.385242000	-1.956162000
1	-4.230806000	1.148268000	-1.263307000
6	-3.339147000	1.073817000	-3.217345000
1	-2.857698000	0.359744000	-3.896380000
1	-4.173929000	1.518348000	-3.768267000
1	-2.610871000	1.860414000	-3.017954000
6	-4.970239000	-0.590028000	-2.312696000
1	-4.736024000	-1.140190000	-3.228611000
1	-5.191421000	-1.331816000	-1.542453000
1	-5.894614000	-0.039483000	-2.512447000
6	1.671418000	3.531415000	-0.071770000
1	2.535777000	3.140658000	0.486188000
6	1.418797000	4.966174000	0.384284000
1	2.311184000	5.570905000	0.194354000
1	0.600569000	5.430642000	-0.173616000
1	1.185136000	5.067200000	1.445414000
6	2.020760000	3.532926000	-1.555929000
1	2.220412000	2.531700000	-1.945766000
1	1.213580000	3.967719000	-2.154565000
1	2.911757000	4.145248000	-1.729621000
7	-0.114181000	2.028342000	-3.721471000
7	0.025811000	1.376537000	-2.701705000
1	0.802879000	2.347492000	-4.109587000

[3c''_{PB}]-Quartet (TE = -3506.526313)

6	-1.641465000	1.080864000	1.694473000
6	-1.814372000	2.039095000	2.708100000
1	-0.933917000	2.457902000	3.193366000
6	-3.072284000	2.455871000	3.129290000
1	-3.161439000	3.193564000	3.923671000
6	-4.213856000	1.927396000	2.537140000
1	-5.202328000	2.240682000	2.864041000
6	-4.079823000	1.010139000	1.500559000
1	-4.975693000	0.628670000	1.014141000
6	-2.818079000	0.593629000	1.069035000
6	0.047307000	-1.034047000	1.789202000
6	-0.730893000	-1.439575000	2.902489000
1	-1.543629000	-0.798702000	3.234733000
6	-0.460995000	-2.586057000	3.632108000
1	-1.062579000	-2.823261000	4.506438000
6	0.577149000	-3.426859000	3.244637000
1	0.801582000	-4.327458000	3.811004000
6	1.320946000	-3.108150000	2.118764000

1	2.115371000	-3.780262000	1.802832000
6	1.085712000	-1.933849000	1.392026000
6	1.049812000	1.498020000	1.655577000
6	1.596895000	1.685823000	2.934197000
1	1.206480000	1.107434000	3.772549000
6	2.637930000	2.579981000	3.153756000
1	3.049147000	2.700505000	4.153650000
6	3.161948000	3.315356000	2.093315000
1	3.978281000	4.013841000	2.260048000
6	2.644227000	3.143499000	0.815933000
1	3.068248000	3.708689000	-0.010686000
6	1.597495000	2.241253000	0.594993000
23	-0.120144000	-0.470008000	-0.828072000
6	-3.456632000	-2.040828000	-0.251610000
1	-4.523231000	-1.825465000	-0.099774000
6	3.779936000	-1.386210000	0.276036000
1	4.074600000	-2.354585000	0.705270000
6	-0.091416000	3.343741000	-1.565248000
1	-0.140932000	3.266715000	-2.662722000
6	0.494641000	4.693846000	-1.169264000
1	-0.162651000	5.493031000	-1.527435000
1	0.549054000	4.790411000	-0.080850000
1	1.487074000	4.891684000	-1.570676000
6	-1.499351000	3.231814000	-1.001112000
1	-1.505331000	3.364719000	0.085429000
1	-2.150546000	4.001443000	-1.427904000
1	-1.943232000	2.260700000	-1.209851000
6	-3.281707000	-2.860014000	-1.526662000
1	-3.615058000	-2.343597000	-2.429977000
1	-2.232746000	-3.127863000	-1.683115000
1	-3.850273000	-3.792647000	-1.458563000
6	-2.941818000	-2.808405000	0.953092000
1	-3.086646000	-2.263086000	1.888727000
1	-3.470310000	-3.763126000	1.041505000
1	-1.873681000	-3.038272000	0.861993000
6	4.616143000	-1.126300000	-0.972051000
1	5.682032000	-1.202183000	-0.736555000
1	4.414170000	-1.824151000	-1.789529000
1	4.447206000	-0.118026000	-1.359784000
6	3.991605000	-0.317328000	1.332382000
1	3.737642000	0.679701000	0.963113000
1	3.399569000	-0.498013000	2.233101000
1	5.045172000	-0.293595000	1.629083000
5	-0.176249000	0.519065000	1.447444000
7	-0.409970000	-1.831418000	-3.537740000
7	-0.295673000	-1.237776000	-2.479129000

1	-0.366082000	-1.185278000	-4.359566000
15	0.915478000	1.851276000	-1.049663000
15	-2.627450000	-0.386407000	-0.461998000
15	1.989515000	-1.646306000	-0.171599000
6	2.399007000	1.787770000	-2.203934000
1	3.190245000	1.404563000	-1.544225000
6	2.871997000	3.108803000	-2.798117000
1	3.726999000	2.922874000	-3.456002000
1	2.101554000	3.585538000	-3.411867000
1	3.201888000	3.832407000	-2.052033000
6	2.170441000	0.775070000	-3.321096000
1	2.016834000	-0.236438000	-2.939376000
1	1.296663000	1.034522000	-3.931440000
1	3.034607000	0.750093000	-3.992840000
6	2.015376000	-3.298090000	-1.083205000
1	2.101717000	-2.968856000	-2.129950000
6	0.692374000	-4.046893000	-0.947610000
1	-0.180253000	-3.399166000	-1.059347000
1	0.621094000	-4.819246000	-1.719036000
1	0.609468000	-4.545041000	0.022489000
6	3.178994000	-4.240174000	-0.791738000
1	3.093389000	-5.123239000	-1.433087000
1	4.160980000	-3.805419000	-0.984619000
1	3.175870000	-4.606920000	0.238986000
6	-3.727006000	0.499938000	-1.716273000
1	-3.763533000	1.524240000	-1.326549000
6	-5.166445000	0.005152000	-1.804322000
1	-5.731149000	0.659882000	-2.475681000
1	-5.243450000	-1.005168000	-2.213516000
1	-5.687892000	0.013087000	-0.844586000
6	-3.077301000	0.534056000	-3.096017000
1	-2.057542000	0.933739000	-3.067816000
1	-3.022605000	-0.462494000	-3.545614000
1	-3.662901000	1.161147000	-3.775947000

[3d''_{sc}]-Triplet (TE = -3334.916108)

6	-0.338962000	1.952622000	0.363712000
6	0.249051000	3.087508000	0.941869000
1	1.126006000	2.967025000	1.572790000
6	-0.275157000	4.362891000	0.756971000
1	0.207632000	5.213031000	1.233247000
6	-1.412427000	4.555409000	-0.019569000
1	-1.828033000	5.549428000	-0.160011000
6	-1.985973000	3.463242000	-0.658907000
1	-2.831637000	3.602046000	-1.328954000
6	-1.450779000	2.189867000	-0.476760000

6	-0.875951000	-0.136558000	1.558067000
6	-1.482169000	0.564940000	2.612566000
1	-1.287730000	1.631542000	2.712340000
6	-2.321249000	-0.056084000	3.528051000
1	-2.763035000	0.525245000	4.333907000
6	-2.604106000	-1.414410000	3.413322000
1	-3.265020000	-1.905453000	4.122496000
6	-2.065742000	-2.130535000	2.353654000
1	-2.322113000	-3.178003000	2.210127000
6	-1.216705000	-1.494250000	1.445800000
6	1.513979000	0.488289000	1.243944000
6	1.727458000	0.750766000	2.606456000
1	0.870527000	0.958135000	3.242024000
6	2.994360000	0.756807000	3.174991000
1	3.105134000	0.964424000	4.236666000
6	4.116264000	0.494365000	2.395114000
1	5.110717000	0.491399000	2.832981000
6	3.945771000	0.197301000	1.051932000
1	4.800571000	-0.068215000	0.434695000
6	2.664888000	0.196350000	0.492805000
16	2.515708000	-0.466038000	-1.166234000
16	-1.989850000	0.863837000	-1.546159000
16	-0.709065000	-2.397332000	-0.005824000
23	0.060579000	-0.508959000	-1.355234000
6	-3.745535000	0.352243000	-1.105834000
1	-4.341374000	1.072692000	-1.677843000
6	0.584190000	-3.618054000	0.584892000
1	-0.026969000	-4.367070000	1.103012000
6	2.765005000	0.977468000	-2.345394000
1	3.077034000	0.448732000	-3.253164000
6	3.862588000	1.896571000	-1.867088000
1	4.035859000	2.677465000	-2.613687000
1	3.590944000	2.393291000	-0.930711000
1	4.807207000	1.370958000	-1.712290000
6	1.453513000	1.697972000	-2.586799000
1	1.090862000	2.202260000	-1.687256000
1	1.566330000	2.468945000	-3.356281000
1	0.669266000	1.032642000	-2.990262000
6	-3.933863000	-1.038668000	-1.674507000
1	-3.670111000	-1.101023000	-2.733482000
1	-3.333947000	-1.776070000	-1.131679000
1	-4.983482000	-1.331938000	-1.578443000
6	-4.065055000	0.463373000	0.363017000
1	-3.788962000	1.434058000	0.783009000
1	-5.145813000	0.346073000	0.495925000
1	-3.574394000	-0.317093000	0.946965000

6	1.201616000	-4.225588000	-0.658183000
1	1.867635000	-5.046053000	-0.376803000
1	0.451461000	-4.629657000	-1.343509000
1	1.802913000	-3.489566000	-1.202480000
6	1.592954000	-3.021679000	1.535172000
1	2.266964000	-2.327282000	1.028906000
1	1.125001000	-2.493820000	2.370220000
1	2.207666000	-3.823477000	1.957125000
6	0.123674000	0.534275000	0.621494000
7	-0.610316000	-2.185400000	-3.809743000
7	-0.206507000	-1.510676000	-2.889983000
1	0.151987000	-2.679451000	-4.324658000

[3e''_{ssi}]-Triplet (TE = -3586.318558)

6	0.823448000	0.771567000	2.073361000
6	1.712314000	1.502426000	2.869627000
1	2.131385000	2.431957000	2.483840000
6	2.089725000	1.056466000	4.131618000
1	2.785625000	1.636995000	4.731950000
6	1.580304000	-0.142069000	4.619075000
1	1.874955000	-0.504218000	5.600847000
6	0.692747000	-0.894711000	3.855529000
1	0.306305000	-1.826538000	4.257210000
6	0.332678000	-0.436579000	2.591472000
6	1.961383000	1.767469000	-0.518806000
6	2.402424000	3.081306000	-0.715841000
1	1.747619000	3.910046000	-0.448462000
6	3.655477000	3.349105000	-1.256629000
1	3.974398000	4.376667000	-1.412603000
6	4.506166000	2.298871000	-1.587100000
1	5.493572000	2.500281000	-1.994659000
6	4.102000000	0.981244000	-1.395884000
1	4.782307000	0.170451000	-1.643079000
6	2.827571000	0.728789000	-0.896211000
6	-1.059942000	2.426811000	0.149727000
6	-1.115797000	3.696277000	0.741221000
1	-0.300460000	4.021173000	1.387275000
6	-2.196690000	4.545037000	0.534434000
1	-2.222209000	5.522060000	1.010416000
6	-3.243482000	4.145039000	-0.291479000
1	-4.084629000	4.809919000	-0.470720000
6	-3.216110000	2.896673000	-0.901368000
1	-4.024343000	2.598963000	-1.563948000
6	-2.141968000	2.041761000	-0.656346000
16	-2.095501000	0.429286000	-1.467793000
16	-0.884219000	-1.288937000	1.564354000

16	2.281942000	-0.985210000	-0.631876000
23	-0.225760000	-1.000359000	-0.794387000
6	-0.845078000	-3.055399000	2.139266000
1	-0.921777000	-2.978966000	3.228879000
6	2.811602000	-1.802332000	-2.227559000
1	3.877987000	-1.568125000	-2.305003000
6	-3.722079000	-0.428145000	-1.032512000
1	-3.384545000	-1.471553000	-1.035983000
6	-4.743911000	-0.220301000	-2.130387000
1	-5.617557000	-0.850679000	-1.935479000
1	-5.099037000	0.812817000	-2.173644000
1	-4.356071000	-0.487294000	-3.115259000
6	-4.220244000	-0.051455000	0.343680000
1	-4.566568000	0.984088000	0.387083000
1	-5.075632000	-0.686879000	0.595093000
1	-3.461505000	-0.189640000	1.116344000
6	-2.099748000	-3.724864000	1.612215000
1	-3.006393000	-3.218490000	1.952452000
1	-2.122413000	-3.760840000	0.520864000
1	-2.141735000	-4.757033000	1.971394000
6	0.442145000	-3.744306000	1.742487000
1	1.325617000	-3.216537000	2.112410000
1	0.466908000	-4.759855000	2.150616000
1	0.528156000	-3.823112000	0.653309000
6	2.634856000	-3.296436000	-2.059399000
1	2.971203000	-3.811770000	-2.963478000
1	3.208787000	-3.689357000	-1.217027000
1	1.583184000	-3.556201000	-1.904049000
6	2.059475000	-1.228902000	-3.409977000
1	0.999079000	-1.514816000	-3.385336000
1	2.128909000	-0.138980000	-3.459633000
1	2.462500000	-1.626146000	-4.347013000
14	0.361188000	1.205748000	0.294261000
7	-1.478326000	-3.520420000	-1.954546000
7	-0.844425000	-2.612346000	-1.448433000
1	-0.879652000	-4.343501000	-2.192761000

[3f'_{SB}]-Quartet (TE = -3321.670568)

6	-0.371067000	2.065468000	0.434447000
6	0.157203000	3.204528000	1.068455000
1	0.989717000	3.082887000	1.760146000
6	-0.369440000	4.475227000	0.864621000
1	0.055637000	5.327289000	1.390012000
6	-1.434076000	4.660966000	-0.012604000
1	-1.844964000	5.652996000	-0.180990000
6	-1.944282000	3.571671000	-0.708427000

1	-2.733986000	3.710050000	-1.443895000
6	-1.419128000	2.301662000	-0.476606000
6	-0.945931000	-0.224605000	1.693251000
6	-1.524086000	0.376785000	2.825510000
1	-1.287311000	1.417883000	3.046693000
6	-2.393727000	-0.308002000	3.665482000
1	-2.813441000	0.192847000	4.534817000
6	-2.743321000	-1.626742000	3.386347000
1	-3.433941000	-2.163912000	4.031101000
6	-2.229009000	-2.243607000	2.253790000
1	-2.531521000	-3.255869000	1.992869000
6	-1.337992000	-1.545145000	1.436801000
6	1.640197000	0.468467000	1.339422000
6	1.920842000	0.766835000	2.685654000
1	1.095910000	1.027770000	3.347945000
6	3.208564000	0.735358000	3.205849000
1	3.374035000	0.975946000	4.253464000
6	4.281664000	0.378582000	2.394670000
1	5.290974000	0.337175000	2.795418000
6	4.046116000	0.040008000	1.070525000
1	4.863754000	-0.292130000	0.435179000
6	2.746539000	0.101229000	0.559067000
16	2.518881000	-0.551929000	-1.103210000
16	-1.927732000	0.959634000	-1.544998000
16	-0.815958000	-2.334111000	-0.081634000
23	0.074182000	-0.497236000	-1.437282000
6	-3.708161000	0.515018000	-1.135080000
1	-4.263725000	1.284150000	-1.684444000
6	0.413224000	-3.636846000	0.467352000
1	-0.238826000	-4.375795000	0.948832000
6	2.874563000	0.869452000	-2.274628000
1	3.004159000	0.326281000	-3.218083000
6	4.147541000	1.591749000	-1.904131000
1	4.361721000	2.360074000	-2.653136000
1	4.058681000	2.094571000	-0.936884000
1	5.007858000	0.920273000	-1.863347000
6	1.675194000	1.791093000	-2.363718000
1	1.454093000	2.274522000	-1.408702000
1	1.845894000	2.585051000	-3.098599000
1	0.766518000	1.279322000	-2.734773000
6	-3.961999000	-0.845009000	-1.749639000
1	-3.712101000	-0.880927000	-2.812862000
1	-3.390015000	-1.626847000	-1.240115000
1	-5.022292000	-1.095606000	-1.651281000
6	-4.028127000	0.594336000	0.336696000
1	-3.717199000	1.541201000	0.785460000

1	-5.113128000	0.514799000	0.462211000
1	-3.569729000	-0.220177000	0.899979000
6	1.023278000	-4.226635000	-0.787531000
1	1.639600000	-5.091124000	-0.525265000
1	0.268081000	-4.563762000	-1.502554000
1	1.675982000	-3.505519000	-1.290980000
6	1.432040000	-3.121276000	1.454442000
1	2.132961000	-2.424667000	0.989054000
1	0.973486000	-2.619477000	2.310301000
1	2.017162000	-3.962204000	1.840684000
5	0.123566000	0.615428000	0.861652000
7	-0.738028000	-2.009185000	-3.941644000
7	-0.236392000	-1.379633000	-3.038891000
1	-0.049873000	-2.306969000	-4.667917000

{[HIPTN₃N]-V-N=NH}⁺ (TE = -2203.381994)

23	-0.007754000	-0.750704000	-0.339660000
6	1.399555000	-3.079468000	1.108205000
6	1.925046000	-2.967528000	-0.306946000
6	-0.800205000	-0.503942000	2.371273000
6	-0.304260000	-1.936217000	2.481107000
6	-0.961536000	-3.431161000	0.621416000
6	-2.191141000	-2.648780000	0.253250000
1	-2.760637000	-2.368687000	1.151654000
1	-2.874102000	-3.244556000	-0.365240000
1	-0.545224000	-3.909071000	-0.271157000
1	-1.172875000	-4.222396000	1.352798000
1	-0.677116000	-0.001653000	3.339265000
1	-1.878371000	-0.475800000	2.148853000
1	0.599295000	-1.958758000	3.093619000
1	-1.038311000	-2.582182000	2.976606000
1	2.032390000	-2.492164000	1.778775000
1	1.390800000	-4.114207000	1.477737000
1	1.438610000	-3.688164000	-0.974940000
1	2.997132000	-3.184155000	-0.349438000
7	-1.755779000	-1.461567000	-0.475290000
7	0.046533000	-2.481081000	1.138091000
7	-0.035605000	0.184029000	1.334616000
7	1.636253000	-1.615642000	-0.782928000
6	-2.770204000	-0.542530000	-0.826792000
6	-2.789655000	-0.009862000	-2.124267000
6	-3.758537000	-0.135875000	0.088326000
6	-3.744548000	0.925778000	-2.488364000
1	-2.041278000	-0.345876000	-2.836963000
6	-4.706964000	0.804964000	-0.281423000
1	-3.776343000	-0.545121000	1.094910000

6	-4.702661000	1.342812000	-1.567495000
1	-3.746086000	1.326525000	-3.498570000
1	-5.455389000	1.123595000	0.439652000
1	-5.450635000	2.078029000	-1.852080000
6	0.104647000	1.572718000	1.459931000
6	-0.872063000	2.380119000	2.062317000
6	1.248683000	2.188558000	0.927503000
6	-0.717075000	3.761770000	2.095834000
1	-1.770421000	1.928042000	2.476390000
6	1.391133000	3.568949000	0.955815000
1	2.025961000	1.561040000	0.494641000
6	0.406237000	4.365800000	1.539149000
1	-1.490437000	4.372972000	2.555143000
1	2.287736000	4.023052000	0.538445000
1	0.520755000	5.445833000	1.570207000
6	2.713699000	-0.727253000	-0.917868000
6	3.768791000	-0.672043000	0.014255000
6	2.718479000	0.167556000	-2.000084000
6	4.756519000	0.289176000	-0.111456000
1	3.788368000	-1.359981000	0.856115000
6	3.708791000	1.132753000	-2.115132000
1	1.946552000	0.068528000	-2.757523000
6	4.725129000	1.204009000	-1.167516000
1	5.553803000	0.338792000	0.625662000
1	3.699260000	1.816228000	-2.960437000
1	5.504336000	1.956241000	-1.256724000
7	-0.164076000	1.848223000	-1.887161000
7	-0.061133000	0.779651000	-1.355474000
1	0.120072000	2.642972000	-1.264415000

Cartesian coordinates of $[4a'_{PC}]-[4f'_{SB}]$, $[4a''_{PC}]-[4f''_{SB}]$ and $[[HIPTN_3N]-V-N=NH]$ along with their total energies (in hartree) including zero point vibrational correction at M06-L-D3(heptane)/6-311+G* level of theory.

$[4a'_{PC}]$ (TE = -3062.653876)

6	-0.588905000	2.266166000	1.951018000
6	0.196758000	1.175238000	2.677953000
6	-2.410077000	-0.691080000	2.044770000
6	-1.046044000	-1.018543000	2.643048000
6	2.679760000	-0.586078000	1.809572000
6	1.405463000	-0.979913000	2.546432000
1	-2.694416000	0.350010000	2.238012000
1	-1.102760000	-0.899928000	3.744916000
1	3.567985000	-1.094111000	2.202815000
1	1.562363000	-0.844486000	3.636573000

1	-0.462083000	3.250776000	2.419103000
1	1.244192000	1.512748000	2.722525000
6	-1.118599000	3.457461000	-0.748024000
1	-0.502000000	4.359124000	-0.871777000
6	-2.605109000	-2.746929000	0.020941000
1	-1.912440000	-3.160748000	0.771602000
6	3.815326000	-0.021524000	-0.820374000
1	3.684479000	1.023694000	-0.501333000
23	0.031889000	-0.200887000	-0.323866000
6	0.146461000	-0.242139000	2.061383000
1	-1.664261000	2.059218000	1.964002000
1	-0.126353000	1.149966000	3.737661000
1	1.258457000	-2.063600000	2.416712000
1	2.874596000	0.491112000	1.908953000
1	-0.867117000	-2.094562000	2.487343000
1	-3.209417000	-1.308297000	2.476547000
6	5.200290000	-0.483862000	-0.389486000
1	5.977555000	0.139579000	-0.846344000
1	5.342644000	-0.437035000	0.694566000
1	5.398819000	-1.513547000	-0.706403000
6	3.647970000	-0.080605000	-2.333495000
1	3.765506000	-1.103133000	-2.712133000
1	2.662339000	0.266484000	-2.655400000
1	4.404969000	0.530808000	-2.837217000
6	-4.009316000	-3.230752000	0.354274000
1	-4.035126000	-4.325234000	0.409508000
1	-4.378257000	-2.850835000	1.311588000
1	-4.728527000	-2.939731000	-0.418063000
6	-2.149833000	-3.253696000	-1.342313000
1	-2.800896000	-2.901547000	-2.148858000
1	-1.134880000	-2.918091000	-1.568128000
1	-2.162624000	-4.349109000	-1.374128000
6	-1.438617000	2.908140000	-2.134507000
1	-0.538914000	2.630568000	-2.691771000
1	-2.051155000	2.001814000	-2.071769000
1	-1.991163000	3.643485000	-2.730677000
6	-2.380136000	3.863730000	0.000309000
1	-2.162646000	4.345382000	0.957946000
1	-2.970420000	4.568027000	-0.596371000
1	-3.030279000	3.006132000	0.208409000
6	2.829404000	-2.715163000	-0.260148000
1	3.452915000	-2.707176000	-1.166814000
6	1.576183000	-3.524292000	-0.568903000
1	0.862572000	-3.496875000	0.264781000
1	1.050196000	-3.131055000	-1.442795000
1	1.823582000	-4.574880000	-0.762088000

6	3.632420000	-3.357866000	0.862740000
1	3.897982000	-4.388414000	0.600651000
1	4.563591000	-2.828644000	1.080733000
1	3.057524000	-3.405602000	1.793788000
6	-3.739696000	0.023857000	-0.469823000
1	-3.363080000	1.056036000	-0.403624000
6	-5.045256000	-0.029112000	0.314270000
1	-5.542277000	-0.998441000	0.235797000
1	-4.905687000	0.183179000	1.378064000
1	-5.747550000	0.718618000	-0.072796000
6	-3.946113000	-0.286642000	-1.947167000
1	-4.398871000	-1.273567000	-2.090426000
1	-4.621721000	0.441500000	-2.409629000
1	-3.006457000	-0.269328000	-2.509666000
6	1.602282000	3.086204000	0.210128000
1	2.258389000	2.369786000	0.727554000
6	1.636334000	4.404728000	0.967906000
1	2.626318000	4.869497000	0.896261000
1	0.918911000	5.129467000	0.565611000
1	1.416084000	4.281453000	2.031634000
6	2.103428000	3.240440000	-1.221226000
1	3.149570000	3.565804000	-1.242053000
1	2.032724000	2.303483000	-1.783860000
1	1.527403000	3.993995000	-1.770329000
15	-2.281663000	-0.915247000	0.222468000
15	-0.058496000	2.225489000	0.191154000
15	2.401413000	-0.898533000	0.018141000
7	0.026460000	-0.757970000	-3.350012000
7	0.022915000	-0.561216000	-2.126329000
1	-0.234437000	-1.751328000	-3.568007000

[4b'_{psi}] (TE = -3314.088377)

6	-0.125228000	2.716802000	1.793554000
6	0.298079000	1.673782000	2.827893000
6	-2.703533000	-0.019778000	2.019304000
6	-1.613159000	-0.703364000	2.841284000
6	2.569530000	-1.449995000	1.815708000
6	1.474512000	-1.219101000	2.860839000
1	-2.686389000	1.065274000	2.193736000
1	-1.742645000	-0.488698000	3.911370000
1	3.192960000	-2.328421000	2.036659000
1	1.913262000	-0.794363000	3.773677000
1	0.127782000	3.748824000	2.075007000
1	1.357700000	1.819978000	3.083877000
6	0.181449000	3.675024000	-0.986518000
1	0.906063000	4.481464000	-0.795686000

6	-2.869884000	-2.042740000	-0.074938000
1	-1.951383000	-2.579312000	0.207519000
6	3.502302000	-1.270490000	-0.883585000
1	3.851946000	-0.324441000	-0.440057000
23	0.015775000	-0.061467000	-0.462984000
1	-1.213450000	2.695640000	1.650755000
1	-0.253688000	1.822031000	3.766942000
1	1.035101000	-2.175387000	3.166603000
1	3.258858000	-0.593752000	1.803175000
1	-1.696489000	-1.795766000	2.738281000
1	-3.719951000	-0.348110000	2.272475000
6	4.587042000	-2.317750000	-0.670718000
1	5.537230000	-1.983309000	-1.102755000
1	4.771171000	-2.533590000	0.385779000
1	4.337328000	-3.263468000	-1.163150000
6	3.263170000	-1.018503000	-2.366463000
1	2.984055000	-1.935869000	-2.895355000
1	2.460787000	-0.292506000	-2.529134000
1	4.172208000	-0.639746000	-2.847863000
6	-4.000366000	-2.582022000	0.791714000
1	-4.168888000	-3.641593000	0.566305000
1	-3.780175000	-2.516356000	1.860720000
1	-4.948470000	-2.066183000	0.617418000
6	-3.110419000	-2.314506000	-1.555353000
1	-4.061199000	-1.889125000	-1.893908000
1	-2.317918000	-1.909728000	-2.190810000
1	-3.166000000	-3.393333000	-1.740328000
6	0.300030000	3.231074000	-2.442058000
1	1.272583000	2.793683000	-2.682559000
1	-0.451315000	2.469572000	-2.677302000
1	0.138422000	4.075932000	-3.121060000
6	-1.219976000	4.208461000	-0.718883000
1	-1.327548000	4.644893000	0.277424000
1	-1.482397000	4.984011000	-1.446888000
1	-1.970574000	3.414721000	-0.818719000
6	1.569765000	-3.385192000	-0.130868000
1	2.545933000	-3.890408000	-0.121594000
6	0.871408000	-3.663052000	-1.455062000
1	-0.113654000	-3.184098000	-1.486704000
1	1.427894000	-3.291901000	-2.319824000
1	0.724182000	-4.739948000	-1.595407000
6	0.746741000	-3.932986000	1.028189000
1	0.442661000	-4.966175000	0.826306000
1	1.298604000	-3.935904000	1.971174000
1	-0.169596000	-3.349951000	1.183446000
6	-3.631321000	0.866337000	-0.560091000

1	-3.416091000	1.808810000	-0.028135000
6	-5.089691000	0.511344000	-0.301617000
1	-5.388092000	-0.389604000	-0.846546000
1	-5.307529000	0.345999000	0.757447000
1	-5.747671000	1.317952000	-0.645647000
6	-3.367805000	1.107123000	-2.041089000
1	-3.599755000	0.228537000	-2.649079000
1	-3.985189000	1.932498000	-2.414182000
1	-2.319716000	1.354274000	-2.231845000
6	2.439715000	2.526715000	0.488712000
1	2.719391000	1.640024000	1.078877000
6	2.766744000	3.772149000	1.300444000
1	3.850753000	3.878844000	1.422304000
1	2.414484000	4.686092000	0.808490000
1	2.331502000	3.749986000	2.302667000
6	3.238907000	2.500571000	-0.807777000
1	4.313910000	2.445521000	-0.602297000
1	2.978612000	1.647247000	-1.441456000
1	3.076550000	3.410926000	-1.395367000
15	-2.354146000	-0.259738000	0.215904000
15	0.609856000	2.255565000	0.161824000
15	1.909877000	-1.551988000	0.075989000
14	0.075960000	-0.123883000	2.139630000
7	-0.348349000	-0.821538000	-3.403820000
7	-0.129899000	-0.498215000	-2.221782000
1	0.513453000	-0.712344000	-3.983225000

[4c'_{pb}] (TE = -3049.421541)

6	-0.556859000	2.283630000	2.038348000
6	0.287562000	1.313184000	2.862976000
6	-2.324896000	-0.771405000	2.091570000
6	-1.026143000	-1.141342000	2.800651000
6	2.775903000	-0.550279000	1.740573000
6	1.677446000	-0.997321000	2.701910000
1	-2.588565000	0.276666000	2.277079000
1	-1.211600000	-1.113712000	3.890892000
1	3.752481000	-0.990990000	1.978907000
1	2.032226000	-0.813303000	3.732485000
1	-0.499595000	3.311720000	2.421127000
1	1.324906000	1.685095000	2.869722000
6	-1.120152000	3.503537000	-0.595750000
1	-0.517618000	4.423104000	-0.621474000
6	-2.434976000	-2.787686000	0.007307000
1	-1.652405000	-3.212846000	0.656210000
6	3.671247000	-0.127787000	-0.982007000
1	3.615616000	0.926107000	-0.666845000

23	0.012538000	-0.116035000	-0.640569000
1	-1.617389000	2.012149000	2.073055000
1	-0.031889000	1.405253000	3.917221000
1	1.563389000	-2.089334000	2.639290000
1	2.914501000	0.538637000	1.793019000
1	-0.802041000	-2.200437000	2.597191000
1	-3.181052000	-1.357863000	2.451249000
6	5.072930000	-0.641408000	-0.683651000
1	5.822061000	-0.036208000	-1.206999000
1	5.322061000	-0.612384000	0.380995000
1	5.205700000	-1.671738000	-1.030378000
6	3.375083000	-0.187960000	-2.474828000
1	3.367388000	-1.221354000	-2.842841000
1	2.398965000	0.244520000	-2.709752000
1	4.139313000	0.348670000	-3.048146000
6	-3.780803000	-3.332006000	0.467582000
1	-3.770334000	-4.428100000	0.464681000
1	-4.056316000	-3.016591000	1.477934000
1	-4.586338000	-3.026452000	-0.207682000
6	-2.135764000	-3.231024000	-1.422262000
1	-2.964621000	-3.003767000	-2.097959000
1	-1.249618000	-2.743649000	-1.835186000
1	-1.978848000	-4.314817000	-1.463044000
6	-1.402109000	3.077788000	-2.032881000
1	-0.487150000	2.859994000	-2.592071000
1	-2.007248000	2.164644000	-2.067774000
1	-1.946613000	3.860648000	-2.573201000
6	-2.411236000	3.822525000	0.146028000
1	-2.234989000	4.247279000	1.137727000
1	-3.006192000	4.548053000	-0.419661000
1	-3.041811000	2.935886000	0.278698000
6	2.624121000	-2.763875000	-0.189527000
1	3.041128000	-2.850172000	-1.205138000
6	1.323093000	-3.555992000	-0.152137000
1	0.820998000	-3.452599000	0.817990000
1	0.618152000	-3.214078000	-0.913122000
1	1.508996000	-4.624349000	-0.313522000
6	3.628025000	-3.348504000	0.797354000
1	3.834096000	-4.396490000	0.551300000
1	4.585884000	-2.824961000	0.808906000
1	3.236843000	-3.335655000	1.819895000
6	-3.611820000	-0.021620000	-0.409655000
1	-3.236056000	1.011430000	-0.356970000
6	-4.898952000	-0.078310000	0.404097000
1	-5.353206000	-1.072232000	0.400830000
1	-4.753282000	0.211875000	1.448167000

1	-5.640342000	0.609952000	-0.018780000
6	-3.854902000	-0.335262000	-1.880642000
1	-4.345667000	-1.306132000	-2.005333000
1	-4.518689000	0.412396000	-2.329353000
1	-2.928436000	-0.352885000	-2.463623000
6	1.617400000	3.050126000	0.270824000
1	2.283041000	2.294366000	0.713482000
6	1.700778000	4.313752000	1.114015000
1	2.691592000	4.774006000	1.026680000
1	0.973574000	5.070536000	0.797267000
1	1.529639000	4.119077000	2.176121000
6	2.076193000	3.298299000	-1.161444000
1	3.124437000	3.616172000	-1.189399000
1	1.982304000	2.402311000	-1.785217000
1	1.492313000	4.092712000	-1.640107000
15	-2.138636000	-0.957343000	0.262650000
15	-0.058497000	2.207595000	0.264086000
15	2.287489000	-0.918293000	-0.001122000
5	0.274258000	-0.257081000	2.542312000
7	-0.421105000	-0.552998000	-3.631627000
7	-0.159218000	-0.361323000	-2.425432000
1	0.446545000	-0.491432000	-4.208521000

[4d'_{sc}]-Quartet (TE = -2877.804475)

6	0.037364000	2.068077000	1.649338000
6	0.290260000	0.866863000	2.554441000
6	-2.481474000	-0.188018000	1.943793000
6	-1.319509000	-1.067565000	2.355681000
6	2.465474000	-1.258004000	1.703127000
6	1.126408000	-1.488586000	2.383130000
1	-2.458877000	0.773148000	2.468682000
1	-1.386695000	-1.195956000	3.458071000
1	3.257602000	-1.905083000	2.094305000
1	1.296581000	-1.443743000	3.478543000
1	0.394172000	3.002359000	2.096875000
1	1.337053000	0.937808000	2.885161000
6	0.469912000	3.113650000	-1.031359000
1	1.207119000	2.994115000	-1.836304000
6	-3.560361000	-0.952586000	-0.667586000
1	-3.111776000	-1.944345000	-0.532465000
6	3.577446000	-0.473877000	-0.798816000
1	3.453306000	0.487736000	-0.285670000
23	-0.035647000	-0.572675000	-0.334013000
16	-2.416342000	0.253016000	0.157528000
16	0.961267000	1.733708000	0.102544000
16	2.261473000	-1.566795000	-0.093628000

6	0.037659000	-0.518152000	1.922147000
1	-1.021779000	2.197440000	1.396552000
1	-0.299960000	1.012680000	3.478929000
1	0.808595000	-2.523852000	2.188297000
1	2.794433000	-0.215706000	1.808760000
1	-1.463081000	-2.073840000	1.932732000
1	-3.458649000	-0.629166000	2.155937000
6	4.954457000	-1.042140000	-0.519639000
1	5.729432000	-0.376396000	-0.915787000
1	5.143872000	-1.161014000	0.550783000
1	5.085524000	-2.020469000	-0.992366000
6	3.296344000	-0.300762000	-2.278662000
1	3.342029000	-1.255472000	-2.812906000
1	2.303519000	0.126287000	-2.455503000
1	4.039905000	0.363261000	-2.731537000
6	-4.954798000	-0.909972000	-0.077885000
1	-5.608621000	-1.593311000	-0.630390000
1	-4.991353000	-1.216775000	0.969881000
1	-5.388761000	0.092344000	-0.151747000
6	-3.559395000	-0.583138000	-2.140009000
1	-4.005641000	0.405339000	-2.295323000
1	-2.551571000	-0.582136000	-2.559344000
1	-4.151315000	-1.308301000	-2.706955000
6	-0.922104000	2.935583000	-1.601645000
1	-1.036276000	1.964759000	-2.093534000
1	-1.691085000	3.004750000	-0.826134000
1	-1.130717000	3.717548000	-2.340589000
6	0.667624000	4.464443000	-0.370634000
1	1.666086000	4.572748000	0.060939000
1	0.529598000	5.267643000	-1.102115000
1	-0.063885000	4.631090000	0.426263000
7	-0.932168000	-2.729558000	-2.350897000
7	-0.563515000	-1.839532000	-1.569681000
1	-0.933323000	-3.664077000	-1.871323000

[4e'_{ssi}]-Quartet (TE = -3129.217811)

6	0.568605000	-0.627420000	2.506636000
6	0.217825000	0.830920000	2.763949000
6	2.749086000	2.023091000	0.743358000
6	1.592281000	2.953848000	1.075017000
6	-2.724435000	1.734989000	0.890926000
6	-1.645598000	2.749782000	1.245046000
1	2.930433000	1.322838000	1.567456000
1	1.806318000	3.461047000	2.025428000
1	-3.728814000	2.170710000	0.860176000
1	-1.866104000	3.156182000	2.241729000

1	0.443647000	-1.270761000	3.385281000
1	-0.725771000	0.876628000	3.325500000
6	-0.217401000	-3.028709000	1.054981000
1	-0.909566000	-3.313012000	0.251088000
6	3.837868000	-0.001853000	-0.967165000
1	4.656143000	0.710135000	-1.139250000
6	-3.584062000	-0.446853000	-0.681707000
1	-3.355136000	-0.942762000	0.271857000
23	-0.018971000	0.180586000	-0.837081000
16	2.325417000	1.056849000	-0.768330000
16	-0.564939000	-1.211979000	1.179396000
16	-2.400439000	0.981094000	-0.764396000
1	1.597724000	-0.738399000	2.142802000
1	0.980923000	1.271507000	3.420444000
1	-1.688332000	3.596937000	0.549017000
1	-2.738169000	0.902539000	1.608504000
1	1.506704000	3.733189000	0.308564000
1	3.693135000	2.540949000	0.534971000
6	-5.024018000	0.027293000	-0.694680000
1	-5.705922000	-0.828310000	-0.634636000
1	-5.257462000	0.685249000	0.145957000
1	-5.254956000	0.568385000	-1.617608000
6	-3.272220000	-1.383577000	-1.832481000
1	-3.407845000	-0.890524000	-2.800988000
1	-2.242431000	-1.751279000	-1.795529000
1	-3.944124000	-2.247746000	-1.808907000
6	4.134101000	-0.843943000	0.255911000
1	5.007017000	-1.481704000	0.076296000
1	4.352877000	-0.244129000	1.143003000
1	3.290819000	-1.500152000	0.489477000
6	3.619218000	-0.844433000	-2.208400000
1	2.752923000	-1.504429000	-2.090779000
1	3.436753000	-0.233301000	-3.095504000
1	4.496076000	-1.470401000	-2.402292000
6	1.200773000	-3.319009000	0.613369000
1	1.453811000	-2.778649000	-0.304074000
1	1.924586000	-3.041882000	1.387281000
1	1.332884000	-4.389340000	0.421156000
6	-0.602507000	-3.757117000	2.328566000
1	-1.624846000	-3.528691000	2.639555000
1	-0.529954000	-4.840622000	2.184656000
1	0.064928000	-3.502709000	3.157774000
14	0.033942000	1.848737000	1.118463000
7	0.236561000	-0.459515000	-3.837850000
7	0.120209000	-0.178262000	-2.637295000
1	-0.142207000	0.313665000	-4.434700000

[4f_{SB}] (TE = -2864.561466)

6	-0.730051000	-2.223349000	1.667266000
6	-0.732555000	-0.949190000	2.497148000
6	2.588181000	-0.939180000	1.349640000
6	1.858935000	-0.047003000	2.339467000
6	-1.594623000	2.075288000	1.891033000
6	-0.205155000	1.726582000	2.389332000
1	2.135832000	-1.933710000	1.276286000
1	1.988913000	-0.515045000	3.332421000
1	-1.911116000	3.090594000	2.152202000
1	-0.209634000	1.898017000	3.483333000
1	-1.430571000	-2.978794000	2.040482000
1	-1.772095000	-0.589370000	2.537182000
6	-0.772729000	-3.254285000	-1.037635000
1	-1.244297000	-3.023629000	-2.001343000
6	3.329640000	1.344410000	-0.208953000
1	2.633358000	1.950307000	0.385951000
6	-3.372031000	1.206869000	-0.164464000
1	-3.385400000	0.303027000	0.460163000
23	0.092757000	0.291167000	-0.605485000
16	2.518372000	-0.322211000	-0.376316000
16	-1.241965000	-1.767948000	-0.036787000
16	-1.677822000	1.928599000	0.054715000
1	0.262224000	-2.685400000	1.617490000
1	-0.511861000	-1.250176000	3.537091000
1	0.511953000	2.467691000	2.005224000
1	-2.348714000	1.386608000	2.287836000
1	2.409879000	0.902609000	2.415808000
1	3.644214000	-1.102323000	1.595564000
6	-4.433875000	2.184233000	0.297707000
1	-5.430743000	1.742090000	0.191040000
1	-4.313716000	2.465494000	1.347335000
1	-4.412668000	3.102172000	-0.298002000
6	-3.525605000	0.821754000	-1.622137000
1	-3.443517000	1.696313000	-2.276303000
1	-2.763124000	0.101872000	-1.934323000
1	-4.508899000	0.372043000	-1.793783000
6	4.670180000	1.236497000	0.488592000
1	5.155170000	2.218201000	0.509897000
1	4.586354000	0.897937000	1.524115000
1	5.341479000	0.551115000	-0.039349000
6	3.449782000	1.931020000	-1.601856000
1	4.109602000	1.325328000	-2.231949000
1	2.482847000	2.013358000	-2.101325000
1	3.883716000	2.934373000	-1.542813000

6	0.72460000	-3.377459000	-1.231569000
1	1.146430000	-2.494512000	-1.717963000
1	1.247016000	-3.519884000	-0.278826000
1	0.957522000	-4.247922000	-1.854728000
6	-1.397106000	-4.509271000	-0.457859000
1	-2.473046000	-4.400362000	-0.299998000
1	-1.240811000	-5.356617000	-1.133491000
1	-0.941858000	-4.777456000	0.500674000
5	0.292948000	0.229930000	2.098168000
7	0.336269000	1.567561000	-3.389843000
7	0.198616000	0.965289000	-2.317714000
1	-0.219666000	1.103094000	-4.147755000

[4a''_{PC}]-Quartet (TE = -3519.926040)

6	1.217672000	-0.630432000	1.763382000
6	1.811855000	-0.099233000	2.919605000
1	1.321268000	0.728883000	3.428516000
6	3.003517000	-0.598700000	3.434444000
1	3.433847000	-0.151388000	4.328929000
6	3.636112000	-1.672216000	2.817641000
1	4.566545000	-2.071767000	3.214875000
6	3.073312000	-2.217160000	1.667350000
1	3.591272000	-3.030998000	1.162222000
6	1.892647000	-1.703978000	1.121249000
6	-0.371883000	1.312618000	1.694729000
6	-1.266221000	1.587784000	2.743580000
1	-1.756214000	0.760119000	3.252010000
6	-1.561248000	2.886379000	3.141509000
1	-2.271309000	3.054885000	3.949356000
6	-0.951647000	3.963615000	2.509316000
1	-1.179695000	4.985073000	2.805746000
6	-0.047113000	3.719034000	1.481412000
1	0.415190000	4.565810000	0.982933000
6	0.242215000	2.417450000	1.060304000
6	-1.263987000	-0.968894000	1.591680000
6	-1.268088000	-1.803885000	2.716252000
1	-0.356800000	-1.898795000	3.305373000
6	-2.404872000	-2.508045000	3.098770000
1	-2.370719000	-3.154934000	3.973834000
6	-3.585806000	-2.375651000	2.376767000
1	-4.480514000	-2.918251000	2.673720000
6	-3.611224000	-1.540726000	1.262543000
1	-4.535137000	-1.439932000	0.698334000
6	-2.467179000	-0.853267000	0.851429000
6	-0.088257000	-0.099042000	1.233176000
23	0.085930000	-0.088585000	-1.135722000

6	2.878185000	-2.479337000	-1.520162000
1	3.490492000	-3.198081000	-0.959721000
6	0.976367000	3.540887000	-1.535664000
1	-0.083812000	3.770599000	-1.343317000
6	-3.395552000	-0.712140000	-2.002396000
1	-3.045290000	-0.192994000	-2.908023000
6	-4.911871000	-0.565818000	-1.947735000
1	-5.359078000	-1.043917000	-2.827129000
1	-5.354498000	-1.049636000	-1.072829000
1	-5.243320000	0.474110000	-1.950847000
6	-2.992643000	-2.176488000	-2.141134000
1	-3.317594000	-2.764462000	-1.275629000
1	-3.458199000	-2.616993000	-3.029116000
1	-1.909282000	-2.294449000	-2.241184000
6	2.539999000	-3.071805000	-2.884239000
1	2.119020000	-4.078611000	-2.820939000
1	1.818801000	-2.446393000	-3.422524000
1	3.439334000	-3.138080000	-3.506212000
6	3.669260000	-1.193529000	-1.679491000
1	3.886374000	-0.715920000	-0.719237000
1	4.625026000	-1.380963000	-2.181945000
1	3.111516000	-0.472822000	-2.287040000
6	1.789514000	4.806598000	-1.276778000
1	1.409864000	5.622695000	-1.902389000
1	1.758749000	5.156990000	-0.244217000
1	2.841551000	4.678137000	-1.541722000
6	1.102214000	3.133489000	-3.001194000
1	2.131968000	2.860055000	-3.257730000
1	0.469149000	2.273969000	-3.234670000
1	0.817406000	3.963012000	-3.658233000
15	-2.336875000	0.108341000	-0.697003000
15	1.226153000	2.038964000	-0.432784000
15	1.307523000	-2.168321000	-0.550058000
6	3.013292000	2.018208000	0.150871000
1	3.089885000	0.999722000	0.559553000
6	3.997541000	2.130903000	-1.008865000
1	4.112517000	3.163364000	-1.348012000
1	4.991604000	1.787590000	-0.701754000
1	3.704902000	1.532388000	-1.874364000
6	3.351670000	2.986900000	1.274702000
1	4.376771000	2.815765000	1.624093000
1	3.293488000	4.031805000	0.954903000
1	2.689162000	2.866461000	2.135733000
6	0.607160000	-3.909722000	-0.504297000
1	0.334908000	-4.079912000	-1.556580000
6	-0.656724000	-4.015881000	0.330466000

1	-0.433417000	-3.921340000	1.396416000
1	-1.394480000	-3.249324000	0.084063000
1	-1.126795000	-4.994685000	0.182740000
6	1.607767000	-4.973689000	-0.071315000
1	1.136757000	-5.963162000	-0.084397000
1	2.490681000	-5.033167000	-0.712431000
1	1.949563000	-4.800999000	0.955118000
6	-3.076699000	1.795390000	-0.376534000
1	-2.284173000	2.280347000	0.207465000
6	-4.341158000	1.831596000	0.469615000
1	-4.608679000	2.868169000	0.706402000
1	-5.204405000	1.382520000	-0.028566000
1	-4.201191000	1.309823000	1.420847000
6	-3.196404000	2.563011000	-1.688409000
1	-3.417468000	3.619204000	-1.499589000
1	-2.265343000	2.520716000	-2.266997000
1	-3.995397000	2.179390000	-2.330637000
7	-0.291306000	-0.504998000	-4.135342000
7	-0.054796000	-0.240932000	-2.947049000
1	0.019165000	0.279219000	-4.754654000

[4b''_{psi}]-Quartet (TE = -3771.336353)

6	1.294863000	-1.351887000	1.962691000
6	1.243951000	-1.994159000	3.206199000
1	0.412837000	-1.789096000	3.882584000
6	2.213145000	-2.916364000	3.588323000
1	2.146801000	-3.414288000	4.554063000
6	3.263172000	-3.209081000	2.723527000
1	4.022624000	-3.934215000	3.009241000
6	3.336117000	-2.583049000	1.482907000
1	4.157012000	-2.837491000	0.816974000
6	2.358287000	-1.663111000	1.091148000
6	0.250061000	1.521193000	2.167225000
6	0.670840000	1.672491000	3.493838000
1	0.824219000	0.786105000	4.111545000
6	0.939206000	2.925942000	4.034593000
1	1.282298000	3.018515000	5.063566000
6	0.779384000	4.061751000	3.247381000
1	0.994663000	5.047129000	3.655950000
6	0.354315000	3.937967000	1.928053000
1	0.249503000	4.838779000	1.330066000
6	0.096000000	2.678958000	1.376175000
6	-1.730551000	-0.767680000	1.851969000
6	-2.248091000	-0.597187000	3.142567000
1	-1.616070000	-0.165460000	3.920161000
6	-3.566427000	-0.917160000	3.448112000

1	-3.951125000	-0.760193000	4.454296000
6	-4.399221000	-1.418589000	2.452288000
1	-5.437820000	-1.656189000	2.673712000
6	-3.905953000	-1.608568000	1.166250000
1	-4.576782000	-1.992102000	0.403232000
6	-2.579358000	-1.290529000	0.853840000
23	0.096817000	0.105205000	-1.219312000
6	3.720965000	0.430315000	-0.370638000
1	4.640804000	-0.134938000	-0.167886000
6	-2.185072000	3.015122000	-0.364043000
1	-2.148505000	4.067883000	-0.051115000
6	-1.518225000	-3.298752000	-1.005602000
1	-1.658839000	-3.492313000	-2.080254000
6	-2.443392000	-4.204425000	-0.203325000
1	-2.231491000	-5.255381000	-0.431657000
1	-2.285104000	-4.069371000	0.871429000
1	-3.503739000	-4.038213000	-0.396409000
6	-0.071444000	-3.608410000	-0.654309000
1	0.147057000	-3.382297000	0.395575000
1	0.145978000	-4.671531000	-0.809729000
1	0.623243000	-3.029975000	-1.265462000
6	3.883144000	1.221098000	-1.661675000
1	4.014100000	0.590069000	-2.546069000
1	2.998078000	1.840593000	-1.840412000
1	4.747482000	1.892256000	-1.605011000
6	3.462942000	1.365829000	0.799798000
1	3.324888000	0.833971000	1.745936000
1	4.303469000	2.057360000	0.927290000
1	2.566169000	1.971480000	0.635320000
6	-2.798991000	2.920233000	-1.753821000
1	-3.823921000	3.308145000	-1.754373000
1	-2.241216000	3.473256000	-2.514746000
1	-2.845229000	1.876773000	-2.084867000
6	-3.025778000	2.244766000	0.640962000
1	-3.139631000	1.198123000	0.344580000
1	-2.599886000	2.252524000	1.648672000
1	-4.032002000	2.674352000	0.702691000
14	-0.017803000	-0.149892000	1.294805000
15	-0.400005000	2.428965000	-0.389709000
15	-1.870255000	-1.450563000	-0.843907000
15	2.358769000	-0.844348000	-0.565266000
6	3.170916000	-2.155956000	-1.670311000
1	2.853471000	-3.096256000	-1.196464000
6	4.695261000	-2.155892000	-1.735489000
1	5.039905000	-3.024732000	-2.307553000
1	5.083213000	-1.271248000	-2.249203000

1	5.185017000	-2.201456000	-0.760188000
6	2.595049000	-2.120170000	-3.080284000
1	1.502494000	-2.156064000	-3.091656000
1	2.874582000	-1.204577000	-3.610977000
1	2.971507000	-2.964379000	-3.669074000
6	-3.326231000	-1.190024000	-2.020644000
1	-3.873776000	-0.351411000	-1.561019000
6	-2.787132000	-0.733409000	-3.373307000
1	-2.168539000	-1.507254000	-3.843012000
1	-3.612162000	-0.517652000	-4.061341000
1	-2.162322000	0.157595000	-3.299281000
6	-4.298395000	-2.343978000	-2.248448000
1	-3.796285000	-3.220621000	-2.670065000
1	-4.831394000	-2.670583000	-1.354907000
1	-5.059986000	-2.042404000	-2.976452000
6	0.471007000	3.849199000	-1.295558000
1	1.428908000	3.926261000	-0.757380000
6	-0.211172000	5.214950000	-1.268579000
1	0.455441000	5.970092000	-1.699868000
1	-1.122674000	5.222069000	-1.873955000
1	-0.487684000	5.565141000	-0.272817000
6	0.772948000	3.474113000	-2.742244000
1	1.348069000	2.550402000	-2.811593000
1	-0.145312000	3.321579000	-3.320899000
1	1.338743000	4.272928000	-3.235061000
7	0.564142000	0.316976000	-4.240465000
7	0.380328000	0.269370000	-3.017434000
1	0.895603000	1.268559000	-4.528102000

[4c''_{PB}] (TE = -3506.679846)

6	1.468285000	-0.617742000	1.906813000
6	1.585443000	-1.361187000	3.095712000
1	0.679015000	-1.623673000	3.641508000
6	2.812015000	-1.780425000	3.599058000
1	2.853273000	-2.357604000	4.521271000
6	3.982973000	-1.466079000	2.918058000
1	4.949660000	-1.790599000	3.297601000
6	3.903729000	-0.746419000	1.731664000
1	4.820759000	-0.527215000	1.189766000
6	2.669908000	-0.330300000	1.219584000
6	-0.442767000	1.336680000	1.944657000
6	-0.005654000	1.809672000	3.194151000
1	0.740483000	1.231734000	3.740937000
6	-0.492748000	2.983690000	3.758548000
1	-0.120451000	3.317794000	4.725695000
6	-1.462946000	3.724358000	3.091456000

1	-1.859737000	4.638620000	3.527789000
6	-1.910714000	3.290690000	1.847997000
1	-2.658558000	3.879957000	1.321577000
6	-1.398470000	2.128992000	1.262338000
6	-1.146297000	-1.215658000	1.679688000
6	-1.858844000	-1.183310000	2.893036000
1	-1.642187000	-0.386679000	3.605690000
6	-2.842865000	-2.111148000	3.207856000
1	-3.374038000	-2.043248000	4.155857000
6	-3.158760000	-3.115848000	2.298980000
1	-3.937494000	-3.842051000	2.522655000
6	-2.476086000	-3.176672000	1.091255000
1	-2.743737000	-3.954226000	0.382051000
6	-1.477377000	-2.246873000	0.773220000
23	0.143122000	0.203170000	-1.157103000
6	3.197594000	2.189310000	-0.193883000
1	4.244149000	2.072381000	0.123293000
6	-3.632029000	1.268070000	-0.474789000
1	-4.127789000	2.207492000	-0.191847000
6	0.472629000	-3.686587000	-0.961671000
1	0.403524000	-4.000905000	-2.013886000
6	0.066729000	-4.850311000	-0.069160000
1	0.751751000	-5.693477000	-0.214290000
1	0.115148000	-4.570655000	0.988358000
1	-0.942990000	-5.216969000	-0.262498000
6	1.914918000	-3.290449000	-0.692214000
1	2.049205000	-2.896596000	0.320631000
1	2.580174000	-4.155059000	-0.797858000
1	2.251141000	-2.524010000	-1.391837000
6	3.157057000	2.946874000	-1.516997000
1	3.839901000	2.533518000	-2.263588000
1	2.160446000	2.927859000	-1.965821000
1	3.434225000	3.996876000	-1.371397000
6	2.449435000	2.923279000	0.908465000
1	2.518822000	2.402486000	1.867798000
1	2.861830000	3.929432000	1.044290000
1	1.385038000	3.033066000	0.682187000
6	-4.053487000	0.884860000	-1.888418000
1	-5.136153000	0.727085000	-1.945122000
1	-3.794032000	1.639523000	-2.637061000
1	-3.572278000	-0.049573000	-2.197982000
6	-4.039965000	0.204686000	0.528458000
1	-3.603881000	-0.769846000	0.290924000
1	-3.734916000	0.456094000	1.547479000
1	-5.129095000	0.082185000	0.527487000
5	0.007974000	-0.123540000	1.476291000

7	0.371873000	1.638350000	-3.846127000
7	0.275535000	0.954120000	-2.818688000
1	0.130208000	1.065252000	-4.689777000
15	-0.669172000	-2.190110000	-0.869843000
15	2.527726000	0.459773000	-0.425463000
15	-1.801924000	1.647962000	-0.458588000
6	-2.025146000	-2.622829000	-2.107182000
1	-2.910158000	-2.117069000	-1.692026000
6	-2.365030000	-4.094081000	-2.320180000
1	-3.157118000	-4.183934000	-3.072046000
1	-1.510684000	-4.663029000	-2.700421000
1	-2.724574000	-4.602537000	-1.424627000
6	-1.687635000	-1.982382000	-3.451485000
1	-1.534586000	-0.903062000	-3.368509000
1	-0.766886000	-2.403753000	-3.874973000
1	-2.487108000	-2.163454000	-4.178756000
6	-1.770338000	3.222247000	-1.496388000
1	-1.690360000	2.813054000	-2.513909000
6	-0.496332000	4.008469000	-1.233358000
1	0.383070000	3.367588000	-1.298031000
1	-0.377177000	4.807938000	-1.972285000
1	-0.502224000	4.471630000	-0.240517000
6	-2.984962000	4.142980000	-1.460425000
1	-2.832769000	4.967033000	-2.166787000
1	-3.918262000	3.653372000	-1.746855000
1	-3.139868000	4.602928000	-0.480325000
6	3.877041000	-0.366193000	-1.460435000
1	3.927774000	-1.376283000	-1.032955000
6	5.279960000	0.229335000	-1.388681000
1	5.982334000	-0.417829000	-1.926010000
1	5.339832000	1.213360000	-1.860869000
1	5.662416000	0.337238000	-0.371334000
6	3.427042000	-0.480886000	-2.914012000
1	2.455976000	-0.978198000	-3.009966000
1	3.320635000	0.502903000	-3.383579000
1	4.157545000	-1.046610000	-3.503368000

[4d''_{sc}] (TE = -3335.065002)

6	0.003135000	1.606611000	1.128891000
6	0.708526000	2.168912000	2.207280000
1	1.382842000	1.532978000	2.777581000
6	0.567175000	3.500276000	2.579692000
1	1.135146000	3.886328000	3.424111000
6	-0.299465000	4.335433000	1.881801000
1	-0.416290000	5.378912000	2.164544000
6	-0.983359000	3.827267000	0.784720000

1	-1.615891000	4.477977000	0.183697000
6	-0.826201000	2.492175000	0.409948000
6	-0.979645000	-0.640432000	1.544237000
6	-1.458538000	-0.233258000	2.801312000
1	-1.098238000	0.704961000	3.218531000
6	-2.364512000	-0.988030000	3.536768000
1	-2.703731000	-0.626830000	4.505862000
6	-2.830968000	-2.201780000	3.042731000
1	-3.539749000	-2.799812000	3.610572000
6	-2.413199000	-2.619001000	1.785184000
1	-2.816422000	-3.530798000	1.348428000
6	-1.516572000	-1.846772000	1.045515000
6	1.456513000	-0.416735000	1.140948000
6	1.736494000	-0.970517000	2.402523000
1	0.932457000	-1.033200000	3.133030000
6	2.995244000	-1.442688000	2.752497000
1	3.156012000	-1.863688000	3.743279000
6	4.042478000	-1.386053000	1.839510000
1	5.027798000	-1.768246000	2.095471000
6	3.800030000	-0.872525000	0.572074000
1	4.584829000	-0.883749000	-0.180357000
6	2.533815000	-0.390854000	0.228843000
16	2.220574000	-0.013191000	-1.494656000
16	-1.495657000	1.974467000	-1.164991000
16	-1.253335000	-2.273157000	-0.670064000
23	-0.258780000	-0.151507000	-1.464628000
6	-3.342739000	1.804911000	-0.896045000
1	-3.689445000	2.841737000	-0.799817000
6	-0.184077000	-3.812394000	-0.648046000
1	-0.863441000	-4.604172000	-0.307923000
6	2.990436000	1.670884000	-1.810395000
1	2.835780000	1.739955000	-2.894967000
6	4.473486000	1.648539000	-1.506675000
1	4.936315000	2.583750000	-1.839755000
1	4.657396000	1.565059000	-0.431061000
1	4.989995000	0.824300000	-2.005625000
6	2.270670000	2.800846000	-1.114106000
1	2.327800000	2.704353000	-0.025580000
1	2.729415000	3.759157000	-1.383674000
1	1.215954000	2.847682000	-1.392972000
6	-3.891408000	1.182582000	-2.163938000
1	-3.623388000	1.748969000	-3.059936000
1	-3.512363000	0.163227000	-2.294263000
1	-4.983659000	1.131309000	-2.113244000
6	-3.695709000	1.017367000	0.341758000
1	-3.236367000	1.428341000	1.244580000

1	-4.781989000	1.025973000	0.487449000
1	-3.382582000	-0.026796000	0.251358000
6	0.215574000	-4.052963000	-2.090071000
1	0.773058000	-4.990915000	-2.176725000
1	-0.647501000	-4.112533000	-2.759200000
1	0.863343000	-3.246020000	-2.452208000
6	1.002333000	-3.703591000	0.277723000
1	1.700210000	-2.932314000	-0.060765000
1	0.709986000	-3.463299000	1.303265000
1	1.545147000	-4.655612000	0.300543000
6	0.085638000	0.131115000	0.786044000
7	-1.284936000	-0.549760000	-4.313719000
7	-0.740252000	-0.372096000	-3.219283000
1	-0.580419000	-0.535196000	-5.085723000

[4e''_{ssi}] (TE = -3586.475151)

6	1.239327000	1.275767000	-1.655806000
6	1.374032000	1.553612000	-3.022929000
1	0.779714000	0.991938000	-3.744267000
6	2.244053000	2.533806000	-3.490529000
1	2.324020000	2.728998000	-4.558179000
6	3.007727000	3.270392000	-2.589529000
1	3.684113000	4.044155000	-2.946095000
6	2.883872000	3.036194000	-1.224401000
1	3.451037000	3.633796000	-0.512850000
6	2.008237000	2.049817000	-0.770504000
6	1.034921000	-1.709314000	-1.098115000
6	1.604099000	-2.154221000	-2.299686000
1	1.549054000	-1.517890000	-3.184036000
6	2.250953000	-3.381782000	-2.397444000
1	2.684885000	-3.697245000	-3.344369000
6	2.353141000	-4.203177000	-1.277279000
1	2.865541000	-5.160617000	-1.342357000
6	1.821305000	-3.784387000	-0.063331000
1	1.928324000	-4.404773000	0.824999000
6	1.168990000	-2.553297000	0.014705000
6	-1.542397000	-0.218068000	-1.730711000
6	-1.735640000	-0.629476000	-3.057303000
1	-0.868307000	-0.819026000	-3.690332000
6	-3.005070000	-0.827691000	-3.589912000
1	-3.119696000	-1.148206000	-4.623645000
6	-4.128979000	-0.639075000	-2.790751000
1	-5.124953000	-0.812965000	-3.192139000
6	-3.975746000	-0.250916000	-1.464722000
1	-4.846324000	-0.137325000	-0.822401000
6	-2.696466000	-0.026589000	-0.950250000

16	-2.567674000	0.433932000	0.797151000
16	1.834102000	1.839347000	1.019947000
16	0.570811000	-2.009697000	1.633542000
23	-0.175181000	0.415548000	1.586534000
6	3.508000000	1.127998000	1.454706000
1	4.215468000	1.928752000	1.204902000
6	-0.838618000	-3.206992000	1.913160000
1	-0.346764000	-4.181397000	2.025927000
6	-2.938377000	2.268745000	0.758972000
1	-2.791063000	2.515404000	1.817424000
6	-4.373636000	2.526994000	0.350771000
1	-4.612161000	3.586475000	0.493595000
1	-4.539288000	2.301505000	-0.707487000
1	-5.085454000	1.942945000	0.939944000
6	-1.944763000	3.033024000	-0.089346000
1	-1.952708000	2.691547000	-1.130968000
1	-2.201978000	4.097906000	-0.092666000
1	-0.925189000	2.936802000	0.292279000
6	3.501720000	0.886899000	2.950267000
1	3.266070000	1.791950000	3.516441000
1	2.764601000	0.122011000	3.220102000
1	4.482917000	0.529707000	3.278508000
6	3.825720000	-0.119990000	0.662875000
1	3.758781000	0.038610000	-0.417216000
1	4.844374000	-0.456281000	0.886696000
1	3.146206000	-0.936071000	0.924195000
6	-1.502775000	-2.808088000	3.214987000
1	-2.294259000	-3.520920000	3.466878000
1	-0.798004000	-2.780759000	4.050406000
1	-1.965316000	-1.817636000	3.133795000
6	-1.802743000	-3.241382000	0.748592000
1	-2.313660000	-2.282367000	0.627966000
1	-1.310419000	-3.480620000	-0.197810000
1	-2.571634000	-4.001971000	0.924214000
14	0.133342000	-0.039393000	-0.840117000
7	-1.145010000	2.378924000	3.703733000
7	-0.633790000	1.467171000	3.036873000
1	-0.905091000	2.274644000	4.716509000

[4f'_{SB}] (TE = -3321.821651)

6	0.841400000	1.409932000	-1.529554000
6	0.638549000	2.021916000	-2.779302000
1	-0.185131000	1.675439000	-3.403667000
6	1.459125000	3.038744000	-3.256306000
1	1.268413000	3.476002000	-4.234691000
6	2.521924000	3.499735000	-2.484428000

1	3.166523000	4.296982000	-2.847330000
6	2.726904000	2.959903000	-1.220096000
1	3.514406000	3.351092000	-0.578127000
6	1.897887000	1.935988000	-0.762218000
6	0.807807000	-1.245762000	-1.353385000
6	1.416964000	-1.442957000	-2.606784000
1	1.402728000	-0.625416000	-3.329094000
6	2.041952000	-2.633725000	-2.958590000
1	2.498308000	-2.738313000	-3.941221000
6	2.095100000	-3.687490000	-2.049847000
1	2.589139000	-4.620713000	-2.310986000
6	1.544544000	-3.520029000	-0.786142000
1	1.628011000	-4.310956000	-0.042290000
6	0.913076000	-2.319441000	-0.454810000
6	-1.530714000	0.044697000	-1.546963000
6	-1.821450000	-0.343202000	-2.869392000
1	-0.993373000	-0.595149000	-3.531949000
6	-3.116929000	-0.442704000	-3.361154000
1	-3.283818000	-0.749049000	-4.392180000
6	-4.200088000	-0.173782000	-2.529480000
1	-5.219761000	-0.266081000	-2.896148000
6	-3.963517000	0.183460000	-1.209836000
1	-4.795512000	0.350814000	-0.528992000
6	-2.651522000	0.302866000	-0.739476000
16	-2.457902000	0.614608000	1.025093000
16	2.027306000	1.433675000	0.955871000
16	0.421149000	-2.066553000	1.252226000
23	-0.060740000	0.287139000	1.506460000
6	3.683366000	0.597628000	1.157705000
1	4.406077000	1.420169000	1.089325000
6	-1.026545000	-3.231996000	1.455425000
1	-0.567030000	-4.227564000	1.412895000
6	-2.602144000	2.477376000	1.166807000
1	-2.529784000	2.604113000	2.254093000
6	-3.953422000	2.952396000	0.678039000
1	-4.066445000	4.022105000	0.882631000
1	-4.056449000	2.817255000	-0.402819000
1	-4.778994000	2.429241000	1.167009000
6	-1.452590000	3.181207000	0.476299000
1	-1.400332000	2.921201000	-0.586034000
1	-1.576715000	4.267534000	0.545146000
1	-0.479571000	2.947023000	0.923909000
6	3.686764000	0.013264000	2.556098000
1	3.480746000	0.762677000	3.324423000
1	2.932123000	-0.773883000	2.656771000
1	4.664884000	-0.429233000	2.769317000

6	3.946441000	-0.426055000	0.078583000
1	3.842674000	-0.010081000	-0.927375000
1	4.969261000	-0.806464000	0.177671000
1	3.265732000	-1.276954000	0.161359000
6	-1.597112000	-2.980558000	2.836097000
1	-2.401168000	-3.693488000	3.044759000
1	-0.844125000	-3.078982000	3.622318000
1	-2.017065000	-1.971210000	2.905453000
6	-2.052329000	-3.085092000	0.355160000
1	-2.554041000	-2.115458000	0.405637000
1	-1.616096000	-3.184239000	-0.642637000
1	-2.821950000	-3.857967000	0.460297000
5	0.005995000	0.121359000	-1.094025000
7	0.166084000	0.131627000	4.487441000
7	-0.022242000	0.213176000	3.246895000
1	-0.733297000	0.079722000	4.995413000

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23	0.082595000	0.013557000	0.441073000
6	1.196589000	0.706964000	3.105226000
6	2.356270000	0.150477000	2.312225000
6	-2.022208000	1.334333000	1.806695000
6	-1.251754000	0.895691000	3.045717000
6	-0.190959000	-1.333014000	3.016890000
6	-1.231262000	-1.955077000	2.117710000
1	-2.233392000	-1.589938000	2.402474000
1	-1.256651000	-3.043226000	2.271555000
1	0.778387000	-1.809929000	2.841856000
1	-0.440403000	-1.454732000	4.082140000
1	-2.595266000	2.242325000	2.041551000
1	-2.765555000	0.570209000	1.520030000
1	-0.897226000	1.774307000	3.591856000
1	-1.884034000	0.327861000	3.738236000
1	1.102120000	1.777268000	2.898189000
1	1.339200000	0.585485000	4.190293000
1	2.690928000	-0.822555000	2.712440000
1	3.216769000	0.823028000	2.431120000
7	-0.913469000	-1.635554000	0.726353000
7	-0.065842000	0.089239000	2.655552000
7	-1.061397000	1.578284000	0.740504000
7	1.952892000	0.008231000	0.921152000
6	-1.585959000	-2.422108000	-0.219447000
6	-1.040005000	-2.636231000	-1.497697000
6	-2.816378000	-3.043307000	0.070566000
6	-1.702941000	-3.404413000	-2.441632000
1	-0.078174000	-2.196024000	-1.739557000

6	-3.473721000	-3.813429000	-0.882451000
1	-3.278178000	-2.909536000	1.044803000
6	-2.928768000	-3.999238000	-2.147358000
1	-1.247357000	-3.549072000	-3.419285000
1	-4.428555000	-4.269753000	-0.627187000
1	-3.444288000	-4.603330000	-2.889831000
6	-1.375758000	2.538691000	-0.211086000
6	-2.685522000	2.986948000	-0.464655000
6	-0.333758000	3.110437000	-0.970314000
6	-2.933768000	3.942561000	-1.444602000
1	-3.520201000	2.559952000	0.085580000
6	-0.592326000	4.055105000	-1.950924000
1	0.689220000	2.800693000	-0.754429000
6	-1.897693000	4.481545000	-2.199480000
1	-3.959099000	4.260136000	-1.625993000
1	0.236504000	4.480496000	-2.514359000
1	-2.099671000	5.227212000	-2.964126000
6	3.001096000	-0.183617000	0.000540000
6	4.116712000	0.667855000	-0.040441000
6	2.934473000	-1.228794000	-0.932206000
6	5.113188000	0.488381000	-0.991071000
1	4.186481000	1.496812000	0.661031000
6	3.927710000	-1.398124000	-1.888034000
1	2.085136000	-1.908710000	-0.890057000
6	5.024907000	-0.542205000	-1.923735000
1	5.961871000	1.169533000	-1.011234000
1	3.848363000	-2.214351000	-2.603110000
1	5.805256000	-0.678096000	-2.668619000
7	0.238062000	0.331173000	-2.538522000
7	0.201960000	0.173209000	-1.330912000
1	0.161325000	1.341840000	-2.791593000

Cartesian coordinates of $[4a'_{PC}]-[4f'_{SB}]$ and $[4a''_{PC}]-[4f''_{SB}]$ along with their total energies (in hartree) including zero point vibrational correction at M06-D3(heptane)/def2-SVP level of theory.

$[4a'_{PC}]$ (TE = -3060.454573)

6	-0.620139000	2.271571000	1.950387000
6	0.186158000	1.192720000	2.669544000
6	-2.392041000	-0.718069000	2.064011000
6	-1.018585000	-1.019481000	2.650402000
6	2.703726000	-0.551354000	1.814052000
6	1.429727000	-0.941165000	2.550921000
1	-2.692432000	0.329600000	2.246022000

1	-1.065986000	-0.901272000	3.760505000
1	3.598254000	-1.054893000	2.218982000
1	1.581157000	-0.788494000	3.647702000
1	-0.500727000	3.265547000	2.419032000
1	1.235242000	1.551145000	2.708285000
6	-1.199741000	3.442248000	-0.761412000
1	-0.580368000	4.345427000	-0.919429000
6	-2.575473000	-2.787949000	0.037461000
1	-1.881387000	-3.189431000	0.804595000
6	3.806596000	0.047546000	-0.833503000
1	3.606163000	1.094654000	-0.528550000
23	0.046815000	-0.209780000	-0.288836000
6	0.159352000	-0.228068000	2.062686000
1	-1.699988000	2.045878000	1.968141000
1	-0.129999000	1.162932000	3.739338000
1	1.295170000	-2.036029000	2.434419000
1	2.896003000	0.536438000	1.894464000
1	-0.824354000	-2.100787000	2.492767000
1	-3.183315000	-1.350800000	2.507555000
6	5.211830000	-0.325031000	-0.392210000
1	5.956575000	0.320593000	-0.889642000
1	5.356679000	-0.216111000	0.695061000
1	5.460205000	-1.365495000	-0.665537000
6	3.638759000	-0.042848000	-2.343101000
1	3.827766000	-1.067596000	-2.710481000
1	2.620418000	0.234473000	-2.662564000
1	4.355900000	0.619712000	-2.857801000
6	-3.975714000	-3.285635000	0.355764000
1	-3.988937000	-4.388864000	0.391780000
1	-4.351156000	-2.922166000	1.326257000
1	-4.696640000	-2.983931000	-0.423086000
6	-2.093082000	-3.285906000	-1.317283000
1	-2.723800000	-2.907679000	-2.140405000
1	-1.060280000	-2.953124000	-1.507283000
1	-2.121515000	-4.388307000	-1.360459000
6	-1.549787000	2.855559000	-2.122349000
1	-0.656391000	2.563282000	-2.697481000
1	-2.159524000	1.941988000	-2.013651000
1	-2.125780000	3.578456000	-2.725515000
6	-2.443459000	3.866613000	0.003127000
1	-2.202512000	4.380283000	0.947430000
1	-3.047798000	4.558640000	-0.608178000

1	-3.092861000	3.007039000	0.247598000
6	2.885043000	-2.687522000	-0.272426000
1	3.530539000	-2.655866000	-1.171614000
6	1.641973000	-3.491966000	-0.620876000
1	0.903952000	-3.462122000	0.203064000
1	1.140871000	-3.087511000	-1.514878000
1	1.896612000	-4.549212000	-0.811805000
6	3.667956000	-3.342331000	0.854448000
1	3.934494000	-4.377469000	0.579213000
1	4.604673000	-2.813856000	1.090958000
1	3.071256000	-3.399521000	1.781152000
6	-3.712061000	-0.005079000	-0.471664000
1	-3.323186000	1.028557000	-0.363851000
6	-5.040140000	-0.075269000	0.265290000
1	-5.522484000	-1.059374000	0.159840000
1	-4.938661000	0.136027000	1.341880000
1	-5.739036000	0.672378000	-0.149397000
6	-3.864805000	-0.281530000	-1.960604000
1	-4.324169000	-1.269230000	-2.139808000
1	-4.521055000	0.470328000	-2.431932000
1	-2.894888000	-0.261877000	-2.487122000
6	1.547828000	3.110094000	0.170863000
1	2.209502000	2.394044000	0.698253000
6	1.582262000	4.436713000	0.908398000
1	2.577079000	4.905948000	0.814337000
1	0.849242000	5.155302000	0.499684000
1	1.376664000	4.323568000	1.984755000
6	2.040075000	3.230494000	-1.264279000
1	3.095358000	3.553417000	-1.294519000
1	1.960023000	2.268049000	-1.799066000
1	1.458737000	3.977210000	-1.833050000
15	-2.262600000	-0.950151000	0.236693000
15	-0.107915000	2.231437000	0.178915000
15	2.425403000	-0.877182000	0.017968000
7	-0.023670000	-0.881081000	-3.269135000
7	0.005788000	-0.620042000	-2.063000000
1	-0.221725000	-1.904814000	-3.417298000

[4b'_{psi}] (TE = -3311.841504)

6	0.219161000	2.693326000	1.945495000
6	0.610939000	1.570960000	2.901101000
6	-2.732295000	0.132001000	2.020981000

6	-1.671954000	-0.529431000	2.894960000
6	2.441482000	-1.640813000	1.807169000
6	1.315276000	-1.455554000	2.821121000
1	-2.683281000	1.233989000	2.124919000
1	-1.783606000	-0.215351000	3.949892000
1	3.055177000	-2.543717000	1.992602000
1	1.732621000	-1.197605000	3.812447000
1	0.602055000	3.693079000	2.228864000
1	1.709751000	1.549778000	3.045210000
6	0.185168000	3.708450000	-0.823306000
1	0.896474000	4.536325000	-0.631899000
6	-2.899196000	-1.984351000	-0.016003000
1	-1.970684000	-2.487536000	0.323552000
6	3.491829000	-1.327910000	-0.846254000
1	3.735667000	-0.303410000	-0.498201000
23	0.000084000	-0.026835000	-0.424938000
1	-0.882160000	2.783620000	1.908220000
1	0.176951000	1.742876000	3.904290000
1	0.760678000	-2.401190000	2.958882000
1	3.140247000	-0.781517000	1.863905000
1	-1.802151000	-1.630136000	2.884765000
1	-3.767576000	-0.153327000	2.286574000
6	4.633915000	-2.249550000	-0.448978000
1	5.560577000	-1.951227000	-0.969842000
1	4.846835000	-2.231029000	0.631053000
1	4.433804000	-3.296319000	-0.737064000
6	3.325397000	-1.278697000	-2.356781000
1	3.183120000	-2.289802000	-2.776861000
1	2.458575000	-0.667648000	-2.659407000
1	4.227882000	-0.856800000	-2.832479000
6	-4.052986000	-2.509836000	0.822451000
1	-4.169753000	-3.594744000	0.654031000
1	-3.894368000	-2.366383000	1.903120000
1	-5.012019000	-2.037122000	0.556370000
6	-3.073227000	-2.311384000	-1.492611000
1	-4.022587000	-1.907692000	-1.885963000
1	-2.250661000	-1.910970000	-2.109195000
1	-3.103425000	-3.404854000	-1.640255000
6	0.204816000	3.351331000	-2.304626000
1	1.187476000	3.004258000	-2.657541000
1	-0.512092000	2.537362000	-2.509807000
1	-0.084526000	4.224090000	-2.914825000
6	-1.213835000	4.153869000	-0.422481000
1	-1.255112000	4.591982000	0.586370000
1	-1.595791000	4.909843000	-1.129302000
1	-1.915163000	3.298248000	-0.451569000

6	1.461301000	-3.419232000	-0.352263000
1	2.434734000	-3.930943000	-0.484910000
6	0.652785000	-3.513244000	-1.637609000
1	-0.310267000	-2.986332000	-1.517987000
1	1.150900000	-3.050262000	-2.502746000
1	0.444536000	-4.567891000	-1.887479000
6	0.712864000	-4.098431000	0.784108000
1	0.436797000	-5.126744000	0.494068000
1	1.302453000	-4.163560000	1.711687000
1	-0.226574000	-3.563299000	1.016963000
6	-3.703379000	0.907198000	-0.582272000
1	-3.498767000	1.866099000	-0.060574000
6	-5.157287000	0.540870000	-0.328167000
1	-5.437348000	-0.386132000	-0.856730000
1	-5.385768000	0.405253000	0.741131000
1	-5.821578000	1.336952000	-0.707408000
6	-3.433056000	1.128869000	-2.062900000
1	-3.602711000	0.214011000	-2.654449000
1	-4.099249000	1.912272000	-2.463826000
1	-2.390322000	1.436873000	-2.240946000
6	2.603550000	2.419509000	0.307898000
1	2.889153000	1.516250000	0.884596000
6	3.108364000	3.646703000	1.047435000
1	4.211851000	3.673313000	1.033768000
1	2.760475000	4.581880000	0.573807000
1	2.795212000	3.666060000	2.102914000
6	3.234235000	2.306853000	-1.072451000
1	4.323467000	2.145651000	-0.990718000
1	2.808553000	1.469359000	-1.652274000
1	3.090204000	3.232919000	-1.655568000
15	-2.401558000	-0.186038000	0.218060000
15	0.733733000	2.242901000	0.217947000
15	1.854002000	-1.620723000	0.032727000
14	0.071244000	-0.143945000	2.169328000
7	-0.394902000	-0.513850000	-3.403613000
7	-0.185621000	-0.234111000	-2.217568000
1	-0.190234000	0.318238000	-4.010010000

[4c'_{PB}] (TE = -3047.245892)

6	-0.449215000	2.350603000	2.132032000
6	0.372869000	1.311740000	2.885113000
6	-2.470023000	-0.535407000	2.030598000
6	-1.241170000	-0.933298000	2.843373000
6	2.670569000	-0.758717000	1.792763000
6	1.468364000	-1.167059000	2.635409000

1	-2.667700000	0.550150000	2.095069000
1	-1.452117000	-0.724308000	3.915113000
1	3.584362000	-1.326770000	2.042536000
1	1.767602000	-1.150524000	3.707454000
1	-0.315689000	3.377208000	2.522469000
1	1.443750000	1.591943000	2.831622000
6	-1.159357000	3.569011000	-0.471007000
1	-0.597095000	4.522642000	-0.447754000
6	-2.274499000	-2.759048000	0.151671000
1	-1.268838000	-3.014410000	0.539926000
6	3.691933000	-0.008832000	-0.834198000
1	3.565574000	1.021273000	-0.442928000
23	-0.004850000	-0.055427000	-0.572214000
1	-1.525940000	2.129812000	2.218026000
1	0.121804000	1.388284000	3.965726000
1	1.214165000	-2.226209000	2.430096000
1	2.919680000	0.308501000	1.953784000
1	-1.127893000	-2.034976000	2.791301000
1	-3.390456000	-1.031828000	2.390564000
6	5.090224000	-0.485354000	-0.476497000
1	5.845586000	0.194140000	-0.908348000
1	5.266286000	-0.522365000	0.610719000
1	5.292874000	-1.487908000	-0.890865000
6	3.493388000	0.036966000	-2.341817000
1	3.600871000	-0.964246000	-2.796234000
1	2.491487000	0.409250000	-2.611777000
1	4.247600000	0.690395000	-2.813712000
6	-3.305039000	-3.456321000	1.024790000
1	-3.184986000	-4.550445000	0.937987000
1	-3.200694000	-3.204713000	2.092092000
1	-4.337902000	-3.220787000	0.721384000
6	-2.339699000	-3.236979000	-1.292250000
1	-3.359493000	-3.132505000	-1.702346000
1	-1.650172000	-2.681929000	-1.951140000
1	-2.077611000	-4.307500000	-1.354155000
6	-1.433617000	3.186571000	-1.918730000
1	-0.513510000	3.007528000	-2.497834000
1	-2.021056000	2.252011000	-1.961203000
1	-2.012144000	3.975155000	-2.430208000
6	-2.466871000	3.768345000	0.279214000
1	-2.324634000	4.173661000	1.292539000
1	-3.118681000	4.468728000	-0.270351000
1	-3.024725000	2.818079000	0.371185000
6	2.557533000	-2.707748000	-0.450675000
1	2.979499000	-2.644447000	-1.473687000
6	1.243267000	-3.467137000	-0.540583000

1	0.778197000	-3.565218000	0.458219000
1	0.525449000	-2.957810000	-1.203129000
1	1.410730000	-4.488541000	-0.924621000
6	3.537936000	-3.447650000	0.447022000
1	3.706927000	-4.467668000	0.060559000
1	4.520056000	-2.958021000	0.525075000
1	3.135342000	-3.555716000	1.469224000
6	-3.711077000	-0.157794000	-0.571138000
1	-3.612936000	0.893521000	-0.225937000
6	-5.061440000	-0.683485000	-0.112105000
1	-5.244071000	-1.703084000	-0.491880000
1	-5.165404000	-0.705801000	0.984692000
1	-5.872794000	-0.047401000	-0.507070000
6	-3.605294000	-0.145318000	-2.089997000
1	-3.782627000	-1.145710000	-2.517635000
1	-4.359057000	0.534531000	-2.523697000
1	-2.607696000	0.180276000	-2.429309000
6	1.641696000	3.088506000	0.254016000
1	2.297384000	2.306804000	0.687101000
6	1.796805000	4.356411000	1.075429000
1	2.805077000	4.782532000	0.933307000
1	1.075019000	5.136064000	0.773008000
1	1.668443000	4.179906000	2.154798000
6	2.059423000	3.298950000	-1.193574000
1	3.127052000	3.573095000	-1.257561000
1	1.906030000	2.388275000	-1.798232000
1	1.487590000	4.117722000	-1.664608000
15	-2.186368000	-0.888989000	0.238229000
15	-0.049679000	2.272894000	0.327017000
15	2.262901000	-0.899473000	-0.007019000
5	0.169591000	-0.239589000	2.518142000
7	0.032756000	-1.116490000	-3.416563000
7	0.000071000	-0.531691000	-2.324641000
1	0.109526000	-0.419285000	-4.195798000

[4d'_{sc}] (TE = -2876.104036)

6	0.177528000	2.267784000	1.547949000
6	0.295833000	1.088256000	2.508267000
6	-2.576415000	0.267648000	1.805262000
6	-1.520999000	-0.653549000	2.373071000
6	2.227300000	-1.358181000	1.895590000
6	0.845333000	-1.355023000	2.523527000
1	-2.425241000	1.310660000	2.131835000
1	-1.639601000	-0.648124000	3.486581000
1	2.897080000	-2.107818000	2.349886000

1	0.975963000	-1.254905000	3.628844000
1	0.585356000	3.195708000	1.984932000
1	1.351825000	1.067024000	2.844614000
6	0.695290000	3.079977000	-1.210416000
1	1.473398000	2.881442000	-1.971459000
6	-3.399854000	-1.167761000	-0.595862000
1	-2.679953000	-1.997154000	-0.481899000
6	3.476097000	-0.847837000	-0.631184000
1	3.464639000	0.166161000	-0.189497000
23	-0.064840000	-0.415327000	-0.288573000
16	-2.507703000	0.361806000	-0.026345000
16	1.144016000	1.813457000	0.059719000
16	2.029119000	-1.724822000	0.108821000
6	-0.098181000	-0.295350000	1.953588000
1	-0.864222000	2.464360000	1.238764000
1	-0.280101000	1.344202000	3.428082000
1	0.400749000	-2.359967000	2.377418000
1	2.717171000	-0.370158000	1.975902000
1	-1.750098000	-1.692349000	2.055739000
1	-3.603786000	0.004064000	2.102912000
6	4.766509000	-1.561033000	-0.288563000
1	5.628150000	-1.023219000	-0.719965000
1	4.926674000	-1.627470000	0.799351000
1	4.765085000	-2.586042000	-0.696370000
6	3.232981000	-0.755849000	-2.124179000
1	3.140865000	-1.761426000	-2.571426000
1	2.304118000	-0.204924000	-2.348303000
1	4.076229000	-0.243983000	-2.616916000
6	-4.662975000	-1.436706000	0.188989000
1	-5.209422000	-2.271899000	-0.280627000
1	-4.466347000	-1.727371000	1.232374000
1	-5.329804000	-0.556543000	0.188660000
6	-3.685207000	-0.939376000	-2.067442000
1	-4.447616000	-0.152294000	-2.199046000
1	-2.778322000	-0.643156000	-2.616747000
1	-4.060496000	-1.869331000	-2.525654000
6	-0.667369000	2.842039000	-1.823595000
1	-0.753823000	1.818926000	-2.227639000
1	-1.476279000	2.981989000	-1.086129000
1	-0.841836000	3.556963000	-2.645808000
6	0.870182000	4.485367000	-0.673122000
1	1.860558000	4.629565000	-0.213504000
1	0.759291000	5.219745000	-1.488420000
1	0.101638000	4.720959000	0.082411000
7	-0.656098000	-2.449310000	-2.482678000
7	-0.406867000	-1.504769000	-1.729676000

1 -0.393002000 -2.202047000 -3.471644000

[4e' ssi] (TE = -3127.468242)

6	0.506686000	0.232234000	-2.684047000
6	0.172701000	-1.253083000	-2.694996000
6	2.718401000	-2.171869000	-0.385046000
6	1.550691000	-3.105909000	-0.649792000
6	-2.749834000	-1.910165000	-0.531434000
6	-1.651127000	-2.926905000	-0.798473000
1	2.942347000	-1.570335000	-1.285142000
1	1.782676000	-3.746214000	-1.520873000
1	-3.732973000	-2.375639000	-0.345296000
1	-1.906882000	-3.500399000	-1.708998000
1	0.349630000	0.720709000	-3.661514000
1	-0.786856000	-1.407921000	-3.225122000
6	-0.195356000	2.833298000	-1.534922000
1	-0.990806000	3.243283000	-0.884565000
6	3.792868000	0.042471000	1.065584000
1	4.615605000	-0.656559000	1.307606000
6	-3.555539000	0.513869000	0.698014000
1	-3.403865000	0.840303000	-0.348820000
23	0.007141000	-0.015910000	0.760763000
16	2.278051000	-1.020925000	0.989049000
16	-0.604282000	1.030689000	-1.448780000
16	-2.349296000	-0.870663000	0.947425000
1	1.551075000	0.414339000	-2.368750000
1	0.940825000	-1.795969000	-3.277467000
1	-1.600463000	-3.653959000	0.033881000
1	-2.860635000	-1.210014000	-1.381447000
1	1.390797000	-3.772418000	0.217676000
1	3.649981000	-2.683214000	-0.081618000
6	-4.978947000	0.041286000	0.906646000
1	-5.683553000	0.875894000	0.749564000
1	-5.262744000	-0.764364000	0.211842000
1	-5.116694000	-0.329774000	1.936359000
6	-3.175974000	1.637737000	1.639879000
1	-3.220686000	1.306462000	2.692293000
1	-2.152218000	2.000676000	1.451655000
1	-3.877115000	2.480604000	1.522775000
6	4.068940000	0.751309000	-0.241388000
1	4.920943000	1.443449000	-0.130587000
1	4.312550000	0.059392000	-1.062478000
1	3.185516000	1.342590000	-0.535841000
6	3.585457000	1.016401000	2.206942000
1	2.735498000	1.688370000	1.995535000

1	3.367826000	0.499698000	3.155109000
1	4.486695000	1.634983000	2.348800000
6	1.151429000	3.146905000	-0.925369000
1	1.225136000	2.735649000	0.096176000
1	1.968873000	2.728213000	-1.538370000
1	1.307710000	4.237758000	-0.872789000
6	-0.360977000	3.383547000	-2.936461000
1	-1.333565000	3.108624000	-3.373717000
1	-0.289918000	4.484154000	-2.922448000
1	0.435088000	3.017634000	-3.606921000
14	0.015116000	-1.983494000	-0.894410000
7	0.186268000	1.467032000	3.435820000
7	0.110449000	0.866887000	2.362263000
1	0.129225000	0.789034000	4.237178000

[4f_{SB}] (TE = -2862.882797)

6	0.498650000	2.412184000	1.609582000
6	0.407287000	1.293918000	2.634230000
6	-2.733924000	0.878552000	1.353037000
6	-2.003148000	0.001291000	2.345885000
6	1.665441000	-1.695542000	2.108713000
6	0.283988000	-1.438740000	2.674091000
1	-2.356025000	1.916265000	1.359588000
1	-2.258518000	0.377710000	3.361713000
1	2.156769000	-2.585019000	2.539726000
1	0.378268000	-1.447098000	3.783223000
1	1.080343000	3.278327000	1.971063000
1	1.439746000	1.048562000	2.954990000
6	1.073579000	3.045130000	-1.162366000
1	1.696585000	2.646024000	-1.984842000
6	-3.247499000	-1.345389000	-0.401186000
1	-2.518714000	-1.993183000	0.124024000
6	3.245324000	-1.448443000	-0.241783000
1	3.414479000	-0.460115000	0.226752000
23	-0.065087000	-0.234288000	-0.515112000
16	-2.494316000	0.359327000	-0.392338000
16	1.334439000	1.737051000	0.122240000
16	1.541531000	-1.948007000	0.290866000
1	-0.496687000	2.776472000	1.300284000
1	-0.076341000	1.723483000	3.537491000
1	-0.370951000	-2.301037000	2.437104000
1	2.336583000	-0.829752000	2.263050000
1	-2.428572000	-1.020293000	2.309052000
1	-3.822208000	0.950256000	1.525663000
6	4.269228000	-2.451708000	0.245342000

1	5.282191000	-2.140166000	-0.061954000
1	4.272691000	-2.550727000	1.342014000
1	4.073497000	-3.447118000	-0.188113000
6	3.250088000	-1.302893000	-1.749476000
1	2.953614000	-2.246879000	-2.240122000
1	2.551107000	-0.518371000	-2.082498000
1	4.263684000	-1.044432000	-2.098167000
6	-4.590811000	-1.363257000	0.295405000
1	-5.046114000	-2.361542000	0.183749000
1	-4.524296000	-1.153390000	1.373542000
1	-5.277478000	-0.629461000	-0.161905000
6	-3.367904000	-1.776018000	-1.849398000
1	-4.061848000	-1.111154000	-2.392446000
1	-2.403432000	-1.782867000	-2.378298000
1	-3.781563000	-2.797423000	-1.891433000
6	-0.364214000	3.128164000	-1.627394000
1	-0.713237000	2.163374000	-2.030282000
1	-1.041946000	3.425922000	-0.807509000
1	-0.461786000	3.888601000	-2.420803000
6	1.629785000	4.378608000	-0.706654000
1	2.662909000	4.288209000	-0.336341000
1	1.626615000	5.096429000	-1.543890000
1	1.012312000	4.815722000	0.096295000
5	-0.401538000	-0.052059000	2.241392000
7	-0.247343000	-1.402127000	-3.321389000
7	-0.121233000	-0.838473000	-2.232124000
1	0.321372000	-0.911280000	-4.055979000

[4a''_{pc}] (TE = -3517.016994)

6	1.103394000	-0.818908000	1.752413000
6	1.769845000	-0.389968000	2.914940000
1	1.403590000	0.501240000	3.436017000
6	2.877280000	-1.061595000	3.426260000
1	3.368109000	-0.685601000	4.329568000
6	3.350861000	-2.210772000	2.799064000
1	4.219345000	-2.746265000	3.193182000
6	2.710727000	-2.661743000	1.646644000
1	3.104808000	-3.546296000	1.134086000
6	1.613868000	-1.979363000	1.107395000
6	-0.153674000	1.351951000	1.704569000
6	-0.975386000	1.758284000	2.773458000
1	-1.601781000	1.015540000	3.278030000
6	-1.029399000	3.080036000	3.205159000
1	-1.689415000	3.351011000	4.035167000
6	-0.245726000	4.050186000	2.586473000

1	-0.282164000	5.093227000	2.913590000
6	0.584689000	3.674531000	1.534243000
1	1.188792000	4.442652000	1.044258000
6	0.633084000	2.350581000	1.082235000
6	-1.408110000	-0.755706000	1.596481000
6	-1.536402000	-1.573184000	2.729978000
1	-0.641661000	-1.812875000	3.315780000
6	-2.771545000	-2.072323000	3.136058000
1	-2.833651000	-2.707574000	4.025413000
6	-3.925841000	-1.753449000	2.424828000
1	-4.900271000	-2.135016000	2.742931000
6	-3.825438000	-0.942101000	1.295585000
1	-4.732427000	-0.694852000	0.735302000
6	-2.586280000	-0.459613000	0.863322000
6	-0.108275000	-0.085178000	1.230524000
23	0.056960000	-0.094200000	-1.097911000
6	2.435575000	-2.870425000	-1.574188000
1	2.968710000	-3.677077000	-1.036955000
6	1.463888000	3.340528000	-1.550432000
1	0.445803000	3.715799000	-1.319286000
6	-3.453964000	-0.216133000	-2.018338000
1	-3.015746000	0.261956000	-2.917991000
6	-4.935572000	0.125183000	-1.979181000
1	-5.435017000	-0.299130000	-2.867627000
1	-5.445197000	-0.298795000	-1.098272000
1	-5.126139000	1.208960000	-1.989718000
6	-3.226836000	-1.714926000	-2.160177000
1	-3.646942000	-2.267994000	-1.301513000
1	-3.719069000	-2.091393000	-3.072346000
1	-2.151072000	-1.949480000	-2.232229000
6	1.980205000	-3.385523000	-2.933957000
1	1.450231000	-4.348905000	-2.875434000
1	1.308439000	-2.659604000	-3.426838000
1	2.850580000	-3.533352000	-3.595609000
6	3.371055000	-1.688569000	-1.741507000
1	3.709068000	-1.281833000	-0.773727000
1	4.267181000	-1.976446000	-2.317936000
1	2.858427000	-0.877051000	-2.289548000
6	2.455711000	4.476333000	-1.332302000
1	2.160407000	5.347208000	-1.942635000
1	2.527402000	4.820098000	-0.289808000
1	3.470597000	4.196268000	-1.656297000
6	1.474639000	2.903695000	-3.010997000
1	2.434080000	2.429611000	-3.285054000
1	0.675487000	2.174537000	-3.218917000
1	1.337633000	3.775424000	-3.673831000

15	-2.307186000	0.456856000	-0.701859000
15	1.532268000	1.827389000	-0.429845000
15	0.942344000	-2.360805000	-0.563368000
6	3.309682000	1.548262000	0.125561000
1	3.230607000	0.518776000	0.529567000
6	4.276081000	1.517510000	-1.051066000
1	4.537038000	2.532170000	-1.392321000
1	5.219469000	1.026157000	-0.756824000
1	3.875284000	0.966020000	-1.916145000
6	3.811149000	2.442852000	1.246018000
1	4.815626000	2.113160000	1.565182000
1	3.899828000	3.496214000	0.930256000
1	3.154297000	2.406868000	2.129382000
6	0.005767000	-3.987726000	-0.478375000
1	-0.281637000	-4.137605000	-1.538015000
6	-1.265621000	-3.881598000	0.341666000
1	-1.033389000	-3.789208000	1.415534000
1	-1.877079000	-3.010664000	0.060027000
1	-1.878324000	-4.789960000	0.212117000
6	0.835857000	-5.171471000	-0.008526000
1	0.225866000	-6.091151000	-0.028120000
1	1.727565000	-5.360035000	-0.626879000
1	1.166038000	-5.027541000	1.035318000
6	-2.772389000	2.243805000	-0.402276000
1	-1.914926000	2.578451000	0.211533000
6	-4.036331000	2.510653000	0.396388000
1	-4.114797000	3.587273000	0.629540000
1	-4.951551000	2.226502000	-0.148206000
1	-4.032030000	1.967702000	1.355563000
6	-2.711287000	3.005870000	-1.718677000
1	-2.714280000	4.094356000	-1.538062000
1	-1.791812000	2.759734000	-2.281556000
1	-3.571649000	2.781901000	-2.372486000
7	-0.331051000	-0.437215000	-4.085278000
7	-0.075705000	-0.231616000	-2.895155000
1	0.235861000	0.203821000	-4.691670000

[4b''_{psi}] (TE = -3768.375289)

6	1.188507000	-1.470883000	1.956481000
6	1.110169000	-2.074739000	3.218882000
1	0.298490000	-1.794193000	3.902455000
6	2.030325000	-3.041290000	3.618429000
1	1.947359000	-3.506528000	4.605668000
6	3.056987000	-3.416251000	2.753204000
1	3.787156000	-4.171907000	3.058520000

6	3.146209000	-2.837706000	1.488912000
1	3.950945000	-3.156607000	0.818730000
6	2.212271000	-1.878457000	1.077515000
6	0.540545000	1.501427000	2.123878000
6	1.043347000	1.602149000	3.427902000
1	1.096784000	0.703915000	4.056305000
6	1.513984000	2.810871000	3.935574000
1	1.915759000	2.862768000	4.952344000
6	1.480075000	3.951915000	3.137312000
1	1.851113000	4.906657000	3.522224000
6	0.981755000	3.876883000	1.838186000
1	0.976337000	4.784772000	1.229502000
6	0.520638000	2.660409000	1.318639000
6	-1.772877000	-0.503838000	1.927139000
6	-2.218351000	-0.228613000	3.227552000
1	-1.499907000	0.117076000	3.981840000
6	-3.563097000	-0.332827000	3.573789000
1	-3.890687000	-0.095938000	4.590869000
6	-4.493324000	-0.720806000	2.611292000
1	-5.554981000	-0.791561000	2.866488000
6	-4.072605000	-1.013891000	1.316427000
1	-4.821837000	-1.309436000	0.577425000
6	-2.720876000	-0.909440000	0.962494000
23	0.067180000	0.064916000	-1.220899000
6	3.756708000	-0.073011000	-0.599824000
1	4.612880000	-0.760015000	-0.464699000
6	-1.780334000	3.262315000	-0.366289000
1	-1.600461000	4.327540000	-0.128945000
6	-1.978900000	-3.098938000	-0.845216000
1	-2.044230000	-3.293581000	-1.935905000
6	-3.068192000	-3.868527000	-0.113532000
1	-2.934363000	-4.951021000	-0.283268000
1	-2.995186000	-3.699901000	0.974497000
1	-4.089746000	-3.612978000	-0.424219000
6	-0.622592000	-3.571968000	-0.350609000
1	-0.505058000	-3.385664000	0.732656000
1	-0.507269000	-4.657356000	-0.513086000
1	0.199846000	-3.055269000	-0.863530000
6	3.888719000	0.663781000	-1.922713000
1	3.843457000	-0.002033000	-2.800848000
1	3.065656000	1.391748000	-2.025038000
1	4.839159000	1.222324000	-1.969320000
6	3.733617000	0.907999000	0.560485000
1	3.697187000	0.405808000	1.540726000
1	4.635509000	1.543411000	0.538462000
1	2.855535000	1.575858000	0.499438000

6	-2.449685000	3.142310000	-1.725974000
1	-3.466684000	3.569944000	-1.701601000
1	-1.894427000	3.651755000	-2.530097000
1	-2.536446000	2.078606000	-2.011392000
6	-2.661499000	2.674252000	0.721431000
1	-2.872557000	1.607629000	0.534442000
1	-2.208390000	2.751663000	1.723008000
1	-3.629816000	3.202635000	0.747098000
14	-0.005422000	-0.137072000	1.299574000
15	-0.082320000	2.453251000	-0.426564000
15	-2.088706000	-1.214870000	-0.755511000
15	2.215031000	-1.143065000	-0.629074000
6	2.709851000	-2.632251000	-1.705381000
1	2.322912000	-3.482711000	-1.111685000
6	4.199467000	-2.852757000	-1.928845000
1	4.352367000	-3.791543000	-2.488573000
1	4.645413000	-2.047087000	-2.535474000
1	4.785713000	-2.931721000	-1.000089000
6	1.977075000	-2.615652000	-3.038983000
1	0.891086000	-2.465664000	-2.921757000
1	2.327890000	-1.798005000	-3.690702000
1	2.145213000	-3.565070000	-3.575936000
6	-3.517658000	-0.774439000	-1.915239000
1	-3.907028000	0.162618000	-1.465988000
6	-2.934484000	-0.450903000	-3.285323000
1	-2.419982000	-1.327832000	-3.719748000
1	-3.734786000	-0.156370000	-3.985442000
1	-2.191824000	0.359508000	-3.244879000
6	-4.671299000	-1.752552000	-2.093291000
1	-4.329630000	-2.697764000	-2.548489000
1	-5.210557000	-1.999269000	-1.167608000
1	-5.411494000	-1.319085000	-2.787559000
6	0.940267000	3.717950000	-1.407375000
1	1.930824000	3.647976000	-0.913642000
6	0.472521000	5.168094000	-1.371767000
1	1.226143000	5.810781000	-1.858269000
1	-0.465146000	5.299224000	-1.937755000
1	0.304694000	5.573443000	-0.363398000
6	1.105528000	3.287138000	-2.858446000
1	1.525219000	2.274823000	-2.942848000
1	0.136962000	3.279235000	-3.390154000
1	1.768485000	3.990734000	-3.390762000
7	0.489470000	0.124080000	-4.230711000
7	0.295679000	0.159172000	-3.013040000
1	0.664299000	1.090606000	-4.600162000

[4c''_{PB}] (TE = -3503.789021)

6	-1.481514000	0.625216000	1.925591000
6	-1.610484000	1.338813000	3.132201000
1	-0.706121000	1.579578000	3.703855000
6	-2.842448000	1.759679000	3.625499000
1	-2.892997000	2.315886000	4.566917000
6	-4.006977000	1.472420000	2.917645000
1	-4.982826000	1.793832000	3.293568000
6	-3.913843000	0.782410000	1.712793000
1	-4.830214000	0.577683000	1.150231000
6	-2.672889000	0.373311000	1.207621000
6	0.413531000	-1.348195000	1.972058000
6	-0.029984000	-1.804491000	3.226583000
1	-0.757938000	-1.199746000	3.781545000
6	0.423187000	-2.994044000	3.790567000
1	0.044870000	-3.315076000	4.766351000
6	1.367601000	-3.766282000	3.118048000
1	1.744855000	-4.694537000	3.557235000
6	1.817066000	-3.350163000	1.867617000
1	2.548258000	-3.966246000	1.334569000
6	1.330835000	-2.175681000	1.279375000
6	1.158098000	1.208063000	1.722177000
6	1.845500000	1.179497000	2.951244000
1	1.584349000	0.405965000	3.684158000
6	2.860277000	2.077869000	3.262800000
1	3.369551000	2.014850000	4.229651000
6	3.236229000	3.045291000	2.333268000
1	4.041980000	3.750963000	2.555831000
6	2.580826000	3.098740000	1.108497000
1	2.895810000	3.849819000	0.379712000
6	1.550893000	2.198871000	0.794955000
23	-0.130878000	-0.195107000	-1.175856000
6	-3.254724000	-2.090229000	-0.285292000
1	-4.315354000	-1.945691000	-0.003307000
6	3.568836000	-1.393525000	-0.504270000
1	4.052298000	-2.353766000	-0.241715000
6	-0.354661000	3.702376000	-0.905374000
1	-0.405979000	3.937416000	-1.988556000
6	0.161237000	4.911993000	-0.142290000
1	-0.535822000	5.757559000	-0.273998000
1	0.210145000	4.695049000	0.938434000
1	1.154949000	5.254788000	-0.461341000
6	-1.751114000	3.357892000	-0.421282000
1	-1.745507000	3.068811000	0.645598000

1	-2.426652000	4.223547000	-0.529509000
1	-2.172993000	2.517869000	-0.988763000
6	-3.186442000	-2.819700000	-1.621672000
1	-3.868128000	-2.387625000	-2.371293000
1	-2.176190000	-2.781791000	-2.061454000
1	-3.463918000	-3.880855000	-1.499640000
6	-2.570419000	-2.852372000	0.838585000
1	-2.747964000	-2.380415000	1.818406000
1	-2.951263000	-3.887004000	0.886185000
1	-1.477068000	-2.902638000	0.700810000
6	3.963619000	-0.994932000	-1.918928000
1	5.050882000	-0.820225000	-1.988339000
1	3.698922000	-1.752237000	-2.674925000
1	3.456841000	-0.057207000	-2.208634000
6	4.008973000	-0.349287000	0.503536000
1	3.556879000	0.633651000	0.288801000
1	3.731267000	-0.619502000	1.534918000
1	5.105088000	-0.227365000	0.467434000
5	-0.012734000	0.127822000	1.514053000
7	-0.343496000	-1.576933000	-3.867497000
7	-0.255652000	-0.908656000	-2.836069000
1	-0.093712000	-0.989264000	-4.700777000
15	0.742738000	2.169685000	-0.856923000
15	-2.520460000	-0.378382000	-0.464382000
15	1.727621000	-1.727525000	-0.460871000
6	2.099534000	2.546056000	-2.117089000
1	2.965001000	1.985380000	-1.709523000
6	2.516615000	3.993121000	-2.340162000
1	3.317445000	4.030100000	-3.098271000
1	1.682554000	4.599692000	-2.732520000
1	2.906405000	4.494774000	-1.442757000
6	1.703024000	1.927202000	-3.453486000
1	1.517053000	0.844380000	-3.370479000
1	0.774831000	2.386019000	-3.843666000
1	2.493029000	2.093550000	-4.205911000
6	1.619050000	-3.318194000	-1.472333000
1	1.530806000	-2.907966000	-2.497180000
6	0.318244000	-4.041427000	-1.174611000
1	-0.526174000	-3.338511000	-1.177687000
1	0.120633000	-4.811526000	-1.939077000
1	0.342094000	-4.538586000	-0.189251000
6	2.794385000	-4.284042000	-1.453140000
1	2.589795000	-5.111436000	-2.154495000
1	3.746083000	-3.829032000	-1.767114000
1	2.949406000	-4.744966000	-0.463625000
6	-3.805802000	0.539077000	-1.513202000

1	-3.839044000	1.533834000	-1.032846000
6	-5.227056000	-0.007125000	-1.525486000
1	-5.880814000	0.685043000	-2.083524000
1	-5.293726000	-0.982781000	-2.033124000
1	-5.665451000	-0.125076000	-0.522640000
6	-3.287161000	0.711074000	-2.935362000
1	-2.286319000	1.176669000	-2.958312000
1	-3.196619000	-0.260208000	-3.452561000
1	-3.976136000	1.339703000	-3.525466000

[4d''_{sc}] (TE = -3332.655948)

6	0.182905000	1.660183000	1.053958000
6	0.965155000	2.209642000	2.087387000
1	1.592573000	1.539849000	2.684857000
6	0.960467000	3.569026000	2.387681000
1	1.584460000	3.942833000	3.205436000
6	0.163910000	4.449377000	1.658251000
1	0.153875000	5.518415000	1.888185000
6	-0.588052000	3.950734000	0.599692000
1	-1.170105000	4.627868000	-0.034883000
6	-0.569601000	2.586747000	0.297471000
6	-1.021139000	-0.455503000	1.581599000
6	-1.451883000	0.059193000	2.818924000
1	-0.994419000	0.981247000	3.192883000
6	-2.427657000	-0.564303000	3.590868000
1	-2.722420000	-0.122109000	4.547592000
6	-3.022975000	-1.746338000	3.154666000
1	-3.789820000	-2.243145000	3.755426000
6	-2.657680000	-2.261257000	1.915612000
1	-3.159102000	-3.148838000	1.514717000
6	-1.685666000	-1.622665000	1.140361000
6	1.424685000	-0.500109000	1.168895000
6	1.653159000	-1.023927000	2.456054000
1	0.847141000	-0.969987000	3.195055000
6	2.859798000	-1.607837000	2.827669000
1	2.981068000	-1.996203000	3.843619000
6	3.904478000	-1.705378000	1.911658000
1	4.851873000	-2.176636000	2.187470000
6	3.707486000	-1.230072000	0.620178000
1	4.486129000	-1.361484000	-0.137053000
6	2.496019000	-0.631562000	0.255340000
16	2.219930000	-0.325843000	-1.492114000
16	-1.296352000	2.068260000	-1.253926000
16	-1.507112000	-2.144474000	-0.561739000
23	-0.265152000	-0.180075000	-1.426172000
6	-3.143463000	2.033575000	-0.987912000

1	-3.432237000	3.101040000	-0.998150000
6	-0.576435000	-3.758655000	-0.527443000
1	-1.315914000	-4.493406000	-0.158667000
6	3.119399000	1.257789000	-1.915005000
1	2.969380000	1.253305000	-3.010921000
6	4.595241000	1.146072000	-1.603820000
1	5.124114000	2.034247000	-1.988567000
1	4.767677000	1.109017000	-0.514648000
1	5.050850000	0.253456000	-2.060426000
6	2.487585000	2.491208000	-1.319082000
1	2.546319000	2.479492000	-0.217031000
1	3.017049000	3.391559000	-1.674901000
1	1.428819000	2.583600000	-1.605887000
6	-3.709861000	1.321392000	-2.198520000
1	-3.382399000	1.779485000	-3.145555000
1	-3.379997000	0.267463000	-2.209835000
1	-4.811558000	1.343495000	-2.167882000
6	-3.565944000	1.392819000	0.309598000
1	-3.108188000	1.874771000	1.187868000
1	-4.661883000	1.467312000	0.413924000
1	-3.296486000	0.323303000	0.325403000
6	-0.234630000	-4.042008000	-1.976238000
1	0.238956000	-5.032882000	-2.070526000
1	-1.124956000	-4.020974000	-2.625721000
1	0.475501000	-3.282637000	-2.351331000
6	0.639925000	-3.745343000	0.362837000
1	1.383723000	-3.018054000	-0.004557000
1	0.395488000	-3.486100000	1.405119000
1	1.110775000	-4.743333000	0.361907000
6	0.116226000	0.168754000	0.796032000
7	-1.467754000	-0.746318000	-4.145264000
7	-0.837250000	-0.495820000	-3.120388000
1	-0.814943000	-0.915698000	-4.947216000

[4e''_{ssi}] (TE = -3584.016690)

6	1.111456000	-1.139409000	1.841338000
6	1.273275000	-1.219605000	3.232603000
1	0.779282000	-0.481854000	3.876955000
6	2.044027000	-2.216430000	3.826532000
1	2.152700000	-2.250038000	4.914858000
6	2.669745000	-3.177114000	3.032652000
1	3.268978000	-3.968898000	3.491724000
6	2.508004000	-3.142805000	1.650768000
1	2.963550000	-3.915688000	1.022320000
6	1.743442000	-2.128206000	1.067289000

6	1.126412000	1.817271000	1.029803000
6	1.592859000	2.390112000	2.222647000
1	1.386331000	1.889608000	3.176884000
6	2.319673000	3.578354000	2.233687000
1	2.665452000	4.000586000	3.182176000
6	2.616861000	4.223539000	1.033416000
1	3.197022000	5.150994000	1.032757000
6	2.191716000	3.669990000	-0.170481000
1	2.448109000	4.149976000	-1.121201000
6	1.445805000	2.487536000	-0.162536000
6	-1.572195000	0.495177000	1.705483000
6	-1.782665000	0.996586000	2.998667000
1	-0.920693000	1.193685000	3.648012000
6	-3.059286000	1.271512000	3.483537000
1	-3.188380000	1.660355000	4.498218000
6	-4.169856000	1.072877000	2.665080000
1	-5.174456000	1.308616000	3.028306000
6	-3.995689000	0.593614000	1.369849000
1	-4.857875000	0.473152000	0.706727000
6	-2.711721000	0.285670000	0.906167000
16	-2.564963000	-0.300897000	-0.804923000
16	1.520981000	-2.183196000	-0.729403000
16	0.954232000	1.804179000	-1.766983000
23	-0.156250000	-0.459873000	-1.517680000
6	3.242192000	-1.803865000	-1.330840000
1	3.853118000	-2.656014000	-0.981057000
6	-0.329599000	3.044899000	-2.306605000
1	0.237991000	3.985404000	-2.429068000
6	-3.055612000	-2.099251000	-0.681563000
1	-2.880618000	-2.407767000	-1.729574000
6	-4.519109000	-2.252247000	-0.329773000
1	-4.812976000	-3.310543000	-0.432478000
1	-4.714377000	-1.960135000	0.716174000
1	-5.168170000	-1.653310000	-0.987589000
6	-2.149864000	-2.885327000	0.238336000
1	-2.175242000	-2.490439000	1.269571000
1	-2.482241000	-3.936489000	0.275241000
1	-1.107122000	-2.875305000	-0.115807000
6	3.170899000	-1.801915000	-2.843559000
1	2.755059000	-2.742232000	-3.239479000
1	2.532630000	-0.972547000	-3.197824000
1	4.177836000	-1.661787000	-3.269667000
6	3.779755000	-0.507654000	-0.772774000
1	3.772627000	-0.486989000	0.328826000
1	4.820209000	-0.358300000	-1.107999000
1	3.184827000	0.346620000	-1.138004000

6	-0.849737000	2.572262000	-3.647492000
1	-1.573956000	3.300049000	-4.048564000
1	-0.040919000	2.448566000	-4.384914000
1	-1.367107000	1.601684000	-3.540528000
6	-1.428062000	3.225568000	-1.286067000
1	-2.012430000	2.296615000	-1.176234000
1	-1.041192000	3.510250000	-0.294592000
1	-2.119290000	4.017841000	-1.620069000
14	0.124388000	0.184441000	0.873942000
7	-1.239485000	-2.314028000	-3.637280000
7	-0.683977000	-1.441261000	-2.968089000
1	-1.082486000	-2.151931000	-4.661131000

[4f'_{SB}] (TE = -3319.434673)

6	-0.144721000	1.821736000	1.152636000
6	0.372518000	2.501008000	2.271768000
1	0.976756000	1.940524000	2.995923000
6	0.160173000	3.859789000	2.490073000
1	0.584642000	4.341691000	3.376307000
6	-0.582937000	4.606903000	1.577618000
1	-0.749830000	5.676242000	1.735569000
6	-1.082009000	3.980768000	0.440510000
1	-1.625558000	4.556035000	-0.316880000
6	-0.863250000	2.614319000	0.239314000
6	-1.043247000	-0.670922000	1.717063000
6	-1.495763000	-0.339302000	3.008228000
1	-1.117192000	0.575848000	3.480193000
6	-2.413436000	-1.119550000	3.706648000
1	-2.733234000	-0.817478000	4.708799000
6	-2.930773000	-2.277386000	3.127941000
1	-3.657978000	-2.893537000	3.664424000
6	-2.537207000	-2.620911000	1.839282000
1	-2.969120000	-3.496168000	1.341870000
6	-1.610193000	-1.828851000	1.154254000
6	1.587860000	-0.262753000	1.309166000
6	1.948125000	-0.612437000	2.624374000
1	1.186333000	-0.556690000	3.411619000
6	3.224334000	-1.053060000	2.963522000
1	3.451722000	-1.315929000	4.001270000
6	4.203209000	-1.180464000	1.980014000
1	5.202809000	-1.547270000	2.229890000
6	3.882231000	-0.867683000	0.663411000
1	4.617296000	-1.016392000	-0.133903000
6	2.601302000	-0.402554000	0.342902000
16	2.218754000	-0.192394000	-1.401972000

16	-1.381742000	1.934042000	-1.340323000
16	-1.312950000	-2.236700000	-0.568741000
23	-0.242179000	-0.245381000	-1.565507000
6	-3.227469000	1.715409000	-1.142499000
1	-3.612461000	2.751910000	-1.166027000
6	-0.215543000	-3.744042000	-0.500541000
1	-0.895972000	-4.553166000	-0.176427000
6	2.954759000	1.466785000	-1.850804000
1	2.526977000	1.588964000	-2.863595000
6	4.463186000	1.370792000	-1.932619000
1	4.875287000	2.304523000	-2.351030000
1	4.903519000	1.241608000	-0.929204000
1	4.792125000	0.534057000	-2.568137000
6	2.492977000	2.588927000	-0.953199000
1	2.798864000	2.414540000	0.093137000
1	2.948170000	3.538449000	-1.281713000
1	1.400387000	2.710782000	-0.970512000
6	-3.697616000	0.951184000	-2.361428000
1	-3.383504000	1.428834000	-3.303239000
1	-3.286271000	-0.073661000	-2.354948000
1	-4.797858000	0.883021000	-2.359569000
6	-3.617482000	1.044264000	0.151021000
1	-3.231862000	1.574574000	1.036103000
1	-4.717496000	1.008697000	0.227748000
1	-3.242638000	0.007386000	0.185399000
6	0.239380000	-3.986345000	-1.924542000
1	0.809665000	-4.927714000	-1.985787000
1	-0.608104000	-4.050309000	-2.626337000
1	0.897615000	-3.165020000	-2.261709000
6	0.933416000	-3.609074000	0.467733000
1	1.615957000	-2.799462000	0.159011000
1	0.594085000	-3.393582000	1.493341000
1	1.509638000	-4.549693000	0.490604000
5	0.088337000	0.240046000	1.034081000
7	-1.223499000	-0.872246000	-4.353810000
7	-0.694676000	-0.598068000	-3.278978000
1	-0.503039000	-0.944388000	-5.110900000

Cartesian coordinates of $[3\text{-V-H}]^+$, along with their total energies (in hartree) including zero point vibrational correction at M06-L-D3(heptane)/6-311+G* level of theory.

$[3\text{a}'_{\text{PC}}\text{-V-H}]^+$ (TE = -3062.522570)

6	-0.410706000	2.175615000	1.943146000
6	0.344230000	1.104044000	2.731607000

6	-2.474542000	-0.549950000	2.067535000
6	-1.190096000	-1.001491000	2.760978000
6	2.595973000	-0.983014000	1.854002000
6	1.316962000	-1.252862000	2.646394000
1	-2.687177000	0.508245000	2.248591000
1	-1.320402000	-0.860126000	3.848583000
1	3.398129000	-1.642308000	2.207061000
1	1.559628000	-1.163311000	3.721118000
1	-0.202645000	3.163226000	2.368009000
1	1.417352000	1.327278000	2.681855000
6	-1.034318000	3.363721000	-0.728712000
1	-0.380257000	4.231528000	-0.887042000
6	-2.852542000	-2.619684000	0.067070000
1	-2.187304000	-3.068230000	0.821030000
6	3.763669000	-0.119151000	-0.666910000
1	3.396152000	0.891984000	-0.451124000
23	-0.008601000	-0.403031000	-0.301743000
6	0.127328000	-0.357022000	2.392790000
1	-1.491764000	2.044019000	2.023242000
1	0.086966000	1.218069000	3.798800000
1	1.012275000	-2.292073000	2.501865000
1	2.959161000	0.037747000	2.031024000
1	-1.085475000	-2.083289000	2.621277000
1	-3.324797000	-1.094422000	2.495549000
6	5.136948000	-0.226120000	-0.011024000
1	5.764263000	0.608990000	-0.341054000
1	5.090553000	-0.174687000	1.080380000
1	5.669452000	-1.140070000	-0.274120000
6	3.825850000	-0.248083000	-2.184854000
1	4.200383000	-1.224221000	-2.505752000
1	2.846527000	-0.106958000	-2.653720000
1	4.499106000	0.504489000	-2.607347000
6	-4.289199000	-2.987293000	0.408314000
1	-4.392190000	-4.075655000	0.467632000
1	-4.622695000	-2.582017000	1.368057000
1	-4.991939000	-2.648957000	-0.358616000
6	-2.432603000	-3.175405000	-1.288665000
1	-2.996526000	-2.731255000	-2.114540000
1	-1.368288000	-3.008676000	-1.476328000
1	-2.609073000	-4.255037000	-1.327317000
6	-1.437203000	2.831790000	-2.099925000
1	-0.568634000	2.564712000	-2.709986000
1	-2.062339000	1.936219000	-2.022867000
1	-2.007112000	3.583641000	-2.654913000
6	-2.228891000	3.841553000	0.084989000
1	-1.931488000	4.327513000	1.018127000

1	-2.805791000	4.571895000	-0.490689000
1	-2.919627000	3.031338000	0.342008000
6	2.708891000	-2.935343000	-0.398683000
1	2.289938000	-3.036662000	-1.411848000
6	1.962237000	-3.897277000	0.520101000
1	2.385956000	-3.889518000	1.530745000
1	0.896479000	-3.672273000	0.589963000
1	2.068333000	-4.920026000	0.145625000
6	4.182277000	-3.323454000	-0.438108000
1	4.273933000	-4.392839000	-0.653789000
1	4.750698000	-2.796110000	-1.204517000
1	4.676533000	-3.153686000	0.524357000
6	-3.817460000	0.224909000	-0.404269000
1	-3.367463000	1.227867000	-0.381329000
6	-5.089704000	0.283045000	0.432851000
1	-5.649690000	-0.653395000	0.411917000
1	-4.899284000	0.531406000	1.480497000
1	-5.755578000	1.058318000	0.038912000
6	-4.109783000	-0.106376000	-1.863787000
1	-4.633297000	-1.061796000	-1.964084000
1	-4.754461000	0.656794000	-2.310874000
1	-3.202082000	-0.165284000	-2.473941000
6	1.717683000	2.924178000	0.101847000
1	2.378980000	2.216259000	0.623121000
6	1.807005000	4.264109000	0.818118000
1	2.801632000	4.700670000	0.682734000
1	1.089356000	4.994725000	0.430495000
1	1.643298000	4.179682000	1.895307000
6	2.166712000	3.024655000	-1.353086000
1	3.222960000	3.303754000	-1.420772000
1	2.037781000	2.081952000	-1.896968000
1	1.603071000	3.791998000	-1.894265000
15	-2.414000000	-0.816698000	0.239876000
15	0.041866000	2.108749000	0.154877000
15	2.366712000	-1.144249000	0.025843000
7	-0.135022000	-0.681469000	-3.427200000
7	-0.087472000	-0.574447000	-2.310980000
1	-0.131822000	-1.997905000	0.296451000

[3b'_{psi} -V-H]⁺ (TE = -3392.492931)

23	0.228421000	-0.447266000	-0.574288000
14	0.224256000	-0.555114000	2.161622000
6	-0.205916000	1.207396000	2.706258000
6	0.287128000	2.294537000	1.746674000

6	-1.719006000	-2.648990000	1.506756000
6	-1.017577000	-1.904497000	2.652109000
6	2.017874000	-0.951484000	2.613248000
6	2.809895000	-1.648029000	1.509808000
1	2.332394000	-2.597377000	1.230695000
1	3.822657000	-1.904438000	1.840885000
1	2.502579000	-0.005871000	2.891434000
1	2.021657000	-1.560068000	3.527910000
1	-2.602168000	-3.186596000	1.873741000
1	-1.047601000	-3.421612000	1.108705000
1	-1.756988000	-1.437618000	3.312224000
1	-0.490908000	-2.632789000	3.281854000
1	-1.287513000	1.296881000	2.853795000
1	0.232635000	1.365386000	3.702231000
1	1.383971000	2.278771000	1.681638000
1	0.021514000	3.293482000	2.110619000
6	4.014704000	0.792034000	0.450567000
1	3.329716000	1.542967000	0.871682000
6	-3.797325000	-0.810689000	0.479377000
1	-3.890473000	0.030531000	-0.220998000
6	0.432692000	3.365255000	-0.994521000
1	-0.151109000	3.346760000	-1.923118000
6	-3.773926000	-0.261294000	1.903349000
1	-4.610582000	0.427819000	2.057571000
1	-3.885665000	-1.067502000	2.635486000
1	-2.860573000	0.281672000	2.154376000
6	-5.032173000	-1.687182000	0.315620000
1	-5.223844000	-1.969669000	-0.719557000
1	-4.971187000	-2.602241000	0.912620000
1	-5.912754000	-1.137865000	0.665390000
6	0.356072000	4.757881000	-0.382926000
1	0.924249000	4.822726000	0.550534000
1	0.791691000	5.492400000	-1.068311000
1	-0.665134000	5.081906000	-0.175675000
6	1.863380000	2.999886000	-1.348747000
1	2.287129000	3.727114000	-2.048605000
1	2.508084000	3.004225000	-0.464175000
1	1.925384000	2.012148000	-1.815311000
6	4.696496000	1.411679000	-0.767574000
1	5.122890000	2.384744000	-0.504267000
1	5.523868000	0.790344000	-1.118197000
1	4.026126000	1.569155000	-1.612737000
6	5.049798000	0.461468000	1.521407000
1	5.639088000	1.356795000	1.745656000
1	4.610109000	0.127742000	2.463899000
1	5.754297000	-0.306907000	1.194915000

7	0.926428000	-3.367038000	-1.553759000
7	0.667902000	-2.342479000	-1.181153000
1	0.239732000	-0.125159000	-2.260472000
15	2.866885000	-0.616236000	-0.024643000
15	-2.154008000	-1.608370000	0.034765000
15	-0.339889000	2.016752000	0.027264000
6	-2.503012000	-2.878876000	-1.293231000
1	-1.500604000	-3.271478000	-1.485387000
6	-3.355771000	-4.093442000	-0.931831000
1	-4.425818000	-3.890362000	-0.936978000
1	-3.183187000	-4.878669000	-1.675086000
1	-3.101404000	-4.521961000	0.041423000
6	-2.958286000	-2.192644000	-2.576719000
1	-3.085096000	-2.929274000	-3.375930000
1	-3.919633000	-1.680793000	-2.462489000
1	-2.227720000	-1.455136000	-2.923372000
6	3.790399000	-1.738523000	-1.196265000
1	3.219333000	-2.670862000	-1.097665000
6	3.664207000	-1.274799000	-2.643805000
1	3.996873000	-2.063979000	-3.325310000
1	2.632633000	-1.018852000	-2.906726000
1	4.283404000	-0.397539000	-2.848697000
6	5.228000000	-2.073777000	-0.817238000
1	5.605098000	-2.863842000	-1.475064000
1	5.904030000	-1.223485000	-0.932719000
1	5.324013000	-2.442209000	0.207753000
6	-2.169418000	2.395314000	0.174484000
1	-2.526843000	1.420146000	0.520162000
6	-2.557261000	3.405881000	1.249227000
1	-2.131815000	4.398570000	1.091071000
1	-3.646568000	3.526289000	1.263419000
1	-2.265792000	3.088258000	2.253261000
6	-2.934216000	2.639857000	-1.151794000
1	-3.985421000	2.441585000	-0.879487000
6	-2.899469000	4.073587000	-1.667830000
1	-1.917330000	4.366753000	-2.047646000
1	-3.599436000	4.185985000	-2.500816000
1	-3.192101000	4.802927000	-0.907873000
6	-2.563243000	1.654789000	-2.250033000
1	-2.582113000	0.618680000	-1.899792000
1	-3.254455000	1.730070000	-3.094884000
1	-1.555994000	1.822436000	-2.646290000

$[3c'_{PB} - V - H]^+ (TE = -3049.312752)$

6	-0.799021000	2.387736000	1.965503000
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6	0.275235000	1.646571000	2.752525000
6	-2.037821000	-0.800902000	1.992389000
6	-0.706625000	-0.978078000	2.722827000
6	2.908519000	0.055526000	1.771973000
6	1.945211000	-0.431811000	2.859306000
1	-2.405242000	0.225978000	2.060129000
1	-0.918089000	-1.007914000	3.809356000
1	3.938723000	-0.254978000	1.979062000
1	2.315118000	-0.043181000	3.821382000
1	-0.814702000	3.456437000	2.213954000
1	1.239001000	2.156014000	2.612932000
6	-1.882442000	3.349520000	-0.562995000
1	-1.430581000	4.350463000	-0.503669000
6	-2.123502000	-3.091552000	0.253033000
1	-1.352259000	-3.373450000	0.987978000
6	3.670238000	0.366883000	-1.006942000
1	3.442582000	1.427319000	-0.815041000
23	0.001315000	-0.071899000	-0.906482000
1	-1.798509000	2.022813000	2.211706000
1	0.071282000	1.797256000	3.828729000
1	2.009904000	-1.523901000	2.948134000
1	2.929575000	1.152379000	1.733266000
1	-0.313211000	-1.985753000	2.528128000
1	-2.822459000	-1.416061000	2.448287000
6	5.136421000	0.132916000	-0.664947000
1	5.764468000	0.829605000	-1.229181000
1	5.365515000	0.281221000	0.393088000
1	5.458548000	-0.874260000	-0.944348000
6	3.423154000	0.090803000	-2.486634000
1	3.549263000	-0.968857000	-2.733205000
1	2.429721000	0.391978000	-2.833642000
1	4.144417000	0.640637000	-3.099015000
6	-3.471782000	-3.578867000	0.772724000
1	-3.424524000	-4.653188000	0.977341000
1	-3.790416000	-3.091625000	1.697314000
1	-4.262006000	-3.435531000	0.030284000
6	-1.785014000	-3.781054000	-1.063582000
1	-2.463691000	-3.494209000	-1.870744000
1	-0.769831000	-3.575203000	-1.401355000
1	-1.868574000	-4.866242000	-0.948462000
6	-2.205945000	3.057111000	-2.023009000
1	-1.320397000	2.974411000	-2.656036000
1	-2.750456000	2.115135000	-2.132714000
1	-2.835687000	3.855490000	-2.429167000
6	-3.157922000	3.371140000	0.274427000
1	-3.003497000	3.758131000	1.283679000

1	-3.901471000	4.015035000	-0.205090000
1	-3.615794000	2.379653000	0.363747000
6	2.909225000	-2.324828000	0.047633000
1	3.190420000	-2.499978000	-1.002141000
6	1.714007000	-3.214186000	0.374129000
1	1.401215000	-3.095018000	1.417035000
1	0.845638000	-3.000168000	-0.251757000
1	1.968923000	-4.269736000	0.236395000
6	4.086833000	-2.695330000	0.942546000
1	4.371497000	-3.737762000	0.768100000
1	4.975911000	-2.085879000	0.779310000
1	3.821910000	-2.615952000	2.001558000
6	-3.490307000	-0.479183000	-0.521293000
1	-3.151447000	0.558076000	-0.664911000
6	-4.728995000	-0.452806000	0.366263000
1	-5.164501000	-1.443519000	0.511352000
1	-4.542569000	-0.026182000	1.355340000
1	-5.501351000	0.165193000	-0.104382000
6	-3.794983000	-1.037405000	-1.905346000
1	-4.204228000	-2.050972000	-1.854164000
1	-4.547148000	-0.419007000	-2.405390000
1	-2.907948000	-1.053752000	-2.545797000
6	1.027982000	3.141829000	-0.147385000
1	1.783483000	2.476684000	0.299502000
6	1.138791000	4.497727000	0.532785000
1	2.104544000	4.958273000	0.300469000
1	0.369340000	5.197641000	0.192554000
1	1.069718000	4.432416000	1.621522000
6	1.307909000	3.237616000	-1.643952000
1	2.338706000	3.553972000	-1.833358000
1	1.152896000	2.287731000	-2.173111000
1	0.656187000	3.972517000	-2.126065000
15	-1.945303000	-1.231972000	0.197436000
15	-0.570797000	2.213831000	0.146228000
15	2.432968000	-0.514031000	0.083560000
5	0.460004000	0.079008000	2.666496000
7	0.601529000	-2.167217000	-3.218771000
7	0.397438000	-1.490603000	-2.355512000
1	-1.058959000	0.459518000	-2.132529000

[3d'_{SC} -V-H]⁺ (TE = -2877.659849)

6	2.603126000	0.904081000	-1.625859000
6	1.312628000	0.860954000	-2.432378000
6	1.413477000	-2.141261000	-0.752496000
6	0.741989000	-1.652344000	-2.027692000

6	-2.034051000	0.939569000	-2.112389000
6	-1.054348000	-0.009511000	-2.787633000
1	2.359950000	-1.638994000	-0.558723000
1	1.446597000	-1.846524000	-2.854975000
1	-2.953809000	1.001229000	-2.699783000
1	-0.885570000	0.373439000	-3.806442000
1	3.295862000	1.616122000	-2.080978000
1	0.830545000	1.844969000	-2.407751000
6	3.773933000	0.916086000	1.039473000
1	3.546327000	1.350755000	2.020987000
6	-1.090043000	-2.848372000	0.489129000
1	-1.571287000	-2.408614000	-0.393902000
6	-3.397556000	1.688957000	0.305437000
1	-2.667940000	2.504124000	0.381856000
23	-0.069735000	0.609506000	0.378110000
16	0.461993000	-1.870162000	0.779731000
16	2.275160000	1.467202000	0.089910000
16	-2.446992000	0.284363000	-0.452161000
6	0.293269000	-0.210267000	-2.126405000
1	3.106745000	-0.067008000	-1.603901000
1	1.601416000	0.712742000	-3.489160000
1	-1.544719000	-0.980742000	-2.915614000
1	-1.618860000	1.941909000	-1.977655000
1	-0.116535000	-2.300676000	-2.232525000
1	1.643834000	-3.207526000	-0.830950000
6	-4.566886000	2.090025000	-0.568485000
1	-5.135027000	2.881811000	-0.070673000
1	-4.256083000	2.483860000	-1.538306000
1	-5.251384000	1.253692000	-0.739263000
6	-3.836273000	1.229068000	1.682557000
1	-4.542920000	0.395703000	1.620731000
1	-2.999327000	0.913945000	2.310662000
1	-4.341366000	2.048214000	2.201477000
6	-0.779092000	-4.310098000	0.249385000
1	-1.711862000	-4.869787000	0.129518000
1	-0.190297000	-4.478030000	-0.655922000
1	-0.237331000	-4.749448000	1.091742000
6	-1.968884000	-2.623404000	1.704318000
1	-1.521138000	-3.048298000	2.607381000
1	-2.156288000	-1.561405000	1.889693000
1	-2.938678000	-3.106720000	1.557557000
6	3.937713000	-0.580588000	1.181358000
1	3.045070000	-1.065579000	1.584937000
1	4.202270000	-1.055857000	0.230764000
1	4.762742000	-0.795134000	1.868147000
6	5.005826000	1.589180000	0.464041000

1	4.886467000	2.671171000	0.380103000
1	5.869502000	1.395952000	1.107161000
1	5.254237000	1.196436000	-0.526940000
7	-0.322112000	1.718749000	3.315558000
7	-0.253445000	1.313760000	2.276598000
1	-0.349897000	2.193175000	-0.214718000

[3e'_{ssi} -V-H]⁺ (TE = -3129.075960)

23	0.078359000	-0.285112000	1.029880000
16	-2.320986000	-1.218472000	0.621603000
16	2.605576000	-0.794482000	0.877607000
16	0.368624000	1.927910000	-0.170294000
14	0.331711000	-0.998762000	-1.616171000
6	0.350926000	0.646514000	-2.551467000
6	-0.381877000	1.770820000	-1.831468000
6	2.590030000	-2.198120000	-0.305137000
6	1.993288000	-1.898705000	-1.674307000
6	-1.268643000	-1.955887000	-1.919783000
6	-1.953955000	-2.472647000	-0.664027000
1	-1.326445000	-3.197334000	-0.133599000
1	-2.889913000	-2.991743000	-0.888263000
1	-1.943063000	-1.285684000	-2.468870000
1	-1.079523000	-2.799488000	-2.598209000
1	3.613114000	-2.579163000	-0.375492000
1	2.012933000	-2.965902000	0.220195000
1	2.681663000	-1.271766000	-2.255783000
1	1.908026000	-2.836992000	-2.237400000
1	1.389900000	0.944668000	-2.736210000
1	-0.099201000	0.499020000	-3.542266000
1	-1.453082000	1.564722000	-1.731197000
1	-0.270247000	2.725618000	-2.352378000
6	-3.660532000	-0.150494000	-0.111204000
1	-3.157093000	0.645018000	-0.673991000
6	3.569080000	0.511999000	-0.016350000
1	2.943674000	0.844112000	-0.856038000
6	-0.541434000	3.322083000	0.639664000
1	0.013521000	3.394995000	1.583017000
6	4.889398000	-0.032391000	-0.519752000
1	5.464794000	0.775911000	-0.981301000
1	5.493086000	-0.439588000	0.296438000
1	4.772420000	-0.813007000	-1.275548000
6	3.748702000	1.653579000	0.966993000
1	2.799833000	2.001883000	1.383183000
1	4.391495000	1.358075000	1.800782000
1	4.222450000	2.502335000	0.465813000

6	-0.373995000	4.599929000	-0.158385000
1	-0.935422000	4.572097000	-1.097079000
1	-0.765403000	5.443716000	0.417461000
1	0.671663000	4.813879000	-0.390265000
6	-1.981597000	2.969673000	0.928731000
1	-2.468624000	3.785619000	1.471865000
1	-2.557627000	2.810394000	0.010497000
1	-2.045199000	2.072522000	1.547122000
6	-4.415523000	0.439573000	1.067079000
1	-5.108242000	1.210709000	0.716975000
1	-5.000577000	-0.330608000	1.576848000
1	-3.759738000	0.898105000	1.809195000
6	-4.581059000	-0.934446000	-1.022791000
1	-5.397743000	-0.283611000	-1.349594000
1	-4.090540000	-1.307839000	-1.924385000
1	-5.035575000	-1.782835000	-0.502675000
7	0.193145000	-2.895541000	2.846389000
7	0.136821000	-1.995414000	2.190362000
1	-0.099559000	0.530910000	2.523623000

$[3\mathbf{f}_{SB} - \mathbf{V} - \mathbf{H}]^+$ (TE = -2864.458604)

6	-0.691616000	2.508939000	-1.337973000
6	-0.535856000	1.595595000	-2.554081000
6	2.572999000	1.234067000	-1.242282000
6	1.933652000	0.410234000	-2.353310000
6	-1.764086000	-1.373789000	-1.924358000
6	-0.276394000	-1.130020000	-2.188134000
1	2.117183000	2.222514000	-1.138638000
1	2.204503000	0.890685000	-3.306760000
1	-2.186268000	-2.146169000	-2.571304000
1	-0.035125000	-1.450774000	-3.221997000
1	-1.455190000	3.273474000	-1.502181000
1	-1.538350000	1.324475000	-2.908368000
6	-1.075106000	2.673758000	1.535819000
1	-1.524074000	2.067817000	2.331505000
6	3.637174000	-0.923095000	0.385585000
1	3.144984000	-1.736867000	-0.161646000
6	-3.569185000	-1.065340000	0.300104000
1	-3.494657000	-0.057051000	-0.122832000
23	0.124173000	-0.608548000	0.452374000
16	2.429595000	0.498747000	0.428599000
16	-1.210666000	1.503272000	0.101306000
16	-1.979660000	-1.893743000	-0.177609000
1	0.240050000	3.022679000	-1.087530000
1	-0.094192000	2.203476000	-3.355042000

1	0.348711000	-1.864500000	-1.641657000
1	-2.356940000	-0.463469000	-2.062248000
1	2.409590000	-0.580208000	-2.381756000
1	3.636900000	1.416149000	-1.411302000
6	-4.740805000	-1.813452000	-0.301129000
1	-5.674756000	-1.301589000	-0.048535000
1	-4.686552000	-1.870940000	-1.391516000
1	-4.808815000	-2.833396000	0.087064000
6	-3.608822000	-0.987860000	1.812118000
1	-3.619389000	-1.981919000	2.269263000
1	-2.750571000	-0.443070000	2.216276000
1	-4.521215000	-0.476058000	2.131555000
6	4.929956000	-0.553910000	-0.308647000
1	5.647223000	-1.371201000	-0.186918000
1	4.810074000	-0.395269000	-1.382600000
1	5.382888000	0.342350000	0.126164000
6	3.856223000	-1.313217000	1.837077000
1	4.447373000	-0.554502000	2.356966000
1	2.924052000	-1.436688000	2.393813000
1	4.403429000	-2.258586000	1.892958000
6	0.358231000	2.994547000	1.893637000
1	0.912398000	2.096982000	2.171272000
1	0.887938000	3.494982000	1.075269000
1	0.379280000	3.679506000	2.747111000
6	-1.924383000	3.902259000	1.274634000
1	-2.947005000	3.651327000	0.983389000
1	-1.977152000	4.507492000	2.184238000
1	-1.493009000	4.539695000	0.497126000
5	0.356698000	0.315105000	-2.296953000
7	1.182983000	-3.469679000	1.370825000
7	0.862710000	-2.459338000	1.029137000
1	-0.132821000	-0.271855000	2.088198000

[3a''_{PC} -V-H]⁺ (TE = -3129.075960)

6	-0.766966000	-1.106788000	1.763028000
6	-0.241280000	-1.933479000	2.779677000
1	0.730196000	-1.690601000	3.203450000
6	-0.964093000	-2.994175000	3.303406000
1	-0.539080000	-3.590930000	4.106509000
6	-2.239008000	-3.268670000	2.821919000
1	-2.821109000	-4.087702000	3.236458000
6	-2.752264000	-2.512966000	1.767644000
1	-3.711599000	-2.799534000	1.343865000
6	-2.040496000	-1.459072000	1.202468000
6	1.392036000	0.247511000	1.817495000

6	1.720352000	1.111183000	2.876766000
1	0.931593000	1.683504000	3.358680000
6	3.023137000	1.235186000	3.339482000
1	3.239132000	1.908135000	4.165534000
6	4.041191000	0.499052000	2.747039000
1	5.066155000	0.590072000	3.097243000
6	3.741919000	-0.344345000	1.682552000
1	4.550938000	-0.886492000	1.202340000
6	2.438188000	-0.478048000	1.199037000
6	-0.779241000	1.414742000	1.548162000
6	-1.603066000	1.609227000	2.664192000
1	-1.809082000	0.767058000	3.322717000
6	-2.121957000	2.864286000	2.959549000
1	-2.752930000	2.995550000	3.835197000
6	-1.827785000	3.946215000	2.139683000
1	-2.227884000	4.931344000	2.365425000
6	-1.020819000	3.765930000	1.017990000
1	-0.808369000	4.617846000	0.379415000
6	-0.494019000	2.513477000	0.703759000
6	-0.046115000	0.124843000	1.422281000
23	-0.103744000	-0.350037000	-1.082366000
6	-3.191712000	-2.356192000	-1.334041000
1	-4.045082000	-2.662689000	-0.717752000
6	3.608774000	-1.101527000	-1.423325000
1	3.930217000	-0.087161000	-1.139459000
6	-0.272626000	3.170480000	-2.225983000
1	0.241699000	2.719337000	-3.089926000
6	0.010658000	4.668334000	-2.259580000
1	-0.345909000	5.082242000	-3.208674000
1	-0.511468000	5.215200000	-1.470945000
1	1.070857000	4.912019000	-2.187184000
6	-1.765745000	2.900096000	-2.381174000
1	-2.337347000	3.332513000	-1.553186000
1	-2.139443000	3.357111000	-3.302516000
1	-2.002023000	1.831710000	-2.422685000
6	-3.720510000	-1.965025000	-2.712079000
1	-4.543025000	-1.247139000	-2.674230000
1	-2.934198000	-1.535324000	-3.341167000
1	-4.094768000	-2.850547000	-3.234756000
6	-2.259234000	-3.552312000	-1.441311000
1	-1.768318000	-3.800853000	-0.495967000
1	-2.837574000	-4.427399000	-1.758998000
1	-1.473535000	-3.390393000	-2.182787000
6	4.780087000	-2.056647000	-1.220398000
1	5.625517000	-1.733442000	-1.836616000
1	5.138170000	-2.113777000	-0.191591000

1	4.534545000	-3.073617000	-1.536499000
6	3.208382000	-1.074833000	-2.896761000
1	2.802484000	-2.036645000	-3.228273000
1	2.452962000	-0.313743000	-3.106596000
1	4.078440000	-0.859337000	-3.525180000
15	0.426705000	2.134742000	-0.833736000
15	2.074596000	-1.347815000	-0.371931000
15	-2.492948000	-0.834471000	-0.478157000
6	1.897184000	-3.151268000	0.074212000
1	0.921554000	-3.131030000	0.581346000
6	1.732700000	-3.993832000	-1.184783000
1	2.667303000	-4.093215000	-1.744651000
1	1.411010000	-5.007166000	-0.924033000
1	0.977488000	-3.573134000	-1.855845000
6	2.922979000	-3.723478000	1.040888000
1	2.591221000	-4.708214000	1.387032000
1	3.904317000	-3.866386000	0.583537000
1	3.055827000	-3.099135000	1.929414000
6	-4.073918000	0.186310000	-0.383961000
1	-4.210725000	0.474383000	-1.437086000
6	-3.932005000	1.461089000	0.426464000
1	-3.908217000	1.243956000	1.496844000
1	-3.033689000	2.028980000	0.180638000
1	-4.794033000	2.113202000	0.251231000
6	-5.313950000	-0.571145000	0.078720000
1	-6.167388000	0.113671000	0.120502000
1	-5.604480000	-1.393114000	-0.577578000
1	-5.187441000	-0.971435000	1.090339000
6	2.184548000	2.700344000	-0.551508000
1	2.597226000	1.878204000	0.049121000
6	2.348699000	3.976809000	0.261545000
1	3.411002000	4.163302000	0.451731000
1	1.955379000	4.861094000	-0.246335000
1	1.854178000	3.907001000	1.234119000
6	2.947525000	2.725254000	-1.871860000
1	4.020886000	2.837503000	-1.689024000
1	2.811277000	1.803474000	-2.447250000
1	2.647456000	3.556876000	-2.514885000
7	-0.273328000	-0.794132000	-4.187028000
7	-0.208462000	-0.634512000	-3.078649000
1	-0.406280000	-1.990002000	-0.826693000

[3b''_{PSi} -V-H]⁺ (TE = -3771.189715)

6	0.626401000	1.579064000	2.008885000
6	1.217002000	1.746449000	3.268039000

1	1.434319000	0.877107000	3.889575000
6	1.558295000	3.013342000	3.729212000
1	2.025957000	3.130469000	4.703799000
6	1.311266000	4.128769000	2.934721000
1	1.580415000	5.120755000	3.289180000
6	0.733213000	3.977311000	1.678370000
1	0.564941000	4.859372000	1.064114000
6	0.393795000	2.707725000	1.204882000
6	-1.604162000	-0.508194000	2.065512000
6	-1.893185000	-0.230886000	3.407733000
1	-1.129934000	0.208888000	4.050378000
6	-3.156697000	-0.475905000	3.933824000
1	-3.368133000	-0.246389000	4.975403000
6	-4.150567000	-0.997381000	3.114222000
1	-5.146543000	-1.179128000	3.510773000
6	-3.879890000	-1.277959000	1.778620000
1	-4.679735000	-1.669967000	1.159305000
6	-2.613458000	-1.036970000	1.239262000
6	1.333889000	-1.473245000	1.740329000
6	1.235142000	-2.232940000	2.913387000
1	0.470378000	-1.993434000	3.652967000
6	2.077945000	-3.315112000	3.134969000
1	1.989250000	-3.899328000	4.047697000
6	3.016916000	-3.661274000	2.169378000
1	3.664083000	-4.521785000	2.320995000
6	3.126281000	-2.916773000	0.999215000
1	3.858243000	-3.218875000	0.256848000
6	2.297188000	-1.815477000	0.771320000
23	-0.056803000	-0.083069000	-1.241386000
6	-2.004219000	3.146580000	-0.376888000
1	-1.864804000	4.219714000	-0.192507000
6	-2.026482000	-3.202487000	-0.574673000
1	-3.009520000	-3.565774000	-0.241179000
6	3.856488000	0.325060000	-0.528826000
1	4.247424000	0.439337000	-1.551258000
6	4.952712000	-0.230081000	0.372047000
1	5.809903000	0.451732000	0.378322000
1	4.602333000	-0.315686000	1.405759000
1	5.322526000	-1.210189000	0.071522000
6	3.435426000	1.696952000	-0.030918000
1	3.087561000	1.660309000	1.005357000
1	4.279272000	2.394152000	-0.062360000
1	2.631980000	2.121152000	-0.634526000
6	-2.728230000	2.944765000	-1.700435000
1	-2.153950000	3.274482000	-2.571760000
1	-2.958928000	1.885557000	-1.846891000

1	-3.678424000	3.487664000	-1.712400000
6	-2.804385000	2.557731000	0.773856000
1	-2.307070000	2.670789000	1.741582000
1	-3.779154000	3.050843000	0.845038000
1	-2.994854000	1.490830000	0.623797000
6	-1.751614000	-3.717804000	-1.980897000
1	-1.717115000	-4.812025000	-1.978610000
1	-2.509871000	-3.422211000	-2.709989000
1	-0.783039000	-3.357850000	-2.342088000
6	-0.972735000	-3.702484000	0.400546000
1	0.026527000	-3.369180000	0.104297000
1	-1.150478000	-3.367892000	1.426953000
1	-0.963687000	-4.797286000	0.411119000
14	0.103086000	-0.110906000	1.392202000
15	-2.188577000	-1.340870000	-0.527805000
15	2.372473000	-0.811329000	-0.770636000
15	-0.284668000	2.429125000	-0.476689000
6	0.677371000	3.683782000	-1.525491000
1	1.593543000	3.828870000	-0.938679000
6	0.020831000	5.049732000	-1.692417000
1	0.704872000	5.713808000	-2.230452000
1	-0.899932000	5.005893000	-2.279884000
1	-0.217482000	5.541023000	-0.746355000
6	1.071094000	3.109814000	-2.880189000
1	1.613507000	2.161422000	-2.794562000
1	0.199327000	2.936267000	-3.518582000
1	1.721077000	3.810733000	-3.413261000
6	2.953143000	-2.012856000	-2.101043000
1	2.434240000	-2.943175000	-1.826882000
6	2.439757000	-1.570270000	-3.466607000
1	2.752915000	-0.549141000	-3.717705000
1	2.835599000	-2.224130000	-4.249667000
1	1.353072000	-1.615758000	-3.518783000
6	4.452207000	-2.280028000	-2.190472000
1	5.021887000	-1.378108000	-2.433570000
1	4.890054000	-2.710440000	-1.290030000
1	4.639068000	-2.992115000	-3.000438000
6	-3.790208000	-1.013682000	-1.470044000
1	-4.210642000	-0.142125000	-0.943825000
6	-4.820867000	-2.141447000	-1.454280000
1	-5.759672000	-1.778064000	-1.884091000
1	-4.502859000	-2.987140000	-2.069514000
1	-5.055057000	-2.535770000	-0.465252000
6	-3.516378000	-0.615438000	-2.917038000
1	-2.898907000	0.278077000	-3.002779000
1	-3.013675000	-1.412646000	-3.473611000

1	-4.458537000	-0.410302000	-3.435011000
7	-0.472406000	0.343421000	-4.348333000
7	-0.311300000	0.175445000	-3.252572000
1	0.278779000	-1.746334000	-1.452614000

[3c''_{PB} -V-H]⁺ (TE = -3506.554073)

6	1.579313000	-1.030844000	1.691869000
6	1.740253000	-1.962445000	2.732313000
1	0.854973000	-2.376495000	3.211600000
6	2.991176000	-2.365667000	3.184916000
1	3.068117000	-3.085359000	3.996770000
6	4.139308000	-1.848312000	2.597818000
1	5.124239000	-2.150887000	2.944918000
6	4.016944000	-0.954597000	1.540192000
1	4.919171000	-0.580491000	1.062332000
6	2.761708000	-0.550850000	1.077095000
6	-0.185434000	1.026003000	1.805134000
6	0.505533000	1.413389000	2.977895000
1	1.330180000	0.797788000	3.329519000
6	0.137208000	2.515999000	3.734350000
1	0.680265000	2.750093000	4.647050000
6	-0.927153000	3.312369000	3.326805000
1	-1.232923000	4.172852000	3.916852000
6	-1.590865000	3.003398000	2.148145000
1	-2.405969000	3.643562000	1.819085000
6	-1.241029000	1.884908000	1.383504000
6	-1.074733000	-1.532900000	1.623427000
6	-1.635156000	-1.743429000	2.890881000
1	-1.331984000	-1.109165000	3.724925000
6	-2.573884000	-2.746287000	3.103618000
1	-3.004480000	-2.887633000	4.092557000
6	-2.960769000	-3.574264000	2.052654000
1	-3.685430000	-4.367550000	2.219307000
6	-2.430685000	-3.376405000	0.783165000
1	-2.754811000	-4.017099000	-0.031299000
6	-1.508074000	-2.346398000	0.561642000
23	0.143057000	0.473723000	-1.000810000
6	3.438070000	2.071912000	-0.114570000
1	4.490619000	1.834724000	0.091866000
6	-3.819337000	1.266383000	0.087459000
1	-4.180068000	2.199356000	0.543878000
6	0.295106000	-3.239412000	-1.600231000
1	0.610584000	-2.928522000	-2.605429000
6	-0.456246000	-4.561594000	-1.690470000
1	0.178236000	-5.318073000	-2.163554000

1	-0.712194000	-4.940200000	-0.696768000
1	-1.377563000	-4.505167000	-2.275059000
6	1.528799000	-3.392611000	-0.725575000
1	1.263987000	-3.646942000	0.306358000
1	2.167303000	-4.196394000	-1.105861000
1	2.126005000	-2.480525000	-0.690238000
6	3.360644000	2.980953000	-1.336127000
1	3.660093000	2.495429000	-2.269012000
1	2.343888000	3.360885000	-1.477639000
1	4.007636000	3.853524000	-1.203682000
6	2.855276000	2.763398000	1.105868000
1	2.948416000	2.159029000	2.011094000
1	3.374851000	3.710312000	1.285143000
1	1.792611000	2.998811000	0.973076000
6	-4.577320000	1.025686000	-1.212947000
1	-5.656444000	1.051833000	-1.033338000
1	-4.361778000	1.765116000	-1.989622000
1	-4.348531000	0.041219000	-1.627972000
6	-4.034821000	0.142210000	1.085182000
1	-3.699414000	-0.823058000	0.696455000
1	-3.510628000	0.315496000	2.028470000
1	-5.101776000	0.047994000	1.311623000
5	0.105699000	-0.497775000	1.422994000
15	2.623784000	0.428809000	-0.463155000
15	-2.021378000	1.623057000	-0.248232000
15	-0.766618000	-1.825021000	-1.024129000
6	-2.074404000	3.328755000	-1.060559000
1	-2.084222000	3.069954000	-2.129605000
6	-0.800532000	4.124415000	-0.781232000
1	-0.672782000	4.912566000	-1.529532000
1	-0.838767000	4.606701000	0.198783000
1	0.109345000	3.517689000	-0.792924000
6	-3.297925000	4.199745000	-0.794828000
1	-3.212749000	5.124696000	-1.374423000
1	-4.240586000	3.732386000	-1.083767000
1	-3.383714000	4.499468000	0.253372000
6	3.815837000	-0.415572000	-1.661433000
1	3.816744000	-1.455734000	-1.309667000
6	5.255464000	0.088316000	-1.628075000
1	5.871430000	-0.540838000	-2.278231000
1	5.346902000	1.110560000	-2.005378000
1	5.714464000	0.061448000	-0.637906000
6	3.286642000	-0.398570000	-3.091157000
1	3.951884000	-0.971596000	-3.744892000
1	2.284007000	-0.824385000	-3.167664000
1	3.241718000	0.616934000	-3.499341000

6	-2.110872000	-1.663203000	-2.340506000
1	-2.331684000	-0.585978000	-2.301144000
6	-1.578926000	-1.959861000	-3.739014000
1	-1.396700000	-3.026960000	-3.894075000
1	-2.319760000	-1.653999000	-4.484304000
1	-0.653093000	-1.422620000	-3.958329000
6	-3.414005000	-2.409360000	-2.088086000
1	-3.295415000	-3.494242000	-2.159734000
1	-3.856283000	-2.188177000	-1.114082000
1	-4.147244000	-2.125503000	-2.851018000
7	0.497265000	2.398076000	-3.514903000
7	0.401006000	1.806194000	-2.574675000
1	0.385110000	-0.437696000	-2.390830000

[3d''_{sc} -V-H]⁺ (TE = -3334.919534)

6	1.161305000	1.029294000	1.024803000
6	2.193852000	1.019144000	1.975992000
1	2.413578000	0.092189000	2.503402000
6	2.872908000	2.184865000	2.305656000
1	3.649033000	2.159353000	3.066240000
6	2.544625000	3.386682000	1.681691000
1	3.067598000	4.301853000	1.945823000
6	1.584956000	3.404928000	0.676246000
1	1.393712000	4.319817000	0.120182000
6	0.909285000	2.234234000	0.339831000
6	-1.055480000	0.087018000	1.633034000
6	-1.015439000	0.609045000	2.937685000
1	-0.054284000	0.897856000	3.357240000
6	-2.157862000	0.715488000	3.715807000
1	-2.084707000	1.101728000	4.729032000
6	-3.390785000	0.323468000	3.201094000
1	-4.292248000	0.406444000	3.802158000
6	-3.470373000	-0.132951000	1.894034000
1	-4.437775000	-0.370843000	1.457529000
6	-2.318306000	-0.249055000	1.113317000
6	0.840272000	-1.475684000	1.006294000
6	0.406923000	-2.382715000	1.998981000
1	-0.420706000	-2.096787000	2.642677000
6	1.052838000	-3.587765000	2.213046000
1	0.710786000	-4.247332000	3.006304000
6	2.142773000	-3.947957000	1.424636000
1	2.647921000	-4.897017000	1.582054000
6	2.550786000	-3.109874000	0.390033000
1	3.330850000	-3.434677000	-0.293230000
6	1.920020000	-1.892213000	0.169241000

16	2.207462000	-1.080574000	-1.403631000
16	-0.040851000	2.132824000	-1.156154000
16	-2.525377000	-0.597968000	-0.624384000
23	-0.226090000	-0.405099000	-1.479719000
6	-1.465690000	3.327446000	-0.985218000
1	-0.984775000	4.310600000	-1.048152000
6	-3.212310000	-2.341048000	-0.670347000
1	-4.227884000	-2.214881000	-0.276013000
6	3.840031000	-0.125049000	-1.344589000
1	4.281070000	-0.472016000	-2.285610000
6	4.702578000	-0.573046000	-0.188358000
1	5.665817000	-0.055453000	-0.239820000
1	4.247492000	-0.321512000	0.774094000
1	4.907503000	-1.645185000	-0.198379000
6	3.653341000	1.373363000	-1.403061000
1	3.379382000	1.784895000	-0.431638000
1	4.600552000	1.839136000	-1.696215000
1	2.902435000	1.679434000	-2.136485000
6	-2.338308000	3.102622000	-2.204250000
1	-1.788242000	3.222195000	-3.141158000
1	-2.784788000	2.102775000	-2.193255000
1	-3.157488000	3.826967000	-2.208606000
6	-2.206467000	3.185790000	0.322856000
1	-1.542300000	3.236040000	1.190091000
1	-2.931471000	4.000901000	0.417050000
1	-2.762137000	2.246548000	0.369761000
6	-3.265059000	-2.740030000	-2.130278000
1	-3.774558000	-3.702965000	-2.225953000
1	-3.809880000	-2.017708000	-2.744675000
1	-2.255930000	-2.854993000	-2.535716000
6	-2.419744000	-3.296435000	0.187156000
1	-1.387064000	-3.371598000	-0.164846000
1	-2.412142000	-3.000254000	1.239533000
1	-2.871355000	-4.292372000	0.131013000
6	0.249516000	-0.141542000	0.931498000
7	-0.920756000	-0.425429000	-4.552457000
7	-0.645557000	-0.420347000	-3.469986000
1	-0.236667000	-2.106889000	-1.569616000

[3e''_{ssi} -V-H]⁺ (TE = -3586.351415)

6	-0.996336000	0.496165000	1.827183000
6	-1.701491000	1.422422000	2.608540000
1	-1.732335000	2.468830000	2.303999000
6	-2.383887000	1.029662000	3.754403000
1	-2.923111000	1.765926000	4.345396000

6	-2.391840000	-0.309591000	4.136809000
1	-2.937568000	-0.622915000	5.023155000
6	-1.714260000	-1.254681000	3.375376000
1	-1.732054000	-2.305190000	3.657567000
6	-1.018943000	-0.841332000	2.238877000
6	1.422060000	1.972465000	0.514856000
6	1.583426000	3.003675000	1.444195000
1	0.756866000	3.266737000	2.103982000
6	2.793236000	3.681154000	1.564267000
1	2.907844000	4.468376000	2.305032000
6	3.859142000	3.342058000	0.737955000
1	4.806890000	3.867431000	0.824367000
6	3.728827000	2.326137000	-0.205141000
1	4.571657000	2.078868000	-0.843719000
6	2.517515000	1.646767000	-0.295158000
6	-1.376369000	1.936812000	-0.789270000
6	-1.560804000	3.323425000	-0.743430000
1	-0.906327000	3.933737000	-0.121198000
6	-2.568082000	3.937886000	-1.481353000
1	-2.695971000	5.016536000	-1.432001000
6	-3.407653000	3.177233000	-2.290682000
1	-4.188100000	3.658142000	-2.874633000
6	-3.235514000	1.799716000	-2.374545000
1	-3.867424000	1.201773000	-3.027709000
6	-2.226853000	1.200828000	-1.622696000
16	-1.964453000	-0.569626000	-1.782585000
16	-0.152058000	-2.091723000	1.281074000
16	2.238947000	0.313410000	-1.475651000
23	0.399840000	-1.212797000	-1.011744000
6	1.410577000	-2.288981000	2.293359000
1	1.014511000	-2.499769000	3.294548000
6	3.939946000	-0.373277000	-1.819246000
1	4.499315000	0.514972000	-2.133749000
6	-3.283891000	-1.406310000	-0.697946000
1	-2.684422000	-2.033597000	-0.027267000
6	-4.149481000	-2.267360000	-1.592671000
1	-4.857494000	-2.836745000	-0.981974000
1	-4.731465000	-1.657181000	-2.289459000
1	-3.570257000	-2.983436000	-2.179676000
6	-4.071550000	-0.400943000	0.107732000
1	-4.693697000	0.234069000	-0.528894000
1	-4.741524000	-0.942482000	0.783166000
1	-3.438648000	0.246138000	0.717775000
6	2.160035000	-3.491601000	1.763171000
1	1.559892000	-4.403778000	1.802468000
1	2.476228000	-3.337237000	0.727764000

1	3.058425000	-3.657439000	2.364918000
6	2.217242000	-1.012460000	2.297227000
1	1.658995000	-0.165426000	2.705807000
1	3.116937000	-1.139191000	2.908683000
1	2.540212000	-0.751897000	1.285119000
6	4.563971000	-1.000821000	-0.595848000
1	5.578143000	-1.339236000	-0.831114000
1	4.635720000	-0.305279000	0.244699000
1	3.988478000	-1.874711000	-0.276268000
6	3.824814000	-1.323790000	-2.991567000
1	3.225936000	-2.200818000	-2.731799000
1	3.385661000	-0.848363000	-3.872016000
1	4.822018000	-1.677526000	-3.267887000
14	-0.123807000	0.946508000	0.214829000
7	-0.711813000	-4.127546000	-1.850621000
7	-0.384114000	-3.104446000	-1.573057000
1	1.743141000	-2.256678000	-1.102611000

$[3f''_{SB} - V - H]^+$ (TE = -3321.709775)

6	-1.295441000	1.435438000	-0.979278000
6	-2.097676000	1.781605000	-2.075379000
1	-2.049921000	1.184143000	-2.985959000
6	-2.953073000	2.876079000	-2.022702000
1	-3.561531000	3.129965000	-2.887275000
6	-3.038507000	3.645767000	-0.864161000
1	-3.712096000	4.497685000	-0.820867000
6	-2.281806000	3.306632000	0.250996000
1	-2.374690000	3.873289000	1.174910000
6	-1.417060000	2.215627000	0.174821000
6	1.229728000	0.830534000	-1.561125000
6	1.271925000	1.672298000	-2.687542000
1	0.335950000	2.033771000	-3.110143000
6	2.466481000	2.032119000	-3.296950000
1	2.455561000	2.665510000	-4.180305000
6	3.676045000	1.590945000	-2.768182000
1	4.617414000	1.877255000	-3.230042000
6	3.680672000	0.818513000	-1.614176000
1	4.625140000	0.533768000	-1.155830000
6	2.472949000	0.438194000	-1.030024000
6	-0.494337000	-1.226389000	-1.177187000
6	0.191951000	-1.832426000	-2.262678000
1	0.983434000	-1.272269000	-2.752767000
6	-0.152020000	-3.072000000	-2.773552000
1	0.378286000	-3.466554000	-3.636346000
6	-1.159701000	-3.814363000	-2.166724000

1	-1.424593000	-4.798433000	-2.545293000
6	-1.797622000	-3.313446000	-1.041437000
1	-2.519313000	-3.924604000	-0.506844000
6	-1.499471000	-2.036921000	-0.559556000
16	-2.165379000	-1.625676000	1.054058000
16	-0.529990000	1.657728000	1.620617000
16	2.520243000	-0.345009000	0.576707000
23	0.168953000	-0.802738000	1.168078000
6	0.697920000	3.023443000	1.968076000
1	0.050220000	3.856888000	2.266278000
6	3.568601000	-1.874741000	0.359359000
1	4.543197000	-1.469268000	0.062097000
6	-3.951397000	-1.057467000	0.853057000
1	-4.147539000	-0.724804000	1.879821000
6	-4.783223000	-2.282998000	0.531992000
1	-5.845016000	-2.021965000	0.581510000
1	-4.590444000	-2.638009000	-0.485131000
1	-4.607840000	-3.107732000	1.225327000
6	-4.173679000	0.063064000	-0.127677000
1	-3.830977000	-0.208876000	-1.130266000
1	-5.247980000	0.264283000	-0.198957000
1	-3.683170000	0.988777000	0.167885000
6	1.536864000	2.576759000	3.147460000
1	0.931735000	2.304764000	4.015998000
1	2.170337000	1.723328000	2.883149000
1	2.202651000	3.389203000	3.451936000
6	1.519800000	3.405964000	0.760023000
1	0.904132000	3.621297000	-0.117295000
1	2.096157000	4.308813000	0.987001000
1	2.232882000	2.622003000	0.493870000
6	3.672940000	-2.524273000	1.724260000
1	4.360873000	-3.372652000	1.671280000
1	4.051927000	-1.838701000	2.486952000
1	2.700930000	-2.907105000	2.048458000
6	3.024085000	-2.796974000	-0.703245000
1	2.028368000	-3.159596000	-0.431050000
1	2.965889000	-2.311496000	-1.681110000
1	3.683239000	-3.665193000	-0.806489000
5	-0.184870000	0.329233000	-1.074330000
7	0.938523000	-0.985403000	4.254015000
7	0.648998000	-0.870078000	3.187721000
1	0.514915000	-2.460898000	1.306284000

Cartesian coordinates of the transition states (TS1) involved during the conversion of **[3-V-H]⁺** to **[3-N_α-H]⁺** along with their total energies (in hartree) including zero point vibrational correction at M06-L-D3(heptane)/6-311+G* level of theory.

a' _{PC} -TS1 (TE = -3062.470313)

6	-0.409088000	2.066397000	1.851183000
6	0.150743000	0.854485000	2.609544000
6	-2.544309000	-0.668930000	1.969238000
6	-1.219112000	-1.268054000	2.418783000
6	2.569096000	-1.088182000	1.761630000
6	1.229520000	-1.392839000	2.424410000
1	-2.665034000	0.351891000	2.350915000
1	-1.223050000	-1.336446000	3.522962000
1	3.359253000	-1.765977000	2.103828000
1	1.346917000	-1.308713000	3.520226000
1	-0.238291000	2.997760000	2.404802000
1	1.211116000	1.068969000	2.808089000
6	-0.325537000	3.483791000	-0.807952000
1	0.262561000	3.445363000	-1.736548000
6	-3.069636000	-2.334336000	-0.345847000
1	-2.341988000	-2.932808000	0.226116000
6	3.914640000	-0.595690000	-0.829424000
1	4.044617000	0.419955000	-0.427534000
23	-0.053242000	-0.317270000	-0.333518000
6	0.045730000	-0.538322000	1.939605000
1	-1.493430000	1.991688000	1.700052000
1	-0.311406000	0.824526000	3.612212000
1	0.997361000	-2.454309000	2.257673000
1	2.913453000	-0.074860000	2.005578000
1	-1.178733000	-2.316864000	2.082400000
1	-3.398406000	-1.236823000	2.356297000
6	5.132411000	-1.424820000	-0.443983000
1	6.044674000	-0.957350000	-0.828084000
1	5.253609000	-1.529238000	0.637767000
1	5.088579000	-2.429363000	-0.876640000
6	3.762520000	-0.494748000	-2.342478000
1	3.589787000	-1.475793000	-2.799673000
1	2.935662000	0.155688000	-2.638889000
1	4.675112000	-0.095853000	-2.795805000
6	-4.466945000	-2.769559000	0.076185000
1	-4.574355000	-3.853224000	-0.036087000
1	-4.699045000	-2.528228000	1.116450000
1	-5.235041000	-2.310954000	-0.553063000
6	-2.844676000	-2.624288000	-1.827180000
1	-3.530212000	-2.061705000	-2.466727000
1	-1.826162000	-2.397820000	-2.161142000

1	-3.013174000	-3.684937000	-2.038945000
6	-1.779425000	3.215668000	-1.169213000
1	-1.928774000	2.216749000	-1.589548000
1	-2.431651000	3.316620000	-0.295009000
1	-2.131554000	3.940744000	-1.909181000
6	-0.168876000	4.864905000	-0.183731000
1	0.872987000	5.178187000	-0.101556000
1	-0.678027000	5.614772000	-0.798027000
1	-0.613245000	4.917166000	0.815663000
6	2.216971000	-2.997924000	-0.454532000
1	2.705124000	-3.090106000	-1.435992000
6	0.747293000	-3.376500000	-0.627391000
1	0.179610000	-3.239714000	0.303250000
1	0.266552000	-2.784058000	-1.418918000
1	0.623527000	-4.425584000	-0.915473000
6	2.913740000	-3.931998000	0.524843000
1	2.871307000	-4.963283000	0.159615000
1	3.966386000	-3.684429000	0.674174000
1	2.432117000	-3.924171000	1.507303000
6	-3.967842000	0.581010000	-0.257481000
1	-3.503262000	1.544857000	-0.009626000
6	-5.220287000	0.457184000	0.603562000
1	-5.804932000	-0.434329000	0.371713000
1	-4.999361000	0.441446000	1.673656000
1	-5.872362000	1.318617000	0.425611000
6	-4.299512000	0.590419000	-1.744677000
1	-4.873546000	-0.296033000	-2.032669000
1	-4.913585000	1.459957000	-1.998846000
1	-3.406505000	0.626503000	-2.379039000
6	2.157250000	2.509795000	0.495487000
1	2.587772000	1.543403000	0.787496000
6	2.439927000	3.481415000	1.634804000
1	3.521333000	3.609072000	1.750906000
1	2.019882000	4.474610000	1.464821000
1	2.057617000	3.123644000	2.594302000
6	2.822186000	2.930473000	-0.810829000
1	3.910712000	2.960827000	-0.697830000
1	2.593280000	2.246853000	-1.635993000
1	2.509858000	3.931577000	-1.123276000
15	-2.581597000	-0.593716000	0.132103000
15	0.368424000	2.079224000	0.190439000
15	2.328379000	-1.170311000	-0.057628000
7	0.500299000	0.829433000	-3.195704000
7	0.001177000	0.013599000	-2.472591000
1	-0.690187000	-0.636537000	-2.945820000

b'_{psi} -TS1 (TE = -3313.897644)

6	0.044060000	2.533336000	1.826847000
6	0.442669000	1.377847000	2.747034000
6	-2.797632000	0.068735000	1.944799000
6	-1.768365000	-0.740302000	2.740271000
6	2.555320000	-1.415410000	1.757188000
6	1.319842000	-1.570837000	2.647191000
1	-2.648411000	1.145897000	2.095903000
1	-1.853537000	-0.509363000	3.809967000
1	3.301383000	-2.199174000	1.933793000
1	1.597850000	-1.426758000	3.699133000
1	0.417660000	3.503727000	2.176260000
1	1.529994000	1.395903000	2.906959000
6	0.105392000	3.607158000	-0.940876000
1	0.612393000	3.428161000	-1.901238000
6	-3.155640000	-2.041277000	-0.002623000
1	-2.283428000	-2.588708000	0.377736000
6	3.727741000	-1.067837000	-0.901609000
1	4.043202000	-0.086711000	-0.515796000
23	-0.100769000	-0.145461000	-0.502185000
1	-1.047386000	2.629961000	1.768491000
1	0.004430000	1.524174000	3.743294000
1	0.938084000	-2.597910000	2.582554000
1	3.066510000	-0.465344000	1.970149000
1	-1.984601000	-1.813858000	2.650900000
1	-3.830270000	-0.134822000	2.251889000
6	4.823622000	-2.077760000	-0.582162000
1	5.776455000	-1.740271000	-1.002490000
1	4.979750000	-2.224396000	0.489215000
1	4.612807000	-3.052965000	-1.030983000
6	3.538045000	-0.949646000	-2.408081000
1	3.185809000	-1.887432000	-2.851255000
1	2.823550000	-0.171181000	-2.683717000
1	4.487111000	-0.707190000	-2.895880000
6	-4.340839000	-2.442899000	0.868543000
1	-4.531089000	-3.514892000	0.751493000
1	-4.163671000	-2.269086000	1.932574000
1	-5.262796000	-1.925824000	0.596204000
6	-3.364147000	-2.452274000	-1.456476000
1	-4.303600000	-2.055437000	-1.852676000
1	-2.560182000	-2.119810000	-2.122731000
1	-3.423287000	-3.542027000	-1.539322000
6	-1.394531000	3.506269000	-1.184649000
1	-1.676777000	2.528515000	-1.584978000
1	-1.967730000	3.670306000	-0.265058000

1	-1.724365000	4.264119000	-1.901836000
6	0.492313000	4.993440000	-0.442800000
1	1.571761000	5.153180000	-0.428927000
1	0.066891000	5.759921000	-1.098830000
1	0.112172000	5.191990000	0.564170000
6	1.640566000	-3.126090000	-0.472669000
1	1.973934000	-3.236193000	-1.515333000
6	0.122880000	-3.272277000	-0.445826000
1	-0.269219000	-3.134933000	0.567243000
1	-0.386004000	-2.567758000	-1.122594000
1	-0.194274000	-4.265569000	-0.781920000
6	2.292857000	-4.208576000	0.377173000
1	2.033105000	-5.198998000	-0.010710000
1	3.381475000	-4.145215000	0.399232000
1	1.941846000	-4.173175000	1.413125000
6	-3.834198000	0.850114000	-0.689860000
1	-3.514570000	1.834260000	-0.313448000
6	-5.291452000	0.647834000	-0.294858000
1	-5.701623000	-0.268807000	-0.728267000
1	-5.443699000	0.605813000	0.786806000
1	-5.901643000	1.473738000	-0.675090000
6	-3.674762000	0.856367000	-2.208806000
1	-4.131499000	-0.023099000	-2.668546000
1	-4.166861000	1.732876000	-2.641783000
1	-2.627993000	0.876009000	-2.529790000
6	2.503680000	2.320895000	0.278026000
1	2.789032000	1.323071000	0.641414000
6	3.034624000	3.333947000	1.285162000
1	4.127351000	3.275322000	1.324866000
1	2.782682000	4.363853000	1.025013000
1	2.670193000	3.153096000	2.298937000
6	3.123915000	2.514052000	-1.100715000
1	4.207673000	2.363108000	-1.069324000
1	2.720386000	1.816305000	-1.842827000
1	2.957055000	3.527252000	-1.479651000
15	-2.594597000	-0.261888000	0.141391000
15	0.647054000	2.179749000	0.126181000
15	2.100064000	-1.364956000	-0.036846000
14	-0.024100000	-0.356027000	2.064301000
7	-0.218250000	-1.166198000	-3.350149000
7	0.189214000	-0.331072000	-2.584150000
1	0.580728000	0.554791000	-3.014406000

c'_{PB} -TS1 (TE = -3049.248700)

6	-0.685243000	2.124512000	1.930419000
6	0.187299000	1.196670000	2.778724000

6	-2.362356000	-0.882788000	2.078292000
6	-1.029928000	-1.307815000	2.691425000
6	2.811773000	-0.524980000	1.873133000
6	1.662381000	-1.072808000	2.722828000
1	-2.632982000	0.132877000	2.382326000
1	-1.172770000	-1.412945000	3.783321000
1	3.767922000	-0.993401000	2.133295000
1	1.944371000	-0.946301000	3.783038000
1	-0.669124000	3.148264000	2.321908000
1	1.202660000	1.616924000	2.809825000
6	-1.194862000	3.403873000	-0.709168000
1	-0.533620000	4.275086000	-0.809589000
6	-2.660953000	-2.729363000	-0.125742000
1	-1.927022000	-3.236200000	0.522376000
6	3.912182000	0.095655000	-0.777018000
1	3.824408000	1.144975000	-0.457132000
23	0.048547000	-0.284749000	-0.551898000
1	-1.737731000	1.825366000	1.939228000
1	-0.160828000	1.288570000	3.823839000
1	1.594116000	-2.160853000	2.592578000
1	2.950837000	0.551125000	2.042933000
1	-0.790076000	-2.333187000	2.373619000
1	-3.189641000	-1.517289000	2.418720000
6	5.283352000	-0.420315000	-0.359431000
1	6.068729000	0.202183000	-0.799654000
1	5.436450000	-0.413103000	0.722833000
1	5.454269000	-1.439585000	-0.718838000
6	3.748092000	0.036966000	-2.291152000
1	3.834453000	-0.986988000	-2.669845000
1	2.784129000	0.423723000	-2.630697000
1	4.530279000	0.621943000	-2.784132000
6	-4.052007000	-3.200660000	0.278992000
1	-4.107994000	-4.292541000	0.224291000
1	-4.331744000	-2.916431000	1.296636000
1	-4.818137000	-2.813521000	-0.399153000
6	-2.355648000	-3.120990000	-1.568265000
1	-3.086252000	-2.706567000	-2.267613000
1	-1.369707000	-2.795419000	-1.908334000
1	-2.393250000	-4.208978000	-1.680340000
6	-1.560067000	2.935070000	-2.111715000
1	-0.674215000	2.704931000	-2.713359000
1	-2.184438000	2.034992000	-2.091851000
1	-2.120140000	3.708592000	-2.646527000
6	-2.418076000	3.857261000	0.077596000
1	-2.159259000	4.296743000	1.043606000
1	-2.959516000	4.620782000	-0.489200000

1	-3.128274000	3.045725000	0.265376000
6	2.710075000	-2.563448000	-0.264062000
1	3.167387000	-2.592207000	-1.263991000
6	1.343697000	-3.237183000	-0.361069000
1	0.767785000	-3.130102000	0.567474000
1	0.750535000	-2.836171000	-1.193635000
1	1.438302000	-4.310536000	-0.554410000
6	3.620753000	-3.296902000	0.711493000
1	3.779526000	-4.325800000	0.373058000
1	4.604694000	-2.835140000	0.813187000
1	3.181527000	-3.357390000	1.711683000
6	-3.702825000	0.131726000	-0.334846000
1	-3.260981000	1.135000000	-0.235131000
6	-4.963730000	0.102095000	0.519460000
1	-5.490348000	-0.852081000	0.452828000
1	-4.765138000	0.296435000	1.576452000
1	-5.660921000	0.874331000	0.177523000
6	-4.008485000	-0.087622000	-1.811902000
1	-4.563646000	-1.016485000	-1.973078000
1	-4.631613000	0.724206000	-2.199976000
1	-3.105010000	-0.133931000	-2.430749000
6	1.531375000	2.941243000	0.224916000
1	2.178778000	2.191251000	0.703107000
6	1.577685000	4.216357000	1.054182000
1	2.576317000	4.662132000	1.009903000
1	0.879094000	4.975610000	0.686119000
1	1.351045000	4.042075000	2.109067000
6	2.028050000	3.165726000	-1.198426000
1	3.075642000	3.482778000	-1.203757000
1	1.954864000	2.259413000	-1.809127000
1	1.459891000	3.951384000	-1.707402000
15	-2.289953000	-0.935032000	0.232394000
15	-0.142281000	2.123792000	0.173746000
15	2.482143000	-0.735770000	0.072320000
5	0.245827000	-0.379888000	2.567482000
7	0.329131000	-1.307529000	-3.445578000
7	0.162536000	-0.563902000	-2.526198000
1	-0.004862000	0.505901000	-2.712820000

d'_{sc} -TS1 (TE = -3049.248700)

6	0.171530000	1.585383000	2.143085000
6	0.219786000	0.163085000	2.682216000
6	-2.792555000	-0.132827000	1.741465000
6	-1.817633000	-1.223373000	2.131281000
6	1.849299000	-2.179650000	1.368106000
6	0.445565000	-2.230502000	1.941177000

1	-2.602254000	0.807742000	2.266689000
1	-1.930502000	-1.394919000	3.218107000
1	2.390180000	-3.119086000	1.507649000
1	0.537897000	-2.514747000	3.005932000
1	0.656542000	2.299944000	2.815261000
1	1.269203000	-0.056766000	2.918975000
6	0.698925000	3.241088000	-0.207342000
1	1.019770000	3.079848000	-1.244816000
6	-3.277970000	-1.291341000	-0.811170000
1	-3.887358000	-1.752110000	-0.025131000
6	3.362039000	-0.906015000	-0.698480000
1	3.388755000	-0.160013000	0.105347000
23	-0.230647000	-0.322088000	-0.372423000
16	-2.673382000	0.298293000	-0.041313000
16	1.055726000	1.576657000	0.541973000
16	1.766398000	-1.818924000	-0.433809000
6	-0.358590000	-0.937239000	1.766002000
1	-0.848913000	1.931269000	1.958603000
1	-0.289575000	0.164261000	3.661077000
1	-0.092118000	-3.071245000	1.477424000
1	2.447744000	-1.377845000	1.815101000
1	-2.145716000	-2.166899000	1.672088000
1	-3.836224000	-0.394643000	1.941687000
6	4.530478000	-1.861479000	-0.575205000
1	5.471283000	-1.314324000	-0.691635000
1	4.562087000	-2.357473000	0.397970000
1	4.499906000	-2.635138000	-1.347551000
6	3.302591000	-0.207452000	-2.040998000
1	3.149907000	-0.914457000	-2.863018000
1	2.508743000	0.544595000	-2.080975000
1	4.248007000	0.307504000	-2.233041000
6	-4.136819000	-0.965056000	-2.015564000
1	-4.506235000	-1.886214000	-2.476684000
1	-4.999364000	-0.352755000	-1.747981000
1	-3.568072000	-0.424845000	-2.779800000
6	-2.120241000	-2.211628000	-1.172329000
1	-1.580970000	-1.853593000	-2.057789000
1	-1.414152000	-2.371982000	-0.341587000
1	-2.476525000	-3.212245000	-1.436014000
6	-0.770098000	3.604359000	-0.185852000
1	-1.401188000	2.828017000	-0.623756000
1	-1.125348000	3.814816000	0.827166000
1	-0.926400000	4.516392000	-0.769827000
6	1.580158000	4.288496000	0.446099000
1	2.639800000	4.030552000	0.393772000
1	1.444917000	5.252466000	-0.053619000

1	1.319567000	4.434376000	1.498740000
7	-0.587902000	1.515441000	-2.879138000
7	-0.317171000	0.440081000	-2.428321000
1	0.018335000	-0.272597000	-3.134976000

e'_{ssi} -TS1 (TE = -2877.624030)

6	0.171530000	1.585383000	2.143085000
6	0.219786000	0.163085000	2.682216000
6	-2.792555000	-0.132827000	1.741465000
6	-1.817633000	-1.223373000	2.131281000
6	1.849299000	-2.179650000	1.368106000
6	0.445565000	-2.230502000	1.941177000
1	-2.602254000	0.807742000	2.266689000
1	-1.930502000	-1.394919000	3.218107000
1	2.390180000	-3.119086000	1.507649000
1	0.537897000	-2.514747000	3.005932000
1	0.656542000	2.299944000	2.815261000
1	1.269203000	-0.056766000	2.918975000
6	0.698925000	3.241088000	-0.207342000
1	1.019770000	3.079848000	-1.244816000
6	-3.277970000	-1.291341000	-0.811170000
1	-3.887358000	-1.752110000	-0.025131000
6	3.362039000	-0.906015000	-0.698480000
1	3.388755000	-0.160013000	0.105347000
23	-0.230647000	-0.322088000	-0.372423000
16	-2.673382000	0.298293000	-0.041313000
16	1.055726000	1.576657000	0.541973000
16	1.766398000	-1.818924000	-0.433809000
6	-0.358590000	-0.937239000	1.766002000
1	-0.848913000	1.931269000	1.958603000
1	-0.289575000	0.164261000	3.661077000
1	-0.092118000	-3.071245000	1.477424000
1	2.447744000	-1.377845000	1.815101000
1	-2.145716000	-2.166899000	1.672088000
1	-3.836224000	-0.394643000	1.941687000
6	4.530478000	-1.861479000	-0.575205000
1	5.471283000	-1.314324000	-0.691635000
1	4.562087000	-2.357473000	0.397970000
1	4.499906000	-2.635138000	-1.347551000
6	3.302591000	-0.207452000	-2.040998000
1	3.149907000	-0.914457000	-2.863018000
1	2.508743000	0.544595000	-2.080975000
1	4.248007000	0.307504000	-2.233041000
6	-4.136819000	-0.965056000	-2.015564000
1	-4.506235000	-1.886214000	-2.476684000
1	-4.999364000	-0.352755000	-1.747981000

1	-3.568072000	-0.424845000	-2.779800000
6	-2.120241000	-2.211628000	-1.172329000
1	-1.580970000	-1.853593000	-2.057789000
1	-1.414152000	-2.371982000	-0.341587000
1	-2.476525000	-3.212245000	-1.436014000
6	-0.770098000	3.604359000	-0.185852000
1	-1.401188000	2.828017000	-0.623756000
1	-1.125348000	3.814816000	0.827166000
1	-0.926400000	4.516392000	-0.769827000
6	1.580158000	4.288496000	0.446099000
1	2.639800000	4.030552000	0.393772000
1	1.444917000	5.252466000	-0.053619000
1	1.319567000	4.434376000	1.498740000
7	-0.587902000	1.515441000	-2.879138000
7	-0.317171000	0.440081000	-2.428321000
1	0.018335000	-0.272597000	-3.134976000

f'_{SB} -TS1 (TE = -2864.385755)

6	-0.361357000	1.785240000	2.040271000
6	0.013495000	0.652394000	2.990420000
6	-2.571758000	-0.846884000	1.686073000
6	-1.280163000	-1.593781000	1.973248000
6	2.509134000	-1.189830000	1.686420000
6	1.359199000	-1.672593000	2.564173000
1	-2.741271000	-0.035656000	2.399660000
1	-1.437352000	-2.225025000	2.871423000
1	3.459075000	-1.662296000	1.949010000
1	1.701206000	-1.575489000	3.606290000
1	-0.172758000	2.767608000	2.482452000
1	0.985304000	0.891503000	3.440715000
6	0.229667000	3.071093000	-0.511291000
1	0.916736000	2.919598000	-1.351333000
6	-3.565565000	-1.348926000	-0.945320000
1	-3.155856000	-2.325648000	-0.653610000
6	3.365411000	-0.645220000	-1.066781000
1	2.912877000	0.348046000	-1.181276000
23	-0.105020000	-0.549965000	-0.397899000
16	-2.578323000	-0.085945000	0.011377000
16	0.686046000	1.610686000	0.546613000
16	2.147621000	-1.638132000	-0.058442000
1	-1.411582000	1.755968000	1.733070000
1	-0.701178000	0.676419000	3.829359000
1	1.208272000	-2.748403000	2.403640000
1	2.637354000	-0.103404000	1.741272000
1	-1.106705000	-2.376591000	1.209399000
1	-3.453601000	-1.491489000	1.733059000

6	4.703758000	-0.541153000	-0.367937000
1	5.400814000	-0.002365000	-1.016887000
1	4.654279000	0.008687000	0.573752000
1	5.138725000	-1.525925000	-0.171569000
6	3.472913000	-1.330308000	-2.415130000
1	3.960373000	-2.305277000	-2.325686000
1	2.503942000	-1.480307000	-2.895886000
1	4.073267000	-0.715453000	-3.091618000
6	-5.027476000	-1.249954000	-0.562779000
1	-5.597931000	-2.029513000	-1.076882000
1	-5.199215000	-1.379745000	0.508428000
1	-5.447005000	-0.283541000	-0.854939000
6	-3.337047000	-1.101626000	-2.422361000
1	-3.624168000	-0.085814000	-2.711653000
1	-2.295981000	-1.254466000	-2.721837000
1	-3.948456000	-1.789494000	-3.012713000
6	-1.197237000	3.017351000	-1.010901000
1	-1.384161000	2.131948000	-1.622827000
1	-1.926730000	3.031082000	-0.195073000
1	-1.397776000	3.894555000	-1.634072000
6	0.561925000	4.356455000	0.219868000
1	1.582651000	4.364183000	0.608529000
1	0.463947000	5.200892000	-0.468857000
1	-0.123401000	4.546935000	1.051229000
5	0.032408000	-0.825107000	2.414696000
7	0.906894000	0.860460000	-2.834635000
7	0.305731000	-0.034710000	-2.300782000
1	-0.116696000	-0.815827000	-2.929719000

a''_{PC} -TS1 (TE = -3519.737201)

6	0.311096000	1.431378000	1.620480000
6	-0.447175000	2.111925000	2.592905000
1	-1.267505000	1.588176000	3.078644000
6	-0.165424000	3.416868000	2.966125000
1	-0.771518000	3.900469000	3.729291000
6	0.899267000	4.099976000	2.382854000
1	1.132324000	5.119591000	2.678321000
6	1.653775000	3.465629000	1.406232000
1	2.461424000	4.015764000	0.927983000
6	1.377757000	2.151954000	1.003192000
6	-1.301071000	-0.510402000	1.799138000
6	-1.350965000	-1.310730000	2.950725000
1	-0.426004000	-1.562602000	3.462606000
6	-2.547380000	-1.802660000	3.457884000
1	-2.537591000	-2.425225000	4.349726000
6	-3.748747000	-1.499332000	2.829684000

1	-4.690603000	-1.880746000	3.215563000
6	-3.731317000	-0.709414000	1.687529000
1	-4.671001000	-0.496427000	1.186806000
6	-2.530954000	-0.220366000	1.160915000
6	1.129942000	-0.941030000	1.638583000
6	1.876628000	-0.773270000	2.810531000
1	1.730396000	0.126956000	3.406794000
6	2.779390000	-1.741245000	3.233528000
1	3.345621000	-1.589520000	4.149941000
6	2.952828000	-2.907394000	2.493762000
1	3.653087000	-3.670086000	2.824825000
6	2.228054000	-3.090228000	1.321241000
1	2.372953000	-3.999317000	0.743495000
6	1.328743000	-2.114456000	0.881979000
6	0.018519000	0.006884000	1.261451000
23	-0.022392000	0.254595000	-0.977675000
6	2.136990000	2.904561000	-1.672466000
1	2.623718000	3.754313000	-1.177934000
6	-3.930244000	-0.036904000	-1.420567000
1	-3.978574000	-1.085208000	-1.088719000
6	1.487906000	-2.968936000	-1.982448000
1	0.955362000	-2.711590000	-2.910569000
6	1.654947000	-4.484306000	-1.955392000
1	2.259369000	-4.797882000	-2.813111000
1	2.174489000	-4.838899000	-1.061817000
1	0.708221000	-5.022475000	-2.021703000
6	2.842280000	-2.266991000	-2.026501000
1	3.453479000	-2.519129000	-1.153820000
1	3.399071000	-2.576366000	-2.916177000
1	2.747713000	-1.176642000	-2.063449000
6	2.894798000	2.573358000	-2.952175000
1	3.968218000	2.453479000	-2.786524000
1	2.529037000	1.649299000	-3.415103000
1	2.772058000	3.372644000	-3.689649000
6	0.692383000	3.290168000	-1.966534000
1	0.103238000	3.449070000	-1.056443000
1	0.636334000	4.215126000	-2.549142000
1	0.189764000	2.524202000	-2.571870000
6	-5.287423000	0.612051000	-1.162679000
1	-6.067866000	0.045299000	-1.680730000
1	-5.567720000	0.654697000	-0.109636000
1	-5.333013000	1.632136000	-1.551827000
6	-3.628423000	-0.034588000	-2.916744000
1	-3.468884000	0.978402000	-3.303055000
1	-2.749590000	-0.638009000	-3.161057000
1	-4.467901000	-0.455664000	-3.478608000

15	0.412592000	-2.167062000	-0.688896000
15	-2.459983000	0.610588000	-0.458497000
15	2.164347000	1.450210000	-0.498485000
6	-2.676273000	2.447158000	-0.160898000
1	-1.687950000	2.725475000	0.237083000
6	-2.871632000	3.199094000	-1.473680000
1	-3.869876000	3.048757000	-1.892438000
1	-2.753426000	4.275996000	-1.316886000
1	-2.148238000	2.905203000	-2.241465000
6	-3.704379000	2.829245000	0.893950000
1	-3.610011000	3.892849000	1.137464000
1	-4.730118000	2.668837000	0.554209000
1	-3.568722000	2.269550000	1.823416000
6	3.992526000	1.159506000	-0.265592000
1	4.299913000	0.826591000	-1.268174000
6	4.299464000	0.048138000	0.722287000
1	4.065248000	0.354343000	1.744695000
1	3.746744000	-0.871369000	0.517715000
1	5.367475000	-0.190177000	0.692819000
6	4.760108000	2.424039000	0.096691000
1	5.831699000	2.205256000	0.142434000
1	4.631707000	3.238106000	-0.620735000
1	4.471735000	2.793636000	1.085724000
6	-1.096933000	-3.227866000	-0.429233000
1	-1.747491000	-2.560510000	0.153182000
6	-0.880141000	-4.484593000	0.402175000
1	-1.840516000	-4.975384000	0.592316000
1	-0.238066000	-5.217473000	-0.092149000
1	-0.435454000	-4.255951000	1.374391000
6	-1.785196000	-3.493646000	-1.763488000
1	-2.769001000	-3.946361000	-1.604627000
1	-1.939166000	-2.572303000	-2.336792000
1	-1.218640000	-4.179824000	-2.399256000
7	0.739032000	-0.381814000	-3.942517000
7	-0.050225000	0.026139000	-3.136956000
1	-0.939312000	0.437460000	-3.537628000

b''_{psi} -TS1 (TE = -3771.148505)

6	-1.784939000	0.991004000	1.907496000
6	-2.009444000	1.302512000	3.255631000
1	-1.181047000	1.274159000	3.963430000
6	-3.277757000	1.632888000	3.717386000
1	-3.433179000	1.865420000	4.768495000
6	-4.352023000	1.662862000	2.831696000
1	-5.345804000	1.925440000	3.186467000
6	-4.157852000	1.346431000	1.493223000

1	-5.010335000	1.365153000	0.816926000
6	-2.883195000	1.001375000	1.026151000
6	0.788441000	-0.741836000	2.187192000
6	1.404217000	-0.459131000	3.413783000
1	1.345986000	0.548724000	3.825816000
6	2.123253000	-1.427713000	4.104580000
1	2.601960000	-1.182733000	5.050084000
6	2.240942000	-2.709451000	3.575092000
1	2.806056000	-3.472015000	4.105620000
6	1.642230000	-3.015430000	2.358815000
1	1.753118000	-4.018657000	1.957941000
6	0.919670000	-2.042500000	1.658866000
6	1.021691000	2.112059000	1.221374000
6	0.861179000	3.176793000	2.115523000
1	0.035552000	3.161067000	2.827099000
6	1.722945000	4.268400000	2.103528000
1	1.574731000	5.089601000	2.801361000
6	2.776022000	4.306136000	1.195794000
1	3.458940000	5.152177000	1.182781000
6	2.956432000	3.260941000	0.296433000
1	3.789022000	3.305645000	-0.397490000
6	2.080463000	2.170256000	0.288237000
23	-0.151235000	-0.192726000	-1.224226000
6	-4.189554000	-0.149912000	-1.312744000
1	-4.921909000	0.659862000	-1.195292000
6	1.368759000	-3.536586000	-0.857324000
1	2.350705000	-3.173409000	-0.518888000
6	2.974522000	1.412924000	-2.489015000
1	2.947128000	0.502512000	-3.108592000
6	4.414701000	1.928398000	-2.489696000
1	4.812589000	1.885149000	-3.508736000
1	4.472359000	2.976099000	-2.186894000
1	5.097765000	1.362873000	-1.856073000
6	2.052907000	2.445815000	-3.127373000
1	1.947468000	3.332817000	-2.492736000
1	2.470090000	2.781368000	-4.081911000
1	1.050465000	2.062621000	-3.337789000
6	-4.124490000	-0.517961000	-2.788611000
1	-3.814772000	0.312438000	-3.429239000
1	-3.433095000	-1.350755000	-2.961557000
1	-5.106230000	-0.847682000	-3.141786000
6	-4.647155000	-1.332631000	-0.471337000
1	-4.684043000	-1.107916000	0.597283000
1	-5.651057000	-1.645203000	-0.775251000
1	-3.992283000	-2.195349000	-0.607674000
6	1.278056000	-5.023552000	-0.525703000

1	2.095376000	-5.556520000	-1.022615000
1	1.353645000	-5.248403000	0.538315000
1	0.349546000	-5.471869000	-0.887146000
6	1.290490000	-3.343480000	-2.371706000
1	0.327787000	-3.676702000	-2.774146000
1	1.431533000	-2.300038000	-2.677089000
1	2.064308000	-3.931950000	-2.875267000
15	2.237952000	0.768196000	-0.890693000
15	0.200514000	-2.341587000	-0.000475000
15	-2.565491000	0.561414000	-0.726920000
6	-1.429351000	-3.201339000	0.301560000
1	-2.063296000	-2.364053000	0.635968000
6	-1.997140000	-3.732590000	-1.010229000
1	-1.405600000	-4.559194000	-1.411631000
1	-3.010454000	-4.119669000	-0.865660000
1	-2.050913000	-2.957823000	-1.784343000
6	-1.434590000	-4.254298000	1.400459000
1	-2.460989000	-4.585064000	1.590432000
1	-0.859193000	-5.142742000	1.130550000
1	-1.037579000	-3.871143000	2.343242000
6	-2.508530000	2.205685000	-1.624357000
1	-2.495386000	1.925560000	-2.687151000
6	-1.196997000	2.911352000	-1.309630000
1	-1.120656000	3.184267000	-0.251616000
1	-0.309897000	2.304851000	-1.545352000
1	-1.094398000	3.829804000	-1.897198000
6	-3.693286000	3.122498000	-1.366172000
1	-3.590593000	4.039817000	-1.954954000
1	-4.651856000	2.676238000	-1.642986000
1	-3.751318000	3.420558000	-0.314703000
6	3.523880000	-0.382149000	-0.153267000
1	2.917625000	-1.040533000	0.481521000
6	4.544132000	0.290010000	0.755677000
1	5.217400000	-0.464744000	1.175932000
1	5.167611000	1.021071000	0.233039000
1	4.068440000	0.805543000	1.593477000
6	4.174500000	-1.249595000	-1.227064000
1	4.720259000	-2.075862000	-0.759898000
1	3.447946000	-1.690768000	-1.915865000
1	4.896826000	-0.697482000	-1.832770000
14	-0.098252000	0.586916000	1.159189000
7	-0.786663000	0.585087000	-4.047353000
7	-0.806294000	-0.289110000	-3.217786000
1	-1.025126000	-1.267973000	-3.555251000

c''_{PB}-TS1 (TE = -3506.492429)

6	1.526440000	-0.395903000	1.964025000
6	1.635368000	-0.991644000	3.234839000
1	0.728027000	-1.189778000	3.804529000
6	2.860808000	-1.332071000	3.794497000
1	2.897917000	-1.785854000	4.782334000
6	4.035101000	-1.101522000	3.086155000
1	4.999649000	-1.368167000	3.511074000
6	3.962184000	-0.541426000	1.817650000
1	4.881380000	-0.387708000	1.255371000
6	2.730695000	-0.190783000	1.253855000
6	-0.407440000	1.541753000	1.741782000
6	0.143455000	2.251932000	2.824272000
1	1.031550000	1.856827000	3.316242000
6	-0.445393000	3.409814000	3.318531000
1	-0.002577000	3.924302000	4.168428000
6	-1.617328000	3.893265000	2.745233000
1	-2.100729000	4.781035000	3.145629000
6	-2.158237000	3.245511000	1.638346000
1	-3.061347000	3.643906000	1.180775000
6	-1.553268000	2.100613000	1.115762000
6	-1.106278000	-1.016067000	1.747713000
6	-1.822036000	-0.898109000	2.954485000
1	-1.615132000	-0.053206000	3.612205000
6	-2.787190000	-1.821967000	3.334879000
1	-3.313644000	-1.698904000	4.278835000
6	-3.092046000	-2.890940000	2.498623000
1	-3.853953000	-3.613495000	2.780356000
6	-2.427118000	-3.017203000	1.286511000
1	-2.691009000	-3.837341000	0.623596000
6	-1.439285000	-2.099102000	0.909284000
23	0.166869000	0.207520000	-1.089444000
6	3.389037000	2.110200000	-0.457809000
1	4.442835000	1.967661000	-0.182806000
6	-3.871601000	1.151734000	-0.473163000
1	-4.286474000	2.141573000	-0.232174000
6	0.454605000	-3.663482000	-0.739457000
1	0.612352000	-3.882366000	-1.807759000
6	-0.092060000	-4.900285000	-0.036880000
1	0.638448000	-5.712256000	-0.112962000
1	-0.243884000	-4.708246000	1.029254000
1	-1.029207000	-5.274590000	-0.445503000
6	1.790175000	-3.288550000	-0.113130000
1	1.682539000	-3.060402000	0.952663000
1	2.503183000	-4.114704000	-0.199101000

1	2.231776000	-2.414874000	-0.588887000
6	3.319637000	2.737384000	-1.846389000
1	3.883379000	3.675184000	-1.869475000
1	3.728190000	2.096868000	-2.632975000
1	2.292514000	2.975838000	-2.135889000
6	2.740663000	2.991493000	0.598069000
1	2.862661000	2.583768000	1.604881000
1	3.192183000	3.988693000	0.586949000
1	1.667359000	3.120705000	0.429224000
6	-4.378410000	0.728592000	-1.845784000
1	-5.471660000	0.685030000	-1.852739000
1	-4.076683000	1.410959000	-2.645871000
1	-4.017453000	-0.269298000	-2.114118000
6	-4.288706000	0.179350000	0.617705000
1	-3.890424000	-0.825392000	0.443278000
1	-3.949360000	0.497181000	1.606852000
1	-5.379531000	0.095425000	0.652090000
5	0.061855000	0.046623000	1.532204000
15	2.651080000	0.397713000	-0.473040000
15	-2.034475000	1.410858000	-0.509061000
15	-0.663303000	-2.162265000	-0.738807000
6	-1.811577000	2.854688000	-1.690713000
1	-1.814855000	2.367971000	-2.678150000
6	-0.426151000	3.445099000	-1.464282000
1	-0.140902000	4.117538000	-2.278656000
1	-0.376228000	4.002226000	-0.523070000
1	0.367219000	2.684105000	-1.421050000
6	-2.870039000	3.946795000	-1.692896000
1	-2.650768000	4.669332000	-2.485932000
1	-3.878582000	3.570406000	-1.878553000
1	-2.885365000	4.508568000	-0.755368000
6	3.936918000	-0.642413000	-1.388770000
1	4.019072000	-1.540032000	-0.763184000
6	5.334100000	-0.043227000	-1.501834000
1	6.004717000	-0.775428000	-1.962756000
1	5.363213000	0.849231000	-2.131734000
1	5.771594000	0.222202000	-0.536774000
6	3.415206000	-1.064526000	-2.757822000
1	4.124905000	-1.735628000	-3.251698000
1	2.459628000	-1.598241000	-2.686240000
1	3.270372000	-0.206897000	-3.424020000
6	-2.079557000	-2.523373000	-1.928382000
1	-2.935611000	-2.042182000	-1.432509000
6	-1.837265000	-1.813925000	-3.257258000
1	-0.921259000	-2.169230000	-3.747379000
1	-2.659033000	-2.008921000	-3.953497000

1	-1.763553000	-0.728083000	-3.144034000
6	-2.429690000	-3.983533000	-2.184980000
1	-1.587040000	-4.543590000	-2.602126000
1	-2.776792000	-4.512498000	-1.296888000
1	-3.239094000	-4.039026000	-2.920009000
7	0.500468000	1.501276000	-3.836093000
7	0.478976000	0.521678000	-3.143793000
1	0.650274000	-0.410541000	-3.617651000

d''_{SC} -TS1 (TE = -3334.882520)

6	-0.449016000	1.801134000	0.704367000
6	0.058070000	2.797268000	1.555885000
1	0.826960000	2.530928000	2.276595000
6	-0.408566000	4.105537000	1.525497000
1	0.005925000	4.837105000	2.215183000
6	-1.403380000	4.480867000	0.628107000
1	-1.773873000	5.501957000	0.603220000
6	-1.890434000	3.540336000	-0.268845000
1	-2.622452000	3.827211000	-1.020794000
6	-1.421312000	2.226851000	-0.235203000
6	-1.115323000	-0.484607000	1.392228000
6	-1.849636000	-0.017654000	2.494392000
1	-1.667240000	0.994992000	2.850962000
6	-2.796238000	-0.802296000	3.139095000
1	-3.333633000	-0.403463000	3.996218000
6	-3.064811000	-2.090970000	2.685823000
1	-3.808724000	-2.709179000	3.181118000
6	-2.400208000	-2.567472000	1.564437000
1	-2.638456000	-3.548906000	1.159905000
6	-1.441642000	-1.772581000	0.932362000
6	1.297525000	0.170534000	1.523480000
6	1.339591000	0.150525000	2.926434000
1	0.407546000	0.233192000	3.479408000
6	2.526987000	0.034072000	3.636767000
1	2.504069000	0.024505000	4.723906000
6	3.739098000	-0.073755000	2.962947000
1	4.673349000	-0.169797000	3.509454000
6	3.737345000	-0.097984000	1.576847000
1	4.665532000	-0.244359000	1.029735000
6	2.536370000	0.022054000	0.871157000
16	2.613802000	-0.312335000	-0.891759000
16	-1.879432000	1.143547000	-1.584445000
16	-0.745952000	-2.357869000	-0.606095000
23	0.183555000	-0.212309000	-1.341276000
6	-3.685891000	0.649297000	-1.405418000
1	-4.203001000	1.494722000	-1.873118000

6	0.457858000	-3.709289000	-0.122081000
1	-0.209159000	-4.528782000	0.171119000
6	3.046648000	1.309344000	-1.726418000
1	3.293941000	0.953268000	-2.733366000
6	4.254436000	1.951402000	-1.085405000
1	4.529972000	2.852862000	-1.641070000
1	4.049287000	2.254305000	-0.054171000
1	5.120947000	1.286581000	-1.081000000
6	1.847920000	2.234827000	-1.780868000
1	1.534446000	2.560014000	-0.785911000
1	2.084266000	3.135574000	-2.357119000
1	0.980057000	1.797443000	-2.306504000
6	-3.863550000	-0.596626000	-2.247233000
1	-3.517122000	-0.461777000	-3.276082000
1	-3.330854000	-1.448214000	-1.811160000
1	-4.923988000	-0.861076000	-2.294435000
6	-4.138468000	0.487210000	0.022691000
1	-3.869541000	1.341734000	0.648931000
1	-5.230266000	0.402198000	0.038520000
1	-3.730694000	-0.416743000	0.477926000
6	1.212987000	-4.080988000	-1.381682000
1	1.853154000	-4.946278000	-1.188603000
1	0.546373000	-4.346091000	-2.207197000
1	1.863880000	-3.263838000	-1.711212000
6	1.355224000	-3.328267000	1.029794000
1	2.080026000	-2.563508000	0.742270000
1	0.797794000	-2.960993000	1.895460000
1	1.920996000	-4.208066000	1.353094000
6	-0.011128000	0.357868000	0.770070000
7	0.497184000	-0.782437000	-3.437780000
7	1.262611000	-0.402862000	-4.274397000
1	-0.211808000	-1.498204000	-3.754672000

e''_{SSi} -TS1 (TE = -3586.285072)

6	-1.074289000	0.391152000	1.909517000
6	-1.761035000	1.236062000	2.792637000
1	-1.814523000	2.304291000	2.582597000
6	-2.388831000	0.742869000	3.931629000
1	-2.912454000	1.421581000	4.600604000
6	-2.358878000	-0.620830000	4.209160000
1	-2.857481000	-1.012138000	5.092293000
6	-1.706721000	-1.490883000	3.343029000
1	-1.700650000	-2.561089000	3.538734000
6	-1.068907000	-0.978953000	2.213217000
6	1.293057000	2.040392000	0.644369000
6	1.411318000	3.081364000	1.572011000

1	0.569538000	3.315427000	2.222990000
6	2.584684000	3.819442000	1.692546000
1	2.654749000	4.617185000	2.427742000
6	3.666634000	3.538224000	0.865220000
1	4.582981000	4.117649000	0.944497000
6	3.587143000	2.512306000	-0.071508000
1	4.435608000	2.308159000	-0.719113000
6	2.415520000	1.764989000	-0.152532000
6	-1.491241000	1.943335000	-0.698283000
6	-1.702780000	3.325722000	-0.627956000
1	-1.131007000	3.919190000	0.085241000
6	-2.619327000	3.962771000	-1.458889000
1	-2.762168000	5.038390000	-1.386147000
6	-3.344027000	3.228142000	-2.392302000
1	-4.051472000	3.724083000	-3.051895000
6	-3.152014000	1.854400000	-2.495132000
1	-3.702268000	1.273390000	-3.231705000
6	-2.238026000	1.228944000	-1.648815000
16	-2.005256000	-0.553390000	-1.839322000
16	-0.258976000	-2.158996000	1.117207000
16	2.246458000	0.423865000	-1.350184000
23	0.340632000	-1.037102000	-1.053004000
6	1.361962000	-2.434608000	2.017762000
1	1.052396000	-2.933114000	2.944116000
6	3.970457000	-0.202054000	-1.695236000
1	4.485960000	0.641779000	-2.167877000
6	-3.280020000	-1.294943000	-0.673683000
1	-2.938690000	-1.025846000	0.332479000
6	-3.232423000	-2.795335000	-0.874770000
1	-3.937467000	-3.276743000	-0.190843000
1	-3.525102000	-3.072286000	-1.892317000
1	-2.245923000	-3.217821000	-0.672120000
6	-4.646174000	-0.705580000	-0.936164000
1	-4.981910000	-0.900079000	-1.959477000
1	-5.370429000	-1.167957000	-0.258214000
1	-4.679422000	0.371660000	-0.762368000
6	2.188388000	-3.380205000	1.172337000
1	1.667860000	-4.315049000	0.954303000
1	2.462231000	-2.922876000	0.213259000
1	3.120068000	-3.622611000	1.692282000
6	2.066198000	-1.132896000	2.324974000
1	1.466948000	-0.466869000	2.950609000
1	2.999699000	-1.335899000	2.860537000
1	2.324350000	-0.592643000	1.408432000
6	4.683198000	-0.638348000	-0.433991000
1	5.716543000	-0.908864000	-0.673808000

1	4.717837000	0.141715000	0.329619000
1	4.207030000	-1.519131000	0.005712000
6	3.809333000	-1.326057000	-2.699412000
1	3.254742000	-2.169652000	-2.270418000
1	3.297059000	-1.004348000	-3.609877000
1	4.792707000	-1.704518000	-2.990664000
14	-0.228726000	0.968656000	0.317158000
7	0.415261000	-4.110513000	-1.553574000
7	0.231238000	-2.988264000	-1.933800000
1	0.089970000	-2.881542000	-2.980337000

f''_{SB}-TS1 (TE = -3321.642146)

6	-1.222255000	0.344563000	1.745427000
6	-1.209503000	0.871995000	3.050760000
1	-0.250390000	1.070853000	3.528387000
6	-2.375572000	1.132447000	3.758639000
1	-2.317359000	1.525537000	4.770776000
6	-3.615400000	0.904712000	3.168362000
1	-4.533762000	1.119170000	3.708577000
6	-3.671724000	0.430750000	1.865981000
1	-4.631863000	0.293491000	1.372858000
6	-2.489630000	0.145896000	1.177364000
6	0.816385000	-1.428109000	1.302529000
6	0.520729000	-2.126733000	2.490258000
1	-0.234070000	-1.719158000	3.161677000
6	1.186891000	-3.291008000	2.849508000
1	0.945905000	-3.785433000	3.787507000
6	2.157819000	-3.828440000	2.008475000
1	2.677507000	-4.743743000	2.279596000
6	2.430245000	-3.212425000	0.793252000
1	3.136363000	-3.660477000	0.097625000
6	1.775456000	-2.029355000	0.453449000
6	1.205657000	1.220171000	0.988581000
6	2.101286000	1.405433000	2.056233000
1	2.127111000	0.667438000	2.858280000
6	2.961794000	2.495965000	2.115354000
1	3.633189000	2.609136000	2.963327000
6	2.984640000	3.426063000	1.080345000
1	3.670435000	4.268639000	1.109833000
6	2.134791000	3.261074000	-0.006722000
1	2.157520000	3.963224000	-0.837216000
6	1.246845000	2.184267000	-0.029206000
16	0.205304000	1.996066000	-1.479475000
16	-2.665756000	-0.346885000	-0.543381000
16	1.965086000	-1.409155000	-1.216968000
23	-0.297002000	-0.403113000	-1.332907000

6	-3.263753000	-2.119718000	-0.398069000
1	-3.986192000	-2.051927000	0.424216000
6	3.695071000	-0.710415000	-1.437499000
1	4.283585000	-1.608461000	-1.656577000
6	-1.363253000	2.935877000	-1.056159000
1	-1.804410000	2.395974000	-0.209900000
6	-2.249403000	2.838563000	-2.281343000
1	-3.229422000	3.273285000	-2.064816000
1	-1.824304000	3.388544000	-3.126191000
1	-2.416711000	1.803513000	-2.596086000
6	-1.040205000	4.356348000	-0.656872000
1	-0.535718000	4.898934000	-1.462269000
1	-1.969587000	4.888766000	-0.432900000
1	-0.413782000	4.405150000	0.236413000
6	-3.971432000	-2.493169000	-1.682791000
1	-4.779102000	-1.800357000	-1.928066000
1	-3.282231000	-2.536895000	-2.530141000
1	-4.407880000	-3.490855000	-1.578559000
6	-2.138009000	-3.059711000	-0.026849000
1	-1.628285000	-2.755663000	0.890676000
1	-2.531392000	-4.068895000	0.133924000
1	-1.394624000	-3.146531000	-0.831748000
6	3.628801000	0.179436000	-2.660639000
1	4.635221000	0.517991000	-2.923500000
1	3.219514000	-0.334172000	-3.535105000
1	3.023015000	1.071312000	-2.467282000
6	4.231308000	-0.014252000	-0.213301000
1	3.748701000	0.951059000	-0.055428000
1	4.119779000	-0.610213000	0.696241000
1	5.301730000	0.169843000	-0.352973000
5	0.187491000	0.005585000	1.095146000
7	-1.097821000	-2.286364000	-3.612465000
7	-0.751082000	-1.223817000	-3.190460000
1	-0.522161000	-0.457482000	-3.894376000

Cartesian coordinates of the intermediate involved during the conversion of **[3-V-H]⁺** to **[3]** along with their total energies (in hartree) including zero point vibrational correction at M06-L-D3(heptane)/6-311+G* level of theory.

[3a'_{PC}-N_α-H]⁺ (TE = -3062.505287)

6	-0.447155000	2.079418000	1.775533000
6	0.145767000	0.886120000	2.536339000
6	-2.506027000	-0.678290000	2.013423000
6	-1.165921000	-1.264110000	2.410822000
6	2.598419000	-1.029792000	1.773765000
6	1.252627000	-1.341980000	2.405265000

1	-2.627443000	0.336561000	2.410039000
1	-1.115992000	-1.327515000	3.513520000
1	3.385075000	-1.711956000	2.113691000
1	1.331002000	-1.238174000	3.502501000
1	-0.297948000	3.020077000	2.319508000
1	1.201980000	1.127453000	2.727335000
6	-0.372968000	3.455507000	-0.916975000
1	0.195576000	3.374316000	-1.855883000
6	-3.018307000	-2.329638000	-0.306476000
1	-2.282976000	-2.927251000	0.255835000
6	3.942086000	-0.507931000	-0.782737000
1	4.035391000	0.520045000	-0.402981000
23	-0.029710000	-0.278855000	-0.474423000
6	0.065795000	-0.515775000	1.873055000
1	-1.529098000	1.977107000	1.623906000
1	-0.307685000	0.851566000	3.542522000
1	1.040592000	-2.408911000	2.246896000
1	2.941993000	-0.018099000	2.027375000
1	-1.126135000	-2.312645000	2.074824000
1	-3.348763000	-1.259729000	2.403869000
6	5.158685000	-1.297738000	-0.313261000
1	6.076307000	-0.812694000	-0.661445000
1	5.228453000	-1.378455000	0.774763000
1	5.164063000	-2.310227000	-0.728713000
6	3.884428000	-0.453271000	-2.303837000
1	3.784818000	-1.453209000	-2.740366000
1	3.052310000	0.143165000	-2.678309000
1	4.812967000	-0.030809000	-2.700558000
6	-4.409592000	-2.774174000	0.126618000
1	-4.512461000	-3.856785000	0.000090000
1	-4.631517000	-2.549696000	1.172746000
1	-5.187527000	-2.311807000	-0.487761000
6	-2.804443000	-2.613254000	-1.790277000
1	-3.499535000	-2.052396000	-2.421533000
1	-1.793593000	-2.375606000	-2.130307000
1	-2.972515000	-3.674193000	-2.000600000
6	-1.835729000	3.179491000	-1.232718000
1	-2.000291000	2.157581000	-1.586199000
1	-2.467953000	3.336777000	-0.352417000
1	-2.199010000	3.862561000	-2.006482000
6	-0.198491000	4.861915000	-0.357041000
1	0.845449000	5.174852000	-0.308914000
1	-0.718170000	5.585482000	-0.993626000
1	-0.623680000	4.958702000	0.647324000
6	2.248702000	-2.919019000	-0.468566000
1	2.750165000	-2.984872000	-1.445205000

6	0.788764000	-3.320154000	-0.667252000
1	0.207087000	-3.204670000	0.256564000
1	0.305570000	-2.733204000	-1.461117000
1	0.693687000	-4.367921000	-0.970998000
6	2.944591000	-3.861714000	0.503946000
1	2.924823000	-4.885458000	0.116147000
1	3.990032000	-3.601733000	0.678945000
1	2.444544000	-3.882985000	1.477028000
6	-3.939723000	0.569793000	-0.196103000
1	-3.482798000	1.543946000	0.021407000
6	-5.164245000	0.447710000	0.705702000
1	-5.733684000	-0.464825000	0.523367000
1	-4.913226000	0.476680000	1.768507000
1	-5.840962000	1.287302000	0.515115000
6	-4.326228000	0.549454000	-1.669477000
1	-4.904025000	-0.345819000	-1.919116000
1	-4.955491000	1.410452000	-1.915936000
1	-3.460121000	0.577410000	-2.338014000
6	2.116946000	2.543446000	0.424125000
1	2.548976000	1.593324000	0.762353000
6	2.381263000	3.563181000	1.525065000
1	3.460759000	3.695162000	1.652465000
1	1.964233000	4.548210000	1.308548000
1	1.984436000	3.243978000	2.492219000
6	2.788438000	2.908708000	-0.895123000
1	3.874652000	2.967118000	-0.772826000
1	2.586264000	2.172520000	-1.681116000
1	2.460445000	3.884238000	-1.266702000
15	-2.535526000	-0.590630000	0.185141000
15	0.336351000	2.089100000	0.122482000
15	2.344198000	-1.097814000	-0.036281000
7	0.617011000	-0.168727000	-2.442479000
7	-0.601513000	-0.086261000	-2.414439000
1	-1.125653000	0.016385000	-3.305171000

[3b' _{PSi} **-N_α-H]⁺ (TE = -3313.935780)**

15	1.277434000	2.093839000	0.080678000
15	1.219626000	-2.100063000	0.264920000
15	-2.571188000	-0.051778000	0.124769000
6	1.137391000	2.591663000	1.855355000
6	1.088672000	1.378779000	2.775691000
6	-2.983621000	-0.027836000	1.926390000
6	-1.882958000	0.613832000	2.761380000
6	1.472418000	-2.171510000	2.097246000
6	0.298747000	-1.578036000	2.867234000
1	-3.968649000	0.430577000	2.076966000

1	-1.966743000	1.706275000	2.731523000
1	1.701457000	-3.203324000	2.390376000
1	-0.559122000	-2.260994000	2.850131000
1	1.932373000	3.305394000	2.107041000
1	0.826373000	1.688677000	3.795945000
6	0.705666000	3.645373000	-0.798600000
1	-0.376824000	3.659091000	-0.606642000
6	3.117542000	2.057506000	-0.252611000
1	3.419171000	3.109843000	-0.354134000
6	-3.844155000	-1.250994000	-0.536743000
1	-3.516996000	-2.223167000	-0.147090000
6	-3.148058000	1.589198000	-0.572413000
1	-4.218570000	1.480737000	-0.793814000
6	0.300121000	-3.691382000	-0.084880000
1	0.681737000	-4.412825000	0.652117000
6	2.968955000	-2.350682000	-0.345090000
1	3.470740000	-1.462888000	0.069762000
23	-0.066395000	-0.029072000	-0.494494000
14	-0.166426000	0.107180000	2.114018000
1	-2.000937000	0.341018000	3.818208000
1	-3.104730000	-1.085133000	2.201545000
1	0.562142000	-1.470286000	3.927843000
1	2.385284000	-1.591490000	2.295643000
1	2.078330000	0.914424000	2.854675000
1	0.197228000	3.156642000	1.928829000
6	0.918703000	3.576649000	-2.305351000
1	0.370004000	4.380479000	-2.805855000
1	1.973084000	3.705026000	-2.568165000
1	0.580115000	2.631770000	-2.742846000
6	1.291959000	4.929430000	-0.223193000
1	2.381498000	4.969033000	-0.319867000
1	0.898832000	5.794431000	-0.766962000
1	1.046346000	5.074791000	0.830656000
6	3.433371000	1.321346000	-1.546904000
1	2.900128000	1.716952000	-2.414114000
1	4.504140000	1.375918000	-1.768648000
1	3.172473000	0.264235000	-1.459066000
6	3.898881000	1.448342000	0.903799000
1	3.806066000	2.017386000	1.831302000
1	3.576751000	0.420880000	1.111338000
1	4.964154000	1.403599000	0.656323000
6	3.639391000	-3.584751000	0.249944000
1	4.672317000	-3.658908000	-0.105188000
1	3.675585000	-3.565152000	1.341118000
1	3.135553000	-4.509034000	-0.049611000
6	3.144330000	-2.307615000	-1.861179000

1	4.181369000	-2.061693000	-2.110309000
1	2.928989000	-3.268763000	-2.329573000
1	2.510195000	-1.562680000	-2.347369000
6	0.528309000	-4.239764000	-1.487185000
1	1.538418000	-4.622009000	-1.639277000
1	-0.158698000	-5.071226000	-1.674826000
1	0.327979000	-3.486110000	-2.257114000
6	-1.193217000	-3.488268000	0.131027000
1	-1.439462000	-3.005023000	1.081112000
1	-1.595258000	-2.867556000	-0.674891000
1	-1.721248000	-4.446880000	0.101508000
6	-5.248445000	-0.991663000	-0.000700000
1	-5.946567000	-1.715627000	-0.433258000
1	-5.316743000	-1.090454000	1.084390000
1	-5.623680000	0.001180000	-0.269531000
6	-3.839287000	-1.311647000	-2.058438000
1	-4.474497000	-2.132346000	-2.405954000
1	-4.251017000	-0.395921000	-2.496319000
1	-2.840922000	-1.464114000	-2.475427000
6	-2.406480000	1.865264000	-1.876004000
1	-2.532370000	1.074692000	-2.620020000
1	-2.735613000	2.806309000	-2.330183000
1	-1.326900000	1.975084000	-1.701381000
6	-2.975345000	2.740425000	0.407588000
1	-3.581468000	2.621646000	1.308808000
1	-1.931867000	2.847454000	0.726670000
1	-3.268381000	3.686698000	-0.059081000
7	-0.507939000	-0.846554000	-2.305184000
7	0.453045000	-0.085641000	-2.426261000
1	0.874329000	0.054921000	-3.363776000

$[3c'_{PB} - N_{\alpha} - H]^+$ (TE = -3049.286752)

6	-0.677346000	2.047665000	2.001431000
6	0.211593000	1.142641000	2.858128000
6	-2.242137000	-0.982042000	2.079836000
6	-0.915787000	-1.400881000	2.695788000
6	2.815209000	-0.522821000	1.795382000
6	1.752126000	-1.078235000	2.740908000
1	-2.530080000	0.017211000	2.415191000
1	-1.066375000	-1.561967000	3.779462000
1	3.798344000	-0.961660000	1.996942000
1	2.102598000	-0.903243000	3.772344000
1	-0.681967000	3.071391000	2.393350000
1	1.215256000	1.590387000	2.900686000
6	-1.212543000	3.375922000	-0.598805000
1	-0.560456000	4.257052000	-0.667728000

6	-2.518059000	-2.767440000	-0.154520000
1	-1.761692000	-3.282341000	0.460398000
6	3.817592000	0.093381000	-0.839155000
1	3.734640000	1.133314000	-0.489674000
23	0.012197000	-0.172460000	-0.872586000
1	-1.724541000	1.730358000	2.010369000
1	-0.150445000	1.224558000	3.898857000
1	1.706255000	-2.170874000	2.646121000
1	2.937859000	0.558886000	1.939028000
1	-0.633083000	-2.400123000	2.333570000
1	-3.065551000	-1.636740000	2.387985000
6	5.196755000	-0.428050000	-0.452829000
1	5.971346000	0.212815000	-0.886039000
1	5.369041000	-0.450960000	0.625678000
1	5.369869000	-1.434962000	-0.844849000
6	3.660003000	0.086907000	-2.353951000
1	3.661934000	-0.931841000	-2.759154000
1	2.738106000	0.569840000	-2.681378000
1	4.494836000	0.613501000	-2.826455000
6	-3.893377000	-3.263975000	0.276006000
1	-3.946183000	-4.352679000	0.172800000
1	-4.138531000	-3.031269000	1.315008000
1	-4.685801000	-2.850492000	-0.354294000
6	-2.255404000	-3.130100000	-1.611726000
1	-2.980337000	-2.670419000	-2.287648000
1	-1.264877000	-2.826150000	-1.955859000
1	-2.328251000	-4.213644000	-1.749649000
6	-1.564214000	2.948518000	-2.019308000
1	-0.677261000	2.687119000	-2.605553000
1	-2.225532000	2.075927000	-2.034187000
1	-2.078707000	3.756876000	-2.548384000
6	-2.445465000	3.794921000	0.191765000
1	-2.197427000	4.218410000	1.167854000
1	-2.995332000	4.562528000	-0.361754000
1	-3.145465000	2.970256000	0.359768000
6	2.707371000	-2.585975000	-0.315426000
1	3.181768000	-2.590763000	-1.308532000
6	1.390137000	-3.344845000	-0.425950000
1	0.801337000	-3.274863000	0.497002000
1	0.768965000	-2.965818000	-1.244026000
1	1.561822000	-4.408258000	-0.621873000
6	3.646323000	-3.273849000	0.668359000
1	3.861269000	-4.291766000	0.327433000
1	4.604525000	-2.765049000	0.784592000
1	3.198738000	-3.362736000	1.662455000
6	-3.619784000	0.067930000	-0.270850000

1	-3.183375000	1.077193000	-0.233825000
6	-4.814573000	0.053923000	0.676194000
1	-5.295157000	-0.925818000	0.728716000
1	-4.558433000	0.351478000	1.695876000
1	-5.572465000	0.760005000	0.320156000
6	-4.049486000	-0.183419000	-1.712047000
1	-4.591060000	-1.129206000	-1.809351000
1	-4.735959000	0.603815000	-2.040622000
1	-3.210219000	-0.205420000	-2.410573000
6	1.516178000	2.921873000	0.299528000
1	2.186567000	2.167645000	0.735764000
6	1.554000000	4.162478000	1.180039000
1	2.540029000	4.635156000	1.129407000
1	0.827209000	4.918059000	0.862459000
1	1.359698000	3.938657000	2.232006000
6	1.989184000	3.218759000	-1.119301000
1	3.035261000	3.540993000	-1.124219000
1	1.910107000	2.346402000	-1.776682000
1	1.410125000	4.025984000	-1.579526000
15	-2.155306000	-0.974646000	0.233203000
15	-0.145305000	2.075023000	0.241037000
15	2.391512000	-0.765246000	0.014105000
5	0.318427000	-0.425508000	2.635231000
7	-0.809446000	-0.387507000	-2.704791000
7	0.420851000	-0.470649000	-2.806483000
1	0.831275000	-0.662231000	-3.739379000

[3d'_{sc}-N_α-H]⁺ (TE = -2877.655083)

6	0.089362000	1.504321000	2.081310000
6	0.245722000	0.076145000	2.582687000
6	-2.669273000	-0.424695000	1.769802000
6	-1.627805000	-1.494393000	1.984911000
6	2.107816000	-2.101931000	1.339537000
6	0.688281000	-2.276670000	1.827001000
1	-2.520414000	0.443685000	2.417523000
1	-1.679417000	-1.828759000	3.037780000
1	2.710991000	-3.005414000	1.459361000
1	0.730575000	-2.566740000	2.892626000
1	0.528514000	2.232637000	2.769384000
1	1.304340000	-0.054558000	2.842813000
6	0.504119000	3.240305000	-0.233284000
1	1.039772000	3.208657000	-1.191605000
6	-3.538421000	-1.177523000	-0.774885000
1	-3.475571000	-2.012321000	-0.066904000
6	3.557007000	-0.607383000	-0.593423000
1	3.487183000	0.100393000	0.241841000

23	-0.112503000	-0.350457000	-0.529429000
16	-2.541971000	0.179099000	0.047911000
16	0.974966000	1.592566000	0.484982000
16	2.036629000	-1.663354000	-0.433117000
6	-0.208308000	-1.047817000	1.620850000
1	-0.951664000	1.789470000	1.903613000
1	-0.284387000	0.003779000	3.547466000
1	0.245386000	-3.145628000	1.319168000
1	2.625823000	-1.281973000	1.849384000
1	-1.900331000	-2.381339000	1.392555000
1	-3.697236000	-0.763763000	1.932834000
6	4.788799000	-1.477800000	-0.447329000
1	5.687248000	-0.853910000	-0.485918000
1	4.809946000	-2.017333000	0.502378000
1	4.860322000	-2.211971000	-1.254577000
6	3.520724000	0.148773000	-1.903832000
1	3.441914000	-0.524848000	-2.763437000
1	2.692624000	0.861442000	-1.943370000
1	4.447544000	0.716590000	-2.025026000
6	-4.975240000	-0.716961000	-0.909554000
1	-5.595384000	-1.531428000	-1.297464000
1	-5.401194000	-0.406166000	0.047378000
1	-5.059998000	0.124621000	-1.602294000
6	-2.929649000	-1.594271000	-2.096505000
1	-2.844448000	-0.758539000	-2.796240000
1	-1.936614000	-2.047557000	-1.983327000
1	-3.563097000	-2.351092000	-2.569130000
6	-0.981245000	3.388573000	-0.480336000
1	-1.376761000	2.612335000	-1.137043000
1	-1.555379000	3.374464000	0.451022000
1	-1.175038000	4.355755000	-0.954764000
6	1.076580000	4.346090000	0.633142000
1	2.146487000	4.224152000	0.814239000
1	0.928400000	5.312887000	0.143283000
1	0.570528000	4.399544000	1.601617000
7	-0.740855000	0.528826000	-2.303546000
7	0.334309000	-0.016905000	-2.482212000
1	0.787952000	0.018436000	-3.414969000

$[3e'_{\text{ssi}} - N_{\alpha} - H]^+$ (TE = -3129.067888)

6	-0.860415000	0.136164000	2.379905000
6	-0.030099000	-1.124486000	2.545960000
6	-2.255091000	-2.556080000	0.412749000
6	-0.940689000	-3.295659000	0.613001000
6	3.108226000	-1.337948000	0.749182000
6	2.226119000	-2.552603000	1.017983000

1	-2.590252000	-2.063051000	1.333017000
1	-1.058395000	-3.981669000	1.461203000
1	4.167380000	-1.595114000	0.661889000
1	2.482063000	-2.960730000	2.003452000
1	-1.001211000	0.682269000	3.317330000
1	0.894929000	-0.876974000	3.082618000
6	-1.172418000	2.642476000	0.918362000
6	-3.620687000	-0.257199000	-0.710954000
6	3.748477000	0.839872000	-1.108001000
23	0.172218000	-0.145386000	-0.847006000
16	-2.063637000	-1.253452000	-0.888169000
16	0.026879000	1.252041000	1.224520000
16	2.601605000	-0.599894000	-0.863315000
1	-1.849532000	-0.069821000	1.955729000
1	-0.572979000	-1.815364000	3.205035000
1	2.451165000	-3.339490000	0.289303000
1	3.007493000	-0.575039000	1.530006000
1	-0.724862000	-3.920245000	-0.261120000
1	-3.062557000	-3.209737000	0.072761000
14	0.413929000	-1.993261000	0.890909000
1	3.520525000	1.108324000	-2.147559000
1	-1.875349000	2.262074000	0.166853000
1	-3.567730000	0.201809000	0.287024000
6	5.197631000	0.406118000	-1.007109000
1	5.848700000	1.220889000	-1.337882000
1	5.481214000	0.174067000	0.023350000
1	5.416224000	-0.465804000	-1.627431000
6	3.407503000	1.998382000	-0.193238000
1	3.530162000	1.736972000	0.862208000
1	4.072736000	2.843984000	-0.395610000
1	2.379343000	2.342714000	-0.332796000
6	-3.588728000	0.818775000	-1.778513000
1	-4.470070000	1.459931000	-1.688508000
1	-2.705153000	1.458298000	-1.698332000
1	-3.597262000	0.386127000	-2.783325000
6	-4.847629000	-1.139789000	-0.813206000
1	-5.749197000	-0.522507000	-0.750750000
1	-4.877969000	-1.672252000	-1.768105000
1	-4.907886000	-1.876891000	-0.010259000
6	-1.916249000	3.030057000	2.178967000
1	-2.556267000	3.892348000	1.968576000
1	-2.562581000	2.233884000	2.554151000
1	-1.231207000	3.323312000	2.980175000
6	-0.370542000	3.794876000	0.345088000
1	-1.040766000	4.608422000	0.052484000
1	0.331192000	4.194027000	1.083159000

1	0.204538000	3.505127000	-0.536960000
7	0.160869000	0.406976000	-2.749426000
7	-0.061791000	1.457838000	-2.162017000
1	-0.207714000	2.315664000	-2.724694000

[3f_{SB}-N_α-H]⁺ (TE = -3129.067888)

6	0.345627000	1.822670000	2.038798000
6	0.535913000	0.415992000	2.584363000
6	-2.744013000	0.374876000	1.319978000
6	-2.056937000	-0.486872000	2.368393000
6	1.422365000	-2.415917000	1.529585000
6	-0.003415000	-2.200535000	1.986433000
1	-2.448686000	1.425082000	1.381495000
1	-2.245085000	-0.002840000	3.339840000
1	1.704940000	-3.471361000	1.499462000
1	-0.130837000	-2.705506000	2.961338000
1	0.960326000	2.553941000	2.570593000
1	1.580113000	0.119584000	2.420414000
6	0.236973000	3.473570000	-0.347762000
1	0.678670000	3.499103000	-1.351834000
6	-2.925969000	-1.819831000	-0.522786000
1	-2.526766000	-2.314459000	0.369695000
6	3.409858000	-1.091540000	-0.023198000
1	3.379587000	-0.405086000	0.834242000
23	0.066316000	-0.024232000	-1.050506000
16	-2.369319000	-0.054374000	-0.418864000
16	0.905140000	1.861696000	0.290582000
16	1.673846000	-1.742749000	-0.166945000
1	-0.692528000	2.162550000	2.090441000
1	0.449202000	0.490309000	3.683263000
1	-0.694330000	-2.755527000	1.336063000
1	2.141188000	-1.903000000	2.176250000
1	-2.582554000	-1.449386000	2.429681000
1	-3.833944000	0.364364000	1.420061000
6	4.365852000	-2.235093000	0.248122000
1	5.379737000	-1.845036000	0.381224000
1	4.113638000	-2.793440000	1.152507000
1	4.388580000	-2.939764000	-0.587848000
6	3.760633000	-0.325321000	-1.280515000
1	3.687876000	-0.957427000	-2.171351000
1	3.119344000	0.546966000	-1.425712000
1	4.793525000	0.028686000	-1.215968000
6	-4.438037000	-1.895966000	-0.527641000
1	-4.760292000	-2.941427000	-0.561468000
1	-4.879699000	-1.452258000	0.368423000
1	-4.862114000	-1.388519000	-1.398328000

6	-2.289649000	-2.423554000	-1.760202000
1	-2.545588000	-1.866578000	-2.667196000
1	-1.196122000	-2.467972000	-1.678380000
1	-2.634434000	-3.451592000	-1.901554000
6	-1.272945000	3.479593000	-0.458222000
1	-1.649233000	2.658571000	-1.073545000
1	-1.753064000	3.432378000	0.524759000
1	-1.605241000	4.414315000	-0.920369000
6	0.779933000	4.623383000	0.478249000
1	1.868332000	4.597894000	0.564691000
1	0.504588000	5.573859000	0.012093000
1	0.357033000	4.631510000	1.487256000
5	-0.495595000	-0.720886000	2.208076000
7	-0.326318000	0.780554000	-2.865319000
7	0.812759000	0.304773000	-2.884513000
1	1.369654000	0.370657000	-3.758096000

[3a''_{PC}-N_α-H]⁺ (TE = -3519.773774)

6	1.319954000	0.450291000	1.722382000
6	1.275400000	1.164615000	2.928839000
1	0.323063000	1.283290000	3.440638000
6	2.417599000	1.716872000	3.496982000
1	2.339883000	2.267858000	4.431785000
6	3.655312000	1.556745000	2.883937000
1	4.552708000	1.981350000	3.326367000
6	3.729161000	0.861817000	1.683004000
1	4.692411000	0.768107000	1.185386000
6	2.581623000	0.324640000	1.090188000
6	-1.188755000	0.381472000	1.719332000
6	-1.852450000	-0.213118000	2.803543000
1	-1.441897000	-1.115255000	3.250951000
6	-3.032423000	0.310184000	3.316718000
1	-3.522883000	-0.184275000	4.152321000
6	-3.586437000	1.457018000	2.759671000
1	-4.516087000	1.868133000	3.144778000
6	-2.942958000	2.071577000	1.692923000
1	-3.396209000	2.953353000	1.251982000
6	-1.755557000	1.548284000	1.169611000
6	0.063484000	-1.696615000	1.406358000
6	0.771672000	-2.298686000	2.452185000
1	1.460575000	-1.699397000	3.045113000
6	0.602658000	-3.644998000	2.756484000
1	1.168766000	-4.087034000	3.573665000
6	-0.294429000	-4.423969000	2.033100000
1	-0.432065000	-5.474860000	2.274113000
6	-1.020337000	-3.844388000	0.997515000

1	-1.729907000	-4.450373000	0.440150000
6	-0.842007000	-2.497681000	0.673023000
6	0.088420000	-0.208041000	1.143674000
23	0.112152000	0.063396000	-1.188595000
6	3.785034000	0.775468000	-1.521862000
1	4.715113000	0.791076000	-0.939588000
6	-2.352247000	3.007606000	-1.285319000
1	-3.195417000	2.330659000	-1.079453000
6	-1.635501000	-2.769992000	-2.198366000
1	-1.922689000	-2.074899000	-3.001905000
6	-2.595697000	-3.951817000	-2.234001000
1	-2.513334000	-4.462725000	-3.199364000
1	-2.374375000	-4.698209000	-1.467039000
1	-3.640054000	-3.657145000	-2.120842000
6	-0.203600000	-3.226014000	-2.464754000
1	0.132600000	-3.948817000	-1.714779000
1	-0.126322000	-3.709262000	-3.443577000
1	0.522736000	-2.400037000	-2.461814000
6	4.093986000	0.220800000	-2.908199000
1	4.680982000	-0.699744000	-2.877920000
1	3.184076000	0.004996000	-3.478951000
1	4.670724000	0.947932000	-3.487771000
6	3.246212000	2.192675000	-1.596322000
1	3.044578000	2.611322000	-0.606326000
1	3.960206000	2.856832000	-2.093579000
1	2.314547000	2.225814000	-2.168495000
6	-2.750828000	4.412162000	-0.832838000
1	-3.694614000	4.691070000	-1.312643000
1	-2.894412000	4.517609000	0.242530000
1	-2.016757000	5.161948000	-1.135089000
6	-2.104958000	3.001199000	-2.790388000
1	-1.204462000	3.562512000	-3.060914000
1	-2.004926000	1.992698000	-3.195672000
1	-2.942540000	3.478908000	-3.308563000
15	-1.636566000	-1.640565000	-0.717285000
15	-0.964316000	2.173448000	-0.341701000
15	2.591107000	-0.328588000	-0.607816000
6	0.282576000	3.467393000	0.185139000
1	1.137601000	2.842347000	0.481049000
6	0.720137000	4.340585000	-0.986763000
1	-0.023221000	5.102473000	-1.230107000
1	1.646079000	4.869735000	-0.740242000
1	0.911299000	3.769696000	-1.899085000
6	-0.115748000	4.293091000	1.400569000
1	0.733088000	4.904254000	1.725583000
1	-0.940173000	4.978133000	1.187924000

1	-0.409177000	3.667791000	2.247553000
6	3.481548000	-1.970850000	-0.710541000
1	3.476422000	-2.168686000	-1.792751000
6	2.760350000	-3.112933000	-0.016672000
1	2.840851000	-3.027264000	1.068658000
1	1.697232000	-3.165650000	-0.260969000
1	3.217087000	-4.066393000	-0.300749000
6	4.923982000	-1.890938000	-0.225283000
1	5.407704000	-2.866393000	-0.338747000
1	5.534630000	-1.167602000	-0.770127000
1	4.969526000	-1.638218000	0.838990000
6	-3.403646000	-1.239897000	-0.299892000
1	-3.307656000	-0.375881000	0.368521000
6	-4.139931000	-2.328511000	0.468503000
1	-5.135141000	-1.971962000	0.754441000
1	-4.281758000	-3.242429000	-0.114087000
1	-3.616334000	-2.598535000	1.389750000
6	-4.135011000	-0.773910000	-1.554797000
1	-5.102889000	-0.338038000	-1.288437000
1	-3.570677000	-0.012662000	-2.104451000
1	-4.336177000	-1.593524000	-2.250552000
7	-0.689039000	0.134726000	-3.047152000
7	0.482447000	0.501416000	-3.115938000
1	0.891433000	0.717045000	-4.042410000

[3b''_{PSi}-N_α-H]⁺ (TE = -3771.191923)

6	-1.764986000	-0.739214000	1.935395000
6	-1.959322000	-1.071675000	3.281597000
1	-1.143836000	-0.944868000	3.993884000
6	-3.177864000	-1.573716000	3.725443000
1	-3.312116000	-1.833914000	4.773075000
6	-4.227387000	-1.750301000	2.826515000
1	-5.179714000	-2.146360000	3.170881000
6	-4.052877000	-1.440049000	1.482965000
1	-4.870688000	-1.617939000	0.786890000
6	-2.825604000	-0.940265000	1.032869000
6	1.363744000	-0.427371000	2.112493000
6	1.693542000	0.036979000	3.391667000
1	0.965968000	0.616711000	3.960307000
6	2.954036000	-0.182124000	3.936803000
1	3.194992000	0.196734000	4.927442000
6	3.917285000	-0.859077000	3.195551000
1	4.914387000	-1.009801000	3.602436000
6	3.612404000	-1.338441000	1.926017000
1	4.388422000	-1.846410000	1.362158000
6	2.337583000	-1.139427000	1.386142000

6	-0.392466000	1.926752000	1.564521000
6	-1.040737000	2.463096000	2.681880000
1	-1.497992000	1.794736000	3.412324000
6	-1.145420000	3.838497000	2.859476000
1	-1.668313000	4.239288000	3.725110000
6	-0.585982000	4.704420000	1.923573000
1	-0.665506000	5.780476000	2.057847000
6	0.073604000	4.194733000	0.810855000
1	0.509524000	4.884038000	0.093518000
6	0.162588000	2.812124000	0.621481000
23	-0.020369000	-0.253539000	-1.322359000
6	-3.284807000	-2.043691000	-1.588948000
1	-4.349750000	-1.953319000	-1.336867000
6	3.423377000	-2.125751000	-1.158067000
1	4.065705000	-1.277110000	-0.875868000
6	0.744651000	3.101963000	-2.320674000
1	1.084541000	2.434723000	-3.127974000
6	1.567122000	4.382810000	-2.418253000
1	1.405726000	4.838283000	-3.401115000
1	1.276969000	5.132780000	-1.679257000
1	2.640325000	4.217888000	-2.318073000
6	-0.738063000	3.384940000	-2.539375000
1	-1.142409000	4.033449000	-1.755432000
1	-0.890147000	3.895838000	-3.495007000
1	-1.339824000	2.471628000	-2.556431000
6	-3.128703000	-1.945546000	-3.099374000
1	-3.437696000	-0.977695000	-3.503984000
1	-2.087841000	-2.101273000	-3.404006000
1	-3.725601000	-2.716840000	-3.595998000
6	-2.785694000	-3.378554000	-1.061118000
1	-2.925045000	-3.486847000	0.017526000
1	-3.319021000	-4.201736000	-1.546946000
1	-1.724606000	-3.517329000	-1.275303000
6	4.127806000	-3.414980000	-0.737010000
1	5.135373000	-3.436439000	-1.165238000
1	4.231825000	-3.538221000	0.341050000
1	3.612341000	-4.301361000	-1.114445000
6	3.264675000	-2.098124000	-2.675126000
1	2.577125000	-2.871058000	-3.031930000
1	2.896254000	-1.137036000	-3.036366000
1	4.229568000	-2.282471000	-3.157848000
15	0.953737000	2.009018000	-0.815533000
15	1.821415000	-1.703416000	-0.279510000
15	-2.469474000	-0.600494000	-0.730648000
6	0.890338000	-3.303849000	0.034617000
1	-0.099324000	-2.927737000	0.343262000

6	0.712610000	-4.074530000	-1.269715000
1	1.650262000	-4.511826000	-1.620399000
1	0.011370000	-4.903680000	-1.135014000
1	0.324652000	-3.447911000	-2.083299000
6	1.412890000	-4.183353000	1.160833000
1	0.704047000	-4.995672000	1.352629000
1	2.371780000	-4.647401000	0.920844000
1	1.533086000	-3.629762000	2.095591000
6	-3.528178000	0.854194000	-1.248359000
1	-3.141927000	1.097719000	-2.249565000
6	-3.281747000	2.039733000	-0.325707000
1	-3.623208000	1.832131000	0.694386000
1	-2.228344000	2.315010000	-0.265559000
1	-3.830422000	2.917499000	-0.681686000
6	-5.018388000	0.560367000	-1.356945000
1	-5.549409000	1.472257000	-1.648216000
1	-5.260537000	-0.198223000	-2.104399000
1	-5.443393000	0.244557000	-0.398792000
6	2.772538000	1.942724000	-0.404814000
1	2.816867000	1.095850000	0.292674000
6	3.321506000	3.155790000	0.333395000
1	4.374240000	2.989180000	0.584755000
1	3.274235000	4.074748000	-0.256214000
1	2.789472000	3.336261000	1.270746000
6	3.583770000	1.569365000	-1.639332000
1	4.608244000	1.302627000	-1.360336000
1	3.152593000	0.711028000	-2.165502000
1	3.655361000	2.389436000	-2.359055000
14	-0.223991000	0.070902000	1.203746000
7	-0.705139000	0.092582000	-3.202165000
7	0.448947000	-0.340077000	-3.258843000
1	0.886874000	-0.490714000	-4.186594000

$[3c''_{PB} - N_{\alpha} - H]^+$ (TE = -3506.525989)

6	0.926998000	-1.417638000	1.771980000
6	0.635568000	-2.261648000	2.857022000
1	-0.313311000	-2.144317000	3.379885000
6	1.535189000	-3.226861000	3.297959000
1	1.279443000	-3.862547000	4.142613000
6	2.762062000	-3.372737000	2.661080000
1	3.476175000	-4.117573000	3.003589000
6	3.062366000	-2.574748000	1.561705000
1	4.011673000	-2.718081000	1.051475000
6	2.154608000	-1.617633000	1.104452000
6	0.510861000	1.249769000	1.895019000
6	1.215567000	1.358030000	3.105825000

1	1.523382000	0.448828000	3.622489000
6	1.516980000	2.591028000	3.673769000
1	2.061287000	2.637062000	4.614392000
6	1.121800000	3.762612000	3.038320000
1	1.348610000	4.731553000	3.476164000
6	0.446059000	3.688263000	1.825194000
1	0.160187000	4.609088000	1.322019000
6	0.147798000	2.451635000	1.247086000
6	-1.583148000	-0.395937000	1.749586000
6	-2.079232000	0.008428000	3.002010000
1	-1.408039000	0.507953000	3.700823000
6	-3.401874000	-0.195754000	3.372302000
1	-3.750559000	0.130774000	4.349454000
6	-4.281706000	-0.795349000	2.478212000
1	-5.325420000	-0.942574000	2.744911000
6	-3.822520000	-1.193190000	1.229411000
1	-4.530528000	-1.634521000	0.533918000
6	-2.483818000	-1.011844000	0.861152000
23	0.135183000	0.093781000	-1.438806000
6	3.964535000	0.234637000	-0.291189000
1	4.722057000	-0.523166000	-0.041450000
6	-2.327746000	2.975629000	-0.319841000
1	-2.183637000	4.048625000	-0.137415000
6	-1.598602000	-3.331064000	-0.761273000
1	-2.143406000	-3.703901000	-1.637021000
6	-2.161160000	-3.997352000	0.485680000
1	-2.021977000	-5.081607000	0.423307000
1	-1.645310000	-3.652457000	1.388040000
1	-3.227290000	-3.811835000	0.633260000
6	-0.133512000	-3.681965000	-0.946113000
1	0.474794000	-3.325169000	-0.109510000
1	-0.000459000	-4.767571000	-1.002149000
1	0.270088000	-3.258704000	-1.870006000
6	4.371926000	0.916436000	-1.592472000
1	4.468428000	0.224323000	-2.431429000
1	3.657094000	1.681391000	-1.898565000
1	5.341214000	1.409618000	-1.468764000
6	3.879011000	1.213425000	0.870226000
1	3.663766000	0.709233000	1.816053000
1	4.830291000	1.742821000	0.985873000
1	3.101477000	1.968622000	0.720712000
6	-3.007863000	2.787226000	-1.670162000
1	-3.973393000	3.301911000	-1.694274000
1	-2.416852000	3.167348000	-2.510349000
1	-3.202935000	1.726499000	-1.862366000
6	-3.172097000	2.430731000	0.816711000

1	-3.436202000	1.381780000	0.668817000
1	-2.672980000	2.515574000	1.785158000
1	-4.108857000	2.994248000	0.878697000
5	-0.031783000	-0.190774000	1.528816000
15	2.393396000	-0.747057000	-0.485220000
15	-0.587253000	2.312271000	-0.414500000
15	-1.875248000	-1.463259000	-0.805525000
6	0.241113000	3.621290000	-1.491335000
1	0.068517000	3.235830000	-2.505198000
6	1.743490000	3.618624000	-1.253681000
1	2.263546000	4.140765000	-2.062600000
1	2.007845000	4.115414000	-0.315558000
1	2.141068000	2.604071000	-1.208655000
6	-0.318221000	5.038615000	-1.450915000
1	0.272320000	5.672679000	-2.120464000
1	-1.354763000	5.107048000	-1.787530000
1	-0.259152000	5.496196000	-0.459577000
6	2.896465000	-2.140906000	-1.661590000
1	2.369468000	-3.006646000	-1.245085000
6	4.376905000	-2.501010000	-1.724484000
1	4.501687000	-3.398368000	-2.339355000
1	4.986439000	-1.720180000	-2.183943000
1	4.813751000	-2.727008000	-0.750486000
6	2.350593000	-1.881221000	-3.061084000
1	2.586191000	-2.715226000	-3.730379000
1	1.257225000	-1.774427000	-3.075376000
1	2.763231000	-0.972758000	-3.511013000
6	-3.409721000	-1.288983000	-1.886596000
1	-3.953558000	-0.457629000	-1.414798000
6	-3.040857000	-0.877064000	-3.306414000
1	-2.347152000	-1.590476000	-3.768673000
1	-3.933649000	-0.845526000	-3.939209000
1	-2.573566000	0.107657000	-3.341250000
6	-4.331849000	-2.506039000	-1.936322000
1	-3.939169000	-3.279912000	-2.602437000
1	-4.513805000	-2.977703000	-0.968979000
1	-5.304681000	-2.213624000	-2.343680000
7	1.033515000	0.964058000	-3.055849000
7	-0.115525000	0.635704000	-3.353506000
1	-0.456081000	0.811235000	-4.318854000

[3d''_{sc} -N_α-H]⁺ (TE = -3334.914743)

6	-0.416765000	1.801982000	0.692745000
6	0.138067000	2.816446000	1.485527000
1	1.031721000	2.608957000	2.068628000
6	-0.444259000	4.077691000	1.573209000

1	0.013194000	4.834221000	2.206468000
6	-1.608297000	4.371490000	0.871753000
1	-2.068648000	5.352874000	0.946224000
6	-2.150895000	3.409272000	0.028016000
1	-3.017552000	3.643699000	-0.586441000
6	-1.552861000	2.155526000	-0.065342000
6	-0.891320000	-0.501661000	1.433644000
6	-1.559910000	-0.023554000	2.572335000
1	-1.430638000	1.019330000	2.856736000
6	-2.375141000	-0.836832000	3.348116000
1	-2.865820000	-0.424884000	4.226823000
6	-2.571367000	-2.170536000	3.001607000
1	-3.214457000	-2.810835000	3.599366000
6	-1.963616000	-2.668353000	1.857693000
1	-2.146483000	-3.692082000	1.538592000
6	-1.136333000	-1.842836000	1.093528000
6	1.468187000	0.263712000	1.284828000
6	1.652223000	0.218479000	2.675378000
1	0.779371000	0.206865000	3.322877000
6	2.913817000	0.192415000	3.255710000
1	3.004962000	0.156533000	4.338740000
6	4.055865000	0.207827000	2.460747000
1	5.045701000	0.181145000	2.908203000
6	3.914402000	0.217611000	1.081576000
1	4.789159000	0.168321000	0.437582000
6	2.638802000	0.245616000	0.512319000
16	2.521462000	-0.037006000	-1.246031000
16	-2.016540000	1.042410000	-1.374740000
16	-0.520517000	-2.472252000	-0.456029000
23	0.071178000	-0.333567000	-1.489790000
6	-3.772371000	0.440584000	-1.097435000
1	-4.369963000	1.276354000	-1.479636000
6	0.854970000	-3.668184000	-0.016303000
1	0.296947000	-4.544275000	0.335106000
6	2.658750000	1.638139000	-2.097871000
1	3.119286000	1.348747000	-3.049310000
6	3.573443000	2.566419000	-1.335695000
1	3.698887000	3.496532000	-1.898391000
1	3.156270000	2.827658000	-0.358366000
1	4.566115000	2.138932000	-1.179076000
6	1.288116000	2.235442000	-2.345916000
1	0.794289000	2.528070000	-1.415642000
1	1.367343000	3.138125000	-2.960784000
1	0.626032000	1.567484000	-2.919757000
6	-3.953389000	-0.772775000	-1.984918000
1	-3.708422000	-0.572937000	-3.030203000

1	-3.331858000	-1.608279000	-1.646560000
1	-4.997015000	-1.097937000	-1.942862000
6	-4.099622000	0.183739000	0.351813000
1	-3.846690000	1.028445000	0.997581000
1	-5.177468000	0.012102000	0.443391000
1	-3.590484000	-0.704625000	0.731340000
6	1.566691000	-3.995996000	-1.312860000
1	2.302024000	-4.787006000	-1.140943000
1	0.882113000	-4.347035000	-2.089889000
1	2.108434000	-3.124961000	-1.697470000
6	1.777088000	-3.168989000	1.068029000
1	2.408224000	-2.348646000	0.719187000
1	1.238543000	-2.830812000	1.957070000
1	2.440496000	-3.983598000	1.376803000
6	0.086211000	0.373980000	0.654898000
7	-0.792459000	-0.954525000	-3.273358000
7	0.410205000	-1.129348000	-3.329391000
1	0.841681000	-1.527700000	-4.184960000

$[3e''_{\text{ssi}} - N_{\alpha} - \mathbf{H}]^+$ (TE = -3586.324718)

6	-0.874803000	0.120286000	2.100973000
6	-1.649675000	0.822554000	3.033290000
1	-2.045862000	1.804087000	2.773235000
6	-1.939142000	0.288031000	4.284375000
1	-2.542068000	0.853643000	4.990682000
6	-1.469376000	-0.976306000	4.629319000
1	-1.702758000	-1.401556000	5.602106000
6	-0.722659000	-1.712519000	3.716710000
1	-0.384536000	-2.716252000	3.964942000
6	-0.433189000	-1.155437000	2.472220000
6	0.917181000	2.074418000	0.477464000
6	0.929253000	3.164157000	1.355445000
1	0.166652000	3.235674000	2.131101000
6	1.906523000	4.150914000	1.274311000
1	1.903515000	4.982178000	1.974884000
6	2.884968000	4.073703000	0.288501000
1	3.642091000	4.849365000	0.205680000
6	2.906786000	3.001860000	-0.597654000
1	3.675009000	2.956636000	-1.364781000
6	1.941412000	2.004844000	-0.475819000
6	-1.953606000	1.562997000	-0.386686000
6	-2.454995000	2.826218000	-0.047951000
1	-1.956236000	3.416311000	0.720716000
6	-3.570270000	3.357496000	-0.686649000
1	-3.942507000	4.339427000	-0.404460000
6	-4.196155000	2.644983000	-1.705532000

1	-5.052205000	3.068342000	-2.224696000
6	-3.707907000	1.400257000	-2.085953000
1	-4.161821000	0.862435000	-2.914172000
6	-2.608462000	0.867954000	-1.411578000
16	-1.946963000	-0.716456000	-1.945550000
16	0.480407000	-2.163706000	1.293191000
16	1.927406000	0.579871000	-1.577757000
23	0.325024000	-1.219323000	-1.034493000
6	2.219712000	-2.040767000	1.964277000
1	2.143769000	-2.540685000	2.937599000
6	3.716506000	0.333067000	-2.056334000
1	3.947672000	1.231620000	-2.639844000
6	-3.153050000	-1.982186000	-1.271729000
1	-2.631262000	-2.905797000	-1.546698000
6	-4.480681000	-1.894602000	-1.993704000
1	-5.103002000	-2.747294000	-1.704762000
1	-5.031596000	-0.991290000	-1.717285000
1	-4.371258000	-1.916176000	-3.080156000
6	-3.290208000	-1.871139000	0.229821000
1	-3.652973000	-0.882820000	0.532287000
1	-4.016839000	-2.606548000	0.589217000
1	-2.348251000	-2.058969000	0.749184000
6	3.109682000	-2.844529000	1.040077000
1	2.777382000	-3.881059000	0.938481000
1	3.140820000	-2.399990000	0.039222000
1	4.133344000	-2.858207000	1.425251000
6	2.656899000	-0.605556000	2.138595000
1	2.009326000	-0.053119000	2.824200000
1	3.673431000	-0.572341000	2.544953000
1	2.665053000	-0.074459000	1.182955000
6	4.650255000	0.212225000	-0.872127000
1	5.685279000	0.201724000	-1.229318000
1	4.558628000	1.038806000	-0.164767000
1	4.484765000	-0.719654000	-0.326405000
6	3.772091000	-0.877450000	-2.964512000
1	3.577182000	-1.796924000	-2.404848000
1	3.062042000	-0.818605000	-3.793539000
1	4.774104000	-0.966494000	-3.392812000
14	-0.425792000	0.748038000	0.374748000
7	-0.058161000	-3.070816000	-1.777187000
7	1.149471000	-2.876072000	-1.851592000
1	1.753337000	-3.600084000	-2.282880000

[3f'_{SB} - N_α-H]⁺ (TE = -3321.675483)

6	-1.108153000	-1.369379000	-1.321349000
6	-1.037507000	-2.064419000	-2.540365000

1	-0.284226000	-1.774087000	-3.272942000
6	-1.912905000	-3.101588000	-2.841294000
1	-1.838996000	-3.612132000	-3.798363000
6	-2.871549000	-3.496588000	-1.912766000
1	-3.549094000	-4.316606000	-2.135915000
6	-2.931902000	-2.866566000	-0.675734000
1	-3.633219000	-3.210082000	0.081646000
6	-2.065737000	-1.809597000	-0.398782000
6	-0.946900000	1.309337000	-1.389833000
6	-1.802203000	1.443949000	-2.496566000
1	-2.047391000	0.560960000	-3.086677000
6	-2.327370000	2.675934000	-2.869348000
1	-2.975157000	2.747936000	-3.739571000
6	-2.037644000	3.812956000	-2.120854000
1	-2.459499000	4.775919000	-2.396991000
6	-1.236511000	3.708081000	-0.989739000
1	-1.052740000	4.579773000	-0.365339000
6	-0.694041000	2.471175000	-0.645692000
6	1.307515000	-0.143130000	-1.506951000
6	1.673928000	0.325295000	-2.781224000
1	0.911184000	0.776458000	-3.416054000
6	2.977129000	0.235508000	-3.255357000
1	3.217610000	0.602121000	-4.250351000
6	3.976111000	-0.290692000	-2.443757000
1	5.004805000	-0.335589000	-2.791557000
6	3.659207000	-0.724922000	-1.162864000
1	4.441309000	-1.078918000	-0.496188000
6	2.336199000	-0.677356000	-0.716171000
16	2.046246000	-1.106006000	0.999680000
16	-2.018310000	-1.172069000	1.271673000
16	0.174048000	2.309649000	0.905716000
23	0.085719000	0.069766000	1.916405000
6	-3.595070000	-0.190736000	1.492194000
1	-4.370508000	-0.963786000	1.545412000
6	1.746364000	3.311468000	0.727541000
1	1.381917000	4.345491000	0.733150000
6	2.019631000	-2.977128000	1.079414000
1	1.868546000	-3.113817000	2.158226000
6	3.370521000	-3.527541000	0.673913000
1	3.396584000	-4.604017000	0.868556000
1	3.552076000	-3.391954000	-0.396281000
1	4.194571000	-3.068959000	1.225106000
6	0.877524000	-3.587808000	0.303748000
1	0.936275000	-3.340298000	-0.760754000
1	0.918506000	-4.678844000	0.387011000
1	-0.096418000	-3.264993000	0.675712000

6	-3.478811000	0.515804000	2.827912000
1	-3.243186000	-0.166040000	3.649442000
1	-2.713901000	1.302563000	2.796804000
1	-4.424441000	1.008382000	3.070380000
6	-3.867334000	0.754094000	0.347048000
1	-3.865261000	0.249295000	-0.622276000
1	-4.854757000	1.208911000	0.479281000
1	-3.131953000	1.562789000	0.310326000
6	2.577070000	3.045539000	1.964711000
1	3.459997000	3.691109000	1.953207000
1	2.032056000	3.242650000	2.890530000
1	2.926445000	2.008714000	1.996449000
6	2.473232000	3.015498000	-0.562292000
1	2.887737000	2.004283000	-0.568157000
1	1.833248000	3.128009000	-1.441250000
1	3.307165000	3.716683000	-0.671610000
5	-0.230140000	-0.074981000	-1.176846000
7	1.011421000	0.480605000	3.678316000
7	0.255289000	-0.478346000	3.839633000
1	0.178026000	-0.901917000	4.783909000

Cartesian coordinates of the transition states (TS2) involved during the conversion of **[3-V-H]⁺** **[3-N_α-H]⁺** to **[3]** along with their total energies (in hartree) including zero point vibrational correction at M06-L-D3(heptane)/6-311+G* level of theory.

a'pc -TS2 (TE = -3062.077849)

6	-0.394995000	2.195523000	1.752465000
6	0.184851000	1.013551000	2.542335000
6	-2.513303000	-0.520804000	1.981488000
6	-1.185940000	-1.115651000	2.427473000
6	2.596710000	-0.969699000	1.820028000
6	1.257535000	-1.236958000	2.490010000
1	-2.619437000	0.514192000	2.325686000
1	-1.174707000	-1.152536000	3.532559000
1	3.381838000	-1.645027000	2.177001000
1	1.354077000	-1.080245000	3.578943000
1	-0.213231000	3.144922000	2.269860000
1	1.245026000	1.243532000	2.720882000
6	-0.332015000	3.468070000	-0.994912000
1	0.281850000	3.389622000	-1.904067000
6	-3.076311000	-2.295428000	-0.235648000
1	-2.315590000	-2.851433000	0.336067000
6	3.894919000	-0.573457000	-0.792503000
1	4.027507000	0.456208000	-0.428624000
23	-0.061207000	-0.261085000	-0.377007000
6	0.088252000	-0.409742000	1.934903000

1	-1.481284000	2.116717000	1.622596000
1	-0.264935000	1.009260000	3.550556000
1	1.025519000	-2.305781000	2.386219000
1	2.954122000	0.048247000	2.023434000
1	-1.153931000	-2.172992000	2.121975000
1	-3.360962000	-1.067037000	2.410767000
6	5.111715000	-1.386492000	-0.366581000
1	6.025266000	-0.926261000	-0.756369000
1	5.223446000	-1.457154000	0.718735000
1	5.076411000	-2.403160000	-0.769645000
6	3.767461000	-0.530373000	-2.309601000
1	3.586736000	-1.525660000	-2.731087000
1	2.954037000	0.116826000	-2.644152000
1	4.695033000	-0.161990000	-2.758777000
6	-4.448159000	-2.728188000	0.265304000
1	-4.539310000	-3.817620000	0.209402000
1	-4.645904000	-2.441262000	1.301257000
1	-5.248084000	-2.315196000	-0.355952000
6	-2.898919000	-2.656176000	-1.707403000
1	-3.657842000	-2.182761000	-2.336355000
1	-1.920550000	-2.373031000	-2.105788000
1	-3.005691000	-3.737083000	-1.844348000
6	-1.768315000	3.147115000	-1.381590000
1	-1.876831000	2.126550000	-1.763533000
1	-2.446287000	3.268175000	-0.530084000
1	-2.118838000	3.830242000	-2.161230000
6	-0.215396000	4.882033000	-0.439851000
1	0.819253000	5.215018000	-0.342487000
1	-0.716065000	5.591436000	-1.106834000
1	-0.690520000	4.978497000	0.542081000
6	2.173279000	-2.951848000	-0.319916000
1	2.617579000	-3.074266000	-1.319069000
6	0.699156000	-3.343261000	-0.414231000
1	0.165581000	-3.139318000	0.523029000
1	0.188466000	-2.827919000	-1.237085000
1	0.581668000	-4.414283000	-0.611058000
6	2.913216000	-3.850106000	0.662740000
1	2.864469000	-4.891737000	0.329072000
1	3.968400000	-3.594618000	0.773522000
1	2.460912000	-3.817208000	1.658819000
6	-3.996688000	0.617681000	-0.270997000
1	-3.534848000	1.597500000	-0.091414000
6	-5.224443000	0.531671000	0.629342000
1	-5.798314000	-0.383080000	0.472949000
1	-4.977321000	0.592047000	1.692155000
1	-5.896131000	1.368370000	0.410844000

6	-4.366623000	0.535029000	-1.746891000
1	-4.947794000	-0.366841000	-1.962258000
1	-4.986393000	1.388482000	-2.038475000
1	-3.491351000	0.525388000	-2.405444000
6	2.154278000	2.574939000	0.359492000
1	2.585161000	1.627327000	0.707010000
6	2.438366000	3.613383000	1.437871000
1	3.519613000	3.751997000	1.541281000
1	2.012703000	4.592771000	1.210846000
1	2.061952000	3.312283000	2.418920000
6	2.812989000	2.918078000	-0.972098000
1	3.901911000	2.956112000	-0.866151000
1	2.581655000	2.183955000	-1.751199000
1	2.498109000	3.899005000	-1.341599000
15	-2.597878000	-0.530250000	0.146694000
15	0.363421000	2.132362000	0.088899000
15	2.310834000	-1.114104000	0.014675000
7	0.548429000	-0.149970000	-2.297327000
7	0.123319000	-1.099565000	-2.938069000
1	-0.045997000	-0.860940000	-3.945845000

b'_{psi} -TS2 (TE = -3313.909631)

15	-2.386810000	-1.114532000	0.017528000
15	-0.181020000	2.089638000	0.020392000
15	2.523683000	-0.626502000	0.113428000
6	-1.976906000	-2.588139000	1.055815000
6	-1.365920000	-2.101502000	2.376582000
6	2.795682000	-0.604939000	1.944894000
6	1.683463000	-1.353335000	2.677943000
6	-0.984947000	2.005839000	1.682385000
6	-0.375852000	0.964090000	2.643177000
1	3.795199000	-0.988562000	2.180350000
1	1.786740000	-2.435327000	2.519281000
1	-1.006105000	3.006043000	2.136471000
1	0.578686000	1.346427000	3.027218000
1	-2.852775000	-3.233454000	1.191981000
1	-0.945731000	-2.951544000	2.926770000
6	-3.404020000	-1.717763000	-1.433966000
1	-4.449496000	-1.669709000	-1.098532000
6	-3.685903000	-0.288433000	1.091168000
1	-3.126076000	0.140053000	1.933468000
6	3.785621000	0.592498000	-0.515572000
1	3.542423000	1.477532000	0.090886000
6	3.015663000	-2.360225000	-0.394250000
1	2.071564000	-2.918555000	-0.298456000
6	1.155022000	3.384404000	0.143952000

1	1.826054000	3.171894000	-0.700705000
6	-1.476761000	2.674230000	-1.177932000
1	-2.109515000	1.775429000	-1.227229000
23	0.089082000	-0.343319000	-0.500307000
14	-0.003297000	-0.818551000	1.979998000
1	1.776092000	-1.204479000	3.761446000
1	2.807579000	0.448673000	2.248264000
1	-1.020589000	0.898844000	3.531279000
1	-2.032285000	1.766373000	1.469632000
1	-2.142073000	-1.683526000	3.029325000
1	-1.243745000	-3.176935000	0.488967000
7	0.208086000	-2.373054000	-2.101090000
7	0.250257000	-1.135962000	-2.182619000
1	0.258027000	-2.846292000	-3.027898000
6	-4.408379000	0.833961000	0.356939000
1	-5.018028000	0.449966000	-0.467363000
1	-5.092055000	1.353610000	1.035211000
1	-3.734200000	1.585760000	-0.058060000
6	-4.693649000	-1.281569000	1.660727000
1	-5.462796000	-0.744654000	2.224775000
1	-5.213788000	-1.843014000	0.877608000
1	-4.243714000	-2.004683000	2.343527000
6	-3.240946000	-0.773018000	-2.620369000
1	-3.897376000	-1.071449000	-3.444057000
1	-3.491471000	0.263194000	-2.368387000
1	-2.213999000	-0.776117000	-3.000355000
6	-3.098521000	-3.161059000	-1.811313000
1	-2.044961000	-3.305124000	-2.065564000
1	-3.340700000	-3.863146000	-1.009735000
1	-3.687772000	-3.452547000	-2.686526000
6	-0.865886000	2.848376000	-2.565198000
1	-1.648917000	3.039596000	-3.305222000
1	-0.170866000	3.692397000	-2.612520000
1	-0.323030000	1.954258000	-2.893140000
6	-2.367122000	3.838860000	-0.760705000
1	-1.872899000	4.805734000	-0.861322000
1	-3.255978000	3.869817000	-1.400070000
1	-2.719362000	3.755883000	0.272120000
6	1.932523000	3.213686000	1.443835000
1	2.245917000	2.184225000	1.624239000
1	2.833873000	3.833775000	1.433459000
1	1.338068000	3.527873000	2.307648000
6	0.665445000	4.822708000	0.027399000
1	1.502450000	5.509553000	0.189080000
1	0.247162000	5.055741000	-0.952487000
1	-0.090464000	5.060636000	0.783001000

6	5.240207000	0.234763000	-0.235749000
1	5.575317000	-0.618830000	-0.830974000
1	5.892921000	1.074782000	-0.495593000
1	5.423495000	-0.000786000	0.816181000
6	3.554087000	0.970522000	-1.975408000
1	4.128357000	1.866707000	-2.231822000
1	3.873074000	0.183195000	-2.662164000
1	2.499695000	1.179751000	-2.189758000
6	4.054418000	-3.028476000	0.498237000
1	4.263540000	-4.037214000	0.127176000
1	5.005958000	-2.489233000	0.505409000
1	3.724424000	-3.133831000	1.534272000
6	3.435953000	-2.422056000	-1.860350000
1	4.444554000	-2.024978000	-2.006243000
1	3.453770000	-3.462328000	-2.200552000
1	2.767253000	-1.871861000	-2.524932000

c'_{PB} -TS2 (TE = -3049.270191)

6	-0.592282000	2.202654000	1.971227000
6	0.254376000	1.257772000	2.826521000
6	-2.343104000	-0.784717000	2.054271000
6	-1.031246000	-1.217955000	2.702073000
6	2.755237000	-0.548400000	1.819106000
6	1.660639000	-1.039812000	2.769645000
1	-2.599332000	0.247008000	2.314026000
1	-1.199753000	-1.315477000	3.791633000
1	3.720949000	-1.010189000	2.051586000
1	2.012785000	-0.857836000	3.799407000
1	-0.543521000	3.228108000	2.355368000
1	1.282747000	1.644603000	2.855710000
6	-1.123990000	3.449224000	-0.678724000
1	-0.475771000	4.329913000	-0.783907000
6	-2.588607000	-2.718700000	-0.087830000
1	-1.810128000	-3.179820000	0.541661000
6	3.788538000	-0.041214000	-0.842806000
1	3.708901000	1.010777000	-0.528402000
23	0.001458000	-0.151279000	-0.729904000
1	-1.652314000	1.933916000	1.990641000
1	-0.089081000	1.366583000	3.871731000
1	1.568131000	-2.131087000	2.696869000
1	2.910944000	0.532935000	1.927175000
1	-0.792797000	-2.247419000	2.398745000
1	-3.186311000	-1.389512000	2.408472000
6	5.167452000	-0.552092000	-0.444314000
1	5.941307000	0.075933000	-0.897342000
1	5.341019000	-0.544174000	0.634827000

1	5.339041000	-1.569425000	-0.808388000
6	3.611351000	-0.100817000	-2.354678000
1	3.651664000	-1.130205000	-2.726828000
1	2.662269000	0.324163000	-2.686931000
1	4.416851000	0.448068000	-2.852351000
6	-3.944312000	-3.235486000	0.376441000
1	-3.954652000	-4.329931000	0.353552000
1	-4.204822000	-2.934726000	1.394432000
1	-4.747273000	-2.901576000	-0.287251000
6	-2.321815000	-3.136887000	-1.531153000
1	-3.114377000	-2.799950000	-2.204235000
1	-1.377491000	-2.754995000	-1.927987000
1	-2.286745000	-4.228405000	-1.605713000
6	-1.477801000	2.951910000	-2.075461000
1	-0.594536000	2.683206000	-2.661369000
1	-2.110408000	2.058118000	-2.036347000
1	-2.026750000	3.719175000	-2.630481000
6	-2.357720000	3.881160000	0.102048000
1	-2.112229000	4.335852000	1.064837000
1	-2.918819000	4.624084000	-0.473055000
1	-3.045973000	3.051298000	0.295218000
6	2.601841000	-2.690397000	-0.197448000
1	3.011422000	-2.766674000	-1.215582000
6	1.266003000	-3.427474000	-0.175609000
1	0.746828000	-3.298696000	0.781712000
1	0.600071000	-3.091167000	-0.975695000
1	1.416387000	-4.502928000	-0.316699000
6	3.581605000	-3.336103000	0.775946000
1	3.759861000	-4.376483000	0.485652000
1	4.553571000	-2.842208000	0.814951000
1	3.182913000	-3.358839000	1.794847000
6	-3.723956000	0.102828000	-0.365018000
1	-3.322224000	1.124480000	-0.280989000
6	-4.980839000	0.035373000	0.493497000
1	-5.464378000	-0.942618000	0.449989000
1	-4.790486000	0.263383000	1.545205000
1	-5.712293000	0.767325000	0.135285000
6	-4.026975000	-0.147657000	-1.837515000
1	-4.537688000	-1.104111000	-1.983873000
1	-4.692175000	0.628421000	-2.228554000
1	-3.126226000	-0.152765000	-2.461569000
6	1.617037000	2.977942000	0.223409000
1	2.267524000	2.221538000	0.687273000
6	1.692072000	4.253270000	1.050516000
1	2.687645000	4.700929000	0.971018000
1	0.978522000	5.010421000	0.707123000

1	1.503121000	4.079082000	2.112884000
6	2.087355000	3.197456000	-1.210991000
1	3.138740000	3.500728000	-1.232305000
1	1.989336000	2.297575000	-1.827328000
1	1.520690000	3.994040000	-1.704211000
15	-2.268478000	-0.904308000	0.213017000
15	-0.066656000	2.183069000	0.209800000
15	2.356659000	-0.846526000	0.041319000
5	0.261925000	-0.318015000	2.641029000
7	0.103724000	-0.178953000	-2.592042000
7	0.377060000	-1.311598000	-3.038081000
1	0.118654000	-1.411861000	-4.041877000

d'_{sc} -TS2 (TE = -2877.649322)

6	-0.016172000	1.574801000	2.050591000
6	0.269710000	0.182093000	2.614673000
6	-2.541360000	-0.650184000	1.885209000
6	-1.405094000	-1.642444000	2.020811000
6	2.406105000	-1.735975000	1.364384000
6	1.039888000	-2.116792000	1.908261000
1	-2.498567000	0.126469000	2.654909000
1	-1.432770000	-2.056168000	3.045687000
1	3.150542000	-2.518374000	1.530682000
1	1.158568000	-2.372817000	2.975826000
1	0.329694000	2.356234000	2.733101000
1	1.327916000	0.170023000	2.903203000
6	0.331091000	3.279941000	-0.360415000
1	1.185913000	3.488828000	-1.015363000
6	-3.806601000	-0.572011000	-0.723291000
1	-4.717888000	-0.287033000	-0.182674000
6	3.565084000	-0.190572000	-0.776581000
1	3.444945000	0.573552000	0.000415000
23	-0.068083000	-0.430190000	-0.333249000
16	-2.466596000	0.237975000	0.278425000
16	0.928351000	1.730772000	0.483001000
16	2.247383000	-1.445109000	-0.436850000
6	-0.032262000	-1.041101000	1.714730000
1	-1.074347000	1.757022000	1.842261000
1	-0.274783000	0.100720000	3.569638000
1	0.713934000	-3.050577000	1.428622000
1	2.787569000	-0.810046000	1.809829000
1	-1.589279000	-2.499260000	1.356276000
1	-3.530688000	-1.109160000	1.961097000
6	4.934168000	-0.831696000	-0.677368000
1	5.710140000	-0.082079000	-0.861868000
1	5.123734000	-1.258029000	0.310975000

1	5.059763000	-1.626766000	-1.417556000
6	3.286489000	0.409322000	-2.141528000
1	3.335393000	-0.344964000	-2.932797000
1	2.300551000	0.884245000	-2.201697000
1	4.035622000	1.171855000	-2.373116000
6	-3.798847000	0.093823000	-2.085675000
1	-4.624369000	-0.292582000	-2.689831000
1	-3.919770000	1.177783000	-2.016890000
1	-2.872943000	-0.109259000	-2.631635000
6	-3.693187000	-2.078603000	-0.785126000
1	-2.772637000	-2.398427000	-1.279501000
1	-3.726535000	-2.543785000	0.203294000
1	-4.536964000	-2.482186000	-1.354210000
6	-0.908354000	3.058106000	-1.200774000
1	-0.784570000	2.238348000	-1.917845000
1	-1.785600000	2.846074000	-0.584633000
1	-1.124779000	3.962776000	-1.778151000
6	0.182950000	4.402005000	0.646151000
1	1.086688000	4.553357000	1.240789000
1	-0.026622000	5.337507000	0.119600000
1	-0.652997000	4.225656000	1.329302000
7	-0.545610000	-1.581672000	-1.754427000
7	-0.419432000	-1.092391000	-2.872917000
1	-0.711523000	-1.738594000	-3.639134000

e'_{ssi} -TS2 (TE = -3129.056635)

6	-0.911700000	0.005096000	2.394341000
6	-0.247894000	-1.361333000	2.405157000
6	-2.530888000	-2.344754000	0.165088000
6	-1.298291000	-3.233619000	0.250708000
6	2.880616000	-1.621221000	0.801993000
6	1.921493000	-2.807570000	0.845404000
1	-2.806575000	-1.935147000	1.144282000
1	-1.481362000	-4.006092000	1.007949000
1	3.929671000	-1.927689000	0.770116000
1	2.067180000	-3.351512000	1.786704000
1	-1.001282000	0.441362000	3.393963000
1	0.682119000	-1.299125000	2.985532000
6	-0.983637000	2.629079000	1.224574000
6	-3.594184000	0.252053000	-0.595779000
6	3.751467000	0.701023000	-0.783198000
23	0.116203000	-0.058158000	-0.822890000
16	-2.205147000	-0.918908000	-0.966201000
16	0.112455000	1.141425000	1.386319000
16	2.530423000	-0.699110000	-0.749131000
1	-1.911986000	-0.017869000	1.946149000

1	-0.888908000	-2.055637000	2.965466000
1	2.162770000	-3.507638000	0.038344000
1	2.748762000	-0.949823000	1.659204000
1	-1.144608000	-3.758895000	-0.698032000
1	-3.404613000	-2.862715000	-0.239081000
14	0.166963000	-2.106368000	0.677415000
1	3.686001000	1.000835000	-1.836344000
1	-1.942815000	2.238076000	0.860490000
1	-3.476973000	0.534048000	0.460117000
6	5.152262000	0.200159000	-0.490859000
1	5.876783000	0.990490000	-0.708647000
1	5.278149000	-0.063180000	0.563256000
1	5.419947000	-0.669285000	-1.095840000
6	3.335853000	1.861412000	0.096643000
1	3.267385000	1.576077000	1.150923000
1	4.073790000	2.667194000	0.023892000
1	2.369556000	2.273929000	-0.207140000
6	-3.391162000	1.463839000	-1.485670000
1	-4.139477000	2.227875000	-1.256628000
1	-2.403947000	1.921277000	-1.355522000
1	-3.500232000	1.203507000	-2.542555000
6	-4.939024000	-0.412260000	-0.805308000
1	-5.739680000	0.309873000	-0.617921000
1	-5.051504000	-0.771147000	-1.832227000
1	-5.101826000	-1.255164000	-0.130220000
6	-1.173388000	3.306290000	2.565734000
1	-1.813093000	4.186216000	2.446669000
1	-1.651356000	2.657464000	3.302925000
1	-0.220082000	3.646264000	2.979687000
6	-0.363804000	3.543992000	0.185474000
1	-1.033532000	4.384019000	-0.019672000
1	0.583139000	3.963168000	0.538834000
1	-0.167027000	3.039040000	-0.767474000
7	0.471802000	0.329442000	-2.639992000
7	0.748123000	1.496743000	-2.898023000
1	0.535999000	1.746081000	-3.890057000

f'_{SB} -TS2 (TE = -2864.405525)

6	0.745708000	1.607537000	2.101941000
6	0.597060000	0.175118000	2.594750000
6	-2.609638000	0.902233000	1.308381000
6	-2.132872000	-0.080264000	2.369155000
6	0.815263000	-2.717126000	1.363588000
6	-0.536878000	-2.190895000	1.802051000
1	-2.061595000	1.847637000	1.335969000
1	-2.196076000	0.448066000	3.332824000

1	0.835654000	-3.806286000	1.277186000
1	-0.836378000	-2.736693000	2.715617000
1	1.499421000	2.157704000	2.671575000
1	1.543422000	-0.352439000	2.418772000
6	1.053630000	3.299226000	-0.241884000
1	1.446565000	3.218728000	-1.261923000
6	-3.404733000	-1.193063000	-0.524325000
1	-3.153435000	-1.777390000	0.368062000
6	3.110007000	-1.684575000	-0.024983000
1	3.141613000	-1.007905000	0.840138000
23	0.040415000	-0.069879000	-1.009720000
16	-2.375250000	0.347903000	-0.421210000
16	1.333253000	1.567637000	0.363966000
16	1.301245000	-2.051658000	-0.284354000
1	-0.189322000	2.172233000	2.157471000
1	0.516681000	0.222036000	3.695687000
1	-1.312215000	-2.494290000	1.083688000
1	1.608545000	-2.432308000	2.060877000
1	-2.864838000	-0.895980000	2.444680000
1	-3.666882000	1.160729000	1.422275000
6	3.852631000	-2.970619000	0.273712000
1	4.907423000	-2.749700000	0.464089000
1	3.468142000	-3.491071000	1.154097000
1	3.806578000	-3.660570000	-0.573431000
6	3.632997000	-0.978052000	-1.257681000
1	3.508438000	-1.590136000	-2.155895000
1	3.139760000	-0.019056000	-1.430747000
1	4.702867000	-0.784197000	-1.138533000
6	-4.876716000	-0.838388000	-0.513989000
1	-5.479004000	-1.751662000	-0.541680000
1	-5.168207000	-0.289335000	0.385143000
1	-5.149630000	-0.233443000	-1.382830000
6	-2.973264000	-1.945922000	-1.767258000
1	-3.098514000	-1.344506000	-2.672965000
1	-1.926696000	-2.266785000	-1.716361000
1	-3.581996000	-2.846156000	-1.889627000
6	-0.411430000	3.677018000	-0.298541000
1	-0.995850000	2.993918000	-0.921369000
1	-0.864205000	3.724099000	0.697517000
1	-0.516161000	4.676198000	-0.732849000
6	1.886939000	4.270228000	0.571221000
1	2.940285000	3.984610000	0.607986000
1	1.827567000	5.268215000	0.127066000
1	1.521414000	4.358442000	1.598967000
5	-0.670525000	-0.667518000	2.175271000
7	0.580844000	1.317157000	-3.068438000

7	0.549693000	0.101098000	-2.799186000
1	0.515797000	1.497457000	-4.092175000

a''_{PC} -TS2 (TE = -3519.746765)

6	-0.649221000	-1.297457000	1.662390000
6	-0.058188000	-2.016896000	2.715767000
1	0.830416000	-1.615101000	3.196979000
6	-0.594879000	-3.209775000	3.180150000
1	-0.111490000	-3.730755000	4.003687000
6	-1.755338000	-3.728460000	2.612941000
1	-2.185966000	-4.655911000	2.980991000
6	-2.344647000	-3.057572000	1.549108000
1	-3.218743000	-3.493336000	1.068572000
6	-1.806299000	-1.864064000	1.055822000
6	1.217116000	0.392458000	1.847119000
6	1.294120000	1.177951000	3.006437000
1	0.378873000	1.547001000	3.461935000
6	2.511103000	1.507099000	3.589952000
1	2.529428000	2.124548000	4.485117000
6	3.697964000	1.050048000	3.030254000
1	4.656277000	1.306346000	3.474667000
6	3.649221000	0.271168000	1.881462000
1	4.582330000	-0.057496000	1.435132000
6	2.428928000	-0.057620000	1.281366000
6	-1.104694000	1.155542000	1.495548000
6	-1.963359000	1.128397000	2.601350000
1	-2.010049000	0.230663000	3.216238000
6	-2.739026000	2.231392000	2.938019000
1	-3.396094000	2.184707000	3.803740000
6	-2.671733000	3.394451000	2.177567000
1	-3.274620000	4.259941000	2.440269000
6	-1.829197000	3.441986000	1.072119000
1	-1.781401000	4.351093000	0.478695000
6	-1.055360000	2.332972000	0.720288000
6	-0.119805000	0.038127000	1.228485000
23	-0.021305000	-0.238706000	-1.061381000
6	-2.420956000	-2.721970000	-1.621685000
1	-3.152259000	-3.406187000	-1.173023000
6	3.925810000	-0.457237000	-1.200999000
1	4.102883000	0.575411000	-0.862045000
6	-0.833302000	3.083125000	-2.179063000
1	-0.222524000	2.736895000	-3.026813000
6	-0.840274000	4.607009000	-2.191682000
1	-1.285970000	4.961622000	-3.127220000
1	-1.437473000	5.034389000	-1.382311000

1	0.158193000	5.042496000	-2.132073000
6	-2.240720000	2.525061000	-2.367357000
1	-2.901853000	2.813044000	-1.543055000
1	-2.683575000	2.914301000	-3.289337000
1	-2.248882000	1.431384000	-2.435342000
6	-2.883606000	-2.347652000	-3.024955000
1	-3.913838000	-1.983114000	-3.045464000
1	-2.254536000	-1.563358000	-3.464181000
1	-2.835773000	-3.213468000	-3.692283000
6	-1.066537000	-3.416106000	-1.637600000
1	-0.755125000	-3.748833000	-0.643705000
1	-1.083611000	-4.295955000	-2.288879000
1	-0.275826000	-2.766744000	-2.040097000
6	5.144668000	-1.299282000	-0.829881000
1	6.041417000	-0.853231000	-1.272191000
1	5.324583000	-1.386508000	0.242156000
1	5.072843000	-2.313546000	-1.229599000
6	3.756813000	-0.430825000	-2.716079000
1	3.509053000	-1.417452000	-3.118502000
1	2.970285000	0.254220000	-3.035096000
1	4.690677000	-0.111992000	-3.190122000
15	-0.009859000	2.205121000	-0.758914000
15	2.316822000	-0.874407000	-0.341792000
15	-2.332806000	-1.191403000	-0.557374000
6	2.237336000	-2.720039000	-0.033221000
1	1.187776000	-2.842800000	0.277443000
6	2.431389000	-3.502523000	-1.329274000
1	3.483848000	-3.557529000	-1.618328000
1	2.082877000	-4.533093000	-1.206343000
1	1.887188000	-3.069059000	-2.174305000
6	3.104057000	-3.241469000	1.103904000
1	2.835637000	-4.279115000	1.329820000
1	4.167211000	-3.233875000	0.852926000
1	2.973425000	-2.663841000	2.023113000
6	-4.094209000	-0.578443000	-0.570506000
1	-4.210480000	-0.237942000	-1.610619000
6	-4.314226000	0.609599000	0.349812000
1	-4.248260000	0.312036000	1.399370000
1	-3.594985000	1.415712000	0.189244000
1	-5.316281000	1.020508000	0.191683000
6	-5.120917000	-1.668963000	-0.291319000
1	-6.129923000	-1.252518000	-0.372808000
1	-5.068028000	-2.510503000	-0.985759000
1	-5.024229000	-2.059658000	0.726456000
6	1.610823000	3.048905000	-0.404612000
1	2.123606000	2.314120000	0.230388000

6	1.507949000	4.341442000	0.393401000
1	2.510681000	4.706304000	0.639706000
1	1.001562000	5.140585000	-0.153766000
1	0.975759000	4.195633000	1.337207000
6	2.415392000	3.191871000	-1.691740000
1	3.442918000	3.495410000	-1.468159000
1	2.465445000	2.252072000	-2.252180000
1	1.999145000	3.948689000	-2.362671000
7	0.339951000	0.049118000	-3.007204000
7	0.633365000	-1.001550000	-3.556550000
1	0.144734000	-1.122119000	-4.479746000

b''_{PSi} -TS2 (TE = -3771.168080)

6	1.821644000	-1.128750000	1.809254000
6	2.060851000	-1.519750000	3.133500000
1	1.237610000	-1.555730000	3.846941000
6	3.340993000	-1.847460000	3.563832000
1	3.511060000	-2.141450000	4.597085000
6	4.408610000	-1.793435000	2.671021000
1	5.411501000	-2.050695000	3.003376000
6	4.196681000	-1.401027000	1.355342000
1	5.043850000	-1.356470000	0.673482000
6	2.909882000	-1.061321000	0.919690000
6	-0.762795000	0.548573000	2.212909000
6	-1.365016000	0.158573000	3.416838000
1	-1.304490000	-0.881980000	3.737352000
6	-2.073542000	1.063249000	4.198847000
1	-2.541958000	0.735971000	5.124317000
6	-2.193138000	2.387073000	3.786411000
1	-2.748551000	3.100927000	4.389864000
6	-1.609596000	2.797917000	2.593917000
1	-1.723503000	3.832701000	2.284686000
6	-0.898360000	1.889929000	1.800961000
6	-0.978205000	-2.233260000	1.059680000
6	-0.798117000	-3.360636000	1.868379000
1	0.038293000	-3.394042000	2.566770000
6	-1.654804000	-4.452924000	1.783140000
1	-1.492781000	-5.325062000	2.412660000
6	-2.720080000	-4.426990000	0.888980000
1	-3.397685000	-5.274478000	0.819745000
6	-2.919946000	-3.316534000	0.075950000
1	-3.762432000	-3.311814000	-0.607478000
6	-2.048894000	-2.224023000	0.140666000
23	0.150547000	0.265715000	-1.229457000
6	4.130985000	0.251564000	-1.376338000
1	4.887139000	-0.541586000	-1.301186000

6	-1.429556000	3.552060000	-0.585003000
1	-2.393346000	3.144985000	-0.244304000
6	-2.930715000	-1.258157000	-2.570221000
1	-2.910910000	-0.302969000	-3.118770000
6	-4.362251000	-1.794084000	-2.620146000
1	-4.753774000	-1.681660000	-3.636406000
1	-4.403500000	-2.862269000	-2.396602000
1	-5.059468000	-1.288827000	-1.951964000
6	-1.987496000	-2.227264000	-3.274080000
1	-1.896389000	-3.167363000	-2.718865000
1	-2.379264000	-2.477842000	-4.264989000
1	-0.985189000	-1.815536000	-3.412970000
6	4.023130000	0.680806000	-2.833082000
1	3.748463000	-0.140527000	-3.501258000
1	3.277822000	1.470822000	-2.963390000
1	4.982972000	1.073297000	-3.183102000
6	4.568707000	1.406845000	-0.488464000
1	4.617857000	1.138662000	0.569992000
1	5.564695000	1.750359000	-0.785032000
1	3.897689000	2.261383000	-0.587797000
6	-1.354814000	5.011923000	-0.145275000
1	-2.201151000	5.560689000	-0.571337000
1	-1.394593000	5.155987000	0.934573000
1	-0.450025000	5.505594000	-0.507454000
6	-1.394196000	3.474552000	-2.110245000
1	-0.440383000	3.824627000	-2.516527000
1	-1.546842000	2.458256000	-2.488639000
1	-2.181699000	4.102697000	-2.539479000
15	-2.221186000	-0.730895000	-0.918103000
15	-0.213776000	2.330927000	0.160172000
15	2.542296000	-0.535816000	-0.797825000
6	1.404631000	3.199756000	0.479194000
1	2.061681000	2.354551000	0.740701000
6	1.920109000	3.821780000	-0.814889000
1	1.317731000	4.679959000	-1.123185000
1	2.940862000	4.193787000	-0.683527000
1	1.927059000	3.110223000	-1.648684000
6	1.421842000	4.176447000	1.645934000
1	2.447591000	4.512879000	1.829089000
1	0.824850000	5.070397000	1.452430000
1	1.059213000	3.723987000	2.572014000
6	2.508086000	-2.135561000	-1.776127000
1	2.430222000	-1.791671000	-2.817051000
6	1.248683000	-2.919370000	-1.437050000
1	1.241860000	-3.245995000	-0.391258000
1	0.329232000	-2.341265000	-1.597886000

1	1.166679000	-3.816012000	-2.060433000
6	3.745260000	-3.005209000	-1.622863000
1	3.649828000	-3.901620000	-2.244243000
1	4.666076000	-2.504015000	-1.931591000
1	3.875425000	-3.345363000	-0.590733000
6	-3.531758000	0.328539000	-0.091229000
1	-2.937577000	0.944081000	0.595965000
6	-4.536954000	-0.437557000	0.758191000
1	-5.223626000	0.266467000	1.240218000
1	-5.147479000	-1.132526000	0.174389000
1	-4.050807000	-1.013435000	1.549210000
6	-4.206287000	1.268241000	-1.086433000
1	-4.759368000	2.045052000	-0.548638000
1	-3.496302000	1.775813000	-1.745090000
1	-4.928030000	0.754559000	-1.725426000
14	0.128448000	-0.702155000	1.096513000
7	0.603961000	0.127745000	-3.042002000
7	0.755750000	1.253350000	-3.529309000
1	0.243581000	1.354223000	-4.434855000

c''_{PB} -TS2 (TE = -3506.505196)

6	-1.563409000	0.101740000	1.980529000
6	-1.708813000	0.577069000	3.297590000
1	-0.817387000	0.764345000	3.895325000
6	-2.953502000	0.815863000	3.867090000
1	-3.020063000	1.178802000	4.890227000
6	-4.108249000	0.603808000	3.122487000
1	-5.087670000	0.795822000	3.553617000
6	-3.998544000	0.158990000	1.811765000
1	-4.904728000	0.020056000	1.226368000
6	-2.747759000	-0.093222000	1.238010000
6	0.546869000	-1.650129000	1.675807000
6	0.115492000	-2.439038000	2.755987000
1	-0.774997000	-2.137090000	3.306784000
6	0.816720000	-3.566560000	3.168107000
1	0.461260000	-4.148230000	4.015646000
6	1.983355000	-3.937150000	2.507921000
1	2.549755000	-4.805537000	2.835422000
6	2.412570000	-3.200688000	1.408036000
1	3.311988000	-3.513588000	0.881946000
6	1.699895000	-2.081602000	0.973022000
6	0.986289000	0.963341000	1.777707000
6	1.710898000	0.828380000	2.978818000
1	1.599531000	-0.084490000	3.564028000
6	2.567236000	1.817405000	3.444883000
1	3.100015000	1.674435000	4.382359000

6	2.760374000	2.974953000	2.699125000
1	3.440374000	3.749611000	3.044586000
6	2.090451000	3.122891000	1.492775000
1	2.271786000	4.012982000	0.895404000
6	1.201264000	2.142755000	1.033820000
23	-0.165254000	-0.114993000	-1.185115000
6	-3.121855000	-2.350426000	-0.587942000
1	-4.178214000	-2.347716000	-0.285464000
6	3.895929000	-0.779697000	-0.507476000
1	4.418479000	-1.736353000	-0.364576000
6	-0.792935000	3.665908000	-0.549796000
1	-0.924319000	3.963523000	-1.601814000
6	-0.384291000	4.876303000	0.280166000
1	-1.176324000	5.630707000	0.234252000
1	-0.261667000	4.605914000	1.333131000
1	0.534682000	5.357843000	-0.051166000
6	-2.113295000	3.119773000	-0.026722000
1	-2.020410000	2.761101000	1.004312000
1	-2.881649000	3.899379000	-0.031736000
1	-2.476243000	2.292631000	-0.634747000
6	-3.011779000	-2.899464000	-2.005189000
1	-3.451190000	-3.900513000	-2.059852000
1	-3.522404000	-2.280544000	-2.748388000
1	-1.969646000	-2.981727000	-2.325237000
6	-2.347273000	-3.200412000	0.406679000
1	-2.467456000	-2.848376000	1.434594000
1	-2.697042000	-4.237154000	0.368658000
1	-1.274309000	-3.215447000	0.191573000
6	4.365580000	-0.152049000	-1.814158000
1	5.456859000	-0.072597000	-1.829713000
1	4.068868000	-0.717623000	-2.702684000
1	3.970571000	0.861215000	-1.928542000
6	4.204438000	0.107320000	0.685948000
1	3.695827000	1.074177000	0.621128000
1	3.912921000	-0.354977000	1.632155000
1	5.279499000	0.309373000	0.733500000
5	-0.071920000	-0.205561000	1.530731000
15	-2.607917000	-0.557182000	-0.521135000
15	2.100801000	-1.260716000	-0.616463000
15	0.459111000	2.279723000	-0.624505000
6	2.131798000	-2.666979000	-1.878743000
1	1.972479000	-2.133852000	-2.827740000
6	0.944806000	-3.595969000	-1.657167000
1	0.816165000	-4.264682000	-2.514025000
1	1.084274000	-4.218463000	-0.768012000
1	0.002605000	-3.057305000	-1.533637000

6	3.418080000	-3.473962000	-1.998940000
1	3.305607000	-4.210140000	-2.801895000
1	4.295032000	-2.871844000	-2.243780000
1	3.642499000	-4.041322000	-1.091696000
6	-4.019020000	0.352915000	-1.377711000
1	-4.181606000	1.221980000	-0.727231000
6	-5.343987000	-0.394265000	-1.478739000
1	-6.103283000	0.271946000	-1.900726000
1	-5.287542000	-1.263196000	-2.139401000
1	-5.725939000	-0.741473000	-0.515857000
6	-3.573070000	0.857482000	-2.745799000
1	-4.346461000	1.491628000	-3.191060000
1	-2.647301000	1.442014000	-2.698305000
1	-3.392099000	0.033296000	-3.443371000
6	1.873189000	2.848571000	-1.730752000
1	2.756781000	2.458371000	-1.204691000
6	1.781831000	2.166474000	-3.091558000
1	0.869757000	2.443942000	-3.629597000
1	2.632849000	2.454946000	-3.717365000
1	1.790871000	1.074180000	-3.014469000
6	2.046906000	4.350928000	-1.912578000
1	1.151530000	4.825937000	-2.325056000
1	2.309884000	4.874140000	-0.992213000
1	2.858141000	4.538028000	-2.623377000
7	-0.475665000	-0.930319000	-2.897498000
7	-0.554076000	-0.017577000	-3.716066000
1	-0.479369000	-0.345085000	-4.705098000

d''_{sc} -TS2 (TE = -3334.901751)

6	-0.562452000	1.697323000	0.857015000
6	-0.051264000	2.623249000	1.778986000
1	0.795617000	2.337529000	2.397583000
6	-0.610340000	3.884160000	1.940472000
1	-0.190807000	4.565563000	2.676650000
6	-1.704264000	4.274732000	1.174551000
1	-2.147818000	5.258389000	1.302164000
6	-2.199090000	3.408945000	0.208678000
1	-3.010393000	3.722342000	-0.444745000
6	-1.638498000	2.142343000	0.045778000
6	-1.091074000	-0.715882000	1.170823000
6	-1.817400000	-0.487829000	2.350479000
1	-1.701661000	0.469574000	2.855648000
6	-2.668862000	-1.440632000	2.890036000
1	-3.192997000	-1.231286000	3.819323000
6	-2.865654000	-2.653420000	2.234947000
1	-3.537804000	-3.402378000	2.644835000

6	-2.227247000	-2.882785000	1.024863000
1	-2.418570000	-3.798073000	0.469034000
6	-1.344441000	-1.930795000	0.507290000
6	1.261498000	0.001230000	1.468719000
6	1.284115000	-0.119627000	2.867186000
1	0.364393000	0.030388000	3.425205000
6	2.441230000	-0.428445000	3.568552000
1	2.407677000	-0.506595000	4.652406000
6	3.633103000	-0.655437000	2.887579000
1	4.538649000	-0.921787000	3.426039000
6	3.647873000	-0.561926000	1.504884000
1	4.556024000	-0.780798000	0.949126000
6	2.482127000	-0.220872000	0.812735000
16	2.565868000	-0.178781000	-0.972866000
16	-2.131827000	1.172083000	-1.375535000
16	-0.647587000	-2.247141000	-1.111501000
23	0.130613000	0.069974000	-1.396183000
6	-3.898213000	0.576054000	-1.151110000
1	-4.469249000	1.443648000	-1.500998000
6	0.559945000	-3.661216000	-0.861018000
1	-0.115324000	-4.512118000	-0.712400000
6	3.385600000	1.482952000	-1.308435000
1	3.150377000	1.611517000	-2.371179000
6	4.882427000	1.367530000	-1.115384000
1	5.363971000	2.289461000	-1.456242000
1	5.142882000	1.246243000	-0.060097000
1	5.316398000	0.537111000	-1.676171000
6	2.770546000	2.594193000	-0.489244000
1	2.938782000	2.441499000	0.581359000
1	3.242301000	3.545161000	-0.756858000
1	1.696977000	2.699580000	-0.658344000
6	-4.077549000	-0.579506000	-2.113365000
1	-3.782341000	-0.328609000	-3.135640000
1	-3.500823000	-1.453357000	-1.793619000
1	-5.131190000	-0.872362000	-2.140387000
6	-4.282887000	0.242004000	0.266181000
1	-3.993823000	1.019442000	0.978219000
1	-5.372145000	0.139790000	0.319421000
1	-3.849197000	-0.704718000	0.589495000
6	1.312371000	-3.816974000	-2.165578000
1	1.966126000	-4.691735000	-2.108465000
1	0.647289000	-3.958402000	-3.020795000
1	1.949342000	-2.948506000	-2.363792000
6	1.457500000	-3.487436000	0.339176000
1	2.224507000	-2.731939000	0.160893000
1	0.910539000	-3.216089000	1.246355000

1	1.973291000	-4.432402000	0.538160000
6	-0.035682000	0.294158000	0.718740000
7	0.651465000	1.122860000	-3.829373000
7	0.574395000	1.444655000	-2.652821000
1	0.800092000	1.936767000	-4.467391000

e''_{SSi} -TS2 (TE = -3586.295926)

6	-1.062806000	0.588780000	1.876557000
6	-1.756210000	1.540062000	2.637750000
1	-1.850237000	2.561128000	2.268150000
6	-2.340681000	1.207275000	3.854972000
1	-2.870262000	1.964201000	4.428405000
6	-2.260054000	-0.097466000	4.334142000
1	-2.724275000	-0.363620000	5.280361000
6	-1.605529000	-1.071742000	3.589514000
1	-1.566105000	-2.100189000	3.941674000
6	-1.011458000	-0.718607000	2.378300000
6	1.289301000	2.041594000	0.415788000
6	1.402271000	3.161680000	1.247530000
1	0.568332000	3.436339000	1.892944000
6	2.564425000	3.925721000	1.281288000
1	2.633319000	4.785049000	1.943512000
6	3.637405000	3.591022000	0.461476000
1	4.543885000	4.190846000	0.472565000
6	3.560351000	2.485752000	-0.379810000
1	4.399868000	2.236572000	-1.023870000
6	2.401541000	1.713788000	-0.372574000
6	-1.510413000	1.827910000	-0.875412000
6	-1.726628000	3.207812000	-0.963308000
1	-1.124732000	3.887289000	-0.360175000
6	-2.691260000	3.730557000	-1.819336000
1	-2.842182000	4.806018000	-1.875167000
6	-3.453294000	2.881002000	-2.616027000
1	-4.196633000	3.288789000	-3.296291000
6	-3.250420000	1.505908000	-2.561823000
1	-3.823198000	0.837679000	-3.200509000
6	-2.290656000	0.995178000	-1.689890000
16	-1.992335000	-0.782512000	-1.684083000
16	-0.218426000	-2.020317000	1.424046000
16	2.241499000	0.276680000	-1.446909000
23	0.374823000	-1.215822000	-0.892758000
6	1.416873000	-2.199632000	2.316125000
1	1.133237000	-2.598663000	3.297369000
6	3.962686000	-0.433784000	-1.618170000
1	4.501445000	0.320035000	-2.203691000
6	-3.241902000	-1.448242000	-0.449517000

1	-2.917578000	-1.071381000	0.527647000
6	-3.142697000	-2.958932000	-0.505071000
1	-3.826914000	-3.394894000	0.228842000
1	-3.428845000	-3.340768000	-1.489747000
1	-2.139025000	-3.324127000	-0.278330000
6	-4.629273000	-0.938813000	-0.767137000
1	-4.952721000	-1.242148000	-1.767818000
1	-5.338010000	-1.364414000	-0.049891000
1	-4.706033000	0.147769000	-0.694884000
6	2.216821000	-3.232597000	1.549316000
1	1.686573000	-4.182070000	1.445156000
1	2.462993000	-2.881034000	0.539584000
1	3.163353000	-3.427962000	2.061796000
6	2.124792000	-0.872576000	2.467295000
1	1.542880000	-0.152389000	3.047924000
1	3.080140000	-1.017506000	2.982802000
1	2.342125000	-0.419777000	1.494180000
6	4.644295000	-0.672476000	-0.289731000
1	5.678237000	-0.986095000	-0.466639000
1	4.676489000	0.216265000	0.343911000
1	4.152967000	-1.470847000	0.272192000
6	3.816558000	-1.702143000	-2.435795000
1	3.291129000	-2.481824000	-1.870984000
1	3.285253000	-1.540476000	-3.377384000
1	4.806862000	-2.096676000	-2.678618000
14	-0.244805000	0.958236000	0.214124000
7	0.115020000	-3.068219000	-1.546907000
7	0.123323000	-3.037287000	-2.766778000
1	0.619584000	-3.857773000	-3.191106000

f''_{SB} -TS2 (TE = -3321.660693)

6	-1.280053000	0.092808000	1.737944000
6	-1.286471000	0.385985000	3.115237000
1	-0.345074000	0.367380000	3.663872000
6	-2.453079000	0.692879000	3.803115000
1	-2.412666000	0.898842000	4.869935000
6	-3.667224000	0.753480000	3.125360000
1	-4.582719000	1.010529000	3.651614000
6	-3.697478000	0.505213000	1.761226000
1	-4.632447000	0.579914000	1.209818000
6	-2.520106000	0.168356000	1.087988000
6	0.749529000	-1.689245000	1.129614000
6	0.422618000	-2.550867000	2.194116000
1	-0.370703000	-2.256546000	2.880597000

6	1.112863000	-3.734383000	2.421017000
1	0.850628000	-4.361105000	3.269861000
6	2.138192000	-4.119909000	1.561257000
1	2.677922000	-5.048088000	1.730344000
6	2.440850000	-3.337046000	0.453215000
1	3.189504000	-3.669202000	-0.262781000
6	1.760262000	-2.138904000	0.246427000
6	1.172580000	0.958630000	1.133744000
6	2.040311000	0.955520000	2.241280000
1	2.039035000	0.095001000	2.910439000
6	2.900751000	2.013778000	2.508448000
1	3.542905000	1.979179000	3.385329000
6	2.963592000	3.099151000	1.640134000
1	3.651213000	3.919354000	1.828516000
6	2.155047000	3.117641000	0.510764000
1	2.217607000	3.939850000	-0.198364000
6	1.254485000	2.074293000	0.285086000
16	0.285301000	2.141047000	-1.221886000
16	-2.663363000	-0.108253000	-0.681548000
16	1.984929000	-1.284600000	-1.309822000
23	-0.277285000	-0.250742000	-1.419124000
6	-3.432615000	-1.820321000	-0.689488000
1	-4.295775000	-1.674046000	-0.028417000
6	3.727049000	-0.595803000	-1.409817000
1	4.305790000	-1.464878000	-1.742246000
6	-1.256191000	3.114677000	-0.770182000
1	-1.771138000	2.513011000	-0.012502000
6	-2.071685000	3.203728000	-2.043717000
1	-3.036531000	3.672511000	-1.830713000
1	-1.566836000	3.814211000	-2.797906000
1	-2.276828000	2.223289000	-2.483326000
6	-0.880741000	4.461961000	-0.199945000
1	-0.310474000	5.059985000	-0.917254000
1	-1.792240000	5.017874000	0.040775000
1	-0.298696000	4.378148000	0.720290000
6	-3.906335000	-2.142340000	-2.089358000
1	-4.548082000	-1.361651000	-2.504069000
1	-3.067748000	-2.302991000	-2.770639000
1	-4.484973000	-3.070479000	-2.068023000
6	-2.496207000	-2.853694000	-0.108569000
1	-2.164903000	-2.590973000	0.899345000
1	-3.004164000	-3.821673000	-0.046267000
1	-1.611113000	-2.989763000	-0.739398000
6	3.690672000	0.451577000	-2.503490000
1	4.706942000	0.796442000	-2.715067000
1	3.272331000	0.071751000	-3.439555000

1	3.105449000	1.324181000	-2.194611000
6	4.262450000	-0.078649000	-0.099363000
1	3.794075000	0.865372000	0.182135000
1	4.132173000	-0.788239000	0.721942000
1	5.337081000	0.104543000	-0.204641000
5	0.131233000	-0.244478000	1.092143000
7	-0.762366000	-1.392180000	-2.859953000
7	-0.788277000	-0.917130000	-3.986504000
1	-0.989022000	-1.629747000	-4.724231000

Cartesian coordinates of the vanadium nitride complexes for $[1a'_{PC}]-[1f'_{SB}]$ and $[1a''_{PC}]-[1f''_{SB}]$, along with their total energies (in hartree) including zero point vibrational correction at M06-L-D3(heptane)/6-311+G* level of theory.

$[1a'_{PC}]\equiv N$ (TE = -3007.310110)

6	-0.611239000	1.773509000	1.678235000
6	0.171196000	0.614582000	2.338052000
6	-2.444127000	-1.021390000	1.901517000
6	-1.104725000	-1.565550000	2.379141000
6	2.683678000	-1.116246000	1.770020000
6	1.345455000	-1.560640000	2.364011000
1	-2.635399000	-0.031099000	2.330196000
1	-1.088212000	-1.544432000	3.488843000
1	3.491805000	-1.824239000	1.994988000
1	1.393871000	-1.444549000	3.466402000
1	-0.550411000	2.661483000	2.319891000
1	1.221856000	0.938577000	2.364970000
6	-1.120793000	3.485961000	-0.744517000
1	-0.442096000	4.323629000	-0.958311000
6	-2.744688000	-2.612632000	-0.467492000
1	-1.958903000	-3.157174000	0.080729000
6	3.918272000	0.210924000	-0.544497000
1	3.586283000	1.208395000	-0.223851000
23	0.058610000	-0.306091000	-0.445708000
6	0.111299000	-0.846280000	1.796555000
1	-1.678431000	1.551790000	1.588062000
1	-0.127361000	0.597979000	3.405266000
1	1.226726000	-2.638160000	2.205042000
1	3.006636000	-0.156387000	2.195548000
1	-1.040920000	-2.633409000	2.118333000
1	-3.285094000	-1.646711000	2.222325000
6	5.254447000	-0.043801000	0.144274000
1	5.969393000	0.744606000	-0.119722000
1	5.166688000	-0.043347000	1.234465000
1	5.709477000	-0.992550000	-0.145107000
6	4.037558000	0.244213000	-2.064144000

1	4.447262000	-0.690049000	-2.460880000
1	3.067477000	0.398175000	-2.548785000
1	4.706076000	1.049571000	-2.388214000
6	-4.096910000	-3.158961000	-0.023864000
1	-4.135756000	-4.241925000	-0.187243000
1	-4.320717000	-2.986210000	1.032350000
1	-4.913312000	-2.727644000	-0.612345000
6	-2.523158000	-2.874944000	-1.952016000
1	-3.323609000	-2.447659000	-2.563330000
1	-1.570865000	-2.465454000	-2.296841000
1	-2.524301000	-3.954615000	-2.141531000
6	-1.715455000	3.022469000	-2.068179000
1	-0.943730000	2.706409000	-2.776225000
1	-2.383329000	2.167186000	-1.930965000
1	-2.296809000	3.823776000	-2.537969000
6	-2.188333000	3.990345000	0.216209000
1	-1.768851000	4.368564000	1.152956000
1	-2.758820000	4.806012000	-0.241307000
1	-2.910103000	3.208051000	0.474756000
6	2.742586000	-2.519287000	-0.829309000
1	2.468402000	-2.324172000	-1.875424000
6	1.756191000	-3.550233000	-0.284408000
1	2.059396000	-3.905421000	0.706359000
1	0.738328000	-3.155635000	-0.217515000
1	1.729882000	-4.425767000	-0.942473000
6	4.157305000	-3.078419000	-0.760739000
1	4.177062000	-4.097728000	-1.164156000
1	4.879355000	-2.496924000	-1.337169000
1	4.527949000	-3.142458000	0.269119000
6	-3.844043000	0.218487000	-0.342886000
1	-3.433075000	1.227192000	-0.174587000
6	-5.069244000	0.077811000	0.552411000
1	-5.551673000	-0.896810000	0.447283000
1	-4.835335000	0.214874000	1.611394000
1	-5.818313000	0.833770000	0.288374000
6	-4.211338000	0.113253000	-1.818162000
1	-4.759623000	-0.811748000	-2.023018000
1	-4.860931000	0.942087000	-2.120926000
1	-3.332650000	0.120805000	-2.471360000
6	1.574814000	3.097956000	0.285226000
1	2.200107000	2.369211000	0.823264000
6	1.427215000	4.338850000	1.153422000
1	2.400820000	4.814359000	1.315964000
1	0.785561000	5.092824000	0.684110000
1	1.010989000	4.118215000	2.140201000
6	2.243470000	3.418457000	-1.046558000

1	3.254515000	3.813653000	-0.898447000
1	2.318925000	2.538542000	-1.692582000
1	1.685245000	4.180989000	-1.602005000
15	-2.368417000	-0.856068000	0.064452000
15	-0.005277000	2.158650000	-0.028588000
15	2.466171000	-0.849370000	-0.038634000
7	0.112395000	-1.092450000	-1.829979000

[1b'_{psi}]=N (TE = -3258.737756)

6	-0.486965000	1.993018000	1.830534000
6	0.222782000	0.799162000	2.488692000
6	-2.677511000	-0.863862000	1.865069000
6	-1.576555000	-1.649838000	2.583899000
6	2.818633000	-1.179186000	1.694439000
6	1.671175000	-1.788318000	2.510456000
1	-2.715714000	0.165179000	2.244466000
1	-1.650159000	-1.504649000	3.670094000
1	3.746609000	-1.760966000	1.754860000
1	1.823451000	-1.597559000	3.581738000
1	-0.366793000	2.907830000	2.426632000
1	1.298322000	1.021538000	2.540235000
6	-0.970361000	3.635872000	-0.635085000
1	-0.305140000	4.507432000	-0.710283000
6	-2.632161000	-2.535135000	-0.468173000
1	-1.860090000	-3.037500000	0.135887000
6	3.797119000	0.047409000	-0.766941000
1	3.511757000	1.081175000	-0.530731000
23	0.021928000	-0.145393000	-0.571178000
1	-1.567925000	1.823555000	1.772047000
1	-0.094121000	0.751859000	3.542783000
1	1.667797000	-2.878512000	2.397063000
1	3.073976000	-0.184274000	2.084020000
1	-1.710157000	-2.725939000	2.411581000
1	-3.678768000	-1.274538000	2.037517000
6	5.164736000	-0.178186000	-0.132052000
1	5.897532000	0.510413000	-0.569694000
1	5.160645000	0.005461000	0.945827000
1	5.550532000	-1.188251000	-0.287206000
6	3.830268000	-0.069690000	-2.285435000
1	4.224893000	-1.039311000	-2.607968000
1	2.830922000	0.038971000	-2.721764000
1	4.476726000	0.699222000	-2.723201000
6	-3.988489000	-3.109171000	-0.076126000
1	-3.994919000	-4.193101000	-0.237982000
1	-4.256336000	-2.941418000	0.970300000
1	-4.791411000	-2.698961000	-0.697188000

6	-2.332268000	-2.841136000	-1.930901000
1	-3.141600000	-2.507494000	-2.586533000
1	-1.409113000	-2.367885000	-2.273650000
1	-2.239615000	-3.924669000	-2.069760000
6	-1.409979000	3.252481000	-2.043843000
1	-0.562423000	3.004800000	-2.689661000
1	-2.058016000	2.369663000	-2.032185000
1	-1.966068000	4.069791000	-2.516788000
6	-2.154865000	4.032215000	0.234195000
1	-1.853811000	4.376660000	1.227693000
1	-2.718733000	4.843888000	-0.238150000
1	-2.856757000	3.202577000	0.373833000
6	2.455331000	-2.594426000	-0.893996000
1	2.360890000	-2.330805000	-1.956931000
6	1.278100000	-3.507026000	-0.564034000
1	1.258852000	-3.798480000	0.491391000
1	0.325991000	-3.031151000	-0.802033000
1	1.352377000	-4.430582000	-1.150930000
6	3.773139000	-3.323340000	-0.670019000
1	3.750846000	-4.300933000	-1.165125000
1	4.634229000	-2.785591000	-1.071225000
1	3.966468000	-3.515491000	0.391514000
6	-3.769592000	0.297581000	-0.572877000
1	-3.379329000	1.312158000	-0.394886000
6	-5.093296000	0.187526000	0.173504000
1	-5.535388000	-0.809484000	0.100073000
1	-4.998280000	0.426304000	1.236023000
1	-5.822504000	0.889903000	-0.247689000
6	-3.951505000	0.141584000	-2.077433000
1	-4.480530000	-0.786031000	-2.318709000
1	-4.549608000	0.963852000	-2.485853000
1	-2.995539000	0.123366000	-2.612139000
6	1.739528000	3.094243000	0.294498000
1	2.362630000	2.311382000	0.754088000
6	1.748303000	4.312222000	1.205930000
1	2.749488000	4.755231000	1.251096000
1	1.073233000	5.098474000	0.849347000
1	1.459185000	4.070465000	2.232158000
6	2.307591000	3.412149000	-1.084558000
1	3.355179000	3.725706000	-1.018946000
1	2.256501000	2.552044000	-1.760667000
1	1.761651000	4.233373000	-1.562967000
15	-2.335625000	-0.749354000	0.035668000
15	0.081584000	2.262086000	0.091627000
15	2.332730000	-0.910172000	-0.080155000
14	0.058036000	-1.037583000	1.818316000

7 0.078863000 -0.684829000 -2.069471000

[1c'_{PB}]≡N (TE = -2994.083858)

6	-0.615954000	1.951994000	1.842006000
6	0.220880000	0.893325000	2.577638000
6	-2.382260000	-1.053848000	1.956457000
6	-1.081550000	-1.560278000	2.571382000
6	2.791253000	-0.831488000	1.721409000
6	1.634497000	-1.398566000	2.545093000
1	-2.618258000	-0.049192000	2.327355000
1	-1.215365000	-1.619799000	3.668613000
1	3.741580000	-1.341919000	1.919042000
1	1.887943000	-1.299705000	3.617241000
1	-0.613241000	2.898002000	2.398125000
1	1.255084000	1.265125000	2.618277000
6	-1.099058000	3.559897000	-0.636079000
1	-0.443026000	4.436627000	-0.731047000
6	-2.507915000	-2.712383000	-0.406736000
1	-1.715482000	-3.221396000	0.165389000
6	3.763001000	0.006296000	-0.899754000
1	3.676639000	1.020229000	-0.477672000
23	0.042192000	-0.150993000	-0.655509000
1	-1.668465000	1.659368000	1.764966000
1	-0.098489000	0.925634000	3.637649000
1	1.566717000	-2.483203000	2.380033000
1	2.963929000	0.226542000	1.962028000
1	-0.914879000	-2.605222000	2.269723000
1	-3.246895000	-1.673544000	2.225617000
6	5.160795000	-0.516468000	-0.596831000
1	5.919076000	0.158559000	-1.010267000
1	5.362918000	-0.611525000	0.474230000
1	5.330390000	-1.494665000	-1.058289000
6	3.526736000	0.096767000	-2.402318000
1	3.676264000	-0.874829000	-2.886900000
1	2.508311000	0.413992000	-2.643240000
1	4.233517000	0.794350000	-2.865655000
6	-3.846521000	-3.318686000	-0.005056000
1	-3.833405000	-4.402434000	-0.167519000
1	-4.107787000	-3.154861000	1.044075000
1	-4.662654000	-2.922455000	-0.617678000
6	-2.233411000	-2.954828000	-1.887846000
1	-3.080503000	-2.644454000	-2.506460000
1	-1.356016000	-2.410110000	-2.245655000
1	-2.080293000	-4.024028000	-2.073624000
6	-1.543863000	3.147393000	-2.034298000
1	-0.701507000	2.867567000	-2.673305000

1	-2.204971000	2.275148000	-1.998527000
1	-2.089361000	3.960574000	-2.526436000
6	-2.284812000	3.961565000	0.229644000
1	-1.986051000	4.339510000	1.211336000
1	-2.863408000	4.750873000	-0.262505000
1	-2.973228000	3.125370000	0.395499000
6	2.606359000	-2.689551000	-0.552153000
1	3.001579000	-2.623152000	-1.577022000
6	1.278619000	-3.436798000	-0.616987000
1	0.800726000	-3.489332000	0.369068000
1	0.576369000	-2.947461000	-1.296531000
1	1.429791000	-4.466160000	-0.963769000
6	3.603629000	-3.452590000	0.311742000
1	3.784410000	-4.447828000	-0.110006000
1	4.573267000	-2.959154000	0.404217000
1	3.218087000	-3.605845000	1.325228000
6	-3.700253000	0.088440000	-0.377591000
1	-3.327480000	1.105206000	-0.171989000
6	-4.978601000	-0.098706000	0.430126000
1	-5.426532000	-1.083992000	0.280180000
1	-4.821802000	0.029857000	1.504422000
1	-5.728646000	0.640338000	0.124689000
6	-3.953748000	-0.009283000	-1.876731000
1	-4.460759000	-0.945536000	-2.132160000
1	-4.602254000	0.805529000	-2.217432000
1	-3.025336000	0.032318000	-2.456740000
6	1.608764000	3.094325000	0.347156000
1	2.246981000	2.324887000	0.808913000
6	1.563204000	4.305194000	1.266825000
1	2.549321000	4.777749000	1.337907000
1	0.872917000	5.073183000	0.899116000
1	1.256886000	4.047689000	2.284468000
6	2.196349000	3.436182000	-1.017174000
1	3.229094000	3.789462000	-0.924330000
1	2.196408000	2.574102000	-1.691978000
1	1.632303000	4.235807000	-1.510792000
15	-2.217587000	-0.937946000	0.118528000
15	-0.023393000	2.215888000	0.113384000
15	2.351770000	-0.890530000	-0.067181000
5	0.224949000	-0.695729000	2.312020000
7	0.037390000	-0.436992000	-2.216255000

[1d'_{sc}]=N (TE = -2822.468249)

6	-0.048784000	-1.374065000	1.836368000
6	-0.410109000	0.050048000	2.276705000
6	2.473607000	0.797314000	1.682782000

6	1.347490000	1.803677000	1.793888000
6	-2.430013000	2.028020000	1.031442000
6	-1.045053000	2.367382000	1.551605000
1	2.379836000	0.004700000	2.432505000
1	1.344491000	2.166902000	2.844093000
1	-3.106071000	2.887598000	1.063592000
1	-1.164776000	2.673274000	2.611941000
1	-0.387548000	-2.092594000	2.589985000
1	-1.497124000	0.048172000	2.436007000
6	-0.157348000	-3.440160000	-0.189493000
1	-0.803526000	-3.731204000	-1.027823000
6	3.547126000	0.989008000	-1.001055000
1	3.049682000	1.965090000	-1.016701000
6	-3.646858000	0.147764000	-0.699730000
1	-3.428762000	-0.512984000	0.149096000
23	0.082179000	0.595005000	-0.690119000
16	2.476471000	-0.080836000	0.067603000
16	-0.883473000	-1.800518000	0.255930000
16	-2.313979000	1.428555000	-0.704228000
6	-0.015034000	1.250094000	1.386049000
1	1.026925000	-1.525509000	1.703483000
1	0.010453000	0.167075000	3.294840000
1	-0.681485000	3.264225000	1.032406000
1	-2.899003000	1.223607000	1.609655000
1	1.581058000	2.680827000	1.175509000
1	3.463023000	1.238045000	1.830730000
6	-5.007224000	0.793212000	-0.522844000
1	-5.793027000	0.029736000	-0.503803000
1	-5.079989000	1.358030000	0.410534000
1	-5.230797000	1.479769000	-1.345335000
6	-3.539131000	-0.635974000	-1.992716000
1	-3.708368000	0.004103000	-2.864566000
1	-2.554432000	-1.099855000	-2.108332000
1	-4.288540000	-1.433498000	-2.019814000
6	4.960396000	1.078191000	-0.463755000
1	5.564287000	1.713712000	-1.120342000
1	5.015636000	1.515624000	0.536020000
1	5.439206000	0.094216000	-0.427048000
6	3.504138000	0.386401000	-2.392243000
1	3.899931000	-0.635954000	-2.400165000
1	2.484745000	0.383060000	-2.783955000
1	4.119606000	0.981648000	-3.074165000
6	1.276213000	-3.343136000	-0.672341000
1	1.385453000	-2.636995000	-1.500204000
1	1.953388000	-3.019649000	0.123193000
1	1.624100000	-4.323628000	-1.016490000

6	-0.325885000	-4.442433000	0.937102000
1	-1.357852000	-4.496255000	1.292271000
1	-0.034174000	-5.442090000	0.598745000
1	0.313467000	-4.197703000	1.790780000
7	0.586367000	1.728017000	-1.674765000

[1e'_{ssi}]=N (TE = -3073.881319)

23	0.194961000	0.267886000	-0.739056000
16	2.667418000	-0.651079000	-0.587542000
16	-0.611005000	-2.246119000	-0.898237000
16	-1.924046000	0.987460000	0.401229000
14	0.617562000	0.101567000	1.707746000
6	-0.528274000	1.211674000	2.770867000
6	-1.350901000	2.055362000	1.800202000
6	0.092766000	-2.696899000	0.741805000
6	-0.095252000	-1.703512000	1.891073000
6	2.452930000	-0.029656000	2.198356000
6	3.100949000	-0.963468000	1.186453000
1	2.785635000	-1.997769000	1.353305000
1	4.193950000	-0.979453000	1.227759000
1	2.927162000	0.959609000	2.163567000
1	2.636052000	-0.427290000	3.206329000
1	-0.317829000	-3.684305000	0.981709000
1	1.147155000	-2.872780000	0.510404000
1	-1.171257000	-1.598383000	2.092486000
1	0.308055000	-2.188679000	2.795221000
1	-1.189767000	0.616663000	3.413339000
1	0.026263000	1.884099000	3.435758000
1	-0.734090000	2.841829000	1.355239000
1	-2.235560000	2.516766000	2.255864000
6	3.565483000	0.944734000	-0.933189000
1	2.931676000	1.726764000	-0.500908000
6	-2.430042000	-2.309580000	-0.553181000
1	-2.592085000	-1.680220000	0.328400000
6	-2.924981000	2.175946000	-0.615918000
1	-3.024720000	1.618025000	-1.555453000
6	-2.886437000	-3.727927000	-0.279756000
1	-3.963142000	-3.744143000	-0.078664000
1	-2.699066000	-4.382296000	-1.136634000
1	-2.393303000	-4.166532000	0.591605000
6	-3.134889000	-1.689337000	-1.743745000
1	-2.770424000	-0.677982000	-1.951277000
1	-2.993680000	-2.284865000	-2.651627000
1	-4.211477000	-1.625632000	-1.555815000

6	-4.294896000	2.382282000	0.002035000
1	-4.227518000	2.876140000	0.976903000
1	-4.909104000	3.024262000	-0.639240000
1	-4.828693000	1.438611000	0.142851000
6	-2.181039000	3.465633000	-0.887590000
1	-2.713565000	4.045677000	-1.649029000
1	-2.122006000	4.093671000	0.007083000
1	-1.168288000	3.268156000	-1.250792000
6	3.603341000	1.104509000	-2.440316000
1	4.056657000	2.067874000	-2.695147000
1	4.203641000	0.318407000	-2.910751000
1	2.597179000	1.094841000	-2.862744000
6	4.952061000	0.962543000	-0.324499000
1	5.472129000	1.870766000	-0.646612000
1	4.944089000	0.973486000	0.768029000
1	5.555314000	0.109759000	-0.654351000
7	0.512553000	1.549088000	-1.614247000

[$\mathbf{1f}_{SB}$]≡N (TE = -2809.229728)

6	-0.107109000	-1.380326000	1.934339000
6	-0.401912000	0.077080000	2.322904000
6	2.661849000	0.638807000	1.660381000
6	1.704306000	1.797503000	1.837256000
6	-2.249962000	2.290855000	1.030715000
6	-0.864746000	2.645983000	1.540140000
1	2.441206000	-0.174335000	2.360593000
1	1.827800000	2.177093000	2.869912000
1	-2.914212000	3.155909000	0.934485000
1	-0.989625000	3.076965000	2.551335000
1	-0.455232000	-2.066880000	2.713088000
1	-1.493618000	0.145399000	2.435131000
6	-0.258823000	-3.450863000	-0.112374000
1	-0.919206000	-3.724736000	-0.944851000
6	3.252918000	1.137308000	-1.126194000
1	2.470542000	1.893770000	-1.264684000
6	-3.604055000	0.439811000	-0.661633000
1	-3.516141000	-0.220403000	0.211965000
23	0.045101000	0.206743000	-0.656433000
16	2.513694000	-0.145520000	0.008410000
16	-0.998230000	-1.824273000	0.384953000
16	-2.093251000	1.512284000	-0.624522000
1	0.956497000	-1.581277000	1.771669000
1	-0.029805000	0.167445000	3.360513000
1	-0.459655000	3.474386000	0.941861000
1	-2.751026000	1.566149000	1.682693000
1	2.016404000	2.637437000	1.199028000

1	3.717977000	0.883417000	1.811038000
6	-4.862815000	1.277589000	-0.558711000
1	-5.748853000	0.633598000	-0.584413000
1	-4.907565000	1.853821000	0.369033000
1	-4.940786000	1.980388000	-1.394101000
6	-3.551818000	-0.382186000	-1.933713000
1	-3.611671000	0.254939000	-2.821619000
1	-2.626980000	-0.960529000	-2.011591000
1	-4.395252000	-1.079329000	-1.967669000
6	4.502327000	1.760871000	-0.541199000
1	4.955032000	2.424951000	-1.284913000
1	4.305128000	2.365053000	0.347396000
1	5.251379000	1.004800000	-0.282240000
6	3.518672000	0.440090000	-2.445700000
1	4.287801000	-0.332119000	-2.337536000
1	2.606695000	-0.011959000	-2.841721000
1	3.876732000	1.166990000	-3.181863000
6	1.162776000	-3.331926000	-0.617299000
1	1.250083000	-2.600218000	-1.424909000
1	1.854627000	-3.035503000	0.176870000
1	1.503675000	-4.302197000	-0.995191000
6	-0.409393000	-4.463474000	1.006759000
1	-1.437385000	-4.531355000	1.371372000
1	-0.112192000	-5.456972000	0.656057000
1	0.235907000	-4.220320000	1.856705000
5	0.169916000	1.428378000	1.599033000
7	0.308016000	0.268008000	-2.213733000

[1a''_{pc}]≡N (TE = -3464.580826)

6	-0.394435000	-1.375701000	1.628544000
6	0.343821000	-2.095400000	2.599100000
1	1.182375000	-1.597460000	3.083188000
6	0.012758000	-3.383623000	2.978649000
1	0.603634000	-3.885554000	3.743541000
6	-1.089686000	-4.029448000	2.412561000
1	-1.364075000	-5.035804000	2.719092000
6	-1.811864000	-3.372584000	1.426506000
1	-2.630128000	-3.900067000	0.938236000
6	-1.476882000	-2.079796000	1.000106000
6	1.231179000	0.547311000	1.763530000
6	1.311789000	1.469747000	2.826552000
1	0.391277000	1.787903000	3.311947000
6	2.518916000	1.982050000	3.278042000
1	2.528328000	2.691383000	4.103932000
6	3.713373000	1.580011000	2.686969000
1	4.667176000	1.970554000	3.033890000

6	3.668988000	0.682810000	1.627008000
1	4.601596000	0.404178000	1.145854000
6	2.456836000	0.177257000	1.142523000
6	-1.179263000	0.998960000	1.548839000
6	-2.031043000	0.885242000	2.659810000
1	-1.960714000	-0.008054000	3.280361000
6	-2.922431000	1.891957000	3.001001000
1	-3.555610000	1.780784000	3.879733000
6	-2.992316000	3.054208000	2.234282000
1	-3.680571000	3.852447000	2.502970000
6	-2.176733000	3.183741000	1.115580000
1	-2.245447000	4.086729000	0.514069000
6	-1.285135000	2.168421000	0.751723000
6	-0.083647000	0.020913000	1.308184000
23	0.007982000	-0.241907000	-1.287002000
6	-2.111132000	-2.939292000	-1.684125000
1	-2.712131000	-3.730184000	-1.216723000
6	3.828138000	-0.108961000	-1.449037000
1	3.866415000	0.956334000	-1.171652000
6	-1.298386000	2.991762000	-2.137800000
1	-0.701034000	2.709419000	-3.017810000
6	-1.442744000	4.508606000	-2.131642000
1	-1.969565000	4.831174000	-3.037301000
1	-2.027217000	4.879092000	-1.285055000
1	-0.483913000	5.030158000	-2.122089000
6	-2.653723000	2.307144000	-2.277596000
1	-3.306343000	2.527111000	-1.425150000
1	-3.167502000	2.655407000	-3.179964000
1	-2.548538000	1.219660000	-2.354050000
6	-2.695085000	-2.591066000	-3.047770000
1	-3.758856000	-2.340864000	-3.002361000
1	-2.163053000	-1.741239000	-3.491016000
1	-2.592725000	-3.436398000	-3.736565000
6	-0.676995000	-3.430321000	-1.821839000
1	-0.232873000	-3.705393000	-0.860599000
1	-0.619003000	-4.308664000	-2.474211000
1	-0.051187000	-2.658832000	-2.294445000
6	5.194854000	-0.727976000	-1.165775000
1	5.964713000	-0.192187000	-1.732372000
1	5.494185000	-0.704092000	-0.116855000
1	5.241122000	-1.770600000	-1.490535000
6	3.520676000	-0.196336000	-2.942340000
1	3.523548000	-1.234751000	-3.290193000
1	2.541475000	0.217725000	-3.194083000
1	4.287130000	0.335280000	-3.517281000
15	-0.321225000	2.143369000	-0.793748000

15	2.356272000	-0.701350000	-0.453237000
15	-2.129238000	-1.430015000	-0.579811000
6	2.563066000	-2.530549000	-0.103528000
1	1.568294000	-2.798541000	0.281684000
6	2.793802000	-3.324216000	-1.385400000
1	3.815974000	-3.213953000	-1.757620000
1	2.634888000	-4.393146000	-1.206022000
1	2.120987000	-3.026070000	-2.194073000
6	3.572053000	-2.875035000	0.982423000
1	3.503205000	-3.939192000	1.235886000
1	4.602020000	-2.685539000	0.667759000
1	3.395530000	-2.308744000	1.901014000
6	-3.957172000	-1.039486000	-0.512140000
1	-4.162264000	-0.711082000	-1.541885000
6	-4.289625000	0.104271000	0.428343000
1	-4.161949000	-0.195509000	1.471523000
1	-3.666988000	0.985923000	0.264241000
1	-5.336094000	0.402853000	0.301166000
6	-4.826534000	-2.250314000	-0.198256000
1	-5.884088000	-1.964275000	-0.212779000
1	-4.707529000	-3.070678000	-0.910077000
1	-4.618631000	-2.639049000	0.804139000
6	1.227086000	3.150901000	-0.524729000
1	1.846739000	2.466109000	0.068363000
6	1.054531000	4.421521000	0.295309000
1	2.031740000	4.874741000	0.498625000
1	0.448404000	5.177609000	-0.211140000
1	0.585942000	4.215979000	1.262045000
6	1.939645000	3.374177000	-1.854171000
1	2.951195000	3.761208000	-1.688745000
1	2.028352000	2.445616000	-2.429129000
1	1.421378000	4.099031000	-2.489504000
7	0.049943000	-0.098585000	-2.873655000

[1b''_{psi}]≡N (TE = -3715.981210)

6	1.718602000	-2.103565000	0.954587000
6	1.980060000	-3.187256000	1.800142000
1	1.158240000	-3.667913000	2.331507000
6	3.278374000	-3.647013000	1.995893000
1	3.467165000	-4.492150000	2.655397000
6	4.340988000	-3.000376000	1.370454000
1	5.362518000	-3.332228000	1.544270000
6	4.096123000	-1.938466000	0.505380000
1	4.937995000	-1.457983000	0.009566000
6	2.789308000	-1.509569000	0.254221000
6	0.569597000	0.388389000	1.944753000

6	1.235103000	0.044983000	3.134701000
1	1.473993000	-1.001453000	3.325454000
6	1.627001000	0.986248000	4.079228000
1	2.141025000	0.668187000	4.984500000
6	1.365220000	2.332696000	3.855868000
1	1.668551000	3.085596000	4.580454000
6	0.708454000	2.709709000	2.692515000
1	0.504083000	3.765023000	2.528027000
6	0.309927000	1.766332000	1.734893000
6	-1.473843000	-1.762612000	1.505881000
6	-1.660378000	-2.279801000	2.793676000
1	-0.795453000	-2.489491000	3.423629000
6	-2.934794000	-2.495460000	3.307643000
1	-3.059559000	-2.892861000	4.313171000
6	-4.052702000	-2.175421000	2.541506000
1	-5.052081000	-2.319346000	2.947271000
6	-3.893925000	-1.670297000	1.255824000
1	-4.777483000	-1.420023000	0.673274000
6	-2.615275000	-1.474010000	0.726126000
23	-0.123426000	0.345780000	-1.258334000
6	3.800429000	0.994038000	-0.790981000
1	4.723134000	0.464034000	-1.074585000
6	-2.147722000	3.014857000	0.943679000
1	-1.849970000	3.845300000	1.601176000
6	-2.209242000	-2.475647000	-1.959473000
1	-2.532521000	-2.158694000	-2.962815000
6	-3.149557000	-3.553384000	-1.430048000
1	-3.193310000	-4.390068000	-2.136600000
1	-2.782995000	-3.954092000	-0.479172000
1	-4.172442000	-3.215794000	-1.261096000
6	-0.805696000	-3.052111000	-2.078862000
1	-0.411564000	-3.357858000	-1.102006000
1	-0.824152000	-3.948209000	-2.710707000
1	-0.110256000	-2.333317000	-2.512506000
6	3.649347000	2.226833000	-1.674455000
1	3.585449000	2.004114000	-2.739010000
1	2.746306000	2.783985000	-1.409333000
1	4.499827000	2.902166000	-1.528264000
6	3.899024000	1.430487000	0.667054000
1	4.056830000	0.600045000	1.358910000
1	4.727098000	2.136077000	0.797346000
1	2.984376000	1.945048000	0.984230000
6	-3.071965000	3.544146000	-0.144380000
1	-3.952730000	4.024846000	0.295460000
1	-2.595718000	4.278205000	-0.800248000
1	-3.431572000	2.731401000	-0.781964000

6	-2.851321000	1.962521000	1.787264000
1	-3.157209000	1.103414000	1.183351000
1	-2.225762000	1.578708000	2.598420000
1	-3.759771000	2.378845000	2.236357000
14	0.139049000	-1.104511000	0.752900000
15	-0.549972000	2.361196000	0.219115000
15	-2.266380000	-0.865619000	-0.977186000
15	2.381226000	-0.215390000	-1.020911000
6	2.767875000	-1.145538000	-2.615206000
1	1.870971000	-1.770008000	-2.717294000
6	3.991806000	-2.049298000	-2.597106000
1	4.119549000	-2.506388000	-3.584923000
1	4.914982000	-1.494345000	-2.391155000
1	3.920236000	-2.860500000	-1.871193000
6	2.821579000	-0.220648000	-3.825455000
1	2.014082000	0.514215000	-3.822756000
1	3.786706000	0.293053000	-3.889644000
1	2.719641000	-0.811337000	-4.742083000
6	-3.840366000	-0.036969000	-1.599767000
1	-4.147243000	0.593495000	-0.750136000
6	-3.459803000	0.873700000	-2.765721000
1	-3.141561000	0.290562000	-3.636719000
1	-4.316777000	1.484331000	-3.072527000
1	-2.624282000	1.537374000	-2.528309000
6	-5.026962000	-0.901702000	-2.012749000
1	-4.770908000	-1.571380000	-2.839770000
1	-5.436038000	-1.515585000	-1.208549000
1	-5.841733000	-0.261599000	-2.370584000
6	0.359416000	3.916290000	-0.324197000
1	1.397731000	3.699282000	-0.030758000
6	-0.047704000	5.244513000	0.303584000
1	0.613344000	6.040968000	-0.055476000
1	-1.065236000	5.535717000	0.027120000
1	0.007103000	5.256097000	1.394250000
6	0.299295000	4.014088000	-1.847991000
1	0.605678000	3.084252000	-2.338730000
1	-0.716362000	4.236072000	-2.195164000
1	0.946647000	4.819598000	-2.212593000
7	-0.141027000	0.175127000	-2.840220000

$[1c''_{PB}] \equiv N (TE = -3451.334767)$

6	-1.556328000	-0.492088000	1.877752000
6	-1.760872000	-0.292245000	3.254854000
1	-0.895092000	-0.137852000	3.899837000
6	-3.029890000	-0.269127000	3.822590000
1	-3.143717000	-0.108597000	4.893260000

6	-4.153369000	-0.439204000	3.018995000
1	-5.151293000	-0.413160000	3.451702000
6	-3.988188000	-0.633874000	1.653405000
1	-4.869288000	-0.752228000	1.025042000
6	-2.710817000	-0.659987000	1.083559000
6	0.858485000	-1.781998000	1.480472000
6	0.605868000	-2.739482000	2.478049000
1	-0.335624000	-2.691660000	3.026301000
6	1.536748000	-3.716415000	2.815419000
1	1.308304000	-4.437261000	3.598820000
6	2.773428000	-3.753293000	2.176884000
1	3.518666000	-4.494459000	2.457496000
6	3.036700000	-2.848272000	1.151426000
1	3.993099000	-2.896909000	0.633464000
6	2.084318000	-1.900663000	0.773035000
6	0.778120000	0.850651000	1.703677000
6	1.534223000	0.717874000	2.889422000
1	1.574387000	-0.257169000	3.374624000
6	2.238479000	1.764648000	3.468365000
1	2.794312000	1.599901000	4.389792000
6	2.247076000	3.011704000	2.854786000
1	2.806064000	3.841420000	3.282162000
6	1.537762000	3.180279000	1.675311000
1	1.564851000	4.149617000	1.185089000
6	0.798637000	2.135495000	1.099316000
23	-0.127858000	-0.004502000	-1.261265000
6	-2.659919000	-2.660888000	-1.027954000
1	-3.712935000	-2.867601000	-0.789445000
6	3.893111000	-0.095050000	-0.732339000
1	4.624122000	-0.911169000	-0.640643000
6	-1.440047000	3.573465000	-0.155461000
1	-1.694421000	4.000193000	-1.138687000
6	-1.166428000	4.701662000	0.831871000
1	-2.059126000	5.330724000	0.923613000
1	-0.952938000	4.304005000	1.828526000
1	-0.341136000	5.355645000	0.552726000
6	-2.621221000	2.757818000	0.346280000
1	-2.387336000	2.255914000	1.292261000
1	-3.491986000	3.398269000	0.524420000
1	-2.909918000	1.988877000	-0.366988000
6	-2.408305000	-2.988343000	-2.494944000
1	-3.123452000	-2.500465000	-3.162929000
1	-1.417054000	-2.660675000	-2.818428000
1	-2.485436000	-4.067732000	-2.667154000
6	-1.800322000	-3.498424000	-0.092465000
1	-2.037785000	-3.313894000	0.959189000

1	-1.958725000	-4.565106000	-0.286776000
1	-0.733398000	-3.300365000	-0.215887000
6	4.127091000	0.636813000	-2.048484000
1	5.125557000	1.086707000	-2.071126000
1	4.040482000	-0.013218000	-2.923741000
1	3.401293000	1.446171000	-2.182605000
6	4.065302000	0.829788000	0.459179000
1	3.362086000	1.666990000	0.426969000
1	3.910073000	0.313414000	1.409987000
1	5.076033000	1.253088000	0.469784000
5	-0.050984000	-0.492554000	1.336469000
15	-2.434178000	-0.829554000	-0.710766000
15	2.222213000	-0.919001000	-0.768306000
15	-0.008856000	2.413899000	-0.520761000
6	2.473579000	-2.209627000	-2.118985000
1	2.244334000	-1.629047000	-3.023478000
6	1.421643000	-3.301399000	-2.000000000
1	1.474220000	-3.980997000	-2.857661000
1	1.558519000	-3.902198000	-1.093590000
1	0.415769000	-2.880052000	-1.983013000
6	3.859409000	-2.825056000	-2.256459000
1	3.871981000	-3.497475000	-3.121806000
1	4.655333000	-2.093943000	-2.415730000
1	4.131267000	-3.434523000	-1.389611000
6	-3.954991000	-0.070312000	-1.529766000
1	-4.274288000	0.694299000	-0.809905000
6	-5.148856000	-0.991520000	-1.755461000
1	-5.996672000	-0.408701000	-2.132505000
1	-4.946105000	-1.765995000	-2.499839000
1	-5.487019000	-1.495416000	-0.846179000
6	-3.549232000	0.627990000	-2.823592000
1	-4.404941000	1.147615000	-3.269305000
1	-2.749150000	1.358577000	-2.664114000
1	-3.167318000	-0.081414000	-3.564487000
6	1.205195000	3.399314000	-1.565897000
1	2.179652000	3.009702000	-1.233955000
6	0.999946000	3.011330000	-3.029198000
1	0.020257000	3.343147000	-3.394610000
1	1.756223000	3.489345000	-3.661780000
1	1.046456000	1.930773000	-3.186763000
6	1.220990000	4.917763000	-1.442251000
1	0.248592000	5.357714000	-1.686409000
1	1.513337000	5.280328000	-0.455124000
1	1.940323000	5.333962000	-2.156208000
7	-0.143634000	-0.355275000	-2.802669000

[1d''_{sc}]≡N (TE = -3279.719386)

6	-0.926914000	-0.928346000	0.905836000
6	-1.919396000	-0.902546000	1.903962000
1	-2.203884000	0.066188000	2.313384000
6	-2.510098000	-2.050337000	2.412239000
1	-3.256270000	-1.970373000	3.200388000
6	-2.134742000	-3.299743000	1.925425000
1	-2.578581000	-4.209764000	2.321491000
6	-1.223955000	-3.364891000	0.882061000
1	-0.989016000	-4.325137000	0.426835000
6	-0.639189000	-2.205023000	0.363620000
6	1.065459000	0.359704000	1.482227000
6	0.945588000	0.241600000	2.877906000
1	-0.048790000	0.141113000	3.308568000
6	2.045414000	0.256548000	3.723521000
1	1.902861000	0.166699000	4.798467000
6	3.329051000	0.381148000	3.196444000
1	4.198643000	0.386136000	3.849469000
6	3.488763000	0.471671000	1.822476000
1	4.484533000	0.528403000	1.386432000
6	2.371811000	0.458429000	0.981831000
6	-1.017628000	1.564604000	0.677199000
6	-0.806736000	2.601494000	1.602936000
1	0.016385000	2.517264000	2.308335000
6	-1.611596000	3.734208000	1.646927000
1	-1.402296000	4.509757000	2.381461000
6	-2.672716000	3.881105000	0.761766000
1	-3.298074000	4.770128000	0.780788000
6	-2.891936000	2.890099000	-0.189049000
1	-3.667725000	3.018738000	-0.940624000
6	-2.092034000	1.750573000	-0.231648000
16	-2.254745000	0.658469000	-1.646109000
16	0.283114000	-2.401709000	-1.160800000
16	2.642737000	0.465729000	-0.784176000
23	0.304231000	0.122985000	-1.598439000
6	1.783867000	-3.416642000	-0.699100000
1	1.368136000	-4.418394000	-0.534574000
6	3.113777000	2.256369000	-1.057015000
1	4.017578000	2.360155000	-0.441750000
6	-3.815991000	-0.377593000	-1.411236000
1	-4.331474000	-0.174158000	-2.357038000
6	-4.672102000	0.106841000	-0.264163000
1	-5.580377000	-0.503539000	-0.208915000
1	-4.150448000	0.009134000	0.692064000
1	-4.980738000	1.148283000	-0.372212000
6	-3.515194000	-1.857786000	-1.323633000

1	-3.163569000	-2.134167000	-0.329429000
1	-4.429831000	-2.429986000	-1.519456000
1	-2.766274000	-2.179152000	-2.053332000
6	2.682320000	-3.428168000	-1.919138000
1	2.168331000	-3.789841000	-2.813544000
1	3.069532000	-2.426248000	-2.131400000
1	3.541498000	-4.082759000	-1.743173000
6	2.486270000	-2.939237000	0.550073000
1	1.800151000	-2.779271000	1.386715000
1	3.219235000	-3.690955000	0.863704000
1	3.028665000	-2.009090000	0.373057000
6	3.452401000	2.425182000	-2.522045000
1	3.794804000	3.449186000	-2.702846000
1	4.246671000	1.745865000	-2.844478000
1	2.567363000	2.248679000	-3.139497000
6	2.039725000	3.204186000	-0.574550000
1	1.118606000	3.075266000	-1.149593000
1	1.809647000	3.060962000	0.484694000
1	2.379629000	4.238351000	-0.700831000
6	-0.160720000	0.347678000	0.581662000
7	0.459863000	1.189612000	-2.758702000

[1e''_{ssi}]=N (TE = -3531.127160)

6	-0.274461000	0.037813000	1.854350000
6	-0.370064000	0.763585000	3.053362000
1	-0.464238000	1.849174000	3.001472000
6	-0.326522000	0.159679000	4.303115000
1	-0.395912000	0.762370000	5.206156000
6	-0.193482000	-1.222979000	4.390464000
1	-0.163605000	-1.715858000	5.359730000
6	-0.109934000	-1.981141000	3.231606000
1	-0.027751000	-3.063645000	3.303545000
6	-0.133048000	-1.358304000	1.979167000
6	1.087307000	2.262450000	0.424788000
6	1.012704000	3.591623000	0.858397000
1	0.039954000	4.027462000	1.082223000
6	2.148242000	4.383494000	0.995280000
1	2.057283000	5.417860000	1.320055000
6	3.402202000	3.845522000	0.722539000
1	4.297682000	4.452753000	0.835622000
6	3.516519000	2.526030000	0.299466000
1	4.499879000	2.110468000	0.090911000
6	2.366836000	1.757371000	0.123755000
6	-2.033302000	1.685626000	-0.075769000
6	-2.599041000	2.819008000	0.522480000
1	-2.039040000	3.360075000	1.284333000

6	-3.867852000	3.276234000	0.178248000
1	-4.276615000	4.162133000	0.659938000
6	-4.604577000	2.609029000	-0.794387000
1	-5.585599000	2.974925000	-1.089119000
6	-4.078746000	1.473684000	-1.402089000
1	-4.639735000	0.957669000	-2.177731000
6	-2.817826000	1.010241000	-1.028117000
16	-2.233805000	-0.526332000	-1.787551000
16	-0.097224000	-2.414626000	0.522897000
16	2.496731000	0.033569000	-0.402134000
23	0.329664000	-0.662340000	-1.547664000
6	1.156406000	-3.728778000	0.900635000
1	0.688536000	-4.383356000	1.646106000
6	3.888547000	0.064446000	-1.643892000
1	4.788722000	0.288115000	-1.057926000
6	-3.275004000	-1.789535000	-0.869066000
1	-2.618995000	-2.667221000	-0.901520000
6	-4.552531000	-2.076985000	-1.633033000
1	-5.094847000	-2.904181000	-1.160670000
1	-5.223047000	-1.212124000	-1.629346000
1	-4.361910000	-2.350479000	-2.673241000
6	-3.540188000	-1.408439000	0.571889000
1	-4.244400000	-0.573603000	0.642023000
1	-3.985396000	-2.257829000	1.101298000
1	-2.635223000	-1.118624000	1.109366000
6	1.334209000	-4.495537000	-0.397297000
1	0.391277000	-4.891950000	-0.783516000
1	1.776502000	-3.856732000	-1.171377000
1	2.012551000	-5.340497000	-0.246820000
6	2.463507000	-3.180438000	1.427302000
1	2.335884000	-2.581423000	2.331639000
1	3.137990000	-4.009120000	1.669557000
1	2.955704000	-2.549454000	0.683312000
6	3.984162000	-1.345254000	-2.196378000
1	4.839355000	-1.422080000	-2.874844000
1	4.115857000	-2.096603000	-1.411170000
1	3.084688000	-1.594188000	-2.770145000
6	3.668878000	1.094412000	-2.728218000
1	2.732277000	0.894617000	-3.257042000
1	3.628648000	2.112520000	-2.334263000
1	4.493261000	1.049691000	-3.448898000
14	-0.287933000	0.990860000	0.175930000
7	0.594311000	-0.084000000	-2.992769000

[$\mathbf{1f}'_{SB}$] \equiv N (TE = -3266.488000)

6	-0.766815000	1.968619000	0.519001000
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6	-0.479397000	3.121869000	1.272516000
1	0.390339000	3.115430000	1.929266000
6	-1.284420000	4.254926000	1.231051000
1	-1.034496000	5.120142000	1.842270000
6	-2.411718000	4.284397000	0.413707000
1	-3.045459000	5.167385000	0.375653000
6	-2.692767000	3.191220000	-0.399650000
1	-3.526495000	3.229763000	-1.098755000
6	-1.876989000	2.063419000	-0.347670000
6	-0.926964000	-0.569373000	1.306843000
6	-1.626933000	-0.185771000	2.471223000
1	-1.555173000	0.852143000	2.796843000
6	-2.405197000	-1.058532000	3.219563000
1	-2.909557000	-0.701694000	4.115491000
6	-2.551930000	-2.380507000	2.811860000
1	-3.168983000	-3.074811000	3.377337000
6	-1.920770000	-2.796154000	1.648831000
1	-2.058854000	-3.813245000	1.286706000
6	-1.116126000	-1.913759000	0.918809000
6	1.487067000	0.623192000	1.318988000
6	1.658978000	0.902334000	2.687540000
1	0.777956000	1.102999000	3.297459000
6	2.907779000	0.917686000	3.297129000
1	2.989968000	1.139960000	4.359368000
6	4.050088000	0.631847000	2.554417000
1	5.030490000	0.626939000	3.025095000
6	3.922884000	0.326557000	1.206594000
1	4.797847000	0.060443000	0.617089000
6	2.660910000	0.336511000	0.604753000
16	2.551651000	-0.183819000	-1.110169000
16	-2.071487000	0.783914000	-1.582704000
16	-0.445715000	-2.580636000	-0.609404000
23	0.140861000	-0.424702000	-1.640632000
6	-3.787308000	0.077706000	-1.347121000
1	-4.438496000	0.825884000	-1.815548000
6	0.940996000	-3.702672000	-0.027061000
1	0.402795000	-4.570854000	0.373489000
6	2.937172000	1.383825000	-2.059452000
1	2.801583000	1.020582000	-3.084684000
6	4.369696000	1.808046000	-1.817680000
1	4.623595000	2.645406000	-2.476050000
1	4.517024000	2.152483000	-0.789091000
1	5.081468000	1.001855000	-2.012879000
6	1.940935000	2.483223000	-1.761212000
1	1.918860000	2.732538000	-0.694828000
1	2.216592000	3.392779000	-2.306206000

1	0.925973000	2.213343000	-2.069169000
6	-3.828524000	-1.207239000	-2.149610000
1	-3.514369000	-1.063600000	-3.186771000
1	-3.177864000	-1.968607000	-1.706523000
1	-4.847298000	-1.607411000	-2.160290000
6	-4.176729000	-0.114293000	0.099659000
1	-4.043625000	0.793916000	0.693327000
1	-5.235317000	-0.393171000	0.154626000
1	-3.599281000	-0.912865000	0.570034000
6	1.718961000	-4.098352000	-1.264856000
1	2.493028000	-4.826185000	-1.002112000
1	1.083193000	-4.549935000	-2.030803000
1	2.216230000	-3.231060000	-1.711218000
6	1.803797000	-3.089001000	1.049495000
1	2.409594000	-2.268025000	0.661204000
1	1.221901000	-2.709350000	1.893652000
1	2.493916000	-3.846232000	1.437733000
5	0.011035000	0.607541000	0.710057000
7	0.376671000	-0.399456000	-3.198147000

Cartesian coordinates of the vanadium hydrazine complexes for $[1a'_{PC}]-[1f'_{SB}]$, $[1a''_{PC}]-[1f''_{SB}]$ and $\{[HIPTN_3N]-V\}$ along with their total energies (in hartree) including zero point vibrational correction at M06-L-D3(heptane)/6-311+G* level of theory.

$[1a'_{PC}]-NH_2-NH_2$ (TE = -3064.380243)

6	-0.043347000	2.536402000	1.893779000
6	0.570418000	1.299334000	2.537027000
6	-2.607971000	0.068982000	1.692065000
6	-1.425287000	-0.220005000	2.618833000
6	2.257151000	-1.243634000	1.927577000
6	0.871236000	-1.160021000	2.563975000
1	-2.682174000	1.141188000	1.463854000
1	-1.559626000	0.371796000	3.545565000
1	2.838998000	-2.093779000	2.311196000
1	1.000681000	-1.095553000	3.666727000
1	0.352581000	3.470766000	2.313481000
1	1.656648000	1.331532000	2.357829000
6	-0.823023000	3.831391000	-0.640503000
1	-0.198358000	4.272382000	-1.433090000
6	-2.644556000	-2.567336000	0.486320000
1	-1.891444000	-2.711057000	1.278371000
6	3.709973000	-0.495106000	-0.494421000
1	3.474549000	0.563668000	-0.306268000
23	0.006112000	-0.027264000	-0.297972000
6	-0.009796000	-0.024807000	2.024505000

1	-1.126466000	2.556903000	2.069915000
1	0.463147000	1.385698000	3.639964000
1	0.355165000	-2.115916000	2.395640000
1	2.843242000	-0.348462000	2.171833000
1	-1.532486000	-1.263874000	2.954182000
1	-3.563467000	-0.213836000	2.156507000
6	5.006383000	-0.796369000	0.250492000
1	5.769607000	-0.051410000	-0.005652000
1	4.882176000	-0.764098000	1.336488000
1	5.426574000	-1.771877000	0.000089000
6	3.866401000	-0.665035000	-1.999724000
1	4.113859000	-1.698201000	-2.269795000
1	2.944574000	-0.404179000	-2.534532000
1	4.666786000	-0.030514000	-2.397601000
6	-4.008656000	-2.918036000	1.064092000
1	-4.016484000	-3.945444000	1.448032000
1	-4.301726000	-2.264137000	1.890683000
1	-4.795148000	-2.863641000	0.303727000
6	-2.275972000	-3.507676000	-0.658265000
1	-3.067535000	-3.566060000	-1.410267000
1	-1.362605000	-3.191395000	-1.173797000
1	-2.114344000	-4.526693000	-0.287605000
6	-2.087156000	3.281984000	-1.287485000
1	-1.868094000	2.519683000	-2.042329000
1	-2.738037000	2.810158000	-0.540657000
1	-2.669625000	4.076723000	-1.768424000
6	-1.187346000	4.927277000	0.354972000
1	-0.322939000	5.351439000	0.869160000
1	-1.705728000	5.752074000	-0.148538000
1	-1.868253000	4.550778000	1.125382000
6	2.298477000	-3.130485000	-0.315230000
1	2.063656000	-3.197803000	-1.390197000
6	1.231636000	-3.908011000	0.447593000
1	1.487266000	-3.981558000	1.510634000
1	0.248738000	-3.433841000	0.380201000
1	1.141641000	-4.931551000	0.066546000
6	3.663366000	-3.765661000	-0.088706000
1	3.608443000	-4.852843000	-0.224213000
1	4.423791000	-3.398023000	-0.780766000
1	4.030400000	-3.592275000	0.929154000
6	-3.773610000	-0.173795000	-0.979458000
1	-3.387313000	0.779213000	-1.368868000
6	-5.070001000	0.136386000	-0.241491000
1	-5.508057000	-0.750390000	0.224757000
1	-4.931695000	0.882949000	0.545212000
1	-5.819684000	0.535854000	-0.935778000

6	-4.016877000	-1.083309000	-2.178132000
1	-4.525820000	-2.007143000	-1.884855000
1	-4.661171000	-0.591486000	-2.916138000
1	-3.089041000	-1.371624000	-2.684533000
6	1.959108000	3.123293000	-0.124633000
1	2.549067000	2.456612000	0.524171000
6	2.187750000	4.558648000	0.323388000
1	3.251381000	4.819823000	0.266071000
1	1.655448000	5.272474000	-0.315154000
1	1.871446000	4.735834000	1.355334000
6	2.431481000	2.921165000	-1.558565000
1	3.487879000	3.189228000	-1.678156000
1	2.316431000	1.878250000	-1.873603000
1	1.865479000	3.545554000	-2.261776000
15	-2.328516000	-0.764008000	0.065548000
15	0.221988000	2.427334000	0.068041000
15	2.106929000	-1.292975000	0.082422000
7	-0.094105000	-0.048237000	-2.583020000
1	-0.969719000	0.354341000	-2.908469000
7	-0.022404000	-1.373143000	-3.156179000
1	0.500193000	-1.343503000	-4.031832000
1	0.533858000	-1.917295000	-2.497038000
1	0.643622000	0.552585000	-2.951193000

[1b'_{PSi}]-NH₂-NH₂ (TE = -3315.808576)

6	-0.079218000	2.670289000	1.848263000
6	0.340349000	1.584058000	2.844710000
6	-2.820416000	-0.272817000	1.980985000
6	-1.674828000	-0.790806000	2.848055000
6	2.495868000	-1.508909000	1.743555000
6	1.370160000	-1.372562000	2.773225000
1	-2.933933000	0.813622000	2.111702000
1	-1.846497000	-0.515982000	3.899010000
1	3.151853000	-2.370990000	1.937355000
1	1.796730000	-1.076347000	3.742271000
1	0.244492000	3.675988000	2.151987000
1	1.420900000	1.666078000	3.036982000
6	-0.025519000	3.736646000	-0.888774000
1	0.478021000	3.577197000	-1.855616000
6	-3.032219000	-2.311704000	-0.051159000
1	-2.497640000	-2.793623000	0.783090000
6	3.500127000	-1.042567000	-0.908511000
1	3.539018000	0.024881000	-0.645032000
23	-0.086697000	-0.085207000	-0.392507000
1	-1.175317000	2.709743000	1.770865000
1	-0.142393000	1.760898000	3.816965000

1	0.904726000	-2.350980000	2.946624000
1	3.152250000	-0.627003000	1.797451000
1	-1.670087000	-1.891309000	2.828420000
1	-3.792950000	-0.710859000	2.248514000
6	4.826989000	-1.648453000	-0.460636000
1	5.659538000	-1.052775000	-0.854884000
1	4.937645000	-1.667857000	0.626914000
1	4.975905000	-2.667125000	-0.822679000
6	3.318486000	-1.116665000	-2.418591000
1	3.152940000	-2.145370000	-2.763278000
1	2.474072000	-0.503098000	-2.752742000
1	4.207281000	-0.748341000	-2.944100000
6	-4.514191000	-2.619536000	0.101703000
1	-4.679713000	-3.701078000	0.178204000
1	-4.956081000	-2.161818000	0.991329000
1	-5.087337000	-2.276261000	-0.765968000
6	-2.482991000	-2.907846000	-1.341237000
1	-2.952214000	-2.461865000	-2.227536000
1	-1.399606000	-2.755036000	-1.418377000
1	-2.672021000	-3.986630000	-1.394149000
6	-1.528193000	3.646865000	-1.131619000
1	-1.817712000	2.679741000	-1.556727000
1	-2.095823000	3.770419000	-0.201417000
1	-1.864969000	4.433052000	-1.817244000
6	0.351271000	5.124278000	-0.386434000
1	1.429724000	5.293550000	-0.391320000
1	-0.094061000	5.899995000	-1.021391000
1	-0.006688000	5.305635000	0.632300000
6	1.642631000	-3.359428000	-0.401852000
1	1.177228000	-3.346455000	-1.401062000
6	0.617091000	-3.922764000	0.577725000
1	1.070133000	-4.096809000	1.559762000
1	-0.231468000	-3.244831000	0.721998000
1	0.228042000	-4.886049000	0.227678000
6	2.866019000	-4.262936000	-0.457972000
1	2.564758000	-5.313467000	-0.554660000
1	3.516245000	-4.039089000	-1.306340000
1	3.471901000	-4.189793000	0.452035000
6	-3.811169000	0.591072000	-0.567459000
1	-3.379520000	1.572629000	-0.315802000
6	-5.220819000	0.566831000	0.014262000
1	-5.797605000	-0.300771000	-0.312172000
1	-5.228064000	0.574869000	1.107201000
1	-5.776572000	1.453681000	-0.314346000
6	-3.839947000	0.487871000	-2.085824000
1	-4.223980000	-0.482616000	-2.421985000

1	-4.487928000	1.253954000	-2.527538000
1	-2.841105000	0.624082000	-2.518615000
6	2.390490000	2.492023000	0.314559000
1	2.689353000	1.506501000	0.704366000
6	2.905104000	3.534698000	1.299434000
1	3.996877000	3.467366000	1.381378000
1	2.675989000	4.558810000	0.996229000
1	2.501712000	3.395417000	2.305524000
6	3.023543000	2.655635000	-1.062280000
1	4.112706000	2.538323000	-1.016137000
1	2.639938000	1.920434000	-1.780404000
1	2.830655000	3.651483000	-1.478060000
15	-2.479780000	-0.521693000	0.169012000
15	0.530180000	2.257147000	0.140018000
15	1.909703000	-1.529709000	-0.028093000
14	0.002718000	-0.182102000	2.128020000
7	-0.242316000	-0.444930000	-2.633654000
1	0.380961000	-1.197346000	-2.917836000
1	-1.186411000	-0.777595000	-2.831746000
7	0.095156000	0.692820000	-3.460539000
1	-0.457735000	0.671208000	-4.318532000
1	-0.213328000	1.507763000	-2.932567000

[1c'_{PB}]-NH₂-NH₂ (TE = -3051.151225)

6	0.108919000	2.502668000	2.032832000
6	0.574055000	1.295604000	2.849439000
6	-2.635887000	0.155535000	1.968069000
6	-1.536419000	-0.486045000	2.813383000
6	2.286437000	-1.339223000	1.789065000
6	1.019879000	-1.381754000	2.640061000
1	-2.562706000	1.250629000	1.989659000
1	-1.708099000	-0.199072000	3.867246000
1	3.037360000	-2.079356000	2.095545000
1	1.324790000	-1.411019000	3.703889000
1	0.444630000	3.464937000	2.447138000
1	1.676774000	1.289408000	2.862466000
6	0.022699000	3.860401000	-0.571756000
1	0.714526000	4.682303000	-0.333683000
6	-2.974327000	-2.123299000	0.190026000
1	-2.058074000	-2.589869000	0.580525000
6	3.515198000	-1.103900000	-0.805419000
1	3.703152000	-0.087457000	-0.426275000
23	-0.043215000	0.034247000	-0.368235000
1	-0.984895000	2.545640000	2.013356000
1	0.295976000	1.477519000	3.903987000
1	0.509541000	-2.344881000	2.475102000

1	2.774426000	-0.357562000	1.878709000
1	-1.692778000	-1.577404000	2.801661000
1	-3.647333000	-0.084680000	2.328414000
6	4.698917000	-1.982037000	-0.427182000
1	5.630348000	-1.578863000	-0.842668000
1	4.836221000	-2.060803000	0.654948000
1	4.592192000	-2.997346000	-0.824494000
6	3.371805000	-1.013913000	-2.317608000
1	3.141225000	-1.989709000	-2.763954000
1	2.572122000	-0.322457000	-2.603064000
1	4.296604000	-0.662084000	-2.789312000
6	-4.116775000	-2.558949000	1.098355000
1	-4.183492000	-3.653803000	1.114106000
1	-3.972975000	-2.237278000	2.133541000
1	-5.090587000	-2.190365000	0.768565000
6	-3.157484000	-2.620276000	-1.238808000
1	-4.085768000	-2.244040000	-1.684317000
1	-2.331259000	-2.312350000	-1.890098000
1	-3.213537000	-3.714892000	-1.270553000
6	-0.007683000	3.658840000	-2.083388000
1	0.954821000	3.346159000	-2.498051000
1	-0.742534000	2.886363000	-2.342895000
1	-0.306986000	4.577548000	-2.600985000
6	-1.370575000	4.233425000	-0.082122000
1	-1.384417000	4.542454000	0.965744000
1	-1.785330000	5.057235000	-0.674047000
1	-2.059507000	3.383221000	-0.186156000
6	1.761929000	-3.395490000	-0.269050000
1	2.248547000	-3.553396000	-1.246291000
6	0.311232000	-3.848310000	-0.384709000
1	-0.201277000	-3.752361000	0.579613000
1	-0.264866000	-3.254409000	-1.101287000
1	0.248170000	-4.901893000	-0.682589000
6	2.476940000	-4.249025000	0.771755000
1	2.427304000	-5.310041000	0.499164000
1	3.530984000	-3.995421000	0.897839000
1	1.999019000	-4.151745000	1.752523000
6	-3.808254000	0.691443000	-0.592626000
1	-3.670345000	1.663631000	-0.093448000
6	-5.237392000	0.240309000	-0.327314000
1	-5.474750000	-0.693028000	-0.847306000
1	-5.436480000	0.085773000	0.736787000
1	-5.951972000	0.991003000	-0.686016000
6	-3.557157000	0.911930000	-2.079350000
1	-3.487150000	-0.029915000	-2.636093000
1	-4.360429000	1.500406000	-2.537719000

1	-2.624432000	1.466575000	-2.233570000
6	2.496501000	2.616859000	0.416750000
1	2.852463000	1.688944000	0.890617000
6	2.905783000	3.786982000	1.299099000
1	3.995099000	3.912547000	1.298217000
1	2.480235000	4.735826000	0.952306000
1	2.600294000	3.650785000	2.339387000
6	3.144467000	2.710809000	-0.958161000
1	4.236675000	2.650505000	-0.885740000
1	2.813532000	1.903273000	-1.622694000
1	2.913870000	3.663500000	-1.448444000
15	-2.436831000	-0.321845000	0.196277000
15	0.645660000	2.303472000	0.276171000
15	1.867783000	-1.519684000	-0.003740000
5	-0.001742000	-0.157780000	2.444371000
7	-0.131928000	0.051214000	-2.638654000
1	0.636803000	0.619909000	-2.997070000
1	-0.984776000	0.508513000	-2.950334000
7	-0.139137000	-1.260094000	-3.245428000
1	0.310915000	-1.216621000	-4.160770000
1	0.462215000	-1.831738000	-2.653687000

[1d'_{sc}]-NH₂-NH₂ (TE = -2879.532095)

6	0.999291000	1.684434000	2.006340000
6	0.727507000	0.271064000	2.492601000
6	-2.468662000	1.057210000	1.268028000
6	-1.762749000	0.078482000	2.199694000
6	0.915119000	-2.652828000	1.502968000
6	-0.324886000	-1.947866000	2.025688000
1	-1.939157000	2.012838000	1.197850000
1	-1.702999000	0.573120000	3.189733000
1	0.854106000	-3.738873000	1.624972000
1	-0.382695000	-2.185855000	3.112247000
1	1.783406000	2.182960000	2.587138000
1	1.671617000	-0.288534000	2.407395000
6	1.337222000	3.320249000	-0.334496000
1	1.692969000	3.238101000	-1.369780000
6	-3.586958000	-1.049649000	-0.288009000
1	-3.160953000	-1.604627000	0.556341000
6	3.040527000	-1.882836000	-0.213677000
1	3.135667000	-1.134052000	0.585248000
23	-0.108469000	-0.189750000	-0.486098000
16	-2.498300000	0.469575000	-0.472884000
16	1.533675000	1.564081000	0.249401000
16	1.201989000	-2.273618000	-0.286262000
6	-0.391798000	-0.446279000	1.735343000

1	0.095287000	2.303274000	2.054810000
1	0.529242000	0.330884000	3.584731000
1	-1.206357000	-2.435614000	1.581658000
1	1.818154000	-2.321672000	2.026681000
1	-2.448835000	-0.765417000	2.369263000
1	-3.492819000	1.283694000	1.591753000
6	3.844666000	-3.123032000	0.113141000
1	4.913052000	-2.887615000	0.188528000
1	3.543928000	-3.575814000	1.062265000
1	3.727998000	-3.883348000	-0.666468000
6	3.429869000	-1.263220000	-1.538586000
1	3.266056000	-1.962531000	-2.367655000
1	2.859907000	-0.350733000	-1.741640000
1	4.492758000	-0.999361000	-1.544582000
6	-5.024003000	-0.665202000	-0.008409000
1	-5.650501000	-1.557207000	0.108731000
1	-5.126375000	-0.078588000	0.908793000
1	-5.443530000	-0.073810000	-0.829038000
6	-3.424344000	-1.872142000	-1.547752000
1	-3.754911000	-1.320370000	-2.436710000
1	-2.374121000	-2.157934000	-1.688590000
1	-4.019659000	-2.789502000	-1.493441000
6	-0.104610000	3.787875000	-0.333204000
1	-0.768830000	3.073790000	-0.833063000
1	-0.483319000	3.928855000	0.684865000
1	-0.197436000	4.754673000	-0.840678000
6	2.248595000	4.254103000	0.438854000
1	3.285955000	3.910428000	0.432190000
1	2.224838000	5.262382000	0.010242000
1	1.933059000	4.344194000	1.483443000
7	-0.022503000	-0.092053000	-2.758338000
7	0.399095000	1.195227000	-3.268481000
1	0.008920000	1.339750000	-4.200954000
1	-0.052917000	1.878238000	-2.662038000
1	0.636043000	-0.773581000	-3.127190000
1	-0.935449000	-0.352893000	-3.134289000

[1e'_{ssi}]-NH₂-NH₂ (TE = -3130.946603)

23	0.051078000	-0.099502000	0.773223000
16	-2.000979000	-1.531278000	0.762932000
16	2.357236000	-1.043552000	1.126297000
16	0.447400000	1.866109000	-0.708032000
14	0.380794000	-1.146242000	-1.474057000
6	0.410517000	0.169330000	-2.881701000
6	-0.257078000	1.442379000	-2.374587000
6	2.453575000	-2.470860000	-0.050663000

6	2.033519000	-2.144120000	-1.479023000
6	-1.085979000	-2.359693000	-1.784063000
6	-1.628330000	-2.870552000	-0.457499000
1	-0.883895000	-3.476574000	0.070994000
1	-2.529260000	-3.489484000	-0.547236000
1	-1.881005000	-1.824864000	-2.324906000
1	-0.829352000	-3.223729000	-2.414887000
1	3.462913000	-2.892948000	0.030744000
1	1.772586000	-3.197050000	0.406821000
1	2.820309000	-1.549933000	-1.965429000
1	1.986900000	-3.085516000	-2.045462000
1	1.451962000	0.397124000	-3.149611000
1	-0.083746000	-0.139475000	-3.813237000
1	-1.339907000	1.304968000	-2.252670000
1	-0.093583000	2.302799000	-3.033385000
6	-3.411168000	-0.650766000	-0.115190000
1	-2.926681000	-0.075389000	-0.916965000
6	3.545653000	0.139294000	0.305060000
1	3.067978000	0.410399000	-0.646741000
6	-0.421846000	3.474739000	-0.330939000
1	0.173657000	3.836656000	0.518997000
6	4.903160000	-0.485579000	0.060747000
1	5.590601000	0.253544000	-0.366780000
1	5.349625000	-0.850153000	0.992097000
1	4.859215000	-1.323197000	-0.639920000
6	3.627376000	1.369117000	1.186853000
1	2.635410000	1.796975000	1.368949000
1	4.083006000	1.135837000	2.155956000
1	4.237903000	2.143253000	0.710840000
6	-0.323149000	4.479648000	-1.462211000
1	-0.972494000	4.209739000	-2.300455000
1	-0.642969000	5.471157000	-1.122076000
1	0.697493000	4.571923000	-1.843901000
6	-1.846009000	3.237024000	0.127852000
1	-2.338706000	4.180147000	0.393273000
1	-2.448107000	2.763426000	-0.656696000
1	-1.875793000	2.578119000	1.001095000
6	-4.018674000	0.296425000	0.899604000
1	-4.742946000	0.964230000	0.420718000
1	-4.545796000	-0.256242000	1.685490000
1	-3.259709000	0.916976000	1.383486000
6	-4.438899000	-1.604212000	-0.687370000
1	-5.292293000	-1.043470000	-1.086316000
1	-4.045481000	-2.213082000	-1.504889000
1	-4.826190000	-2.280751000	0.082345000
7	-0.125289000	0.611657000	2.933252000

7	-1.422944000	0.469199000	3.554025000
1	-1.808059000	-0.400680000	3.191338000
1	-1.307276000	0.337697000	4.558700000
1	0.594900000	0.124076000	3.468618000
1	0.105977000	1.599937000	2.992466000

[1f_{SB}]-NH₂-NH₂ (TE = -2866.294036)

6	1.050907000	2.175460000	1.683465000
6	0.800920000	0.907148000	2.485690000
6	-2.540482000	1.409492000	1.022010000
6	-1.924897000	0.677325000	2.207877000
6	0.884824000	-2.292137000	1.940452000
6	-0.383353000	-1.566605000	2.348140000
1	-1.978107000	2.315250000	0.771019000
1	-1.905766000	1.409389000	3.035377000
1	0.882190000	-3.356999000	2.197118000
1	-0.492806000	-1.725191000	3.439889000
1	1.832251000	2.813514000	2.113128000
1	1.740523000	0.332007000	2.510256000
6	1.380304000	3.285379000	-0.958118000
1	1.827555000	3.020542000	-1.926068000
6	-3.502864000	-1.036959000	-0.074112000
1	-3.048897000	-1.407099000	0.852578000
6	3.035978000	-1.849169000	0.145703000
1	3.165866000	-0.984789000	0.812021000
23	-0.077316000	-0.118779000	-0.500030000
16	-2.479328000	0.454692000	-0.551716000
16	1.586735000	1.693213000	-0.015643000
16	1.185569000	-2.155797000	0.113123000
1	0.136440000	2.775017000	1.590008000
1	0.649208000	1.227602000	3.533935000
1	-1.246871000	-2.095007000	1.914991000
1	1.766988000	-1.845003000	2.412869000
1	-2.645312000	-0.085105000	2.545028000
1	-3.579006000	1.721859000	1.193218000
6	3.773918000	-3.056793000	0.684224000
1	4.852525000	-2.865552000	0.731152000
1	3.447912000	-3.327305000	1.692097000
1	3.620126000	-3.930204000	0.041602000
6	3.470297000	-1.479974000	-1.256407000
1	3.274062000	-2.296706000	-1.961622000
1	2.949138000	-0.585687000	-1.613296000
1	4.545446000	-1.274315000	-1.287722000
6	-4.949858000	-0.657042000	0.158513000
1	-5.540002000	-1.537440000	0.438223000

1	-5.064279000	0.074949000	0.962844000
1	-5.399702000	-0.232890000	-0.745317000
6	-3.325965000	-2.072087000	-1.163988000
1	-3.701105000	-1.711974000	-2.129270000
1	-2.269867000	-2.332875000	-1.295037000
1	-3.876212000	-2.986498000	-0.918172000
6	-0.073527000	3.655649000	-1.167028000
1	-0.642850000	2.828951000	-1.605727000
1	-0.559437000	3.925329000	-0.223111000
1	-0.160325000	4.524461000	-1.829416000
6	2.184764000	4.404955000	-0.326055000
1	3.226328000	4.118319000	-0.159382000
1	2.178465000	5.294129000	-0.966236000
1	1.761869000	4.703906000	0.638196000
5	-0.458255000	0.009911000	2.031438000
7	0.007861000	-0.368508000	-2.753210000
1	-0.776393000	0.122278000	-3.176784000
1	0.848210000	0.077519000	-3.121363000
7	-0.086049000	-1.740140000	-3.205114000
1	0.470310000	-1.861079000	-4.050843000
1	0.354969000	-2.301994000	-2.478827000

[1a''_{PC}]-NH₂-NH₂ (TE = -3521.660077)

6	1.243699000	-0.300564000	1.841511000
6	1.579483000	0.336741000	3.047909000
1	0.828961000	0.953227000	3.539661000
6	2.829322000	0.193312000	3.641355000
1	3.046362000	0.710291000	4.574820000
6	3.787800000	-0.625673000	3.056296000
1	4.764227000	-0.757906000	3.517585000
6	3.490394000	-1.256000000	1.851255000
1	4.262875000	-1.855025000	1.372330000
6	2.254837000	-1.083371000	1.217056000
6	-0.890001000	1.011064000	1.755580000
6	-1.844493000	0.909260000	2.782725000
1	-2.039058000	-0.065386000	3.226008000
6	-2.556330000	2.009644000	3.245866000
1	-3.294465000	1.882764000	4.036262000
6	-2.318592000	3.266955000	2.703602000
1	-2.867464000	4.138305000	3.054892000
6	-1.372993000	3.397396000	1.691451000
1	-1.208676000	4.380831000	1.260884000
6	-0.669702000	2.293215000	1.197304000
6	-0.957065000	-1.431393000	1.493750000
6	-0.724430000	-2.287599000	2.579553000
1	0.131955000	-2.095517000	3.224701000

6	-1.557806000	-3.365816000	2.857729000
1	-1.341308000	-4.011660000	3.707331000
6	-2.674687000	-3.606583000	2.065560000
1	-3.338801000	-4.440950000	2.281023000
6	-2.934990000	-2.764791000	0.987068000
1	-3.809112000	-2.957155000	0.370155000
6	-2.085691000	-1.699520000	0.675961000
6	-0.134126000	-0.195013000	1.252660000
23	0.144981000	0.002700000	-1.056202000
6	3.715958000	-1.349162000	-1.267426000
1	4.420062000	-1.951577000	-0.680853000
6	-0.398371000	3.816865000	-1.260565000
1	-1.465447000	3.692198000	-1.017329000
6	-2.978655000	-1.765824000	-2.187081000
1	-2.808217000	-1.135168000	-3.075719000
6	-4.467282000	-2.097353000	-2.173479000
1	-4.729423000	-2.670299000	-3.071347000
1	-4.759816000	-2.710442000	-1.317548000
1	-5.099908000	-1.208375000	-2.169442000
6	-2.144930000	-3.031607000	-2.360536000
1	-2.299072000	-3.727254000	-1.528958000
1	-2.420513000	-3.558828000	-3.280835000
1	-1.070088000	-2.818301000	-2.396249000
6	3.742876000	-1.851308000	-2.705531000
1	3.554010000	-2.925266000	-2.787977000
1	2.990275000	-1.337825000	-3.317926000
1	4.715262000	-1.657713000	-3.172138000
6	4.162355000	0.099887000	-1.195584000
1	4.156653000	0.487729000	-0.172590000
1	5.176938000	0.219282000	-1.593266000
1	3.499370000	0.744091000	-1.781222000
6	0.004758000	5.245710000	-0.907720000
1	-0.628375000	5.957073000	-1.451617000
1	-0.083831000	5.486295000	0.152762000
1	1.035022000	5.462943000	-1.200972000
6	-0.241552000	3.594018000	-2.760285000
1	0.804593000	3.661545000	-3.077657000
1	-0.596731000	2.606875000	-3.067491000
1	-0.801026000	4.348373000	-3.326297000
15	-2.220702000	-0.686594000	-0.840996000
15	0.363614000	2.368809000	-0.317914000
15	1.995434000	-1.580369000	-0.533239000
6	2.067396000	2.899238000	0.285389000
1	2.460508000	1.932760000	0.636321000
6	2.945570000	3.364665000	-0.870984000
1	2.739527000	4.401701000	-1.149585000

1	4.007014000	3.312596000	-0.603774000
1	2.807952000	2.755564000	-1.770532000
6	2.112477000	3.864828000	1.460086000
1	3.140614000	3.969972000	1.827306000
1	1.766877000	4.867159000	1.190376000
1	1.502149000	3.517647000	2.298118000
6	1.907769000	-3.468634000	-0.618954000
1	1.785103000	-3.647954000	-1.699542000
6	0.677058000	-4.014203000	0.084452000
1	0.782243000	-3.940767000	1.170168000
1	-0.237426000	-3.481302000	-0.185463000
1	0.534930000	-5.074157000	-0.156788000
6	3.147158000	-4.211167000	-0.136787000
1	2.994228000	-5.294493000	-0.209642000
1	4.049882000	-3.980330000	-0.708035000
1	3.353059000	-3.994078000	0.917048000
6	-3.493473000	0.643821000	-0.481733000
1	-2.911144000	1.329841000	0.146852000
6	-4.715386000	0.229906000	0.325533000
1	-5.299433000	1.113508000	0.609733000
1	-5.388012000	-0.437053000	-0.220144000
1	-4.429148000	-0.277275000	1.251495000
6	-3.834195000	1.398664000	-1.760951000
1	-4.403320000	2.308086000	-1.538166000
1	-2.927047000	1.706796000	-2.296537000
1	-4.440603000	0.806193000	-2.454357000
7	0.271533000	-0.107432000	-3.330959000
1	0.464430000	-1.090368000	-3.527223000
1	-0.630183000	0.089119000	-3.759557000
7	1.226136000	0.749897000	-3.996329000
1	1.973321000	0.899606000	-3.319781000
1	1.640838000	0.255394000	-4.785597000

[1b''_{psi}]-NH₂-NH₂ (TE = -3773.066706)

6	1.156692000	-1.367631000	2.035019000
6	1.029996000	-1.936915000	3.308434000
1	0.243020000	-1.582032000	3.975789000
6	1.861211000	-2.968289000	3.734715000
1	1.735463000	-3.403415000	4.724831000
6	2.848623000	-3.448532000	2.880994000
1	3.501300000	-4.259953000	3.197819000
6	2.995761000	-2.898932000	1.610437000
1	3.766265000	-3.302717000	0.959351000
6	2.155207000	-1.869154000	1.173056000
6	0.499360000	1.628467000	2.068896000
6	0.960077000	1.808635000	3.378593000

1	0.995338000	0.952494000	4.054785000
6	1.414174000	3.043652000	3.831760000
1	1.782936000	3.154838000	4.850208000
6	1.405604000	4.134576000	2.968994000
1	1.765452000	5.104745000	3.306828000
6	0.944674000	3.983395000	1.664054000
1	0.959341000	4.848401000	1.006641000
6	0.499434000	2.740947000	1.200110000
6	-1.756119000	-0.414421000	1.960261000
6	-2.202972000	-0.097207000	3.249682000
1	-1.493858000	0.301947000	3.976869000
6	-3.538217000	-0.228718000	3.615301000
1	-3.864163000	0.039931000	4.618867000
6	-4.460045000	-0.685969000	2.678954000
1	-5.511974000	-0.777890000	2.943143000
6	-4.038845000	-1.017791000	1.395648000
1	-4.781743000	-1.361076000	0.682389000
6	-2.695434000	-0.890062000	1.021357000
23	0.070082000	0.020280000	-1.162664000
6	3.784504000	-0.040383000	-0.354280000
1	4.617297000	-0.704416000	-0.087024000
6	-1.757215000	3.293395000	-0.492196000
1	-1.578002000	4.344575000	-0.227384000
6	-2.002667000	-3.129619000	-0.751065000
1	-2.263008000	-3.370624000	-1.794796000
6	-2.957509000	-3.859796000	0.183530000
1	-2.895813000	-4.942760000	0.022605000
1	-2.694967000	-3.673459000	1.229985000
1	-4.001984000	-3.571848000	0.058730000
6	-0.580069000	-3.609328000	-0.498114000
1	-0.240299000	-3.349133000	0.511182000
1	-0.515764000	-4.699946000	-0.592930000
1	0.132162000	-3.162210000	-1.197617000
6	4.086411000	0.644181000	-1.679925000
1	4.178025000	-0.052852000	-2.519898000
1	3.286931000	1.352821000	-1.927638000
1	5.020618000	1.215294000	-1.629741000
6	3.622678000	0.994883000	0.745921000
1	3.376650000	0.549123000	1.714230000
1	4.547566000	1.570235000	0.869749000
1	2.825728000	1.705396000	0.506268000
6	-2.428717000	3.219464000	-1.855945000
1	-3.382314000	3.760270000	-1.856035000
1	-1.819840000	3.635805000	-2.664835000
1	-2.645032000	2.177490000	-2.117266000
6	-2.653866000	2.677010000	0.569041000

1	-2.876721000	1.630611000	0.339857000
1	-2.208142000	2.701220000	1.567773000
1	-3.610354000	3.210277000	0.618725000
14	-0.006101000	-0.046074000	1.309072000
15	-0.063905000	2.465936000	-0.547881000
15	-2.098052000	-1.235222000	-0.704586000
15	2.262687000	-1.139202000	-0.530090000
6	2.991405000	-2.601761000	-1.518220000
1	2.537958000	-3.472936000	-1.023230000
6	4.505408000	-2.789214000	-1.521871000
1	4.766082000	-3.728367000	-2.024170000
1	5.014975000	-1.990743000	-2.070200000
1	4.953333000	-2.825441000	-0.527022000
6	2.482611000	-2.582134000	-2.952762000
1	1.392159000	-2.519388000	-2.990716000
1	2.888402000	-1.730959000	-3.516582000
1	2.783556000	-3.486068000	-3.494889000
6	-3.641546000	-0.861280000	-1.751685000
1	-4.066193000	0.018187000	-1.242045000
6	-3.214437000	-0.440160000	-3.152489000
1	-2.870108000	-1.297922000	-3.739417000
1	-4.055794000	0.001386000	-3.699303000
1	-2.395498000	0.283843000	-3.146850000
6	-4.729068000	-1.923415000	-1.889712000
1	-4.337964000	-2.850029000	-2.322920000
1	-5.227312000	-2.188453000	-0.956771000
1	-5.509648000	-1.567807000	-2.572835000
6	0.953732000	3.760567000	-1.506572000
1	1.913097000	3.760324000	-0.966047000
6	0.429003000	5.192629000	-1.562785000
1	1.171236000	5.846933000	-2.034953000
1	-0.481113000	5.267102000	-2.166103000
1	0.198101000	5.624592000	-0.587577000
6	1.225404000	3.279229000	-2.926926000
1	1.708423000	2.298437000	-2.935645000
1	0.299529000	3.205915000	-3.511744000
1	1.882644000	3.974386000	-3.461840000
7	0.413795000	0.041792000	-3.438903000
1	1.428954000	-0.051306000	-3.493671000
7	-0.231145000	-0.927655000	-4.298715000
1	0.453513000	-1.296293000	-4.957101000
1	-0.485309000	-1.704003000	-3.688884000
1	0.199450000	0.952504000	-3.836240000

[1c''_{PB}]-NH₂-NH₂ (TE = -3508.414634)

6	0.886801000	-1.237011000	1.894568000
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6	0.612429000	-2.031848000	3.023045000
1	-0.348476000	-1.911338000	3.525004000
6	1.513967000	-2.967673000	3.520046000
1	1.254643000	-3.564979000	4.392838000
6	2.746367000	-3.135634000	2.898370000
1	3.464384000	-3.861112000	3.275991000
6	3.044687000	-2.377063000	1.771326000
1	4.000173000	-2.531588000	1.273804000
6	2.131304000	-1.451157000	1.255759000
6	0.072043000	1.365530000	1.971772000
6	0.579210000	1.551066000	3.269783000
1	0.902120000	0.674232000	3.833083000
6	0.681400000	2.805031000	3.863220000
1	1.087346000	2.900817000	4.869186000
6	0.252222000	3.933960000	3.173491000
1	0.312305000	4.919821000	3.630335000
6	-0.245275000	3.789488000	1.882460000
1	-0.568075000	4.676406000	1.340046000
6	-0.314575000	2.534256000	1.268024000
6	-1.717781000	-0.579167000	1.619023000
6	-2.411444000	-0.208426000	2.785050000
1	-1.891415000	0.391116000	3.533383000
6	-3.740516000	-0.549039000	3.008087000
1	-4.240411000	-0.231744000	3.922036000
6	-4.433175000	-1.278176000	2.047790000
1	-5.480387000	-1.535781000	2.194614000
6	-3.774584000	-1.671206000	0.888447000
1	-4.332513000	-2.228081000	0.139546000
6	-2.431452000	-1.341578000	0.667034000
23	0.142157000	0.085493000	-1.060295000
6	3.886516000	0.514974000	0.090955000
1	4.694300000	-0.153735000	0.420821000
6	-2.568095000	2.840825000	-0.619533000
1	-2.620293000	3.904276000	-0.348521000
6	-1.169900000	-3.602367000	-0.781874000
1	-1.551907000	-4.027088000	-1.719602000
6	-1.853026000	-4.304527000	0.382917000
1	-1.619615000	-5.375784000	0.372005000
1	-1.507329000	-3.904686000	1.342499000
1	-2.941077000	-4.204732000	0.371268000
6	0.328738000	-3.853048000	-0.746382000
1	0.789658000	-3.437800000	0.155199000
1	0.538659000	-4.929367000	-0.755256000
1	0.833741000	-3.408728000	-1.607735000
6	4.368797000	1.306099000	-1.118580000
1	4.490284000	0.698838000	-2.020070000

1	3.665912000	2.105788000	-1.369886000
1	5.331230000	1.788406000	-0.912904000
6	3.535064000	1.437774000	1.248250000
1	3.277911000	0.881445000	2.153815000
1	4.378527000	2.095689000	1.488335000
1	2.676387000	2.077198000	1.016084000
6	-3.033060000	2.659155000	-2.059178000
1	-4.061801000	3.011476000	-2.194600000
1	-2.410009000	3.191787000	-2.787027000
1	-3.015698000	1.595152000	-2.329766000
6	-3.458708000	2.064324000	0.332547000
1	-3.468648000	0.996931000	0.092932000
1	-3.137045000	2.158814000	1.372868000
1	-4.492307000	2.423837000	0.268055000
5	-0.187590000	-0.133310000	1.471990000
15	2.446124000	-0.608907000	-0.349936000
15	-0.762719000	2.342902000	-0.500609000
15	-1.571989000	-1.746599000	-0.908850000
6	0.030366000	3.810840000	-1.414591000
1	0.051866000	3.437836000	-2.452385000
6	1.473751000	4.002969000	-0.970949000
1	2.034611000	4.609231000	-1.691730000
1	1.531849000	4.509370000	-0.002667000
1	1.992739000	3.048541000	-0.852648000
6	-0.696156000	5.151423000	-1.443606000
1	-0.119733000	5.872394000	-2.035617000
1	-1.690553000	5.097419000	-1.892003000
1	-0.809906000	5.589364000	-0.447901000
6	3.304708000	-1.962028000	-1.373075000
1	2.883521000	-2.881713000	-0.945902000
6	4.823809000	-2.074520000	-1.296026000
1	5.158715000	-2.956555000	-1.854454000
1	5.331503000	-1.213671000	-1.740275000
1	5.205669000	-2.183101000	-0.278242000
6	2.860487000	-1.874543000	-2.829303000
1	3.263309000	-2.710341000	-3.413671000
1	1.768048000	-1.903893000	-2.913957000
1	3.189023000	-0.944508000	-3.304461000
6	-2.984224000	-1.744818000	-2.169201000
1	-3.648613000	-0.954166000	-1.788873000
6	-2.453139000	-1.303408000	-3.528134000
1	-1.674240000	-1.985217000	-3.895568000
1	-3.248532000	-1.288741000	-4.282313000
1	-2.020743000	-0.299923000	-3.481754000
6	-3.794481000	-3.027156000	-2.338240000
1	-3.241849000	-3.779765000	-2.909829000

1	-4.088572000	-3.496370000	-1.397210000
1	-4.712658000	-2.824956000	-2.901488000
7	0.454181000	0.588687000	-3.260046000
1	-0.353584000	1.150283000	-3.532751000
1	0.438398000	-0.230045000	-3.863705000
7	1.686569000	1.283844000	-3.553724000
1	1.522745000	1.979935000	-4.280603000
1	1.919800000	1.794723000	-2.703985000

[1d''_{sc}]-NH₂-NH₂ (TE = -3336.805302)

6	-0.055848000	-1.258575000	-1.485813000
6	0.575351000	-1.551889000	-2.707972000
1	1.150859000	-0.766097000	-3.194421000
6	0.487346000	-2.798200000	-3.318585000
1	0.997205000	-2.972303000	-4.264614000
6	-0.254004000	-3.816011000	-2.728131000
1	-0.329071000	-4.794996000	-3.196094000
6	-0.868427000	-3.576170000	-1.504010000
1	-1.404741000	-4.374991000	-0.994490000
6	-0.761344000	-2.328133000	-0.889183000
6	-1.189957000	0.952292000	-1.298586000
6	-1.772621000	0.812370000	-2.570659000
1	-1.376596000	0.049799000	-3.239460000
6	-2.824287000	1.608995000	-3.008890000
1	-3.238638000	1.456533000	-4.004057000
6	-3.340199000	2.601640000	-2.182646000
1	-4.162691000	3.231663000	-2.513874000
6	-2.814221000	2.751585000	-0.904458000
1	-3.241753000	3.481314000	-0.218825000
6	-1.771108000	1.935122000	-0.463935000
6	1.297162000	0.817533000	-1.191083000
6	1.423160000	1.656492000	-2.312698000
1	0.548820000	1.811007000	-2.942424000
6	2.610070000	2.297945000	-2.646617000
1	2.648489000	2.939448000	-3.525483000
6	3.741093000	2.124146000	-1.857779000
1	4.673452000	2.630177000	-2.098073000
6	3.653283000	1.320826000	-0.726694000
1	4.507670000	1.223541000	-0.060861000
6	2.458672000	0.675488000	-0.394403000
16	2.362072000	-0.099846000	1.227352000
16	-1.326253000	-2.174388000	0.806830000
16	-1.343340000	1.997353000	1.279771000
23	-0.104818000	-0.116482000	1.362006000
6	-3.211794000	-2.150996000	0.676282000
1	-3.474883000	-3.171574000	0.371355000

6	-0.397894000	3.624420000	1.457021000
1	-1.163130000	4.398564000	1.318593000
6	3.257086000	-1.756602000	1.063809000
1	3.273185000	-2.051511000	2.121287000
6	4.671892000	-1.565365000	0.563024000
1	5.221387000	-2.512312000	0.612907000
1	4.683752000	-1.241849000	-0.482589000
1	5.225216000	-0.828144000	1.151466000
6	2.482399000	-2.771687000	0.259499000
1	2.382769000	-2.466347000	-0.786765000
1	2.997380000	-3.739763000	0.272980000
1	1.475587000	-2.921410000	0.658387000
6	-3.709552000	-1.875174000	2.079149000
1	-3.328132000	-2.599158000	2.807107000
1	-3.401972000	-0.871948000	2.401760000
1	-4.803012000	-1.910907000	2.116898000
6	-3.715966000	-1.146462000	-0.328825000
1	-3.303371000	-1.316671000	-1.326650000
1	-4.808328000	-1.202819000	-0.405350000
1	-3.454660000	-0.126098000	-0.031856000
6	0.117964000	3.643308000	2.880102000
1	0.628145000	4.587971000	3.094360000
1	-0.682820000	3.522907000	3.616784000
1	0.845218000	2.835067000	3.032071000
6	0.704071000	3.775563000	0.438913000
1	1.468267000	3.002722000	0.568093000
1	0.333122000	3.707145000	-0.587005000
1	1.193150000	4.750382000	0.552434000
6	-0.003666000	0.117851000	-0.859745000
7	-0.153796000	-0.518903000	3.596782000
1	-1.091796000	-0.370120000	3.971243000
7	0.334391000	-1.841134000	3.915627000
1	-0.092132000	-2.166774000	4.782993000
1	-0.012324000	-2.448366000	3.174395000
1	0.451398000	0.133463000	4.089027000

[1e''_{ssi}]-NH₂-NH₂ (TE = -3588.208615)

6	0.848715000	-1.345212000	1.790791000
6	0.738721000	-1.684953000	3.146682000
1	0.096969000	-1.086428000	3.794897000
6	1.415926000	-2.771206000	3.693650000
1	1.303470000	-3.010931000	4.749619000
6	2.232552000	-3.556228000	2.884819000
1	2.761220000	-4.411336000	3.301111000
6	2.352756000	-3.259316000	1.530881000
1	2.965564000	-3.886124000	0.884695000

6	1.666540000	-2.169088000	0.995711000
6	0.827410000	1.714490000	1.420106000
6	1.181549000	2.084695000	2.725609000
1	0.942331000	1.413952000	3.552094000
6	1.843532000	3.277173000	3.003411000
1	2.108908000	3.529647000	4.028604000
6	2.175602000	4.142716000	1.965222000
1	2.701029000	5.073192000	2.170404000
6	1.855379000	3.801845000	0.655006000
1	2.137687000	4.458041000	-0.166984000
6	1.192015000	2.602977000	0.392948000
6	-1.862580000	0.214279000	1.413868000
6	-2.341794000	0.742960000	2.620643000
1	-1.630198000	1.010737000	3.402803000
6	-3.697377000	0.968971000	2.845728000
1	-4.031355000	1.393888000	3.790797000
6	-4.622314000	0.670364000	1.851131000
1	-5.681881000	0.861872000	2.007838000
6	-4.185274000	0.143419000	0.639061000
1	-4.898261000	-0.067722000	-0.155370000
6	-2.824762000	-0.087521000	0.429556000
16	-2.329449000	-0.709449000	-1.211076000
16	1.819751000	-1.888207000	-0.796169000
16	0.862893000	2.200237000	-1.351153000
23	0.113241000	-0.191368000	-1.525167000
6	3.592885000	-1.255091000	-0.854276000
1	4.195709000	-2.097395000	-0.491981000
6	-0.528511000	3.425522000	-1.677950000
1	-0.068188000	4.409077000	-1.521552000
6	-2.645450000	-2.558170000	-0.985203000
1	-2.304069000	-2.928712000	-1.962140000
6	-4.119075000	-2.856072000	-0.807704000
1	-4.292960000	-3.937833000	-0.837815000
1	-4.481424000	-2.501447000	0.162035000
1	-4.732810000	-2.395421000	-1.586779000
6	-1.791639000	-3.145034000	0.114305000
1	-2.032984000	-2.703831000	1.087815000
1	-1.958594000	-4.225314000	0.194394000
1	-0.727513000	-2.979361000	-0.069114000
6	3.903422000	-0.971242000	-2.308123000
1	3.757217000	-1.847469000	-2.945266000
1	3.256076000	-0.170806000	-2.688834000
1	4.940546000	-0.637807000	-2.418384000
6	3.790191000	-0.043477000	0.027419000
1	3.519345000	-0.233309000	1.069991000
1	4.840366000	0.270211000	0.008274000

1	3.186733000	0.798918000	-0.324814000
6	-0.926629000	3.256289000	-3.128557000
1	-1.696389000	3.984122000	-3.404505000
1	-0.081386000	3.386298000	-3.811533000
1	-1.348953000	2.255889000	-3.291372000
6	-1.695078000	3.227705000	-0.737164000
1	-2.156697000	2.246918000	-0.890041000
1	-1.402463000	3.295759000	0.314514000
1	-2.461951000	3.989404000	-0.919603000
14	-0.028332000	0.087898000	0.881071000
7	0.105371000	-0.515428000	-3.781297000
1	-0.845715000	-0.365694000	-4.119613000
1	0.684475000	0.160844000	-4.273536000
7	0.593167000	-1.821238000	-4.168359000
1	0.335858000	-2.446411000	-3.405276000
1	0.091235000	-2.143916000	-4.994980000

[1f'_{SB}]-NH₂-NH₂ (TE = -3323.566068)

6	-0.283363000	1.458274000	1.507937000
6	0.175959000	1.901299000	2.761885000
1	0.798650000	1.228722000	3.353889000
6	-0.121336000	3.160562000	3.271907000
1	0.260612000	3.456573000	4.247522000
6	-0.899394000	4.044244000	2.530111000
1	-1.133146000	5.035144000	2.913606000
6	-1.350177000	3.658230000	1.273223000
1	-1.921656000	4.352230000	0.658767000
6	-1.044849000	2.389510000	0.776941000
6	-1.087918000	-1.111340000	1.453421000
6	-1.602773000	-1.085403000	2.763042000
1	-1.258055000	-0.303150000	3.440599000
6	-2.539256000	-2.003131000	3.226578000
1	-2.906773000	-1.935215000	4.249130000
6	-3.013011000	-3.000435000	2.379981000
1	-3.752382000	-3.719354000	2.726416000
6	-2.552340000	-3.048651000	1.069846000
1	-2.942496000	-3.793637000	0.378206000
6	-1.610745000	-2.120001000	0.621524000
6	1.547604000	-0.539016000	1.276022000
6	1.857685000	-1.194479000	2.482337000
1	1.057718000	-1.349884000	3.207283000
6	3.127579000	-1.677263000	2.780152000
1	3.308613000	-2.183630000	3.726805000
6	4.157535000	-1.532374000	1.857403000
1	5.150657000	-1.925102000	2.064799000
6	3.895828000	-0.901497000	0.646898000

1	4.676601000	-0.818434000	-0.106027000
6	2.619655000	-0.402699000	0.369308000
16	2.342059000	0.252435000	-1.291566000
16	-1.505527000	2.032200000	-0.927184000
16	-1.196172000	-2.152787000	-1.130777000
23	-0.116323000	0.043892000	-1.414745000
6	-3.367877000	1.782760000	-0.802163000
1	-3.753382000	2.777141000	-0.543504000
6	-0.078995000	-3.669314000	-1.237450000
1	-0.749431000	-4.510131000	-1.019427000
6	3.060892000	1.998789000	-1.185722000
1	2.868191000	2.343594000	-2.211388000
6	4.552221000	1.960274000	-0.929971000
1	4.980127000	2.963601000	-1.036378000
1	4.770410000	1.626259000	0.088935000
1	5.077036000	1.297108000	-1.623303000
6	2.319653000	2.866847000	-0.198272000
1	2.379552000	2.457731000	0.815984000
1	2.752824000	3.873607000	-0.173069000
1	1.261895000	2.961420000	-0.452892000
6	-3.832637000	1.382158000	-2.186269000
1	-3.547704000	2.109852000	-2.951053000
1	-3.400029000	0.414335000	-2.470115000
1	-4.922078000	1.274864000	-2.207232000
6	-3.749057000	0.774438000	0.254634000
1	-3.341864000	1.024832000	1.238129000
1	-4.840139000	0.722281000	0.348185000
1	-3.390483000	-0.225199000	-0.007398000
6	0.402498000	-3.739446000	-2.670872000
1	1.007399000	-4.637530000	-2.831788000
1	-0.423426000	-3.760545000	-3.389070000
1	1.036043000	-2.873168000	-2.902613000
6	1.058261000	-3.622631000	-0.246537000
1	1.734965000	-2.791038000	-0.465188000
1	0.709281000	-3.503029000	0.782677000
1	1.641583000	-4.549552000	-0.296148000
5	0.039409000	-0.040964000	1.045473000
7	-0.187286000	0.111329000	-3.668252000
1	0.701679000	-0.244667000	-4.021163000
1	-0.904259000	-0.504780000	-4.044912000
7	-0.466286000	1.427906000	-4.197106000
1	-0.065223000	2.083819000	-3.527873000
1	0.036469000	1.557804000	-5.074048000

{[HIPTN₃N]-V-NH₂-NH₂} (TE = -2205.341284)

23	0.184440000	0.173246000	0.450626000
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7	2.126640000	0.597070000	0.449301000
7	-0.555853000	-1.406238000	1.362625000
7	-1.099110000	1.676442000	0.367860000
6	2.370365000	1.763950000	1.286942000
1	3.446040000	1.943999000	1.423998000
1	1.969224000	2.693106000	0.847223000
6	1.753274000	1.501159000	2.654063000
1	2.385926000	0.788348000	3.190130000
1	1.705885000	2.414319000	3.263086000
6	-0.917765000	2.654606000	1.437339000
1	-0.084399000	3.353384000	1.247875000
1	-1.811743000	3.283535000	1.554823000
6	-0.681316000	1.884317000	2.720295000
1	-1.594122000	1.333640000	2.965979000
1	-0.450921000	2.543531000	3.570767000
6	-0.855120000	-1.195499000	2.769753000
1	-1.854689000	-0.747005000	2.916343000
1	-0.876517000	-2.147209000	3.323838000
6	0.217744000	-0.308525000	3.364964000
1	-0.005523000	-0.037948000	4.408739000
1	1.167682000	-0.850668000	3.355295000
7	0.401880000	0.895807000	2.523092000
6	-1.281708000	-2.399498000	0.719068000
6	-0.824876000	-2.894705000	-0.521332000
6	-2.476228000	-2.947153000	1.230889000
6	-1.547734000	-3.841152000	-1.230248000
1	0.125072000	-2.538076000	-0.916124000
6	-3.187855000	-3.904146000	0.515004000
1	-2.863541000	-2.607806000	2.187822000
6	-2.742230000	-4.354323000	-0.723422000
1	-1.159306000	-4.198325000	-2.182775000
1	-4.111527000	-4.299024000	0.935373000
1	-3.304002000	-5.102984000	-1.276382000
6	3.165399000	0.154300000	-0.348311000
6	3.233612000	-1.216010000	-0.681695000
6	4.182668000	0.991679000	-0.854822000
6	4.238720000	-1.712144000	-1.497562000
1	2.472367000	-1.883336000	-0.276939000
6	5.194515000	0.481816000	-1.659882000
1	4.161114000	2.056934000	-0.635304000
6	5.232822000	-0.869452000	-1.994462000
1	4.255707000	-2.774521000	-1.733995000
1	5.959439000	1.156706000	-2.040975000
1	6.027442000	-1.261593000	-2.624165000
6	-2.011290000	2.015538000	-0.623682000
6	-2.807329000	1.008563000	-1.207529000

6	-2.202769000	3.335456000	-1.078633000
6	-3.707412000	1.297245000	-2.223586000
1	-2.737142000	-0.003930000	-0.806173000
6	-3.115450000	3.618798000	-2.087622000
1	-1.611741000	4.140208000	-0.645765000
6	-3.867556000	2.605612000	-2.676922000
1	-4.312372000	0.496030000	-2.644184000
1	-3.234900000	4.647647000	-2.423147000
1	-4.581174000	2.833982000	-3.464484000
7	0.853591000	-0.806725000	-2.613930000
7	-0.106866000	-0.148899000	-1.763458000
1	0.699110000	-0.507089000	-3.575140000
1	1.772277000	-0.465404000	-2.344774000
1	-0.962223000	-0.696051000	-1.849511000
1	-0.350413000	0.776165000	-2.125926000

Cartesian coordinates of $[5c''_{PB}]-[14c''_{PB}]$, along with their total energies (in hartree) including zero point vibrational correction at M06-L-D3(heptane)/6-311+G* level of theory.

$[5c''_{PB}]_{alt}$ (TE = -3507.096581)

6	-1.495518000	0.475696000	1.977352000
6	-1.570112000	1.059471000	3.255232000
1	-0.652409000	1.199750000	3.825422000
6	-2.773288000	1.466605000	3.818915000
1	-2.783570000	1.913528000	4.810755000
6	-3.961446000	1.310083000	3.112127000
1	-4.907903000	1.628993000	3.541828000
6	-3.923885000	0.753822000	1.840720000
1	-4.851795000	0.652008000	1.280891000
6	-2.711567000	0.343422000	1.274646000
6	0.319297000	-1.558876000	1.773746000
6	-0.243656000	-2.216016000	2.881596000
1	-1.085834000	-1.753901000	3.396206000
6	0.268836000	-3.414316000	3.364859000
1	-0.186207000	-3.889522000	4.231381000
6	1.381521000	-3.992590000	2.760233000
1	1.804749000	-4.914678000	3.151097000
6	1.940689000	-3.389468000	1.638556000
1	2.802358000	-3.852328000	1.161378000
6	1.402707000	-2.204738000	1.128394000
6	1.158812000	0.952711000	1.756183000
6	1.844404000	0.808513000	2.977306000
1	1.571595000	-0.012980000	3.640739000
6	2.864926000	1.668158000	3.362235000
1	3.367580000	1.521762000	4.316013000
6	3.254267000	2.705608000	2.520236000

1	4.058012000	3.379354000	2.806864000
6	2.616600000	2.861994000	1.297867000
1	2.941736000	3.657688000	0.632093000
6	1.578635000	2.001893000	0.914809000
23	-0.176911000	-0.183813000	-1.124571000
6	-3.474027000	-1.933405000	-0.419655000
1	-4.513600000	-1.727578000	-0.129138000
6	3.764532000	-1.363061000	-0.451803000
1	4.111948000	-2.382545000	-0.226959000
6	-0.233714000	3.665763000	-0.721560000
1	-0.370041000	3.914333000	-1.786312000
6	0.359443000	4.861673000	0.013652000
1	-0.333302000	5.707021000	-0.052664000
1	0.490137000	4.639273000	1.076599000
1	1.317342000	5.202043000	-0.375588000
6	-1.591011000	3.340472000	-0.115738000
1	-1.504980000	3.089142000	0.946579000
1	-2.265543000	4.199096000	-0.194370000
1	-2.066377000	2.496072000	-0.611058000
6	-3.467314000	-2.572339000	-1.804166000
1	-3.873792000	-1.920132000	-2.581798000
1	-2.461136000	-2.851700000	-2.125233000
1	-4.070348000	-3.485870000	-1.801996000
6	-2.861253000	-2.841243000	0.635308000
1	-2.945580000	-2.418140000	1.639587000
1	-3.368720000	-3.811253000	0.639462000
1	-1.799311000	-3.031039000	0.454844000
6	4.301697000	-0.954174000	-1.816867000
1	5.395051000	-0.996723000	-1.824943000
1	3.947073000	-1.594655000	-2.630005000
1	4.021347000	0.074386000	-2.063881000
6	4.246860000	-0.439863000	0.654814000
1	3.925472000	0.593656000	0.492856000
1	3.879116000	-0.744315000	1.637967000
1	5.340775000	-0.438985000	0.694753000
5	-0.066032000	-0.042426000	1.489990000
7	-0.685275000	-1.430542000	-3.833526000
7	-0.409387000	-0.376433000	-3.164629000
1	-0.828939000	-1.195731000	-4.828899000
15	0.819857000	2.116810000	-0.737097000
15	-2.650168000	-0.260300000	-0.442473000
15	1.915372000	-1.518915000	-0.481537000
6	2.262878000	2.449222000	-1.905168000
1	3.098966000	1.941342000	-1.402037000
6	2.656955000	3.902208000	-2.141338000
1	3.470853000	3.942939000	-2.872411000

1	1.833168000	4.492650000	-2.554312000
1	3.015844000	4.409717000	-1.245690000
6	2.028757000	1.764599000	-3.247822000
1	1.900299000	0.683143000	-3.148807000
1	1.145673000	2.170119000	-3.759032000
1	2.879282000	1.930518000	-3.916696000
6	1.607042000	-2.904722000	-1.706137000
1	1.656684000	-2.395079000	-2.680593000
6	0.178317000	-3.388698000	-1.505141000
1	-0.553382000	-2.567427000	-1.444762000
1	-0.156721000	-4.009235000	-2.340738000
1	0.077330000	-3.963623000	-0.579129000
6	2.578537000	-4.074493000	-1.723938000
1	2.314811000	-4.761686000	-2.534850000
1	3.615168000	-3.771859000	-1.889793000
1	2.539672000	-4.654377000	-0.798232000
6	-3.873319000	0.834351000	-1.378701000
1	-3.901711000	1.745015000	-0.767560000
6	-5.304471000	0.317428000	-1.476329000
1	-5.933709000	1.084131000	-1.939636000
1	-5.392021000	-0.577987000	-2.096247000
1	-5.749318000	0.088181000	-0.505546000
6	-3.332881000	1.203087000	-2.755613000
1	-2.347755000	1.680818000	-2.694706000
1	-3.234402000	0.324907000	-3.403146000
1	-4.006802000	1.902796000	-3.260038000
1	-0.380477000	0.491041000	-3.724497000

$[5c''_{PB}]_{dis}$ (TE = -3507.115363)

6	-1.367274000	0.849906000	1.929672000
6	-1.501373000	1.723303000	3.025512000
1	-0.604175000	2.111885000	3.506713000
6	-2.743273000	2.095479000	3.525507000
1	-2.806654000	2.764184000	4.380844000
6	-3.899695000	1.619676000	2.919347000
1	-4.878748000	1.906502000	3.295462000
6	-3.796587000	0.790801000	1.808647000
1	-4.708938000	0.454984000	1.321619000
6	-2.550837000	0.401364000	1.306515000
6	0.552212000	-1.073747000	2.082102000
6	0.150917000	-1.456855000	3.373905000
1	-0.573726000	-0.841805000	3.907152000
6	0.661578000	-2.589213000	3.998723000
1	0.330310000	-2.852049000	5.000749000
6	1.591953000	-3.382204000	3.338575000
1	2.000650000	-4.268542000	3.817464000

6	1.986183000	-3.043984000	2.048330000
1	2.698601000	-3.682033000	1.531617000
6	1.473425000	-1.911378000	1.410653000
6	1.224118000	1.487891000	1.593386000
6	2.022740000	1.636128000	2.739311000
1	1.910306000	0.928800000	3.561675000
6	2.965845000	2.651323000	2.846472000
1	3.569810000	2.738549000	3.746855000
6	3.154642000	3.537583000	1.791110000
1	3.906174000	4.320456000	1.857091000
6	2.386897000	3.405490000	0.640045000
1	2.558814000	4.083629000	-0.193146000
6	1.416656000	2.402665000	0.539770000
23	-0.202745000	-0.375525000	-1.379169000
6	-3.097557000	-2.230838000	0.165307000
1	-4.125496000	-2.046874000	0.507006000
6	3.685215000	-1.147972000	-0.363117000
1	4.155874000	-2.073247000	-0.001641000
6	-0.628071000	3.557497000	-1.282611000
1	-0.838300000	3.518948000	-2.363316000
6	-0.053419000	4.921262000	-0.923151000
1	-0.788852000	5.699280000	-1.152962000
1	0.156927000	4.988676000	0.148382000
1	0.859941000	5.176468000	-1.459843000
6	-1.931031000	3.339080000	-0.526581000
1	-1.774174000	3.356356000	0.557149000
1	-2.650511000	4.128981000	-0.764184000
1	-2.389914000	2.381991000	-0.772774000
6	-3.141026000	-3.136693000	-1.059508000
1	-3.585337000	-2.661426000	-1.937990000
1	-2.138948000	-3.457976000	-1.348557000
1	-3.722652000	-4.039065000	-0.845204000
6	-2.328126000	-2.868944000	1.311771000
1	-2.362226000	-2.260698000	2.219660000
1	-2.753309000	-3.848594000	1.553692000
1	-1.273005000	-3.023999000	1.064997000
6	4.165409000	-0.873163000	-1.783717000
1	5.259205000	-0.869788000	-1.823045000
1	3.818265000	-1.607019000	-2.516896000
1	3.835166000	0.110671000	-2.129237000
6	4.082815000	-0.030510000	0.583889000
1	3.660138000	0.933931000	0.287013000
1	3.767457000	-0.226586000	1.611434000
1	5.171999000	0.082315000	0.588944000
5	0.107047000	0.373722000	1.647167000
7	-0.858926000	-2.091291000	-3.774926000

7	-0.719413000	-1.403532000	-2.648037000
1	-1.626453000	-1.788925000	-4.372002000
15	0.501855000	2.094308000	-1.008186000
15	-2.436046000	-0.540808000	-0.263458000
15	1.861538000	-1.555012000	-0.341240000
6	1.816273000	2.151290000	-2.353888000
1	2.729776000	1.854540000	-1.820044000
6	2.075881000	3.478680000	-3.048630000
1	2.799643000	3.335518000	-3.857990000
1	1.171738000	3.895186000	-3.503252000
1	2.494835000	4.234365000	-2.381895000
6	1.481723000	1.065406000	-3.374307000
1	1.469320000	0.052363000	-2.934085000
1	0.512996000	1.231198000	-3.858271000
1	2.234888000	1.016205000	-4.168176000
6	1.862176000	-3.204635000	-1.264833000
1	1.739009000	-2.868495000	-2.305737000
6	0.633496000	-4.023044000	-0.899223000
1	-0.274038000	-3.419504000	-0.937228000
1	0.510645000	-4.862719000	-1.591655000
1	0.709130000	-4.443761000	0.108199000
6	3.117479000	-4.068559000	-1.202436000
1	2.972977000	-4.950293000	-1.835682000
1	4.017518000	-3.568315000	-1.563221000
1	3.327015000	-4.444614000	-0.197657000
6	-3.839188000	0.224954000	-1.292032000
1	-3.945303000	1.220358000	-0.843699000
6	-5.205965000	-0.448576000	-1.199937000
1	-5.942651000	0.161398000	-1.732946000
1	-5.223948000	-1.437048000	-1.664652000
1	-5.574565000	-0.563936000	-0.178653000
6	-3.444179000	0.413172000	-2.751392000
1	-2.503612000	0.961925000	-2.866679000
1	-3.323619000	-0.547017000	-3.263293000
1	-4.223292000	0.968032000	-3.284588000
1	-0.854114000	-3.104205000	-3.660295000

[6c''_{PB}]_{atl} (TE = -3507.237814)

6	-0.284574000	1.549541000	1.838538000
6	0.315302000	2.175650000	2.946648000
1	1.157103000	1.682387000	3.433432000
6	-0.127742000	3.395118000	3.447860000
1	0.370645000	3.846029000	4.304552000
6	-1.213990000	4.029553000	2.856294000
1	-1.581452000	4.977924000	3.243101000
6	-1.816008000	3.447924000	1.745422000

1	-2.649332000	3.964068000	1.276643000
6	-1.353977000	2.238103000	1.217860000
6	-0.758469000	-1.109346000	1.956651000
6	-1.334603000	-1.003368000	3.234724000
1	-1.213193000	-0.071100000	3.788288000
6	-2.055104000	-2.040672000	3.817139000
1	-2.489727000	-1.912455000	4.807266000
6	-2.218133000	-3.242577000	3.135247000
1	-2.776648000	-4.062033000	3.582950000
6	-1.668456000	-3.381128000	1.865813000
1	-1.808136000	-4.316536000	1.326678000
6	-0.962484000	-2.330905000	1.269726000
6	1.750468000	-0.218088000	1.660655000
6	2.151284000	-0.802946000	2.875794000
1	1.385044000	-1.067500000	3.605515000
6	3.479769000	-1.080922000	3.172013000
1	3.742920000	-1.542469000	4.122414000
6	4.468514000	-0.784138000	2.239917000
1	5.512415000	-1.011915000	2.446141000
6	4.108518000	-0.200681000	1.031512000
1	4.889003000	0.008939000	0.304541000
6	2.770806000	0.090603000	0.734702000
23	-0.134798000	-0.008097000	-1.171893000
6	-3.764303000	1.181336000	-0.064770000
1	-4.233202000	2.112973000	0.285661000
6	1.020841000	-3.651599000	-0.472109000
1	0.545440000	-4.615769000	-0.245557000
6	2.674206000	2.598132000	-0.861763000
1	3.236370000	2.773570000	-1.788478000
6	3.539176000	3.008964000	0.320816000
1	3.780378000	4.076769000	0.264425000
1	3.016308000	2.841380000	1.268697000
1	4.483040000	2.460936000	0.376721000
6	1.412562000	3.444196000	-0.923182000
1	0.792879000	3.308836000	-0.030725000
1	1.663541000	4.509462000	-0.989413000
1	0.797459000	3.191029000	-1.791861000
6	-4.450172000	0.734472000	-1.352467000
1	-4.580725000	1.552965000	-2.064407000
1	-3.880707000	-0.037782000	-1.876725000
1	-5.445701000	0.328081000	-1.141130000
6	-3.886962000	0.147815000	1.044811000
1	-3.454256000	0.505293000	1.983514000
1	-4.940069000	-0.091184000	1.231806000
1	-3.377436000	-0.787581000	0.796484000
6	1.627464000	-3.702538000	-1.868747000

1	2.365208000	-4.508487000	-1.950611000
1	0.885141000	-3.855425000	-2.659276000
1	2.146144000	-2.762526000	-2.091533000
6	2.090195000	-3.401685000	0.575566000
1	2.648077000	-2.483247000	0.374595000
1	1.675897000	-3.316836000	1.583667000
1	2.812238000	-4.226336000	0.580408000
5	0.194529000	0.078711000	1.452527000
7	-1.658543000	-0.545356000	-3.658691000
7	-0.496100000	-0.223271000	-3.160603000
1	-1.589746000	-0.587774000	-4.689035000
15	2.264514000	0.747370000	-0.904665000
15	-1.967969000	1.592760000	-0.392192000
15	-0.367257000	-2.396823000	-0.453888000
6	3.591829000	0.069006000	-2.066547000
1	3.825382000	-0.913110000	-1.628303000
6	4.887152000	0.864620000	-2.203763000
1	5.648121000	0.262621000	-2.712950000
1	4.744686000	1.761581000	-2.814827000
1	5.315310000	1.191387000	-1.253990000
6	2.989604000	-0.157698000	-3.448734000
1	2.161814000	-0.871828000	-3.419455000
1	2.607924000	0.779265000	-3.876301000
1	3.738486000	-0.545865000	-4.148427000
6	-1.653846000	-3.294996000	-1.497520000
1	-1.388889000	-2.954093000	-2.509927000
6	-3.046769000	-2.759484000	-1.210755000
1	-3.063756000	-1.670700000	-1.249682000
1	-3.760907000	-3.124844000	-1.956654000
1	-3.410567000	-3.067423000	-0.224567000
6	-1.647523000	-4.819536000	-1.497612000
1	-2.436494000	-5.186615000	-2.164058000
1	-0.709537000	-5.252251000	-1.852809000
1	-1.852619000	-5.245205000	-0.510459000
6	-2.104624000	3.163151000	-1.447369000
1	-1.271175000	3.772290000	-1.073577000
6	-3.377260000	3.997046000	-1.322067000
1	-3.251732000	4.936970000	-1.871641000
1	-4.245863000	3.497065000	-1.758073000
1	-3.640910000	4.264806000	-0.297886000
6	-1.845267000	2.853047000	-2.917271000
1	-0.883311000	2.355998000	-3.069345000
1	-2.609967000	2.188867000	-3.334002000
1	-1.849237000	3.774181000	-3.511513000
1	0.240182000	-0.095973000	-3.868540000

[6c''_{pg}]_{dis} (TE = -3507.269012)

6	-1.508997000	0.523736000	1.928466000
6	-1.681433000	1.240955000	3.126699000
1	-0.797232000	1.550577000	3.684553000
6	-2.935641000	1.579237000	3.623071000
1	-3.020110000	2.139507000	4.552829000
6	-4.080033000	1.206900000	2.925444000
1	-5.067538000	1.469308000	3.299546000
6	-3.947025000	0.508653000	1.731054000
1	-4.843966000	0.241065000	1.176033000
6	-2.685171000	0.174091000	1.227717000
6	0.536270000	-1.285955000	1.983676000
6	0.134161000	-1.782234000	3.235810000
1	-0.652869000	-1.257853000	3.779357000
6	0.706387000	-2.913719000	3.807424000
1	0.359603000	-3.268721000	4.776728000
6	1.729411000	-3.584751000	3.145090000
1	2.192489000	-4.464431000	3.587402000
6	2.145037000	-3.126569000	1.898938000
1	2.934373000	-3.662547000	1.375369000
6	1.548673000	-2.009508000	1.306105000
6	1.055513000	1.304134000	1.680124000
6	1.772016000	1.346702000	2.890938000
1	1.613488000	0.551526000	3.620622000
6	2.691285000	2.346404000	3.181786000
1	3.228965000	2.334628000	4.128574000
6	2.935125000	3.351930000	2.251538000
1	3.663313000	4.133788000	2.457374000
6	2.245887000	3.340814000	1.046024000
1	2.454999000	4.119970000	0.318614000
6	1.313396000	2.337183000	0.752525000
23	-0.130076000	-0.264436000	-1.189543000
6	-3.045700000	-2.362810000	-0.175072000
1	-4.102676000	-2.302813000	0.121349000
6	3.701836000	-0.995828000	-0.446660000
1	4.261998000	-1.899052000	-0.166116000
6	-0.734091000	3.629232000	-0.954315000
1	-0.778006000	3.876852000	-2.026547000
6	-0.337260000	4.871817000	-0.168687000
1	-1.087786000	5.658317000	-0.309294000
1	-0.291481000	4.657318000	0.903789000
1	0.626970000	5.290642000	-0.458846000
6	-2.115676000	3.170255000	-0.519522000
1	-2.130622000	2.872082000	0.533954000
1	-2.849804000	3.974821000	-0.642475000
1	-2.452140000	2.315972000	-1.106119000

6	-2.938712000	-3.133865000	-1.484638000
1	-3.545763000	-2.703452000	-2.285768000
1	-1.906504000	-3.146997000	-1.843044000
1	-3.257767000	-4.174044000	-1.354585000
6	-2.277025000	-3.045858000	0.945814000
1	-2.394371000	-2.524275000	1.899899000
1	-2.631252000	-4.074020000	1.081971000
1	-1.203524000	-3.092820000	0.740218000
6	4.087774000	-0.585614000	-1.862797000
1	5.159900000	-0.369545000	-1.929842000
1	3.858872000	-1.347673000	-2.613706000
1	3.553257000	0.322106000	-2.162022000
6	4.042248000	0.093129000	0.553743000
1	3.540308000	1.035101000	0.316443000
1	3.758527000	-0.176680000	1.574329000
1	5.120778000	0.288701000	0.547965000
5	-0.018822000	0.129981000	1.495188000
7	-0.135753000	-1.676694000	-3.906298000
7	-0.209633000	-1.006896000	-2.725904000
1	-0.402094000	-1.081158000	-4.692023000
15	0.495349000	2.202789000	-0.879579000
15	-2.474237000	-0.596994000	-0.417178000
15	1.902359000	-1.505920000	-0.419805000
6	1.803081000	2.704161000	-2.145060000
1	2.725596000	2.269215000	-1.731851000
6	2.044117000	4.188374000	-2.397092000
1	2.800060000	4.309076000	-3.181355000
1	1.142567000	4.697304000	-2.753089000
1	2.408511000	4.733971000	-1.525492000
6	1.493642000	2.013435000	-3.471555000
1	1.407251000	0.928749000	-3.366430000
1	0.545396000	2.370713000	-3.893855000
1	2.274040000	2.228850000	-4.210228000
6	1.998677000	-3.087476000	-1.445744000
1	1.862210000	-2.688598000	-2.461274000
6	0.809021000	-3.988019000	-1.154754000
1	-0.125725000	-3.427644000	-1.183594000
1	0.741678000	-4.792975000	-1.895710000
1	0.882049000	-4.456404000	-0.167100000
6	3.290040000	-3.897967000	-1.423486000
1	3.195007000	-4.747832000	-2.109398000
1	4.169156000	-3.334994000	-1.743715000
1	3.509818000	-4.321059000	-0.438787000
6	-3.878367000	0.135478000	-1.457549000
1	-4.027828000	1.124095000	-1.005111000
6	-5.227382000	-0.576306000	-1.424377000

1	-5.971118000	0.020311000	-1.964779000
1	-5.199683000	-1.554592000	-1.911588000
1	-5.617109000	-0.730007000	-0.415379000
6	-3.416306000	0.335597000	-2.897511000
1	-2.490220000	0.917352000	-2.957204000
1	-3.212422000	-0.620796000	-3.391909000
1	-4.184723000	0.851357000	-3.484966000
1	-0.744024000	-2.497587000	-3.915352000

[7c''_{PB}]_{dis} (TE = -3507.777762)

6	1.328621000	-0.823942000	1.925655000
6	1.299690000	-1.621519000	3.084602000
1	0.347339000	-1.782942000	3.588109000
6	2.440825000	-2.212408000	3.613597000
1	2.369837000	-2.822022000	4.511870000
6	3.669263000	-2.028247000	2.989433000
1	4.569471000	-2.487969000	3.390002000
6	3.733482000	-1.265635000	1.830402000
1	4.692382000	-1.154213000	1.331964000
6	2.584642000	-0.673508000	1.294438000
6	-0.279722000	1.401168000	1.902738000
6	0.249996000	1.876716000	3.114754000
1	0.965593000	1.256871000	3.655482000
6	-0.129833000	3.098881000	3.655885000
1	0.297733000	3.431661000	4.599452000
6	-1.070835000	3.889996000	3.002106000
1	-1.384170000	4.839936000	3.428218000
6	-1.605799000	3.457407000	1.794194000
1	-2.342736000	4.077438000	1.288026000
6	-1.206481000	2.238554000	1.236521000
6	-1.346047000	-1.006426000	1.664847000
6	-2.059032000	-0.893529000	2.872588000
1	-1.738341000	-0.153316000	3.606543000
6	-3.163313000	-1.685658000	3.156952000
1	-3.687129000	-1.570203000	4.103549000
6	-3.609539000	-2.613420000	2.220361000
1	-4.482588000	-3.228723000	2.423843000
6	-2.939835000	-2.735768000	1.010856000
1	-3.316708000	-3.441164000	0.274792000
6	-1.813818000	-1.950161000	0.732553000
23	0.187503000	0.223833000	-1.146947000
6	3.530449000	1.787694000	0.011802000
1	4.518971000	1.461009000	0.363742000
6	-3.603507000	1.666337000	-0.416492000
1	-3.881600000	2.707200000	-0.192822000
6	0.043129000	-3.599986000	-0.930571000

1	-0.217643000	-4.058614000	-1.893100000
6	-0.301784000	-4.570247000	0.190137000
1	0.286256000	-5.487567000	0.082636000
1	-0.067831000	-4.142730000	1.170706000
1	-1.355131000	-4.857976000	0.207211000
6	1.533237000	-3.302511000	-0.946054000
1	1.860826000	-2.838743000	-0.010145000
1	2.108149000	-4.226770000	-1.067052000
1	1.806291000	-2.637250000	-1.769917000
6	3.720111000	2.621753000	-1.250145000
1	4.113609000	2.053220000	-2.096352000
1	2.784963000	3.088170000	-1.572134000
1	4.422139000	3.439689000	-1.059985000
6	2.881242000	2.593225000	1.123745000
1	2.818077000	2.028019000	2.056438000
1	3.464429000	3.498234000	1.323160000
1	1.865287000	2.910054000	0.868844000
6	-4.134153000	1.299580000	-1.795708000
1	-5.222508000	1.408326000	-1.827821000
1	-3.722642000	1.920107000	-2.597507000
1	-3.909255000	0.256602000	-2.039915000
6	-4.180197000	0.778051000	0.672387000
1	-3.948906000	-0.277659000	0.504195000
1	-3.805958000	1.041839000	1.664639000
1	-5.270509000	0.874044000	0.692775000
5	-0.033420000	-0.116272000	1.494084000
7	0.795255000	1.524268000	-3.889260000
7	0.377567000	0.486793000	-3.039441000
1	1.342740000	1.150203000	-4.664405000
15	-0.971425000	-2.014752000	-0.885138000
15	2.632828000	0.180117000	-0.319541000
15	-1.747016000	1.697984000	-0.418923000
6	-2.390814000	-2.336359000	-2.083214000
1	-3.241821000	-1.859364000	-1.575586000
6	-2.731630000	-3.803862000	-2.326573000
1	-3.702150000	-3.878712000	-2.827097000
1	-2.003890000	-4.282501000	-2.988418000
1	-2.788146000	-4.407906000	-1.419408000
6	-2.176427000	-1.635311000	-3.417928000
1	-2.069713000	-0.552642000	-3.309938000
1	-1.286737000	-2.021237000	-3.932963000
1	-3.023624000	-1.815956000	-4.087433000
6	-1.346588000	3.104843000	-1.590734000
1	-1.420304000	2.625238000	-2.577988000
6	0.109410000	3.487401000	-1.371307000
1	0.775296000	2.610260000	-1.299617000

1	0.490190000	4.110556000	-2.187179000
1	0.248190000	4.036432000	-0.434507000
6	-2.240925000	4.334593000	-1.584827000
1	-1.918912000	5.028916000	-2.368186000
1	-3.289390000	4.100845000	-1.783443000
1	-2.190305000	4.883033000	-0.640673000
6	3.881955000	-0.782603000	-1.358354000
1	3.757909000	-1.809756000	-0.991987000
6	5.349536000	-0.398713000	-1.181785000
1	5.975435000	-1.119324000	-1.717769000
1	5.576354000	0.584242000	-1.602737000
1	5.691024000	-0.393783000	-0.145605000
6	3.525202000	-0.756420000	-2.841263000
1	2.497061000	-1.070190000	-3.034214000
1	3.637539000	0.246464000	-3.267532000
1	4.193930000	-1.416475000	-3.402852000
1	0.023808000	-0.250368000	-3.647779000
1	1.413715000	2.143220000	-3.371418000

[7c''_{PB}]_{dis} (TE = -3507.749426)

6	-1.331320000	0.821132000	1.953798000
6	-1.344952000	1.621868000	3.109982000
1	-0.402996000	1.843480000	3.610515000
6	-2.521008000	2.141539000	3.638394000
1	-2.487752000	2.758084000	4.534168000
6	-3.735866000	1.879332000	3.015282000
1	-4.662299000	2.284034000	3.415770000
6	-3.753937000	1.111330000	1.857716000
1	-4.704317000	0.939433000	1.359523000
6	-2.571256000	0.589560000	1.323739000
6	0.368775000	-1.309080000	1.997485000
6	-0.089464000	-1.708132000	3.264032000
1	-0.775554000	-1.056540000	3.805561000
6	0.313065000	-2.901511000	3.853459000
1	-0.065508000	-3.177170000	4.835607000
6	1.205140000	-3.737490000	3.190578000
1	1.533177000	-4.668554000	3.646564000
6	1.667204000	-3.377955000	1.929139000
1	2.355434000	-4.041312000	1.410574000
6	1.246759000	-2.189838000	1.324439000
6	1.313822000	1.155009000	1.630693000
6	2.049267000	1.104498000	2.828871000
1	1.792763000	0.350600000	3.573596000
6	3.102416000	1.970946000	3.089461000
1	3.648763000	1.897846000	4.027569000
6	3.467619000	2.917714000	2.138410000

1	4.300589000	3.592648000	2.320508000
6	2.766323000	2.986799000	0.942139000
1	3.076517000	3.715214000	0.199665000
6	1.693187000	2.125093000	0.682073000
23	-0.190432000	-0.248774000	-1.256497000
6	-3.340345000	-1.920028000	0.006974000
1	-4.359078000	-1.689659000	0.347803000
6	3.528801000	-1.515122000	-0.446426000
1	3.935596000	-2.496211000	-0.164483000
6	-0.198025000	3.657154000	-1.039800000
1	-0.142846000	3.929282000	-2.104408000
6	0.323784000	4.815217000	-0.201692000
1	-0.303931000	5.699288000	-0.356320000
1	0.290283000	4.576181000	0.866014000
1	1.348619000	5.102169000	-0.440733000
6	-1.653163000	3.376804000	-0.707081000
1	-1.780053000	3.050743000	0.329906000
1	-2.261464000	4.277542000	-0.842480000
1	-2.062339000	2.600493000	-1.354169000
6	-3.427135000	-2.712845000	-1.291064000
1	-3.959237000	-2.179619000	-2.084050000
1	-2.427580000	-2.953312000	-1.664395000
1	-3.948095000	-3.662803000	-1.133803000
6	-2.639671000	-2.705644000	1.103240000
1	-2.627390000	-2.160974000	2.050710000
1	-3.151264000	-3.658559000	1.275159000
1	-1.599520000	-2.931844000	0.850216000
6	3.964038000	-1.185005000	-1.869099000
1	5.055511000	-1.137954000	-1.938674000
1	3.624084000	-1.916394000	-2.608508000
1	3.579003000	-0.208665000	-2.181113000
6	4.057639000	-0.498095000	0.547696000
1	3.736021000	0.518744000	0.308737000
1	3.738572000	-0.712518000	1.570336000
1	5.152746000	-0.503112000	0.535029000
5	0.060932000	0.179043000	1.529931000
7	-0.946542000	-1.621445000	-3.978229000
7	-0.515870000	-0.941178000	-2.823751000
1	-1.341711000	-0.983870000	-4.681838000
15	0.836263000	2.090797000	-0.931758000
15	-2.535003000	-0.261820000	-0.290168000
15	1.677652000	-1.756823000	-0.396024000
6	2.192115000	2.379760000	-2.208680000
1	3.051557000	1.839923000	-1.784294000
6	2.616428000	3.819192000	-2.481864000
1	3.402632000	3.828059000	-3.244093000

1	1.794587000	4.424053000	-2.876443000
1	3.018876000	4.339465000	-1.612551000
6	1.798237000	1.715184000	-3.524561000
1	1.582196000	0.649994000	-3.407730000
1	0.901062000	2.180446000	-3.952288000
1	2.598081000	1.823143000	-4.264956000
6	1.526960000	-3.338955000	-1.421268000
1	1.483041000	-2.929178000	-2.441983000
6	0.204212000	-4.032731000	-1.139994000
1	-0.631488000	-3.333495000	-1.188499000
1	0.020858000	-4.834870000	-1.863839000
1	0.189045000	-4.488004000	-0.144590000
6	2.673357000	-4.343295000	-1.376079000
1	2.449282000	-5.176756000	-2.050864000
1	3.632342000	-3.931110000	-1.694534000
1	2.813331000	-4.782256000	-0.385137000
6	-3.851993000	0.646951000	-1.305195000
1	-3.813474000	1.659102000	-0.884119000
6	-5.290874000	0.154720000	-1.167708000
1	-5.961942000	0.850398000	-1.682267000
1	-5.447008000	-0.824956000	-1.626814000
1	-5.640011000	0.084920000	-0.136207000
6	-3.478714000	0.735112000	-2.781119000
1	-2.459934000	1.101870000	-2.940642000
1	-3.552893000	-0.244787000	-3.267820000
1	-4.167048000	1.402197000	-3.310632000
1	-1.670897000	-2.326562000	-3.779516000
1	-0.177020000	-2.120808000	-4.441660000

$[8c''_{PB}]_{alt}$ (TE = -3507.842418)

6	0.845096000	-1.283197000	1.849064000
6	0.521727000	-2.100409000	2.948655000
1	-0.451612000	-1.975074000	3.423406000
6	1.395594000	-3.055505000	3.456134000
1	1.099506000	-3.669995000	4.304836000
6	2.650776000	-3.214041000	2.880795000
1	3.353056000	-3.947729000	3.271285000
6	2.994527000	-2.435891000	1.779941000
1	3.969239000	-2.585809000	1.324571000
6	2.106157000	-1.498022000	1.243900000
6	0.237515000	1.354290000	1.931650000
6	0.825658000	1.520280000	3.197660000
1	1.107287000	0.632081000	3.765394000
6	1.060537000	2.774905000	3.749635000
1	1.523527000	2.859582000	4.731588000
6	0.699734000	3.922667000	3.049575000

1	0.875711000	4.908460000	3.475127000
6	0.119883000	3.796323000	1.791854000
1	-0.152596000	4.694657000	1.239841000
6	-0.096745000	2.535439000	1.226989000
6	-1.714555000	-0.448818000	1.673763000
6	-2.312036000	-0.052731000	2.884201000
1	-1.712549000	0.505875000	3.604230000
6	-3.639705000	-0.325725000	3.187834000
1	-4.063182000	0.004976000	4.134846000
6	-4.429558000	-1.008509000	2.268248000
1	-5.476084000	-1.216117000	2.482196000
6	-3.871532000	-1.414371000	1.062485000
1	-4.505744000	-1.927641000	0.344138000
6	-2.530145000	-1.148344000	0.758091000
23	0.128658000	0.044895000	-1.194356000
6	3.964570000	0.388303000	0.057109000
1	4.718574000	-0.323740000	0.422712000
6	-2.458152000	2.925360000	-0.500336000
1	-2.375441000	4.005298000	-0.313821000
6	-1.418282000	-3.405422000	-0.846082000
1	-1.886004000	-3.799041000	-1.757786000
6	-2.006347000	-4.127377000	0.357420000
1	-1.794596000	-5.201384000	0.300450000
1	-1.568899000	-3.756721000	1.290984000
1	-3.089537000	-4.008668000	0.443691000
6	0.077143000	-3.662016000	-0.949564000
1	0.607437000	-3.295488000	-0.064817000
1	0.279998000	-4.736474000	-1.031965000
1	0.515845000	-3.170650000	-1.823858000
6	4.519537000	1.090866000	-1.176612000
1	4.649583000	0.424517000	-2.034316000
1	3.869573000	1.908233000	-1.500376000
1	5.498002000	1.535129000	-0.962305000
6	3.666405000	1.375328000	1.174540000
1	3.363741000	0.869704000	2.095238000
1	4.552022000	1.980089000	1.401303000
1	2.857914000	2.064890000	0.909916000
6	-3.058985000	2.696633000	-1.881475000
1	-4.039572000	3.177432000	-1.968781000
1	-2.433120000	3.074827000	-2.696388000
1	-3.204869000	1.625421000	-2.060149000
6	-3.339323000	2.330022000	0.583279000
1	-3.508218000	1.261128000	0.426733000
1	-2.911461000	2.449783000	1.582130000
1	-4.320484000	2.818511000	0.580149000
5	-0.167064000	-0.120093000	1.455376000

7	1.443051000	0.977886000	-3.774434000
7	0.381983000	0.291475000	-3.094308000
1	1.893264000	0.321190000	-4.419432000
15	-1.802965000	-1.550455000	-0.878153000
15	2.463164000	-0.658095000	-0.359526000
15	-0.700018000	2.291456000	-0.477718000
6	-3.292382000	-1.468180000	-2.036916000
1	-3.900634000	-0.663672000	-1.596253000
6	-4.156240000	-2.720701000	-2.160729000
1	-5.105267000	-2.478080000	-2.651846000
1	-3.673410000	-3.480885000	-2.782888000
1	-4.396878000	-3.195487000	-1.207121000
6	-2.842398000	-1.022696000	-3.423500000
1	-2.369540000	-0.037219000	-3.401715000
1	-2.120210000	-1.726925000	-3.855740000
1	-3.691329000	-0.968316000	-4.114491000
6	0.149779000	3.561254000	-1.581422000
1	0.035178000	3.099741000	-2.573440000
6	1.639053000	3.605364000	-1.277239000
1	2.052098000	2.599209000	-1.178148000
1	2.186585000	4.116572000	-2.076699000
1	1.849458000	4.131367000	-0.339789000
6	-0.428524000	4.969655000	-1.641723000
1	0.161689000	5.578252000	-2.336373000
1	-1.461285000	5.000056000	-1.996312000
1	-0.396565000	5.481674000	-0.674816000
6	3.246580000	-2.061110000	-1.378688000
1	2.711821000	-2.942340000	-1.000280000
6	4.743070000	-2.318417000	-1.216846000
1	5.017090000	-3.223934000	-1.770264000
1	5.349805000	-1.507810000	-1.630132000
1	5.068960000	-2.469981000	-0.186928000
6	2.927706000	-1.922187000	-2.863099000
1	1.870035000	-1.710544000	-3.044689000
1	3.507668000	-1.111239000	-3.319302000
1	3.194261000	-2.839756000	-3.400295000
1	-0.360438000	0.200453000	-3.786139000
1	2.152013000	1.162255000	-3.063201000

$[8c''_{PB}]_{dis}$ (TE = -3451.334767)

6	1.556328000	0.492088000	1.877752000
6	1.760872000	0.292245000	3.254854000
1	0.895092000	0.137852000	3.899837000
6	3.029890000	0.269127000	3.822590000
1	3.143717000	0.108597000	4.893260000
6	4.153369000	0.439204000	3.018995000

1	5.151293000	0.413160000	3.451702000
6	3.988188000	0.633874000	1.653405000
1	4.869288000	0.752228000	1.025042000
6	2.710817000	0.659987000	1.083559000
6	-0.858485000	1.781998000	1.480472000
6	-0.605868000	2.739482000	2.478049000
1	0.335624000	2.691660000	3.026301000
6	-1.536748000	3.716415000	2.815419000
1	-1.308304000	4.437261000	3.598820000
6	-2.773428000	3.753293000	2.176884000
1	-3.518666000	4.494459000	2.457496000
6	-3.036700000	2.848272000	1.151426000
1	-3.993099000	2.896909000	0.633464000
6	-2.084318000	1.900663000	0.773035000
6	-0.778120000	-0.850651000	1.703677000
6	-1.534223000	-0.717874000	2.889422000
1	-1.574387000	0.257169000	3.374624000
6	-2.238479000	-1.764648000	3.468365000
1	-2.794312000	-1.599901000	4.389792000
6	-2.247076000	-3.011704000	2.854786000
1	-2.806064000	-3.841420000	3.282162000
6	-1.537762000	-3.180279000	1.675311000
1	-1.564851000	-4.149617000	1.185089000
6	-0.798637000	-2.135495000	1.099316000
23	0.127858000	0.004502000	-1.261265000
6	2.659919000	2.660888000	-1.027954000
1	3.712935000	2.867601000	-0.789445000
6	-3.893111000	0.095050000	-0.732339000
1	-4.624122000	0.911169000	-0.640643000
6	1.440047000	-3.573465000	-0.155461000
1	1.694421000	-4.000193000	-1.138687000
6	1.166428000	-4.701662000	0.831871000
1	2.059127000	-5.330724000	0.923613000
1	0.952938000	-4.304005000	1.828526000
1	0.341137000	-5.355645000	0.552726000
6	2.621221000	-2.757818000	0.346280000
1	2.387336000	-2.255914000	1.292261000
1	3.491986000	-3.398269000	0.524420000
1	2.909918000	-1.988877000	-0.366988000
6	2.408305000	2.988343000	-2.494944000
1	3.123452000	2.500465000	-3.162929000
1	1.417054000	2.660675000	-2.818428000
1	2.485436000	4.067732000	-2.667154000
6	1.800322000	3.498424000	-0.092465000
1	2.037785000	3.313894000	0.959189000
1	1.958725000	4.565106000	-0.286776000

1	0.733398000	3.300365000	-0.215887000
6	-4.127091000	-0.636813000	-2.048484000
1	-5.125557000	-1.086707000	-2.071126000
1	-4.040482000	0.013218000	-2.923741000
1	-3.401293000	-1.446171000	-2.182605000
6	-4.065302000	-0.829788000	0.459179000
1	-3.362086000	-1.666990000	0.426969000
1	-3.910073000	-0.313414000	1.409987000
1	-5.076033000	-1.253088000	0.469784000
5	0.050984000	0.492554000	1.336469000
15	2.434178000	0.829554000	-0.710766000
15	-2.222213000	0.919001000	-0.768306000
15	0.008856000	-2.413899000	-0.520761000
6	-2.473579000	2.209627000	-2.118985000
1	-2.244334000	1.629047000	-3.023478000
6	-1.421643000	3.301399000	-2.000000000
1	-1.474220000	3.980997000	-2.857661000
1	-1.558519000	3.902198000	-1.093590000
1	-0.415769000	2.880052000	-1.983013000
6	-3.859409000	2.825056000	-2.256459000
1	-3.871981000	3.497475000	-3.121806000
1	-4.655333000	2.093943000	-2.415730000
1	-4.131267000	3.434523000	-1.389611000
6	3.954991000	0.070312000	-1.529766000
1	4.274288000	-0.694299000	-0.809905000
6	5.148856000	0.991520000	-1.755461000
1	5.996672000	0.408702000	-2.132505000
1	4.946105000	1.765995000	-2.499839000
1	5.487019000	1.495416000	-0.846179000
6	3.549232000	-0.627990000	-2.823592000
1	4.404941000	-1.147615000	-3.269305000
1	2.749150000	-1.358577000	-2.664114000
1	3.167318000	0.081414000	-3.564487000
6	-1.205195000	-3.399314000	-1.565897000
1	-2.179652000	-3.009702000	-1.233955000
6	-0.999946000	-3.011330000	-3.029198000
1	-0.020257000	-3.343147000	-3.394610000
1	-1.756223000	-3.489345000	-3.661780000
1	-1.046456000	-1.930773000	-3.186763000
6	-1.220990000	-4.917763000	-1.442251000
1	-0.248591000	-5.357714000	-1.686409000
1	-1.513336000	-5.280328000	-0.455124000
1	-1.940322000	-5.333962000	-2.156208000
7	0.143634000	0.355275000	-2.802669000

$[9c''_{PB}]_{alt}$ (TE = -3508.283230)

6	1.068067000	-1.521385000	1.589754000
6	0.857233000	-2.520683000	2.558094000
1	-0.115646000	-2.582343000	3.043955000
6	1.850950000	-3.415129000	2.937241000
1	1.644964000	-4.167927000	3.695382000
6	3.110956000	-3.335807000	2.355144000
1	3.904545000	-4.016571000	2.653691000
6	3.341472000	-2.388374000	1.364932000
1	4.321201000	-2.354368000	0.896591000
6	2.337248000	-1.502484000	0.960408000
6	0.314245000	1.030550000	2.009308000
6	0.998849000	1.069116000	3.237671000
1	1.387686000	0.138359000	3.651950000
6	1.186411000	2.249367000	3.946419000
1	1.718953000	2.234566000	4.895259000
6	0.687729000	3.449096000	3.446974000
1	0.821362000	4.376265000	3.999078000
6	0.023044000	3.452316000	2.227337000
1	-0.356526000	4.393211000	1.833546000
6	-0.153214000	2.266386000	1.505602000
6	-1.561889000	-0.847000000	1.709069000
6	-2.018939000	-0.712605000	3.032341000
1	-1.353767000	-0.271182000	3.774987000
6	-3.291152000	-1.106890000	3.426048000
1	-3.604314000	-0.980689000	4.460403000
6	-4.167965000	-1.649181000	2.491727000
1	-5.171215000	-1.950678000	2.783147000
6	-3.754115000	-1.789938000	1.174450000
1	-4.454978000	-2.189483000	0.446934000
6	-2.467970000	-1.399774000	0.779579000
23	0.048748000	0.100810000	-1.108664000
6	4.002265000	0.679211000	-0.095164000
1	4.832851000	-0.008237000	0.118601000
6	-2.674165000	2.764883000	0.048580000
1	-2.608532000	3.807456000	0.389566000
6	-1.374208000	-3.189099000	-1.355811000
1	-1.750701000	-3.368623000	-2.372937000
6	-1.943607000	-4.240970000	-0.417103000
1	-1.629565000	-5.242470000	-0.729794000
1	-1.585001000	-4.089277000	0.606203000
1	-3.035432000	-4.236437000	-0.381677000
6	0.145659000	-3.261849000	-1.402934000
1	0.592550000	-3.118834000	-0.414813000
1	0.484587000	-4.235645000	-1.772720000
1	0.570806000	-2.509962000	-2.081298000
6	4.397693000	1.563710000	-1.271996000

1	4.508401000	1.016632000	-2.211556000
1	3.665321000	2.355968000	-1.445932000
1	5.353031000	2.058626000	-1.070225000
6	3.726625000	1.488981000	1.161875000
1	3.536091000	0.848956000	2.026821000
1	4.587822000	2.122145000	1.399686000
1	2.857894000	2.145908000	1.051591000
6	-3.386950000	2.723985000	-1.296905000
1	-4.387271000	3.161904000	-1.222424000
1	-2.856992000	3.267084000	-2.087184000
1	-3.513997000	1.691232000	-1.637897000
6	-3.428977000	1.977875000	1.105774000
1	-3.595182000	0.940709000	0.804996000
1	-2.905819000	1.961202000	2.065454000
1	-4.412582000	2.429085000	1.272409000
5	-0.052798000	-0.406830000	1.408959000
15	2.575823000	-0.444863000	-0.522930000
15	-0.897172000	2.240894000	-0.156260000
15	-1.939573000	-1.440302000	-0.963434000
6	-0.174978000	3.706303000	-1.099629000
1	-0.325965000	3.412904000	-2.151456000
6	1.325414000	3.789550000	-0.848311000
1	1.824680000	4.397094000	-1.611240000
1	1.543499000	4.243988000	0.122415000
1	1.798797000	2.803016000	-0.831713000
6	-0.827686000	5.072026000	-0.922168000
1	-0.306236000	5.809694000	-1.541525000
1	-1.877520000	5.092989000	-1.221092000
1	-0.769558000	5.434155000	0.107661000
6	3.342331000	-1.653950000	-1.770659000
1	2.892041000	-2.612886000	-1.478816000
6	4.859727000	-1.815649000	-1.721108000
1	5.156586000	-2.627646000	-2.392801000
1	5.383329000	-0.919888000	-2.065308000
1	5.254205000	-2.065573000	-0.735855000
6	2.925603000	-1.340353000	-3.203795000
1	3.353346000	-2.078178000	-3.890837000
1	1.841609000	-1.362802000	-3.350591000
1	3.261935000	-0.353119000	-3.528991000
6	-3.488682000	-1.237461000	-2.000471000
1	-4.088519000	-0.507419000	-1.436639000
6	-3.103992000	-0.621646000	-3.342631000
1	-2.429466000	-1.278277000	-3.906861000
1	-3.986749000	-0.462442000	-3.969727000
1	-2.607210000	0.345482000	-3.223177000
6	-4.334680000	-2.485211000	-2.235934000

1	-3.802578000	-3.235110000	-2.828769000
1	-4.670040000	-2.974217000	-1.320786000
1	-5.232805000	-2.220573000	-2.803321000
7	0.137838000	0.847769000	-3.253797000
1	-0.699385000	1.415887000	-3.403073000
1	0.053630000	0.077258000	-3.915061000
7	1.327033000	1.569629000	-3.640586000
1	1.103033000	2.207069000	-4.403471000
1	1.586812000	2.149412000	-2.847467000

[9c''_{pg}]_{dis} (TE = -3451.783734)

6	-0.812057000	-1.225549000	1.885145000
6	-1.240039000	-1.236099000	3.223004000
1	-0.869422000	-0.473750000	3.909369000
6	-2.133759000	-2.192802000	3.692467000
1	-2.452635000	-2.174284000	4.732266000
6	-2.626262000	-3.169157000	2.830422000
1	-3.326072000	-3.918301000	3.192507000
6	-2.231515000	-3.172423000	1.498430000
1	-2.640294000	-3.923367000	0.826462000
6	-1.338047000	-2.207099000	1.025882000
6	1.816110000	-0.474107000	1.709780000
6	2.182880000	-1.144891000	2.887277000
1	1.407216000	-1.609032000	3.495464000
6	3.504321000	-1.209227000	3.317164000
1	3.748388000	-1.727804000	4.241696000
6	4.512257000	-0.602356000	2.574058000
1	5.544619000	-0.637391000	2.913107000
6	4.191416000	0.023583000	1.374483000
1	4.986619000	0.457674000	0.768321000
6	2.867783000	0.075603000	0.931560000
6	-0.047477000	1.390569000	1.433360000
6	0.704690000	2.109879000	2.399455000
1	1.458800000	1.577650000	2.974307000
6	0.486457000	3.444362000	2.686413000
1	1.040971000	3.923451000	3.489862000
6	-0.403995000	4.179526000	1.906491000
1	-0.542904000	5.244441000	2.076076000
6	-1.120971000	3.537931000	0.914137000
1	-1.808071000	4.121266000	0.310762000
6	-1.024672000	2.146802000	0.713327000
23	-0.021004000	0.292499000	-1.099835000
6	0.361226000	-3.507811000	-0.958865000
1	-0.279971000	-4.398122000	-0.959748000
6	3.014386000	2.385942000	-1.012376000
1	4.109876000	2.332828000	-1.038563000

6	-3.816676000	1.067777000	0.503740000
1	-4.555071000	1.327637000	-0.267273000
6	-3.956607000	2.032608000	1.673931000
1	-4.955360000	1.936804000	2.111876000
1	-3.231425000	1.802868000	2.461835000
1	-3.819310000	3.079793000	1.399660000
6	-4.099182000	-0.352210000	0.958037000
1	-3.445813000	-0.657093000	1.776790000
1	-5.128314000	-0.414121000	1.326698000
1	-3.999548000	-1.085522000	0.156266000
6	1.021368000	-3.397193000	-2.329563000
1	0.296149000	-3.526419000	-3.138969000
1	1.496307000	-2.423604000	-2.484484000
1	1.790398000	-4.165573000	-2.457922000
6	1.327271000	-3.656751000	0.208940000
1	0.804872000	-3.958245000	1.120847000
1	2.076922000	-4.423403000	-0.012158000
1	1.860105000	-2.735276000	0.448748000
6	2.496967000	2.882776000	-2.359916000
1	2.967897000	3.835603000	-2.621398000
1	2.678612000	2.187819000	-3.184670000
1	1.414528000	3.049217000	-2.321417000
6	2.611015000	3.334783000	0.097521000
1	1.525241000	3.452458000	0.146317000
1	2.960042000	3.007078000	1.079701000
1	3.032999000	4.327724000	-0.090128000
5	0.279429000	-0.173565000	1.432825000
15	-0.800925000	-2.075188000	-0.709881000
15	2.440105000	0.633068000	-0.747287000
15	-2.197606000	1.326830000	-0.428878000
6	3.551267000	-0.334278000	-1.936237000
1	2.898990000	-0.466248000	-2.811223000
6	3.924979000	-1.709141000	-1.397278000
1	4.325345000	-2.328677000	-2.206088000
1	4.699030000	-1.639003000	-0.628363000
1	3.087610000	-2.246151000	-0.959787000
6	4.821432000	0.379509000	-2.387634000
1	5.370022000	-0.273945000	-3.073617000
1	4.645114000	1.317370000	-2.916228000
1	5.496797000	0.587079000	-1.551124000
6	-2.299735000	-2.532378000	-1.753815000
1	-3.135584000	-2.154160000	-1.150817000
6	-2.510809000	-4.027137000	-1.972957000
1	-3.481561000	-4.188167000	-2.452262000
1	-1.757583000	-4.449979000	-2.644723000
1	-2.504464000	-4.621118000	-1.056957000

6	-2.318003000	-1.806404000	-3.091927000
1	-3.230175000	-2.058083000	-3.642863000
1	-2.279762000	-0.724463000	-2.974112000
1	-1.470294000	-2.092414000	-3.723380000
6	-2.636859000	2.622591000	-1.716424000
1	-1.692236000	3.170636000	-1.851132000
6	-2.976362000	1.929121000	-3.032375000
1	-3.842914000	1.264523000	-2.929894000
1	-3.236252000	2.670792000	-3.793853000
1	-2.137998000	1.340347000	-3.407606000
6	-3.746128000	3.612369000	-1.367969000
1	-4.722963000	3.125209000	-1.298708000
1	-3.593642000	4.165255000	-0.440663000
1	-3.828729000	4.352333000	-2.170077000
7	0.140622000	0.338240000	-2.758320000
1	0.382863000	0.145560000	-3.733861000

[10c''_{PB}]_{alt} (TE = -3508.414634)

6	0.886801000	-1.237011000	1.894568000
6	0.612429000	-2.031848000	3.023045000
1	-0.348476000	-1.911338000	3.525004000
6	1.513967000	-2.967673000	3.520046000
1	1.254643000	-3.564979000	4.392838000
6	2.746367000	-3.135634000	2.898370000
1	3.464384000	-3.861112000	3.275991000
6	3.044687000	-2.377063000	1.771326000
1	4.000173000	-2.531588000	1.273804000
6	2.131304000	-1.451157000	1.255759000
6	0.072043000	1.365530000	1.971772000
6	0.579210000	1.551066000	3.269783000
1	0.902120000	0.674232000	3.833083000
6	0.681400000	2.805031000	3.863220000
1	1.087346000	2.900817000	4.869186000
6	0.252222000	3.933960000	3.173491000
1	0.312305000	4.919821000	3.630335000
6	-0.245275000	3.789488000	1.882460000
1	-0.568075000	4.676406000	1.340046000
6	-0.314575000	2.534256000	1.268024000
6	-1.717781000	-0.579167000	1.619023000
6	-2.411444000	-0.208426000	2.785050000
1	-1.891415000	0.391116000	3.533383000
6	-3.740516000	-0.549039000	3.008087000
1	-4.240411000	-0.231744000	3.922036000
6	-4.433175000	-1.278176000	2.047790000
1	-5.480387000	-1.535781000	2.194614000
6	-3.774584000	-1.671206000	0.888447000

1	-4.332513000	-2.228081000	0.139546000
6	-2.431452000	-1.341578000	0.667034000
23	0.142157000	0.085493000	-1.060295000
6	3.886516000	0.514974000	0.090955000
1	4.694300000	-0.153735000	0.420821000
6	-2.568095000	2.840825000	-0.619533000
1	-2.620293000	3.904276000	-0.348521000
6	-1.169900000	-3.602367000	-0.781874000
1	-1.551907000	-4.027088000	-1.719602000
6	-1.853026000	-4.304527000	0.382917000
1	-1.619615000	-5.375784000	0.372005000
1	-1.507329000	-3.904686000	1.342499000
1	-2.941077000	-4.204732000	0.371268000
6	0.328738000	-3.853048000	-0.746382000
1	0.789658000	-3.437800000	0.155199000
1	0.538659000	-4.929367000	-0.755256000
1	0.833741000	-3.408728000	-1.607735000
6	4.368797000	1.306099000	-1.118580000
1	4.490284000	0.698838000	-2.020070000
1	3.665912000	2.105788000	-1.369886000
1	5.331230000	1.788406000	-0.912904000
6	3.535064000	1.437774000	1.248250000
1	3.277911000	0.881445000	2.153815000
1	4.378527000	2.095689000	1.488335000
1	2.676387000	2.077198000	1.016084000
6	-3.033060000	2.659155000	-2.059178000
1	-4.061801000	3.011476000	-2.194600000
1	-2.410009000	3.191787000	-2.787027000
1	-3.015698000	1.595152000	-2.329766000
6	-3.458708000	2.064324000	0.332547000
1	-3.468648000	0.996931000	0.092932000
1	-3.137045000	2.158814000	1.372868000
1	-4.492307000	2.423837000	0.268055000
5	-0.187590000	-0.133310000	1.471990000
15	2.446124000	-0.608907000	-0.349936000
15	-0.762719000	2.342902000	-0.500609000
15	-1.571989000	-1.746599000	-0.908850000
6	0.030366000	3.810840000	-1.414591000
1	0.051866000	3.437836000	-2.452385000
6	1.473751000	4.002969000	-0.970949000
1	2.034611000	4.609231000	-1.691730000
1	1.531849000	4.509370000	-0.002667000
1	1.992739000	3.048541000	-0.852648000
6	-0.696156000	5.151423000	-1.443606000
1	-0.119733000	5.872394000	-2.035617000
1	-1.690553000	5.097419000	-1.892003000

1	-0.809906000	5.589364000	-0.447901000
6	3.304708000	-1.962028000	-1.373075000
1	2.883521000	-2.881713000	-0.945902000
6	4.823809000	-2.074520000	-1.296026000
1	5.158715000	-2.956555000	-1.854454000
1	5.331503000	-1.213671000	-1.740275000
1	5.205669000	-2.183101000	-0.278242000
6	2.860487000	-1.874543000	-2.829303000
1	3.263309000	-2.710341000	-3.413671000
1	1.768048000	-1.903893000	-2.913957000
1	3.189023000	-0.944508000	-3.304461000
6	-2.984224000	-1.744818000	-2.169201000
1	-3.648613000	-0.954166000	-1.788873000
6	-2.453139000	-1.303408000	-3.528134000
1	-1.674240000	-1.985217000	-3.895568000
1	-3.248532000	-1.288741000	-4.282313000
1	-2.020743000	-0.299923000	-3.481754000
6	-3.794481000	-3.027156000	-2.338240000
1	-3.241849000	-3.779765000	-2.909829000
1	-4.088572000	-3.496370000	-1.397210000
1	-4.712658000	-2.824956000	-2.901488000
7	0.454181000	0.588687000	-3.260046000
1	-0.353584000	1.150283000	-3.532751000
1	0.438398000	-0.230045000	-3.863705000
7	1.686569000	1.283844000	-3.553724000
1	1.522745000	1.979935000	-4.280603000
1	1.919800000	1.794723000	-2.703985000

[10c''_{PB}]_{dis} (TE = -3451.944309)

6	-1.438834000	0.472202000	1.850028000
6	-1.566249000	1.175739000	3.062044000
1	-0.662042000	1.445837000	3.608135000
6	-2.799584000	1.544173000	3.587441000
1	-2.849920000	2.092975000	4.526411000
6	-3.966494000	1.211722000	2.908188000
1	-4.939326000	1.493557000	3.305682000
6	-3.877097000	0.532402000	1.698663000
1	-4.793207000	0.305132000	1.160235000
6	-2.636597000	0.172735000	1.160479000
6	0.470323000	-1.471939000	1.783870000
6	0.054152000	-2.010143000	3.013549000
1	-0.671099000	-1.455231000	3.610315000
6	0.534500000	-3.222987000	3.495397000
1	0.180061000	-3.608451000	4.450096000
6	1.473956000	-3.939870000	2.760723000
1	1.862310000	-4.886077000	3.131665000

6	1.902193000	-3.440164000	1.535419000
1	2.624830000	-4.010671000	0.955008000
6	1.398821000	-2.235148000	1.035218000
6	1.174214000	1.089684000	1.670759000
6	1.911396000	0.986219000	2.864901000
1	1.706333000	0.151260000	3.536039000
6	2.908285000	1.890425000	3.207646000
1	3.460401000	1.768058000	4.138075000
6	3.212852000	2.939424000	2.345947000
1	4.006044000	3.643762000	2.588216000
6	2.501084000	3.073224000	1.160706000
1	2.766105000	3.882097000	0.485314000
6	1.485292000	2.170991000	0.820110000
23	-0.120875000	-0.144881000	-1.349415000
6	-3.103233000	-2.281312000	-0.393010000
1	-4.147443000	-2.204281000	-0.057553000
6	3.592334000	-1.212154000	-0.667373000
1	4.106981000	-2.168865000	-0.503127000
6	-0.603874000	3.678006000	-0.670876000
1	-0.413646000	4.264609000	-1.578900000
6	-0.380292000	4.569630000	0.541650000
1	-1.086417000	5.407807000	0.530176000
1	-0.541624000	4.018619000	1.474470000
1	0.626980000	4.990107000	0.589090000
6	-2.044378000	3.200429000	-0.729086000
1	-2.303882000	2.591461000	0.142768000
1	-2.733482000	4.052861000	-0.748558000
1	-2.232066000	2.601379000	-1.623457000
6	-3.070262000	-2.951317000	-1.763966000
1	-3.844562000	-2.571669000	-2.435023000
1	-2.114266000	-2.789435000	-2.271185000
1	-3.220640000	-4.032878000	-1.674468000
6	-2.332336000	-3.066277000	0.656778000
1	-2.408389000	-2.606793000	1.646314000
1	-2.722824000	-4.087495000	0.732018000
1	-1.267145000	-3.138368000	0.422589000
6	3.969366000	-0.666982000	-2.039404000
1	5.051318000	-0.512035000	-2.115405000
1	3.672724000	-1.322728000	-2.863929000
1	3.487594000	0.301255000	-2.215387000
6	4.019821000	-0.262936000	0.436424000
1	3.583904000	0.731494000	0.311175000
1	3.734119000	-0.622376000	1.428259000
1	5.109316000	-0.143491000	0.426682000
5	0.023490000	0.013596000	1.402739000
15	-2.473638000	-0.525291000	-0.526186000

15	1.769894000	-1.634636000	-0.651413000
15	0.613132000	2.233359000	-0.790770000
6	1.770585000	-3.133140000	-1.801945000
1	1.643842000	-2.644295000	-2.778201000
6	0.541162000	-3.995872000	-1.567678000
1	0.449326000	-4.756270000	-2.351074000
1	0.585047000	-4.519513000	-0.606624000
1	-0.370935000	-3.399644000	-1.578948000
6	3.025290000	-3.997190000	-1.863461000
1	2.875036000	-4.801233000	-2.592981000
1	3.917337000	-3.451349000	-2.178135000
1	3.255225000	-4.484437000	-0.911202000
6	-3.857169000	0.314645000	-1.506588000
1	-3.907668000	1.309430000	-1.045419000
6	-5.250410000	-0.304095000	-1.417225000
1	-5.976261000	0.360698000	-1.898846000
1	-5.312771000	-1.261661000	-1.940893000
1	-5.603099000	-0.472325000	-0.397973000
6	-3.466641000	0.484246000	-2.970871000
1	-4.222415000	1.073728000	-3.502723000
1	-2.496635000	0.972044000	-3.092879000
1	-3.389047000	-0.482473000	-3.480308000
6	1.918656000	2.898983000	-1.977850000
1	2.846310000	2.450553000	-1.590216000
6	1.671030000	2.368577000	-3.385492000
1	0.724097000	2.749250000	-3.788748000
1	2.465195000	2.695489000	-4.066738000
1	1.607296000	1.278588000	-3.417128000
6	2.099054000	4.414308000	-2.036903000
1	1.287564000	4.892207000	-2.594399000
1	2.149837000	4.905167000	-1.063153000
1	3.023809000	4.658527000	-2.571114000
7	-0.236832000	-0.530458000	-2.993888000
1	-0.343961000	-0.755337000	-3.983688000

[11c''_{PB}]_{alt} (TE = -3508.790101)

6	-1.331513000	0.727816000	1.892268000
6	-1.433652000	1.585094000	3.003640000
1	-0.517572000	1.922661000	3.488656000
6	-2.654787000	2.022195000	3.504589000
1	-2.683532000	2.689308000	4.363901000
6	-3.836843000	1.604599000	2.903985000
1	-4.800298000	1.935603000	3.284989000
6	-3.774873000	0.769063000	1.794996000
1	-4.704192000	0.466178000	1.319120000
6	-2.546168000	0.342422000	1.279108000

6	0.606557000	-1.207780000	1.982540000
6	0.261558000	-1.589936000	3.290421000
1	-0.439134000	-0.967839000	3.848621000
6	0.788619000	-2.721960000	3.902104000
1	0.491151000	-2.980693000	4.916555000
6	1.707991000	-3.513778000	3.221940000
1	2.141434000	-4.391381000	3.695949000
6	2.061754000	-3.174808000	1.920973000
1	2.774178000	-3.802021000	1.388589000
6	1.507300000	-2.055350000	1.290793000
6	1.274116000	1.340713000	1.582573000
6	2.082827000	1.350716000	2.733070000
1	1.932819000	0.576832000	3.486471000
6	3.080125000	2.296643000	2.936541000
1	3.686179000	2.264525000	3.839982000
6	3.312402000	3.271814000	1.972716000
1	4.101049000	4.008580000	2.108415000
6	2.529546000	3.292889000	0.825276000
1	2.732718000	4.050348000	0.072428000
6	1.513789000	2.350241000	0.625408000
23	-0.096019000	-0.160930000	-1.033891000
6	-3.177940000	-2.267851000	0.205940000
1	-4.197491000	-2.056593000	0.556990000
6	3.622381000	-1.276056000	-0.651154000
1	4.181281000	-2.179503000	-0.373208000
6	-0.702186000	3.701889000	-0.844844000
1	-0.512126000	4.293297000	-1.748864000
6	-0.512440000	4.599062000	0.369585000
1	-1.244772000	5.413762000	0.356876000
1	-0.657293000	4.042492000	1.301917000
1	0.481358000	5.050970000	0.417364000
6	-2.132361000	3.194201000	-0.922179000
1	-2.393287000	2.599016000	-0.042065000
1	-2.836865000	4.032062000	-0.971723000
1	-2.296081000	2.569993000	-1.806762000
6	-3.263336000	-3.222376000	-0.977435000
1	-3.742462000	-2.782713000	-1.860088000
1	-2.267498000	-3.574178000	-1.271885000
1	-3.838248000	-4.118801000	-0.722739000
6	-2.393781000	-2.884445000	1.353163000
1	-2.406911000	-2.250932000	2.243507000
1	-2.813397000	-3.857570000	1.630105000
1	-1.341677000	-3.040200000	1.091878000
6	3.908838000	-0.929890000	-2.107678000
1	4.978115000	-0.763087000	-2.273619000
1	3.596716000	-1.711752000	-2.810997000

1	3.392682000	-0.002660000	-2.389326000
6	4.055744000	-0.149220000	0.268353000
1	3.551788000	0.790320000	0.023362000
1	3.845654000	-0.366656000	1.318338000
1	5.133262000	0.022964000	0.173052000
5	0.127740000	0.231157000	1.474776000
15	-2.466876000	-0.604150000	-0.291959000
15	1.808904000	-1.702394000	-0.479168000
15	0.546805000	2.278060000	-0.931712000
6	1.787223000	-3.389273000	-1.368895000
1	1.585549000	-3.097344000	-2.418178000
6	0.620091000	-4.243607000	-0.890235000
1	0.406681000	-5.060314000	-1.589403000
1	0.834437000	-4.699952000	0.080021000
1	-0.294474000	-3.658645000	-0.746909000
6	3.065276000	-4.220834000	-1.401794000
1	2.893979000	-5.142562000	-1.968913000
1	3.905717000	-3.708218000	-1.873178000
1	3.385858000	-4.526961000	-0.402838000
6	-3.884058000	0.126082000	-1.327128000
1	-3.904331000	1.169139000	-0.988468000
6	-5.286274000	-0.449813000	-1.156711000
1	-6.005748000	0.147325000	-1.727587000
1	-5.367965000	-1.475370000	-1.528169000
1	-5.634451000	-0.456490000	-0.122961000
6	-3.518064000	0.139386000	-2.807438000
1	-4.202172000	0.765731000	-3.389941000
1	-2.502553000	0.525344000	-2.973477000
1	-3.605519000	-0.867452000	-3.248838000
6	1.778374000	2.892961000	-2.224302000
1	2.741200000	2.524207000	-1.840341000
6	1.516597000	2.218613000	-3.566070000
1	0.498699000	2.420621000	-3.927532000
1	2.206374000	2.580909000	-4.335949000
1	1.645864000	1.133635000	-3.495623000
6	1.877620000	4.403021000	-2.427217000
1	1.050583000	4.783548000	-3.034720000
1	1.879093000	4.977051000	-1.498256000
1	2.797694000	4.652774000	-2.965996000
7	-0.047988000	-0.798482000	-3.230546000
1	0.899472000	-1.113535000	-3.446149000
1	-0.317318000	-0.154747000	-3.976931000
7	-0.904479000	-1.982396000	-3.384826000
1	-0.813455000	-2.490899000	-4.278969000
1	-0.691146000	-2.594131000	-2.574245000
1	-1.877831000	-1.671646000	-3.247857000

[11c''_{PB}]_{dis} (TE = -3452.390430)

6	1.719438000	-0.901713000	1.649391000
6	1.937352000	-1.791229000	2.716124000
1	1.078313000	-2.221031000	3.228721000
6	3.213245000	-2.123271000	3.157170000
1	3.337359000	-2.809001000	3.992292000
6	4.327496000	-1.573777000	2.533454000
1	5.330092000	-1.817557000	2.876278000
6	4.149240000	-0.727656000	1.444229000
1	5.026076000	-0.332596000	0.935295000
6	2.870096000	-0.399405000	0.988710000
6	-0.065855000	1.149438000	1.597935000
6	0.713719000	1.650275000	2.670565000
1	1.589798000	1.092298000	2.988969000
6	0.368530000	2.786550000	3.387637000
1	0.980849000	3.097732000	4.230656000
6	-0.758187000	3.515723000	3.028799000
1	-1.046965000	4.401986000	3.588724000
6	-1.506554000	3.107443000	1.933771000
1	-2.367481000	3.699743000	1.633695000
6	-1.190360000	1.948347000	1.217589000
6	-0.950560000	-1.412931000	1.710966000
6	-1.456419000	-1.532710000	3.014127000
1	-1.067600000	-0.886258000	3.801869000
6	-2.454979000	-2.449943000	3.319525000
1	-2.837419000	-2.518439000	4.335590000
6	-2.971327000	-3.277720000	2.325255000
1	-3.751534000	-3.997232000	2.561132000
6	-2.494537000	-3.171565000	1.025192000
1	-2.915098000	-3.807922000	0.250368000
6	-1.495147000	-2.241944000	0.716519000
23	0.105527000	0.470717000	-0.965402000
6	3.428608000	2.150739000	-0.501695000
1	4.500538000	1.974079000	-0.339257000
6	-3.856182000	1.292897000	0.126055000
1	-4.171032000	2.251138000	0.563958000
6	0.165284000	-3.363454000	-1.462583000
1	0.175046000	-3.322070000	-2.563120000
6	-0.350064000	-4.720783000	-0.998776000
1	0.332329000	-5.504927000	-1.342925000
1	-0.372707000	-4.775903000	0.093759000
1	-1.342592000	-4.976679000	-1.365288000
6	1.585066000	-3.171713000	-0.951479000
1	1.634613000	-3.274826000	0.137363000
1	2.257628000	-3.920641000	-1.382133000

1	1.973701000	-2.186468000	-1.200175000
6	3.234229000	2.879426000	-1.827909000
1	3.585027000	2.310184000	-2.693277000
1	2.177274000	3.107614000	-1.998045000
1	3.778728000	3.828817000	-1.825562000
6	2.898058000	2.985917000	0.650369000
1	3.057918000	2.507796000	1.619773000
1	3.405242000	3.956006000	0.673890000
1	1.825056000	3.186033000	0.548944000
6	-4.702117000	1.015110000	-1.111634000
1	-5.766534000	1.053374000	-0.860531000
1	-4.535469000	1.727550000	-1.924812000
1	-4.505448000	0.017090000	-1.512968000
6	-4.023408000	0.214684000	1.181430000
1	-3.736092000	-0.772237000	0.808826000
1	-3.429581000	0.412796000	2.077454000
1	-5.072694000	0.151745000	1.487365000
5	0.233671000	-0.416645000	1.387481000
15	2.635179000	0.466470000	-0.605481000
15	-2.077137000	1.589732000	-0.343896000
15	-0.882625000	-1.895258000	-0.962875000
6	-2.158921000	3.233383000	-1.270775000
1	-2.279710000	2.890601000	-2.310659000
6	-0.835833000	3.987884000	-1.186820000
1	-0.820802000	4.800348000	-1.919903000
1	-0.691019000	4.439025000	-0.200797000
1	0.024481000	3.346688000	-1.395804000
6	-3.322167000	4.168634000	-0.957893000
1	-3.284615000	5.026906000	-1.636725000
1	-4.304994000	3.711449000	-1.083372000
1	-3.272975000	4.577306000	0.055172000
6	3.783542000	-0.476831000	-1.778645000
1	3.839478000	-1.467348000	-1.310948000
6	5.210513000	0.047823000	-1.890249000
1	5.799050000	-0.638807000	-2.507333000
1	5.264630000	1.026708000	-2.373678000
1	5.723949000	0.126007000	-0.929663000
6	3.163035000	-0.639811000	-3.162321000
1	3.750430000	-1.342516000	-3.762179000
1	2.133867000	-1.011114000	-3.124962000
1	3.150417000	0.305818000	-3.715919000
6	-2.417398000	-1.934222000	-2.051260000
1	-3.187499000	-1.543940000	-1.370088000
6	-2.286097000	-0.977360000	-3.230602000
1	-1.429945000	-1.224243000	-3.867619000
1	-3.183421000	-1.025659000	-3.856093000

1	-2.164033000	0.057558000	-2.906224000
6	-2.872738000	-3.299525000	-2.552527000
1	-2.122314000	-3.775565000	-3.190986000
1	-3.128472000	-3.998414000	-1.755734000
1	-3.772277000	-3.175644000	-3.164229000
7	0.268146000	1.120703000	-2.748397000
1	1.124764000	1.185170000	-3.291267000
1	-0.491697000	1.374879000	-3.376290000

[12c''_{PB}] (TE = -3452.541427)

6	-1.533800000	0.200426000	1.871805000
6	-1.727398000	0.786433000	3.137239000
1	-0.852402000	1.087774000	3.713379000
6	-2.988049000	1.007516000	3.680040000
1	-3.084984000	1.467965000	4.661914000
6	-4.122629000	0.646320000	2.961625000
1	-5.116665000	0.818736000	3.369269000
6	-3.971812000	0.074062000	1.704469000
1	-4.863001000	-0.186399000	1.137803000
6	-2.703304000	-0.145100000	1.154961000
6	0.684517000	-1.420603000	1.744682000
6	0.351505000	-2.068444000	2.947489000
1	-0.506524000	-1.706136000	3.515336000
6	1.087338000	-3.136536000	3.448481000
1	0.792621000	-3.610103000	4.383742000
6	2.214063000	-3.583534000	2.765147000
1	2.812836000	-4.402434000	3.158485000
6	2.557711000	-2.980959000	1.559750000
1	3.430561000	-3.342912000	1.020676000
6	1.793884000	-1.936468000	1.029006000
6	0.951245000	1.203983000	1.685141000
6	1.677819000	1.193867000	2.891202000
1	1.607030000	0.318208000	3.537623000
6	2.495789000	2.246265000	3.280473000
1	3.043419000	2.193109000	4.220147000
6	2.623489000	3.362406000	2.459214000
1	3.268391000	4.190883000	2.744923000
6	1.927348000	3.403209000	1.258525000
1	2.047067000	4.270653000	0.616263000
6	1.099258000	2.343427000	0.864851000
23	-0.145227000	-0.200491000	-1.253793000
6	-2.894597000	-2.600839000	-0.401170000
1	-3.940384000	-2.657504000	-0.066197000
6	3.833946000	-0.639979000	-0.665136000
1	4.475869000	-1.493578000	-0.404180000
6	-1.043131000	3.581883000	-0.799732000

1	-1.059705000	3.913782000	-1.849450000
6	-0.777797000	4.782299000	0.097671000
1	-1.586915000	5.514481000	-0.005663000
1	-0.742311000	4.485343000	1.150776000
1	0.156316000	5.299578000	-0.127277000
6	-2.399711000	2.977408000	-0.478107000
1	-2.434937000	2.576953000	0.540365000
1	-3.191804000	3.730339000	-0.562150000
1	-2.639668000	2.161266000	-1.160682000
6	-2.762221000	-3.289531000	-1.753546000
1	-3.426846000	-2.869862000	-2.514579000
1	-1.743239000	-3.201203000	-2.141217000
1	-2.997522000	-4.356608000	-1.670776000
6	-2.022785000	-3.270642000	0.649477000
1	-2.140656000	-2.813862000	1.635943000
1	-2.281452000	-4.331823000	0.740016000
1	-0.959738000	-3.213655000	0.397190000
6	4.192673000	-0.152697000	-2.064057000
1	5.234558000	0.183485000	-2.107430000
1	4.066257000	-0.919468000	-2.834464000
1	3.565007000	0.697037000	-2.355029000
6	4.057419000	0.447089000	0.370950000
1	3.452963000	1.335695000	0.166948000
1	3.808019000	0.114371000	1.381758000
1	5.107516000	0.761053000	0.372289000
5	-0.023542000	-0.036255000	1.387521000
7	-0.265353000	-1.027995000	-3.009758000
15	0.296048000	2.260614000	-0.775641000
15	-2.501437000	-0.775857000	-0.551572000
15	2.084217000	-1.297538000	-0.667812000
6	1.562677000	2.924509000	-2.001858000
1	2.508303000	2.495516000	-1.637935000
6	1.732952000	4.434460000	-2.123535000
1	2.485259000	4.659697000	-2.888028000
1	0.808766000	4.927012000	-2.442733000
1	2.065526000	4.919060000	-1.204421000
6	1.259772000	2.336529000	-3.377752000
1	1.207174000	1.244036000	-3.367989000
1	0.295334000	2.693744000	-3.760627000
1	2.022758000	2.638097000	-4.104504000
6	2.295656000	-2.837274000	-1.748158000
1	2.146748000	-2.424224000	-2.757144000
6	1.168578000	-3.826579000	-1.490830000
1	0.193668000	-3.340821000	-1.554289000
1	1.186863000	-4.634162000	-2.231373000
1	1.255234000	-4.286962000	-0.500828000

6	3.641563000	-3.553939000	-1.749572000
1	3.622472000	-4.357841000	-2.494628000
1	4.485362000	-2.909463000	-2.005124000
1	3.865689000	-4.030154000	-0.791453000
6	-4.008544000	-0.111121000	-1.483136000
1	-4.212354000	0.839954000	-0.973499000
6	-5.290133000	-0.936647000	-1.441332000
1	-6.103071000	-0.385041000	-1.927337000
1	-5.192089000	-1.884415000	-1.978059000
1	-5.627025000	-1.174191000	-0.429618000
6	-3.626175000	0.196352000	-2.928152000
1	-2.712624000	0.797348000	-2.999787000
1	-3.447627000	-0.722229000	-3.499203000
1	-4.429309000	0.737312000	-3.441149000
1	-1.114718000	-1.195823000	-3.542986000
1	0.500245000	-1.386675000	-3.576496000

[13c''_{PB}] (TE = -3452.987807)

6	1.554535000	-0.272491000	1.900747000
6	1.683864000	-0.791264000	3.202781000
1	0.783670000	-0.953898000	3.794892000
6	2.914493000	-1.109656000	3.764200000
1	2.962523000	-1.508808000	4.775245000
6	4.081970000	-0.925654000	3.030306000
1	5.050587000	-1.175494000	3.456559000
6	3.994269000	-0.430387000	1.736517000
1	4.907053000	-0.306283000	1.156286000
6	2.754404000	-0.109267000	1.171578000
6	-0.414768000	1.617622000	1.623369000
6	0.115445000	2.369948000	2.687648000
1	0.992794000	1.990705000	3.211375000
6	-0.468306000	3.554364000	3.120540000
1	-0.034162000	4.100566000	3.955530000
6	-1.627293000	4.024958000	2.509238000
1	-2.109868000	4.932353000	2.864389000
6	-2.157187000	3.329333000	1.428321000
1	-3.058320000	3.704819000	0.947903000
6	-1.547921000	2.159877000	0.962441000
6	-1.064928000	-0.947206000	1.756755000
6	-1.757129000	-0.796252000	2.972873000
1	-1.539205000	0.070565000	3.598346000
6	-2.718218000	-1.704472000	3.398140000
1	-3.229626000	-1.551007000	4.346308000
6	-3.037835000	-2.801670000	2.603213000
1	-3.795747000	-3.513455000	2.921571000
6	-2.389482000	-2.970584000	1.387886000

1	-2.659571000	-3.815437000	0.758665000
6	-1.411701000	-2.060791000	0.964412000
23	0.166827000	0.174555000	-1.112063000
6	3.371530000	2.142996000	-0.602713000
1	4.426552000	2.027374000	-0.319797000
6	-3.880902000	1.101278000	-0.528238000
1	-4.306841000	2.091890000	-0.310479000
6	0.489996000	-3.672913000	-0.631588000
1	0.615183000	-3.954030000	-1.689694000
6	-0.030692000	-4.868806000	0.156040000
1	0.697971000	-5.684684000	0.104464000
1	-0.152710000	-4.615951000	1.213287000
1	-0.979856000	-5.264873000	-0.202503000
6	1.843118000	-3.259378000	-0.071847000
1	1.765551000	-2.947194000	0.974994000
1	2.551139000	-4.093539000	-0.112131000
1	2.273875000	-2.427416000	-0.626843000
6	3.300238000	2.738417000	-2.004848000
1	3.700610000	2.077824000	-2.780300000
1	2.269971000	2.987468000	-2.280606000
1	3.868648000	3.672284000	-2.058562000
6	2.697408000	3.043242000	0.420673000
1	2.810271000	2.664040000	1.439308000
1	3.130754000	4.048222000	0.389358000
1	1.623137000	3.146268000	0.235058000
6	-4.415080000	0.621629000	-1.871530000
1	-5.505283000	0.531775000	-1.840759000
1	-4.171705000	1.296469000	-2.698062000
1	-4.020507000	-0.367110000	-2.128020000
6	-4.256227000	0.160895000	0.605086000
1	-3.850766000	-0.844403000	0.453346000
1	-3.890843000	0.514051000	1.572670000
1	-5.344714000	0.067132000	0.674355000
5	0.080725000	0.118701000	1.414042000
15	2.653198000	0.420270000	-0.571658000
15	-2.046409000	1.381346000	-0.615086000
15	-0.639282000	-2.178975000	-0.681906000
6	-1.894261000	2.771830000	-1.873286000
1	-1.967227000	2.235820000	-2.832932000
6	-0.495485000	3.364232000	-1.752510000
1	-0.231743000	3.976156000	-2.622054000
1	-0.408827000	3.995402000	-0.862641000
1	0.290678000	2.599744000	-1.655743000
6	-2.944756000	3.872273000	-1.885326000
1	-2.778014000	4.538630000	-2.738659000
1	-3.964616000	3.491238000	-1.976045000

1	-2.895342000	4.495410000	-0.989455000
6	3.944786000	-0.620687000	-1.475211000
1	4.034590000	-1.508505000	-0.837070000
6	5.338773000	-0.019512000	-1.610351000
1	6.011904000	-0.754786000	-2.063120000
1	5.359575000	0.863074000	-2.255137000
1	5.780449000	0.266043000	-0.653036000
6	3.412372000	-1.067884000	-2.833394000
1	4.095533000	-1.780897000	-3.305828000
1	2.432373000	-1.555009000	-2.752579000
1	3.311228000	-0.224781000	-3.527520000
6	-2.046504000	-2.619371000	-1.854375000
1	-2.914279000	-2.128574000	-1.388772000
6	-1.799242000	-1.960471000	-3.208516000
1	-0.865769000	-2.312574000	-3.666704000
1	-2.605924000	-2.195176000	-3.910623000
1	-1.746147000	-0.870849000	-3.123348000
6	-2.376040000	-4.093309000	-2.050149000
1	-1.523550000	-4.660490000	-2.436883000
1	-2.718600000	-4.586187000	-1.139686000
1	-3.181544000	-4.194970000	-2.784947000
7	0.417470000	0.570148000	-3.342410000
1	-0.377556000	0.961747000	-3.843650000
1	1.198237000	1.185482000	-3.563620000
1	0.629018000	-0.300314000	-3.825517000

[14c''_{PB}] (TE = -3453.112714)

6	1.418563000	-0.557239000	1.832685000
6	1.541898000	-1.289400000	3.028031000
1	0.636352000	-1.538007000	3.582706000
6	2.769137000	-1.713302000	3.527601000
1	2.813500000	-2.283536000	4.454251000
6	3.936762000	-1.404304000	2.839277000
1	4.905819000	-1.724702000	3.217109000
6	3.851309000	-0.694343000	1.646322000
1	4.767638000	-0.478107000	1.101915000
6	2.616808000	-0.285356000	1.129336000
6	-0.417567000	1.456226000	1.808522000
6	0.013520000	1.939723000	3.056347000
1	0.690354000	1.322172000	3.648700000
6	-0.388169000	3.171122000	3.564256000
1	-0.020850000	3.507614000	4.532704000
6	-1.267835000	3.965126000	2.836883000
1	-1.601707000	4.924750000	3.226754000
6	-1.709635000	3.522120000	1.594207000
1	-2.389156000	4.151663000	1.023382000

6	-1.279159000	2.301333000	1.063073000
6	-1.225122000	-1.088124000	1.683929000
6	-1.956707000	-0.963555000	2.878922000
1	-1.707055000	-0.149651000	3.561082000
6	-3.003767000	-1.815517000	3.210992000
1	-3.548545000	-1.674679000	4.143366000
6	-3.364305000	-2.834130000	2.335763000
1	-4.194900000	-3.497969000	2.568261000
6	-2.655811000	-2.992276000	1.150583000
1	-2.959079000	-3.782126000	0.467639000
6	-1.591714000	-2.144003000	0.818814000
23	0.080412000	0.090178000	-1.144174000
6	3.304115000	2.137876000	-0.322125000
1	4.335982000	1.947799000	0.007062000
6	-3.529920000	1.484799000	-0.656945000
1	-4.007460000	2.446960000	-0.425280000
6	0.418021000	-3.769486000	-0.637799000
1	0.217411000	-4.360836000	-1.541311000
6	0.136483000	-4.634462000	0.582211000
1	0.800398000	-5.507055000	0.593206000
1	0.312250000	-4.078604000	1.509605000
1	-0.891090000	-5.003260000	0.623730000
6	1.882753000	-3.364844000	-0.674182000
1	2.152843000	-2.737215000	0.181237000
1	2.529577000	-4.250150000	-0.649479000
1	2.121404000	-2.801413000	-1.579877000
6	3.339114000	2.892454000	-1.644870000
1	3.896763000	2.366599000	-2.424993000
1	2.327991000	3.057193000	-2.031100000
1	3.800465000	3.879541000	-1.526405000
6	2.596093000	2.939591000	0.759343000
1	2.636754000	2.438556000	1.730576000
1	3.054971000	3.928599000	0.873479000
1	1.536841000	3.091512000	0.527488000
6	-3.952882000	1.028375000	-2.047552000
1	-5.039407000	0.900982000	-2.112368000
1	-3.660505000	1.725057000	-2.841272000
1	-3.497258000	0.057636000	-2.281821000
6	-3.963288000	0.477560000	0.391903000
1	-3.539793000	-0.512419000	0.198349000
1	-3.656774000	0.768833000	1.399866000
1	-5.054508000	0.372031000	0.391994000
5	-0.037421000	-0.049084000	1.411994000
15	2.489984000	0.459971000	-0.548100000
15	-1.678308000	1.794184000	-0.654766000
15	-0.724659000	-2.257400000	-0.800911000

6	-1.629271000	3.369471000	-1.718205000
1	-1.547897000	2.946373000	-2.732797000
6	-0.353052000	4.153704000	-1.455856000
1	-0.204206000	4.931439000	-2.213528000
1	-0.376403000	4.648104000	-0.479391000
1	0.524000000	3.503163000	-1.461252000
6	-2.836864000	4.301233000	-1.729958000
1	-2.658776000	5.127140000	-2.429057000
1	-3.760225000	3.812565000	-2.048350000
1	-3.028028000	4.758187000	-0.755199000
6	3.818977000	-0.477405000	-1.533637000
1	3.814897000	-1.464868000	-1.053742000
6	5.253336000	0.041560000	-1.508865000
1	5.915794000	-0.671185000	-2.014106000
1	5.363743000	0.994046000	-2.034893000
1	5.653083000	0.184680000	-0.503020000
6	3.359632000	-0.660720000	-2.976273000
1	4.050838000	-1.302215000	-3.535278000
1	2.365547000	-1.118874000	-3.023140000
1	3.309747000	0.296165000	-3.511464000
6	-2.072556000	-2.910183000	-1.958741000
1	-2.984407000	-2.440809000	-1.558972000
6	-1.833558000	-2.363292000	-3.361777000
1	-0.869451000	-2.703945000	-3.763526000
1	-2.609280000	-2.700347000	-4.059406000
1	-1.825362000	-1.269732000	-3.369744000
6	-2.289458000	-4.418597000	-2.035307000
1	-1.492506000	-4.911488000	-2.601506000
1	-2.340101000	-4.912237000	-1.062719000
1	-3.224767000	-4.642034000	-2.561331000
7	0.152782000	0.553012000	-3.376369000
1	-0.751525000	0.825970000	-3.753891000
1	0.772707000	1.338321000	-3.559839000
1	0.480970000	-0.197673000	-3.978577000

Cartesian coordinates of $[5f''_{SB}]-[14f''_{SB}]$, along with their total energies (in hartree) including zero point vibrational correction at M06-L-D3(heptane)/6-311+G* level of theory.

$[5f''_{SB}]_{alt}$ (TE = -3322.249460)

6	1.430079000	0.268980000	1.582946000
6	1.737640000	-0.139990000	2.892937000
1	0.951743000	-0.587288000	3.502066000
6	3.008733000	0.008304000	3.436366000
1	3.202333000	-0.316401000	4.456084000

6	4.035806000	0.557093000	2.673873000
1	5.035042000	0.664519000	3.087743000
6	3.782764000	0.938601000	1.362958000
1	4.584288000	1.326390000	0.737770000
6	2.494993000	0.800128000	0.841598000
6	-1.094087000	1.294478000	1.419771000
6	-1.015247000	2.008933000	2.626298000
1	-0.156528000	1.847937000	3.277947000
6	-2.012660000	2.892536000	3.023774000
1	-1.923829000	3.419083000	3.971160000
6	-3.124146000	3.107294000	2.212932000
1	-3.902895000	3.801983000	2.516676000
6	-3.214289000	2.461112000	0.985498000
1	-4.045766000	2.668347000	0.315212000
6	-2.209607000	1.571572000	0.611920000
6	-0.721619000	-1.326726000	1.220943000
6	-1.583363000	-1.576272000	2.304365000
1	-1.829793000	-0.755653000	2.977936000
6	-2.136448000	-2.829608000	2.541441000
1	-2.792374000	-2.977965000	3.396321000
6	-1.868652000	-3.887294000	1.678252000
1	-2.311736000	-4.865469000	1.846141000
6	-1.035629000	-3.680434000	0.585173000
1	-0.827376000	-4.489228000	-0.111641000
6	-0.464598000	-2.423714000	0.380910000
16	0.540322000	-2.204142000	-1.086440000
16	2.272536000	1.172558000	-0.898827000
16	-2.177289000	0.934394000	-1.059175000
23	0.094136000	0.173710000	-1.553816000
6	2.111185000	3.038285000	-0.959505000
1	3.106026000	3.379363000	-0.648707000
6	-3.680259000	-0.143978000	-1.334717000
1	-4.494733000	0.576304000	-1.471730000
6	2.298308000	-2.505130000	-0.504322000
1	2.507536000	-1.712472000	0.220012000
6	3.183329000	-2.365000000	-1.725724000
1	4.232639000	-2.465927000	-1.433517000
1	2.974110000	-3.144489000	-2.464918000
1	3.075791000	-1.391813000	-2.214092000
6	2.396230000	-3.858799000	0.160063000
1	2.125306000	-4.668543000	-0.524710000
1	3.427993000	-4.030020000	0.482632000
1	1.761567000	-3.932121000	1.046219000
6	1.859760000	3.410136000	-2.406374000
1	2.614234000	3.000576000	-3.082722000
1	0.877434000	3.070340000	-2.753865000

1	1.874861000	4.498397000	-2.513941000
6	1.058603000	3.560344000	-0.011261000
1	1.217876000	3.223983000	1.016212000
1	1.081146000	4.655010000	-0.007717000
1	0.049774000	3.256271000	-0.311578000
6	-3.424311000	-0.891431000	-2.627427000
1	-4.308300000	-1.477752000	-2.893442000
1	-3.206036000	-0.222110000	-3.463738000
1	-2.585752000	-1.589319000	-2.517223000
6	-3.958739000	-1.050416000	-0.161069000
1	-3.183789000	-1.813017000	-0.049355000
1	-4.037323000	-0.503669000	0.781879000
1	-4.911760000	-1.564248000	-0.324524000
5	-0.076792000	0.123676000	1.099376000
7	-0.104522000	0.849947000	-4.352709000
7	0.161406000	-0.121691000	-3.562682000
1	-0.041447000	0.549588000	-5.338135000
1	0.388606000	-1.021099000	-4.016462000

$[5f'_{SB}]_{dis}$ (TE = -3322.260350)

6	-0.140609000	1.317143000	-1.668972000
6	-0.882531000	1.735071000	-2.788713000
1	-1.655847000	1.076975000	-3.185708000
6	-0.645238000	2.952613000	-3.415942000
1	-1.229391000	3.235707000	-4.288087000
6	0.325000000	3.813410000	-2.914122000
1	0.507223000	4.775106000	-3.386754000
6	1.033121000	3.457981000	-1.772800000
1	1.744113000	4.154470000	-1.333032000
6	0.812438000	2.219310000	-1.170087000
6	0.749860000	-1.224066000	-1.656042000
6	1.060701000	-1.323801000	-3.022840000
1	0.635629000	-0.599867000	-3.718717000
6	1.885035000	-2.330404000	-3.511949000
1	2.097192000	-2.386493000	-4.576785000
6	2.452518000	-3.253241000	-2.638103000
1	3.110221000	-4.033486000	-3.012276000
6	2.209477000	-3.148262000	-1.274583000
1	2.698710000	-3.823988000	-0.576369000
6	1.356593000	-2.151381000	-0.800591000
6	-1.810055000	-0.719688000	-1.025850000
6	-2.355695000	-1.563894000	-2.006971000
1	-1.726910000	-1.885200000	-2.837137000
6	-3.676790000	-1.992174000	-1.950966000
1	-4.072508000	-2.633132000	-2.734907000
6	-4.481695000	-1.627205000	-0.876553000

1	-5.505273000	-1.986400000	-0.808604000
6	-3.958746000	-0.836901000	0.140402000
1	-4.555809000	-0.613761000	1.020155000
6	-2.647523000	-0.370106000	0.044653000
16	-1.917846000	0.470918000	1.448405000
16	1.611072000	1.940325000	0.409551000
16	1.234099000	-1.923078000	0.969139000
23	0.486495000	0.295945000	1.852657000
6	3.413134000	1.676297000	-0.019648000
1	3.709614000	2.653670000	-0.419195000
6	0.240884000	-3.381801000	1.586371000
1	0.922544000	-4.229443000	1.449154000
6	-2.698493000	2.169152000	1.555521000
1	-2.145124000	2.565813000	2.416512000
6	-4.173107000	2.073215000	1.883113000
1	-4.556918000	3.071981000	2.112637000
1	-4.748952000	1.701324000	1.031171000
1	-4.373243000	1.433294000	2.745369000
6	-2.419213000	2.992102000	0.319427000
1	-2.837939000	2.523293000	-0.576975000
1	-2.888991000	3.975870000	0.421327000
1	-1.351599000	3.146338000	0.154313000
6	4.141857000	1.404690000	1.279436000
1	3.974655000	2.187984000	2.023075000
1	3.828062000	0.449836000	1.713968000
1	5.217670000	1.346677000	1.089868000
6	3.623563000	0.601504000	-1.058272000
1	3.031415000	0.769940000	-1.961507000
1	4.677828000	0.583948000	-1.354423000
1	3.375915000	-0.388888000	-0.667386000
6	0.004540000	-3.146327000	3.065170000
1	-0.451787000	-4.033921000	3.512463000
1	0.926687000	-2.937079000	3.613412000
1	-0.692167000	-2.316077000	3.233993000
6	-1.032874000	-3.596679000	0.804495000
1	-1.742144000	-2.778695000	0.959219000
1	-0.853348000	-3.691041000	-0.269620000
1	-1.515835000	-4.520246000	1.140431000
5	-0.352579000	-0.179551000	-1.253156000
7	1.941771000	0.991978000	4.412208000
7	1.363151000	0.784095000	3.240963000
1	1.836867000	1.930324000	4.790439000
1	2.894399000	0.643683000	4.495430000

[6f''_{SB}]_{alt} (TE = -3322.393810)

6	0.448473000	-1.571308000	1.327472000
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6	0.003729000	-2.250029000	2.476138000
1	-0.784569000	-1.795605000	3.077685000
6	0.534450000	-3.471647000	2.877179000
1	0.160309000	-3.958071000	3.776317000
6	1.540094000	-4.073693000	2.126681000
1	1.957773000	-5.032288000	2.426527000
6	1.981620000	-3.454802000	0.962767000
1	2.728673000	-3.938679000	0.335674000
6	1.443065000	-2.226951000	0.576279000
6	0.920738000	1.050363000	1.485602000
6	1.444326000	0.989796000	2.790584000
1	1.213957000	0.117564000	3.404078000
6	2.248480000	1.989782000	3.324469000
1	2.627836000	1.897473000	4.340559000
6	2.579718000	3.103034000	2.556181000
1	3.216134000	3.886934000	2.960638000
6	2.119199000	3.184119000	1.248757000
1	2.411509000	4.018883000	0.613867000
6	1.304725000	2.173110000	0.734282000
6	-1.625449000	0.207640000	1.335376000
6	-1.951241000	0.618862000	2.642287000
1	-1.145257000	0.727445000	3.368133000
6	-3.248515000	0.913067000	3.044482000
1	-3.440689000	1.229388000	4.068161000
6	-4.295824000	0.823456000	2.133117000
1	-5.313361000	1.070292000	2.427419000
6	-4.020438000	0.442636000	0.826957000
1	-4.815899000	0.412221000	0.085437000
6	-2.712351000	0.128491000	0.444358000
16	-2.451911000	-0.207430000	-1.306418000
16	1.889086000	-1.577796000	-1.037612000
16	0.892905000	2.232999000	-1.009916000
23	0.021817000	-0.022140000	-1.540627000
6	3.687875000	-1.097384000	-0.860020000
1	4.210261000	-2.058675000	-0.772475000
6	-0.371862000	3.605633000	-1.116552000
1	0.206165000	4.514980000	-0.909429000
6	-2.902054000	-2.022092000	-1.474237000
1	-2.691130000	-2.181723000	-2.540135000
6	-4.376785000	-2.233288000	-1.202612000
1	-4.656706000	-3.265388000	-1.439299000
1	-4.611774000	-2.071738000	-0.146065000
1	-5.009623000	-1.568898000	-1.796761000
6	-2.019399000	-2.912534000	-0.629822000
1	-2.107101000	-2.667777000	0.433889000
1	-2.315385000	-3.960397000	-0.752019000

1	-0.964011000	-2.827634000	-0.903005000
6	4.070250000	-0.416577000	-2.158068000
1	3.863679000	-1.039209000	-3.031167000
1	3.512291000	0.516910000	-2.289433000
1	5.137294000	-0.171012000	-2.151686000
6	3.956548000	-0.246418000	0.358707000
1	3.587964000	-0.706984000	1.279449000
1	5.036120000	-0.093479000	0.472124000
1	3.490651000	0.738262000	0.268675000
6	-0.866877000	3.619007000	-2.548847000
1	-1.570057000	4.444303000	-2.698523000
1	-0.053800000	3.735406000	-3.270458000
1	-1.395499000	2.688024000	-2.787237000
6	-1.488794000	3.454131000	-0.110544000
1	-2.109232000	2.582479000	-0.334126000
1	-1.119303000	3.346279000	0.912962000
1	-2.137037000	4.337145000	-0.139740000
5	-0.086587000	-0.103408000	1.001844000
7	1.051084000	-0.784216000	-4.216988000
7	-0.023033000	-0.531563000	-3.502314000
1	0.766295000	-1.083368000	-5.162988000
1	-0.905522000	-0.641398000	-4.021888000

$[6f'_{SB}]_{dis}$ (TE = -3322.418409)

6	-1.407438000	-0.404570000	1.505664000
6	-2.107240000	0.141004000	2.598130000
1	-1.740363000	1.067790000	3.041527000
6	-3.247204000	-0.451817000	3.129350000
1	-3.753459000	0.006323000	3.977046000
6	-3.748155000	-1.623680000	2.569165000
1	-4.645307000	-2.090421000	2.969607000
6	-3.108778000	-2.175816000	1.466109000
1	-3.512355000	-3.064777000	0.984383000
6	-1.958788000	-1.572792000	0.951357000
6	1.282700000	-0.138182000	1.746228000
6	1.305429000	-0.312482000	3.141481000
1	0.369391000	-0.222631000	3.694060000
6	2.473976000	-0.590720000	3.841897000
1	2.442994000	-0.715395000	4.922812000
6	3.681739000	-0.716569000	3.160965000
1	4.600256000	-0.942367000	3.698058000
6	3.696882000	-0.588684000	1.777522000
1	4.622123000	-0.737632000	1.223284000
6	2.515397000	-0.303415000	1.091145000
6	-0.201675000	1.894825000	0.829910000
6	0.246902000	2.775108000	1.829915000

1	0.736526000	2.358609000	2.711094000
6	0.106503000	4.155688000	1.728090000
1	0.475998000	4.798742000	2.525020000
6	-0.492415000	4.715949000	0.604265000
1	-0.593814000	5.794686000	0.508911000
6	-0.945582000	3.880430000	-0.411387000
1	-1.394274000	4.297455000	-1.310879000
6	-0.804211000	2.498051000	-0.288657000
16	-1.269686000	1.474967000	-1.689074000
16	-1.281402000	-2.229001000	-0.574684000
16	2.552365000	-0.356270000	-0.703070000
23	0.237723000	-0.503204000	-1.495801000
6	-0.351212000	-3.752130000	-0.008111000
1	-1.147119000	-4.434748000	0.315905000
6	3.490241000	1.195972000	-1.173649000
1	4.492930000	1.036716000	-0.756867000
6	-3.053019000	1.024031000	-1.313798000
1	-3.018888000	0.447357000	-0.384041000
6	-3.526220000	0.151128000	-2.457888000
1	-4.534985000	-0.220790000	-2.251441000
1	-3.566633000	0.711645000	-3.397712000
1	-2.878564000	-0.716537000	-2.612884000
6	-3.894011000	2.265880000	-1.125086000
1	-3.891164000	2.894752000	-2.021915000
1	-4.932915000	1.983553000	-0.922189000
1	-3.550501000	2.872903000	-0.283694000
6	0.354196000	-4.310123000	-1.227278000
1	-0.327246000	-4.482829000	-2.064821000
1	1.132593000	-3.619451000	-1.570060000
1	0.834711000	-5.261863000	-0.978978000
6	0.596027000	-3.469274000	1.134119000
1	0.099875000	-2.991233000	1.983205000
1	1.037117000	-4.406985000	1.490738000
1	1.415534000	-2.817496000	0.817147000
6	3.547287000	1.213033000	-2.687414000
1	4.132332000	2.070569000	-3.034486000
1	4.002468000	0.306643000	-3.097195000
1	2.539650000	1.301810000	-3.110433000
6	2.867807000	2.444202000	-0.597537000
1	1.864930000	2.606829000	-1.005273000
1	2.780104000	2.400322000	0.491072000
1	3.477080000	3.319846000	-0.849676000
5	-0.065157000	0.317407000	1.024139000
7	0.912821000	-1.745739000	-4.209243000
7	0.591328000	-1.126179000	-3.042755000
1	1.057468000	-1.070291000	-4.960205000

1 1.767354000 -2.296445000 -4.112198000

[7f'_{SB}]_{alt} (TE = -3322.850322)

6 -1.395247000 0.158804000 1.701261000
6 -1.589286000 0.760501000 2.958125000
1 -0.737435000 1.228592000 3.452078000
6 -2.825444000 0.774218000 3.592940000
1 -2.928408000 1.246256000 4.567312000
6 -3.933541000 0.196287000 2.979311000
1 -4.905368000 0.209950000 3.465720000
6 -3.796539000 -0.365836000 1.717995000
1 -4.662517000 -0.772877000 1.199954000
6 -2.541767000 -0.383737000 1.103995000
6 1.018081000 -1.086379000 1.639473000
6 0.911126000 -1.568068000 2.955660000
1 0.099639000 -1.203359000 3.584239000
6 1.821781000 -2.473949000 3.488599000
1 1.711293000 -2.810053000 4.517040000
6 2.871298000 -2.955317000 2.710859000
1 3.581347000 -3.668953000 3.120509000
6 2.982683000 -2.548630000 1.386599000
1 3.761409000 -2.961363000 0.748249000
6 2.068776000 -1.628070000 0.877783000
6 0.849700000 1.490343000 0.976460000
6 1.718452000 1.887012000 2.009101000
1 1.883032000 1.207045000 2.845262000
6 2.383249000 3.107873000 1.995377000
1 3.041781000 3.374389000 2.819100000
6 2.223082000 3.979965000 0.922855000
1 2.752507000 4.928844000 0.896326000
6 1.386205000 3.621572000 -0.126793000
1 1.260034000 4.280681000 -0.982796000
6 0.705417000 2.403804000 -0.081336000
16 -0.307662000 1.979919000 -1.500097000
16 -2.483176000 -0.947370000 -0.601397000
16 2.075464000 -1.281740000 -0.878239000
23 -0.181209000 -0.474632000 -1.391499000
6 -2.487491000 -2.811798000 -0.496767000
1 -3.308507000 -3.033495000 0.194689000
6 3.658845000 -0.375944000 -1.306261000
1 4.408331000 -1.175769000 -1.304341000
6 -2.031628000 2.550187000 -1.029975000
1 -2.330354000 1.918893000 -0.186209000
6 -2.908530000 2.291929000 -2.238452000
1 -3.948315000 2.531607000 -1.997846000
1 -2.615560000 2.919477000 -3.085620000

1	-2.883727000	1.247244000	-2.562030000
6	-2.002190000	4.000834000	-0.607255000
1	-1.635999000	4.649765000	-1.408986000
1	-3.017078000	4.325381000	-0.357465000
1	-1.380708000	4.163365000	0.276118000
6	-2.800651000	-3.332981000	-1.884263000
1	-3.760581000	-2.971080000	-2.257754000
1	-2.030186000	-3.042353000	-2.607214000
1	-2.836871000	-4.426079000	-1.870172000
6	-1.177043000	-3.330046000	0.052132000
1	-0.925475000	-2.898405000	1.023736000
1	-1.213722000	-4.418303000	0.167096000
1	-0.343549000	-3.123453000	-0.638672000
6	3.473464000	0.162885000	-2.709248000
1	4.407733000	0.614670000	-3.054686000
1	3.198617000	-0.615998000	-3.425705000
1	2.700889000	0.938949000	-2.735359000
6	4.011520000	0.684018000	-0.292459000
1	3.316315000	1.525683000	-0.329908000
1	4.026701000	0.298337000	0.729904000
1	5.012862000	1.067939000	-0.513840000
5	0.088086000	0.097823000	1.124233000
7	0.035753000	-1.866049000	-4.085270000
7	-0.155014000	-0.729965000	-3.296690000
1	0.650838000	-1.670919000	-4.874498000
1	0.476706000	-2.591848000	-3.525193000
1	-0.383418000	0.036966000	-3.930553000

[7F'_{SB}]_{dis} (TE = -3322.818914)

6	-0.408187000	1.673604000	1.311348000
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6	-0.455233000	3.641161000	2.763611000
1	-0.074390000	4.163670000	3.638222000
6	-1.444594000	4.227479000	1.979280000
1	-1.840340000	5.208152000	2.231009000
6	-1.897608000	3.566464000	0.844426000
1	-2.629080000	4.036925000	0.190449000
6	-1.384994000	2.307999000	0.531898000
6	-0.891528000	-0.940907000	1.658766000
6	-1.429117000	-0.769712000	2.946873000
1	-1.253923000	0.170730000	3.469642000
6	-2.170113000	-1.762274000	3.577617000
1	-2.561958000	-1.592384000	4.577939000
6	-2.421871000	-2.966524000	2.926667000
1	-3.011514000	-3.742652000	3.407997000

6	-1.944271000	-3.157172000	1.636260000
1	-2.178242000	-4.070758000	1.093244000
6	-1.186697000	-2.156754000	1.026756000
6	1.634673000	-0.105579000	1.311463000
6	2.052095000	-0.507360000	2.593003000
1	1.298989000	-0.671898000	3.363675000
6	3.390117000	-0.711185000	2.908299000
1	3.668548000	-1.018318000	3.913885000
6	4.368800000	-0.550118000	1.932602000
1	5.415221000	-0.734512000	2.162005000
6	3.993822000	-0.188062000	0.645444000
1	4.738713000	-0.119113000	-0.143427000
6	2.648180000	0.049960000	0.354898000
16	2.202595000	0.336982000	-1.357387000
16	-1.829067000	1.572274000	-1.036672000
16	-0.741043000	-2.361222000	-0.692663000
23	-0.195146000	-0.164817000	-1.686156000
6	-3.613226000	1.047421000	-0.838330000
1	-4.144102000	2.003418000	-0.753627000
6	0.584620000	-3.683940000	-0.681898000
1	0.029215000	-4.586643000	-0.399995000
6	2.628840000	2.132685000	-1.685560000
1	2.339023000	2.206901000	-2.741814000
6	4.120039000	2.352863000	-1.542783000
1	4.376301000	3.359862000	-1.886601000
1	4.435075000	2.282904000	-0.497609000
1	4.707681000	1.640692000	-2.127007000
6	1.812710000	3.088515000	-0.847558000
1	1.977477000	2.926299000	0.222377000
1	2.104797000	4.120338000	-1.070094000
1	0.741706000	2.998169000	-1.040035000
6	-4.004752000	0.352049000	-2.126088000
1	-3.841464000	0.984968000	-3.003719000
1	-3.436747000	-0.575795000	-2.258596000
1	-5.066167000	0.088924000	-2.100622000
6	-3.852501000	0.203289000	0.389471000
1	-3.482298000	0.679926000	1.300595000
1	-4.927822000	0.038002000	0.515829000
1	-3.374609000	-0.776140000	0.303197000
6	1.085582000	-3.806522000	-2.106008000
1	1.807433000	-4.625343000	-2.176705000
1	0.279901000	-4.010773000	-2.816422000
1	1.596468000	-2.890728000	-2.424146000
6	1.686330000	-3.412688000	0.313357000
1	2.294557000	-2.555482000	0.014097000
1	1.305016000	-3.222107000	1.319879000

1	2.348258000	-4.283455000	0.370000000
5	0.086353000	0.181780000	1.101664000
7	-0.865281000	-0.162473000	-4.757960000
7	-0.473132000	-0.230642000	-3.405565000
1	-0.066439000	-0.009849000	-5.385535000
1	-1.324719000	-1.025657000	-5.074048000
1	-1.526656000	0.604632000	-4.934935000

[8f''_{SB}]_{alt} (TE = -3322.999688)

6	-0.517402000	1.347502000	1.518235000
6	-0.083285000	1.909095000	2.732507000
1	0.739045000	1.428780000	3.263864000
6	-0.666395000	3.044673000	3.284305000
1	-0.298585000	3.439737000	4.229619000
6	-1.716665000	3.678575000	2.626758000
1	-2.175105000	4.571935000	3.044900000
6	-2.151213000	3.180284000	1.403924000
1	-2.933593000	3.696261000	0.849791000
6	-1.560485000	2.035546000	0.867926000
6	-0.873613000	-1.289083000	1.316558000
6	-1.413060000	-1.434657000	2.608254000
1	-1.233808000	-0.645156000	3.339720000
6	-2.169681000	-2.538018000	2.984917000
1	-2.564064000	-2.606780000	3.997153000
6	-2.433664000	-3.550115000	2.065154000
1	-3.031932000	-4.413560000	2.347373000
6	-1.955577000	-3.427474000	0.767098000
1	-2.196212000	-4.181167000	0.019080000
6	-1.189730000	-2.315134000	0.412277000
6	1.630312000	-0.331315000	1.321107000
6	1.958694000	-0.879140000	2.576445000
1	1.150993000	-1.096534000	3.275506000
6	3.261718000	-1.173400000	2.959012000
1	3.455913000	-1.597946000	3.942363000
6	4.313276000	-0.944186000	2.077256000
1	5.336263000	-1.188046000	2.354672000
6	4.036167000	-0.426093000	0.819727000
1	4.836652000	-0.284051000	0.096761000
6	2.721180000	-0.114368000	0.458751000
16	2.464752000	0.411767000	-1.244299000
16	-2.011464000	1.555422000	-0.802921000
16	-0.751214000	-2.100744000	-1.312926000
23	-0.001338000	0.252687000	-1.539919000
6	-3.783458000	0.983979000	-0.659016000
1	-4.336097000	1.896196000	-0.400706000
6	0.557478000	-3.403831000	-1.600343000

1	0.006392000	-4.350259000	-1.532963000
6	2.848471000	2.245393000	-1.193069000
1	2.625174000	2.524803000	-2.230383000
6	4.315165000	2.475711000	-0.894758000
1	4.555260000	3.538836000	-1.002956000
1	4.559540000	2.194766000	0.134426000
1	4.970378000	1.913778000	-1.565363000
6	1.935622000	2.992040000	-0.246914000
1	2.034062000	2.621668000	0.778928000
1	2.193460000	4.056951000	-0.238580000
1	0.884862000	2.902685000	-0.535514000
6	-4.187568000	0.513071000	-2.041517000
1	-4.066807000	1.294664000	-2.797318000
1	-3.591071000	-0.353028000	-2.351126000
1	-5.237949000	0.205688000	-2.045633000
6	-3.984724000	-0.065439000	0.407936000
1	-3.603764000	0.256214000	1.380866000
1	-5.053907000	-0.278181000	0.522510000
1	-3.484888000	-1.001907000	0.147552000
6	1.067511000	-3.197960000	-3.012344000
1	1.801048000	-3.970251000	-3.263991000
1	0.267348000	-3.241140000	-3.756026000
1	1.564978000	-2.226240000	-3.111915000
6	1.657916000	-3.363592000	-0.565964000
1	2.255143000	-2.453071000	-0.657157000
1	1.274697000	-3.409802000	0.457143000
1	2.331684000	-4.215854000	-0.708520000
5	0.083544000	-0.038136000	1.007255000
7	-0.984299000	1.742542000	-4.011279000
7	0.101340000	1.234271000	-3.207064000
1	-1.447601000	2.477331000	-3.472916000
1	-1.678166000	0.999149000	-4.079396000
1	0.949306000	1.459233000	-3.724493000

$[8f'_{SB}]_{dis}$ (TE = -3266.488000)

6	-0.766815000	1.968619000	0.519001000
6	-0.479397000	3.121869000	1.272516000
1	0.390339000	3.115430000	1.929266000
6	-1.284420000	4.254926000	1.231051000
1	-1.034496000	5.120142000	1.842270000
6	-2.411718000	4.284397000	0.413707000
1	-3.045459000	5.167385000	0.375653000
6	-2.692767000	3.191220000	-0.399650000
1	-3.526495000	3.229763000	-1.098755000
6	-1.876989000	2.063419000	-0.347670000
6	-0.926964000	-0.569373000	1.306843000

6	-1.626933000	-0.185771000	2.471223000
1	-1.555173000	0.852143000	2.796843000
6	-2.405197000	-1.058532000	3.219563000
1	-2.909557000	-0.701694000	4.115491000
6	-2.551930000	-2.380507000	2.811860000
1	-3.168983000	-3.074811000	3.377337000
6	-1.920770000	-2.796154000	1.648831000
1	-2.058854000	-3.813245000	1.286706000
6	-1.116126000	-1.913759000	0.918809000
6	1.487067000	0.623192000	1.318988000
6	1.658978000	0.902334000	2.687540000
1	0.777956000	1.102999000	3.297459000
6	2.907779000	0.917686000	3.297129000
1	2.989968000	1.139960000	4.359368000
6	4.050088000	0.631847000	2.554417000
1	5.030490000	0.626939000	3.025095000
6	3.922884000	0.326557000	1.206594000
1	4.797847000	0.060443000	0.617089000
6	2.660910000	0.336511000	0.604753000
16	2.551651000	-0.183819000	-1.110169000
16	-2.071487000	0.783914000	-1.582704000
16	-0.445715000	-2.580636000	-0.609404000
23	0.140861000	-0.424702000	-1.640632000
6	-3.787308000	0.077706000	-1.347121000
1	-4.438496000	0.825884000	-1.815548000
6	0.940996000	-3.702672000	-0.027061000
1	0.402795000	-4.570854000	0.373489000
6	2.937172000	1.383825000	-2.059452000
1	2.801583000	1.020582000	-3.084684000
6	4.369696000	1.808046000	-1.817680000
1	4.623595000	2.645406000	-2.476050000
1	4.517024000	2.152483000	-0.789091000
1	5.081468000	1.001855000	-2.012879000
6	1.940935000	2.483223000	-1.761212000
1	1.918860000	2.732538000	-0.694828000
1	2.216592000	3.392779000	-2.306206000
1	0.925973000	2.213343000	-2.069169000
6	-3.828524000	-1.207239000	-2.149610000
1	-3.514369000	-1.063600000	-3.186771000
1	-3.177864000	-1.968607000	-1.706523000
1	-4.847298000	-1.607411000	-2.160290000
6	-4.176729000	-0.114293000	0.099659000
1	-4.043625000	0.793916000	0.693327000
1	-5.235317000	-0.393171000	0.154626000
1	-3.599281000	-0.912865000	0.570034000
6	1.718961000	-4.098352000	-1.264856000

1	2.493028000	-4.826185000	-1.002112000
1	1.083193000	-4.549935000	-2.030803000
1	2.216230000	-3.231060000	-1.711218000
6	1.803797000	-3.089001000	1.049495000
1	2.409594000	-2.268025000	0.661204000
1	1.221901000	-2.709350000	1.893652000
1	2.493916000	-3.846232000	1.437733000
5	0.011035000	0.607541000	0.710057000
7	0.376671000	-0.399456000	-3.198147000

$[9f'_{SB}]_{alt}$ (TE = -3323.442488)

6	0.232717000	2.089619000	-0.410606000
6	-0.376993000	3.215365000	-0.995645000
1	-1.199924000	3.060797000	-1.692720000
6	0.045830000	4.513555000	-0.734615000
1	-0.445282000	5.351555000	-1.224349000
6	1.091346000	4.743268000	0.155025000
1	1.423576000	5.755686000	0.370166000
6	1.687062000	3.665038000	0.797276000
1	2.469466000	3.830482000	1.535326000
6	1.266142000	2.366183000	0.510157000
6	0.898810000	-0.143132000	-1.736598000
6	1.397492000	0.504156000	-2.882031000
1	1.062657000	1.519462000	-3.096501000
6	2.312246000	-0.094412000	-3.739430000
1	2.665654000	0.443341000	-4.616396000
6	2.792359000	-1.372917000	-3.467144000
1	3.519562000	-1.843172000	-4.124064000
6	2.355218000	-2.035043000	-2.327889000
1	2.749865000	-3.017758000	-2.077282000
6	1.416770000	-1.424362000	-1.493038000
6	-1.722610000	0.412503000	-1.317667000
6	-2.051592000	0.727891000	-2.649488000
1	-1.258232000	1.062716000	-3.317295000
6	-3.341591000	0.621439000	-3.153778000
1	-3.539654000	0.879029000	-4.191851000
6	-4.374324000	0.169373000	-2.338075000
1	-5.385314000	0.069446000	-2.724417000
6	-4.092698000	-0.184227000	-1.026996000
1	-4.875448000	-0.584617000	-0.386583000
6	-2.792112000	-0.049878000	-0.530371000
16	-2.518414000	-0.711853000	1.127496000
16	1.929680000	1.030099000	1.508811000
16	0.958628000	-2.291026000	0.009355000
23	-0.055205000	-0.467397000	1.315269000
6	3.719611000	0.783239000	0.981005000

1	4.241609000	1.553944000	1.559624000
6	-0.178811000	-3.653662000	-0.580363000
1	0.504662000	-4.331760000	-1.105271000
6	-2.936914000	0.691817000	2.294504000
1	-2.935728000	0.164756000	3.257486000
6	-4.311147000	1.255514000	2.015832000
1	-4.561124000	2.010878000	2.767108000
1	-4.350759000	1.743361000	1.037806000
1	-5.086396000	0.486721000	2.044537000
6	-1.855513000	1.753301000	2.273598000
1	-1.771321000	2.229248000	1.293265000
1	-2.068808000	2.540838000	3.004064000
1	-0.857571000	1.372685000	2.558132000
6	4.133937000	-0.590857000	1.461312000
1	3.932587000	-0.742630000	2.524322000
1	3.616911000	-1.375901000	0.898287000
1	5.207798000	-0.725882000	1.300148000
6	3.946381000	0.998050000	-0.495041000
1	3.526949000	1.940785000	-0.855064000
1	5.024831000	1.027059000	-0.684275000
1	3.527824000	0.186378000	-1.092437000
6	-0.727355000	-4.330337000	0.658976000
1	-1.308275000	-5.213191000	0.377883000
1	0.063139000	-4.661078000	1.339390000
1	-1.402055000	-3.662766000	1.206621000
6	-1.250910000	-3.159664000	-1.521210000
1	-1.975330000	-2.522183000	-1.008712000
1	-0.841966000	-2.595251000	-2.363084000
1	-1.798374000	-4.014433000	-1.931572000
5	-0.201161000	0.623149000	-0.863264000
7	1.528102000	-1.923703000	3.532695000
7	0.179137000	-1.442600000	3.342755000
1	1.537797000	-2.620056000	4.277038000
1	1.783021000	-2.412866000	2.677112000
1	-0.505604000	-2.189767000	3.481390000
1	0.015685000	-0.783825000	4.102354000

$[9f'_{SB}]_{dis}$ (TE = -3266.933760)

6	0.035250000	1.474626000	1.007565000
6	0.981715000	2.004982000	1.924329000
1	1.626913000	1.311452000	2.457885000
6	1.075190000	3.352504000	2.221588000
1	1.782574000	3.690551000	2.974799000
6	0.273747000	4.273059000	1.548306000
1	0.350225000	5.335852000	1.762909000
6	-0.612376000	3.824340000	0.584754000

1	-1.214230000	4.531897000	0.020406000
6	-0.754838000	2.453243000	0.327078000
6	-1.410470000	-0.901844000	1.204522000
6	-2.017443000	-1.027892000	2.464416000
1	-1.607200000	-0.480367000	3.312797000
6	-3.145157000	-1.818403000	2.652458000
1	-3.592314000	-1.896997000	3.640473000
6	-3.715951000	-2.494822000	1.576367000
1	-4.605898000	-3.102333000	1.718173000
6	-3.152977000	-2.376823000	0.311769000
1	-3.602717000	-2.878917000	-0.542546000
6	-2.004580000	-1.601057000	0.148583000
6	1.256909000	-0.881843000	1.429050000
6	1.295204000	-1.617840000	2.625837000
1	0.390275000	-1.699511000	3.224848000
6	2.454119000	-2.234158000	3.079230000
1	2.446560000	-2.776792000	4.021353000
6	3.615433000	-2.180785000	2.314296000
1	4.518764000	-2.686550000	2.645369000
6	3.601690000	-1.523086000	1.091414000
1	4.474295000	-1.562851000	0.446430000
6	2.445880000	-0.859185000	0.675230000
16	2.351232000	-0.281225000	-1.017242000
16	-1.832621000	2.027428000	-1.036200000
16	-1.304098000	-1.408752000	-1.488956000
23	0.099295000	0.608058000	-1.457607000
6	-3.629646000	1.863512000	-0.448765000
1	-3.951856000	2.903524000	-0.573171000
6	-0.469729000	-3.048536000	-1.830599000
1	-1.327395000	-3.720510000	-1.958429000
6	3.586751000	1.101210000	-1.284457000
1	3.381899000	1.298684000	-2.344018000
6	5.009968000	0.611698000	-1.117829000
1	5.697029000	1.371173000	-1.503282000
1	5.264077000	0.461349000	-0.065350000
1	5.205067000	-0.315573000	-1.660976000
6	3.294013000	2.330789000	-0.457556000
1	3.395754000	2.125503000	0.611869000
1	4.014316000	3.117179000	-0.706336000
1	2.294201000	2.736397000	-0.635984000
6	-4.332122000	0.979403000	-1.454711000
1	-4.176679000	1.304325000	-2.486461000
1	-4.004089000	-0.060288000	-1.367743000
1	-5.409383000	1.002913000	-1.262941000
6	-3.813767000	1.433265000	0.981727000
1	-3.119337000	1.922653000	1.670390000

1	-4.826246000	1.707208000	1.297000000
1	-3.717840000	0.354711000	1.096408000
6	0.269706000	-2.895608000	-3.143395000
1	0.682429000	-3.862278000	-3.445799000
1	-0.377598000	-2.543029000	-3.950194000
1	1.105912000	-2.195859000	-3.046341000
6	0.404252000	-3.525618000	-0.695851000
1	1.307267000	-2.918305000	-0.599991000
1	-0.113745000	-3.524245000	0.266808000
1	0.722894000	-4.553908000	-0.895703000
5	-0.060654000	-0.107706000	1.027021000
7	0.497500000	0.827777000	-3.064605000
1	0.846256000	0.671689000	-4.014328000

[10f'_{SB}]_{alt} (TE = -3323.566068)

6	-0.283363000	1.458274000	1.507937000
6	0.175959000	1.901299000	2.761885000
1	0.798650000	1.228722000	3.353889000
6	-0.121336000	3.160562000	3.271907000
1	0.260612000	3.456573000	4.247522000
6	-0.899394000	4.044244000	2.530111000
1	-1.133146000	5.035144000	2.913606000
6	-1.350177000	3.658230000	1.273223000
1	-1.921656000	4.352230000	0.658767000
6	-1.044849000	2.389510000	0.776941000
6	-1.087918000	-1.111340000	1.453421000
6	-1.602773000	-1.085403000	2.763042000
1	-1.258055000	-0.303150000	3.440599000
6	-2.539256000	-2.003131000	3.226578000
1	-2.906773000	-1.935215000	4.249130000
6	-3.013011000	-3.000435000	2.379981000
1	-3.752382000	-3.719354000	2.726416000
6	-2.552340000	-3.048651000	1.069846000
1	-2.942496000	-3.793637000	0.378206000
6	-1.610745000	-2.120001000	0.621524000
6	1.547604000	-0.539016000	1.276022000
6	1.857685000	-1.194479000	2.482337000
1	1.057718000	-1.349884000	3.207283000
6	3.127579000	-1.677263000	2.780152000
1	3.308613000	-2.183630000	3.726805000
6	4.157535000	-1.532374000	1.857403000
1	5.150657000	-1.925102000	2.064799000
6	3.895828000	-0.901497000	0.646898000
1	4.676601000	-0.818434000	-0.106027000
6	2.619655000	-0.402699000	0.369308000
16	2.342059000	0.252435000	-1.291566000

16	-1.505527000	2.032200000	-0.927184000
16	-1.196172000	-2.152787000	-1.130777000
23	-0.116323000	0.043892000	-1.414745000
6	-3.367877000	1.782760000	-0.802163000
1	-3.753382000	2.777141000	-0.543504000
6	-0.078995000	-3.669314000	-1.237450000
1	-0.749431000	-4.510131000	-1.019427000
6	3.060892000	1.998789000	-1.185722000
1	2.868191000	2.343594000	-2.211388000
6	4.552221000	1.960274000	-0.929971000
1	4.980127000	2.963601000	-1.036378000
1	4.770410000	1.626259000	0.088935000
1	5.077036000	1.297108000	-1.623303000
6	2.319653000	2.866847000	-0.198272000
1	2.379552000	2.457731000	0.815984000
1	2.752824000	3.873607000	-0.173069000
1	1.261895000	2.961420000	-0.452892000
6	-3.832637000	1.382158000	-2.186269000
1	-3.547704000	2.109852000	-2.951053000
1	-3.400029000	0.414335000	-2.470115000
1	-4.922078000	1.274864000	-2.207232000
6	-3.749057000	0.774438000	0.254634000
1	-3.341864000	1.024832000	1.238129000
1	-4.840139000	0.722281000	0.348185000
1	-3.390483000	-0.225199000	-0.007398000
6	0.402498000	-3.739446000	-2.670872000
1	1.007399000	-4.637530000	-2.831788000
1	-0.423426000	-3.760545000	-3.389070000
1	1.036043000	-2.873168000	-2.902613000
6	1.058261000	-3.622631000	-0.246537000
1	1.734965000	-2.791038000	-0.465188000
1	0.709281000	-3.503029000	0.782677000
1	1.641583000	-4.549552000	-0.296148000
5	0.039409000	-0.040964000	1.045473000
7	-0.187286000	0.111329000	-3.668252000
1	0.701679000	-0.244667000	-4.021163000
1	-0.904259000	-0.504780000	-4.044912000
7	-0.466286000	1.427906000	-4.197106000
1	-0.065223000	2.083819000	-3.527873000
1	0.036469000	1.557804000	-5.074048000

[10f''_{SB}]_{dis} (TE = -3267.093000)

6	-0.362894000	1.710071000	1.099358000
6	0.050991000	2.379653000	2.265124000
1	0.691392000	1.850567000	2.971902000
6	-0.323229000	3.688418000	2.548506000

1	0.020222000	4.165227000	3.464760000
6	-1.128167000	4.392499000	1.657138000
1	-1.417796000	5.420232000	1.864145000
6	-1.529159000	3.780174000	0.476137000
1	-2.114428000	4.332231000	-0.257269000
6	-1.150738000	2.462800000	0.213366000
6	-1.123120000	-0.838521000	1.440894000
6	-1.693735000	-0.611571000	2.706995000
1	-1.417164000	0.293473000	3.249296000
6	-2.599074000	-1.490549000	3.290063000
1	-3.012939000	-1.271209000	4.272624000
6	-2.984499000	-2.644927000	2.613929000
1	-3.699819000	-3.334596000	3.056243000
6	-2.473268000	-2.889362000	1.345852000
1	-2.803319000	-3.758283000	0.779074000
6	-1.559992000	-1.997843000	0.779623000
6	1.490237000	-0.246039000	1.299686000
6	1.756392000	-0.638454000	2.624616000
1	0.926326000	-0.690552000	3.329824000
6	3.029043000	-0.980514000	3.066137000
1	3.182485000	-1.279844000	4.101382000
6	4.101235000	-0.963263000	2.179258000
1	5.097469000	-1.252457000	2.506099000
6	3.878648000	-0.607589000	0.855307000
1	4.691802000	-0.646397000	0.133977000
6	2.597348000	-0.239911000	0.434057000
16	2.346252000	0.019670000	-1.325393000
16	-1.526408000	1.787325000	-1.403728000
16	-1.087467000	-2.263358000	-0.928966000
23	-0.073176000	-0.179073000	-1.785929000
6	-3.369844000	1.468150000	-1.333971000
1	-3.800086000	2.476688000	-1.288130000
6	0.073284000	-3.728447000	-0.827074000
1	-0.578253000	-4.546376000	-0.494026000
6	2.985380000	1.752003000	-1.640615000
1	2.776160000	1.838317000	-2.714365000
6	4.478386000	1.822928000	-1.396099000
1	4.864528000	2.790326000	-1.734580000
1	4.710919000	1.741080000	-0.329895000
1	5.026248000	1.039713000	-1.926366000
6	2.219351000	2.803813000	-0.872576000
1	2.286892000	2.641583000	0.208509000
1	2.632239000	3.796911000	-1.082359000
1	1.161977000	2.819332000	-1.142523000
6	-3.742303000	0.801329000	-2.642001000
1	-3.437985000	1.389453000	-3.511809000

1	-3.270479000	-0.183830000	-2.726805000
1	-4.826192000	0.657647000	-2.693738000
6	-3.788343000	0.665441000	-0.125397000
1	-3.432855000	1.102147000	0.811807000
1	-4.882067000	0.615117000	-0.076125000
1	-3.413356000	-0.359940000	-0.179298000
6	0.566280000	-3.993094000	-2.234554000
1	1.202793000	-4.883497000	-2.247080000
1	-0.253282000	-4.154594000	-2.939727000
1	1.162017000	-3.151662000	-2.605246000
6	1.196923000	-3.517879000	0.159716000
1	1.880816000	-2.735153000	-0.179352000
1	0.835595000	-3.239090000	1.153363000
1	1.777624000	-4.441558000	0.262902000
5	-0.001860000	0.167923000	0.901240000
7	-0.081397000	-0.324720000	-3.472010000
1	-0.072708000	-0.405743000	-4.489001000

$[11f'_{SB}]_{alt}$ (TE = -3323.941554)

6	-0.309543000	-1.317628000	-1.558709000
6	0.210350000	-1.747659000	-2.792861000
1	0.917053000	-1.099479000	-3.311792000
6	-0.136307000	-2.963159000	-3.373061000
1	0.293733000	-3.248519000	-4.330849000
6	-1.026754000	-3.816849000	-2.729378000
1	-1.300215000	-4.771328000	-3.172315000
6	-1.549787000	-3.446135000	-1.496110000
1	-2.222917000	-4.114129000	-0.961925000
6	-1.192663000	-2.220357000	-0.934904000
6	-1.034184000	1.265871000	-1.308130000
6	-1.553137000	1.366826000	-2.612173000
1	-1.243175000	0.630398000	-3.354838000
6	-2.445445000	2.362841000	-2.990751000
1	-2.814946000	2.401077000	-4.013415000
6	-2.872879000	3.304828000	-2.059460000
1	-3.576248000	4.084455000	-2.341813000
6	-2.415448000	3.220714000	-0.750927000
1	-2.774876000	3.920529000	0.001298000
6	-1.510925000	2.219447000	-0.390755000
6	1.582683000	0.628499000	-1.237165000
6	1.890919000	1.345508000	-2.407968000
1	1.090807000	1.547271000	-3.120331000
6	3.164812000	1.827729000	-2.685367000
1	3.347538000	2.379026000	-3.605400000
6	4.197191000	1.627322000	-1.775335000

1	5.192340000	2.020915000	-1.967508000
6	3.936269000	0.939889000	-0.597265000
1	4.718839000	0.813401000	0.147143000
6	2.656733000	0.436369000	-0.347596000
16	2.385808000	-0.322996000	1.268802000
16	-1.775368000	-1.846560000	0.726203000
16	-1.086947000	2.078464000	1.351537000
23	-0.074576000	-0.195400000	1.404560000
6	-3.624461000	-1.503620000	0.533658000
1	-4.044229000	-2.481871000	0.270940000
6	0.078640000	3.517301000	1.635882000
1	-0.563260000	4.400574000	1.533226000
6	3.069006000	-2.067055000	1.027756000
1	2.875733000	-2.488432000	2.027334000
6	4.560370000	-2.035158000	0.774707000
1	4.965367000	-3.052331000	0.792032000
1	4.783513000	-1.619971000	-0.212224000
1	5.098732000	-1.446064000	1.521502000
6	2.310685000	-2.838825000	-0.024541000
1	2.404843000	-2.363579000	-1.005993000
1	2.706528000	-3.856417000	-0.113764000
1	1.242275000	-2.902299000	0.204116000
6	-4.104055000	-1.072801000	1.902933000
1	-3.895538000	-1.823483000	2.674725000
1	-3.634260000	-0.127424000	2.201891000
1	-5.185373000	-0.908619000	1.896785000
6	-3.909195000	-0.491044000	-0.546478000
1	-3.464923000	-0.771363000	-1.504982000
1	-4.991058000	-0.404847000	-0.695677000
1	-3.530061000	0.498465000	-0.278858000
6	0.567917000	3.391459000	3.063584000
1	1.217374000	4.233972000	3.319151000
1	-0.252460000	3.374413000	3.787091000
1	1.159402000	2.475001000	3.188716000
6	1.205785000	3.562071000	0.632900000
1	1.879678000	2.709825000	0.755177000
1	0.847706000	3.559129000	-0.399997000
1	1.794474000	4.474490000	0.777661000
5	0.071557000	0.141447000	-1.021431000
7	-0.389583000	-0.947476000	3.548829000
1	0.283812000	-0.667202000	4.262550000
1	-1.315810000	-0.737185000	3.924303000
7	-0.314752000	-2.410638000	3.465315000
1	0.609272000	-2.635465000	3.061417000
1	-0.479659000	-2.922051000	4.346477000
1	-0.995766000	-2.689677000	2.724732000

[11f''_{SB}]_{dis} (TE = -3267.535660)

6	-0.716988000	1.939178000	0.586044000
6	-0.329269000	3.065319000	1.336187000
1	0.574750000	3.004880000	1.940792000
6	-1.085163000	4.229698000	1.360628000
1	-0.767252000	5.071111000	1.971347000
6	-2.249049000	4.320717000	0.601570000
1	-2.843122000	5.230940000	0.611672000
6	-2.626507000	3.259437000	-0.213536000
1	-3.492024000	3.354136000	-0.865568000
6	-1.870935000	2.089400000	-0.218825000
6	-0.920651000	-0.664931000	1.219475000
6	-1.590449000	-0.323495000	2.416154000
1	-1.523694000	0.699965000	2.782220000
6	-2.318670000	-1.241600000	3.160181000
1	-2.787914000	-0.926625000	4.089079000
6	-2.469836000	-2.546349000	2.704247000
1	-3.054332000	-3.269021000	3.267155000
6	-1.889998000	-2.908533000	1.498053000
1	-2.039778000	-3.908412000	1.096871000
6	-1.109412000	-1.993753000	0.784575000
6	1.501370000	0.486764000	1.368577000
6	1.690316000	0.648534000	2.752045000
1	0.830884000	0.872527000	3.383341000
6	2.940247000	0.520327000	3.345586000
1	3.044476000	0.657483000	4.419235000
6	4.051496000	0.198399000	2.572379000
1	5.028374000	0.076251000	3.032779000
6	3.901091000	0.014967000	1.204871000
1	4.751585000	-0.269313000	0.589885000
6	2.643472000	0.175567000	0.618774000
16	2.502387000	-0.108073000	-1.146811000
16	-2.223366000	0.845520000	-1.457943000
16	-0.491092000	-2.566341000	-0.797113000
23	0.012996000	-0.286205000	-1.516285000
6	-3.937402000	0.166463000	-1.132809000
1	-4.590532000	0.947888000	-1.537817000
6	0.927638000	-3.730546000	-0.384225000
1	0.394637000	-4.641727000	-0.088421000
6	3.026092000	1.558515000	-1.844820000
1	2.808273000	1.417095000	-2.909027000
6	4.513609000	1.753964000	-1.643811000
1	4.834717000	2.657910000	-2.170733000
1	4.760791000	1.896531000	-0.587953000
1	5.102957000	0.917481000	-2.026027000

6	2.200633000	2.694139000	-1.285942000
1	2.326993000	2.785009000	-0.202332000
1	2.530777000	3.638965000	-1.729685000
1	1.135674000	2.580546000	-1.500569000
6	-4.051356000	-1.087747000	-1.974854000
1	-3.822903000	-0.911335000	-3.029177000
1	-3.383278000	-1.873465000	-1.606041000
1	-5.072699000	-1.475054000	-1.920773000
6	-4.239888000	-0.065456000	0.326374000
1	-4.021507000	0.806905000	0.947667000
1	-5.306741000	-0.287113000	0.436194000
1	-3.684843000	-0.918273000	0.721614000
6	1.677729000	-3.961144000	-1.678934000
1	2.447855000	-4.722284000	-1.524962000
1	1.028640000	-4.310139000	-2.485877000
1	2.182997000	-3.048738000	-2.012653000
6	1.800953000	-3.245312000	0.745536000
1	2.410537000	-2.390267000	0.448223000
1	1.232177000	-2.968309000	1.636961000
1	2.488056000	-4.047822000	1.032877000
5	0.028343000	0.573312000	0.789386000
7	0.284086000	0.438142000	-3.226053000
1	1.121517000	0.423579000	-3.800319000
1	-0.496528000	0.725030000	-3.811108000

[12f'_{SB}] (TE = -3267.691925)

6	-1.444903000	0.467209000	1.433116000
6	-1.518172000	0.840781000	2.789073000
1	-0.637014000	0.700719000	3.415631000
6	-2.658892000	1.389492000	3.361628000
1	-2.661305000	1.660821000	4.415729000
6	-3.792967000	1.603066000	2.583006000
1	-4.689133000	2.043086000	3.014685000
6	-3.757807000	1.273362000	1.235401000
1	-4.619889000	1.469321000	0.599908000
6	-2.604162000	0.713536000	0.679099000
6	0.176116000	-1.715504000	1.143460000
6	-0.363524000	-2.352831000	2.276766000
1	-1.040959000	-1.788285000	2.917883000
6	-0.054360000	-3.664609000	2.619253000
1	-0.491199000	-4.109697000	3.511545000
6	0.811344000	-4.408723000	1.822935000
1	1.056085000	-5.437145000	2.078913000
6	1.331327000	-3.834985000	0.668373000
1	1.964975000	-4.419511000	0.003457000
6	1.017101000	-2.516080000	0.339471000

6	1.212579000	0.745359000	1.169594000
6	1.899139000	0.585903000	2.387227000
1	1.563947000	-0.190629000	3.076424000
6	2.999818000	1.360534000	2.734426000
1	3.498414000	1.200408000	3.688700000
6	3.481370000	2.322718000	1.850497000
1	4.356661000	2.917688000	2.101469000
6	2.850587000	2.494666000	0.624432000
1	3.243421000	3.204627000	-0.100594000
6	1.726413000	1.727647000	0.306969000
16	1.004839000	1.898009000	-1.326981000
16	-2.637889000	0.416569000	-1.098806000
16	1.542540000	-1.896406000	-1.259188000
23	-0.289714000	-0.201502000	-1.645027000
6	-3.693847000	-1.132202000	-1.120073000
1	-4.565813000	-0.832846000	-0.524461000
6	3.401646000	-1.687850000	-1.164675000
1	3.782736000	-2.699126000	-1.353898000
6	0.035121000	3.502320000	-1.244147000
1	-0.708371000	3.335037000	-2.033791000
6	0.933418000	4.665436000	-1.615793000
1	0.345251000	5.586709000	-1.691803000
1	1.696907000	4.835659000	-0.849994000
1	1.441140000	4.510466000	-2.570466000
6	-0.652757000	3.704909000	0.086618000
1	0.072779000	3.807494000	0.900108000
1	-1.243096000	4.627261000	0.058784000
1	-1.323305000	2.884714000	0.342399000
6	-4.113357000	-1.422148000	-2.544680000
1	-4.581141000	-0.559760000	-3.027243000
1	-3.255169000	-1.736745000	-3.144118000
1	-4.836643000	-2.243934000	-2.556560000
6	-2.985461000	-2.296359000	-0.465272000
1	-2.664016000	-2.064417000	0.553649000
1	-3.655094000	-3.162725000	-0.415484000
1	-2.100023000	-2.588647000	-1.041002000
6	3.778498000	-0.776629000	-2.315659000
1	4.867881000	-0.708844000	-2.401920000
1	3.391231000	-1.132380000	-3.274983000
1	3.393364000	0.236149000	-2.155256000
6	3.907865000	-1.192345000	0.168981000
1	3.641443000	-0.147736000	0.339176000
1	3.523800000	-1.779975000	1.007174000
1	5.001544000	-1.263598000	0.189563000
5	-0.077780000	-0.163721000	0.886603000
7	-0.689231000	-1.072180000	-3.341018000

1	-1.476649000	-0.927291000	-3.966571000
1	-0.072878000	-1.736514000	-3.803193000

[13f''_{SB}] (TE = -3268.143326)

6	-0.459245000	1.893438000	0.730601000
6	0.014633000	2.896142000	1.597545000
1	0.804365000	2.644867000	2.304578000
6	-0.502861000	4.186434000	1.601690000
1	-0.115646000	4.922335000	2.302940000
6	-1.510573000	4.539728000	0.708985000
1	-1.916387000	5.548105000	0.701805000
6	-1.970357000	3.598750000	-0.203466000
1	-2.718840000	3.873112000	-0.944169000
6	-1.454400000	2.302854000	-0.182595000
6	-1.022134000	-0.618006000	1.484250000
6	-1.645178000	-0.272109000	2.697538000
1	-1.414285000	0.694019000	3.147484000
6	-2.554149000	-1.107208000	3.335544000
1	-3.006406000	-0.798632000	4.275469000
6	-2.900705000	-2.329047000	2.764419000
1	-3.620838000	-2.982858000	3.249714000
6	-2.339931000	-2.693647000	1.548078000
1	-2.632913000	-3.623547000	1.064398000
6	-1.411491000	-1.849683000	0.934607000
6	1.564922000	0.188263000	1.402450000
6	1.785158000	0.232332000	2.792227000
1	0.928051000	0.363948000	3.452114000
6	3.046059000	0.104736000	3.361048000
1	3.158788000	0.146950000	4.442096000
6	4.159676000	-0.094568000	2.550901000
1	5.149847000	-0.208494000	2.984450000
6	3.987842000	-0.179708000	1.177501000
1	4.837538000	-0.383769000	0.529975000
6	2.713774000	-0.027583000	0.621174000
16	2.595126000	-0.345605000	-1.152765000
16	-1.936030000	1.188879000	-1.504789000
16	-0.814719000	-2.324433000	-0.688983000
23	0.138668000	-0.203422000	-1.486112000
6	-3.727430000	0.703633000	-1.216955000
1	-4.276682000	1.557330000	-1.630564000
6	0.407427000	-3.699651000	-0.350906000
1	-0.237048000	-4.538219000	-0.060909000
6	2.985178000	1.290230000	-1.975193000
1	3.115598000	0.970452000	-3.017085000
6	4.273104000	1.884058000	-1.453373000

1	4.514600000	2.793132000	-2.012523000
1	4.186189000	2.162958000	-0.399441000
1	5.115372000	1.196232000	-1.555311000
6	1.812279000	2.244077000	-1.861284000
1	1.589204000	2.494766000	-0.820869000
1	2.020509000	3.182380000	-2.386398000
1	0.890559000	1.860393000	-2.335700000
6	-3.975893000	-0.528080000	-2.062085000
1	-3.707714000	-0.377003000	-3.112152000
1	-3.415942000	-1.389005000	-1.682301000
1	-5.038073000	-0.788404000	-2.032828000
6	-4.075700000	0.517638000	0.239085000
1	-3.778283000	1.370844000	0.853951000
1	-5.161798000	0.410765000	0.331434000
1	-3.617327000	-0.380675000	0.655939000
6	1.088127000	-4.002996000	-1.670272000
1	1.753034000	-4.864246000	-1.559769000
1	0.373619000	-4.240028000	-2.463990000
1	1.703702000	-3.158229000	-1.999697000
6	1.371552000	-3.372945000	0.763865000
1	2.061124000	-2.574308000	0.481125000
1	0.862873000	-3.068587000	1.682149000
1	1.972702000	-4.257772000	0.997173000
5	0.063471000	0.393322000	0.883704000
7	0.074212000	-0.668607000	-3.696189000
1	-0.159508000	0.115879000	-4.302239000
1	0.929464000	-1.060618000	-4.085651000
1	-0.643780000	-1.365704000	-3.887504000

[14f'_{SB}] (TE = -3268.265203)

6	-0.300869000	1.708221000	1.125344000
6	0.138954000	2.334809000	2.305795000
1	0.734064000	1.752822000	3.011228000
6	-0.141129000	3.664126000	2.604535000
1	0.226104000	4.102614000	3.530939000
6	-0.882698000	4.434676000	1.714435000
1	-1.102380000	5.477808000	1.931764000
6	-1.315860000	3.863672000	0.523395000
1	-1.860127000	4.461956000	-0.205658000
6	-1.026569000	2.527692000	0.239655000
6	-1.135341000	-0.835670000	1.456882000
6	-1.681551000	-0.599014000	2.732156000
1	-1.348955000	0.281537000	3.283545000
6	-2.633526000	-1.429385000	3.314265000
1	-3.025379000	-1.197266000	4.303175000
6	-3.090304000	-2.550161000	2.628289000

1	-3.840548000	-3.204005000	3.067904000
6	-2.597796000	-2.809297000	1.354771000
1	-2.973826000	-3.656601000	0.783512000
6	-1.642476000	-1.965208000	0.784891000
6	1.506259000	-0.319204000	1.248368000
6	1.786102000	-0.777139000	2.549333000
1	0.971383000	-0.807266000	3.274009000
6	3.044420000	-1.218516000	2.944759000
1	3.202562000	-1.569384000	3.963237000
6	4.091933000	-1.232115000	2.030627000
1	5.076233000	-1.596640000	2.316847000
6	3.859563000	-0.799543000	0.730156000
1	4.654099000	-0.846718000	-0.011364000
6	2.594876000	-0.338863000	0.352017000
16	2.351537000	0.050468000	-1.394948000
16	-1.466874000	1.912979000	-1.395675000
16	-1.190475000	-2.275928000	-0.930625000
23	-0.112419000	-0.145384000	-1.534235000
6	-3.337121000	1.699958000	-1.250615000
1	-3.718644000	2.725653000	-1.170430000
6	-0.081506000	-3.797277000	-0.777574000
1	-0.761722000	-4.595047000	-0.453629000
6	3.101669000	1.779594000	-1.544596000
1	2.894958000	1.986022000	-2.603672000
6	4.597009000	1.746150000	-1.310064000
1	5.041222000	2.716220000	-1.561056000
1	4.827828000	1.551898000	-0.258108000
1	5.096672000	0.982694000	-1.912873000
6	2.397075000	2.789262000	-0.671282000
1	2.473447000	2.521290000	0.388117000
1	2.848942000	3.780729000	-0.792703000
1	1.336234000	2.870204000	-0.915175000
6	-3.788669000	1.070930000	-2.551546000
1	-3.495898000	1.662785000	-3.424850000
1	-3.357902000	0.066800000	-2.659416000
1	-4.877985000	0.964077000	-2.571658000
6	-3.738551000	0.887035000	-0.044021000
1	-3.347254000	1.303767000	0.888037000
1	-4.831121000	0.850184000	0.039283000
1	-3.376111000	-0.142022000	-0.123767000
6	0.434108000	-4.078323000	-2.172759000
1	1.051172000	-4.982518000	-2.182841000
1	-0.375409000	-4.219223000	-2.896326000
1	1.062536000	-3.247894000	-2.520990000
6	1.031104000	-3.604333000	0.223091000
1	1.715323000	-2.813754000	-0.098902000

1	0.657503000	-3.334416000	1.214557000
1	1.612877000	-4.528015000	0.325306000
5	0.009378000	0.150549000	0.909999000
7	-0.278852000	-0.446516000	-3.773462000
1	-0.659789000	0.358686000	-4.265203000
1	0.608118000	-0.648590000	-4.228878000
1	-0.889172000	-1.224450000	-4.014187000

Cartesian coordinates of the intermediate and TS involved in the conversion of [4]→[5]_{alt} for the catalysts [**1c''_{PB}**] and [**1f''_{SB}**], along with their total energies (in hartree) including zero point vibrational correction at M06-L-D3(heptane)/6-311+G* level of theory.

For catalyst [**1c''_{PB}**]

[**4c''_{PB}** -V-H]⁺ (TE= -3507.088650)

6	1.567069000	-0.653872000	1.844241000
6	1.848572000	-1.579368000	2.866937000
1	1.023541000	-2.119171000	3.330452000
6	3.141170000	-1.809021000	3.324580000
1	3.316074000	-2.522805000	4.125823000
6	4.203390000	-1.129002000	2.744624000
1	5.220822000	-1.297200000	3.089153000
6	3.963603000	-0.250426000	1.692119000
1	4.811676000	0.233638000	1.215202000
6	2.669712000	-0.004616000	1.228848000
6	-0.576924000	1.060156000	1.918802000
6	-0.131889000	1.541101000	3.166861000
1	0.763534000	1.112153000	3.614003000
6	-0.834588000	2.512723000	3.873995000
1	-0.473760000	2.840141000	4.845920000
6	-1.988618000	3.059743000	3.332597000
1	-2.549449000	3.814146000	3.878767000
6	-2.410833000	2.658485000	2.066212000
1	-3.289987000	3.128605000	1.628802000
6	-1.725689000	1.679787000	1.351369000
6	-0.976574000	-1.561202000	1.655962000
6	-1.741231000	-1.740741000	2.820049000
1	-1.659614000	-1.014173000	3.629224000
6	-2.604487000	-2.819652000	2.962709000
1	-3.180294000	-2.939246000	3.877402000
6	-2.749559000	-3.728047000	1.919849000
1	-3.439654000	-4.563256000	2.010443000
6	-2.024114000	-3.553966000	0.747387000
1	-2.181472000	-4.250029000	-0.072104000
6	-1.126301000	-2.490326000	0.609116000
23	0.091819000	0.499402000	-1.169572000

6	2.821207000	2.708411000	0.048189000
1	3.890290000	2.707809000	0.301538000
6	-3.851486000	0.629362000	-0.430268000
1	-4.515629000	1.460855000	-0.163390000
6	1.146124000	-3.426724000	-1.059748000
1	1.004479000	-3.888123000	-2.044349000
6	1.049743000	-4.512202000	0.002343000
1	1.854317000	-5.241244000	-0.138893000
1	1.157092000	-4.097935000	1.010533000
1	0.105653000	-5.060828000	-0.022446000
6	2.519759000	-2.780745000	-1.053344000
1	2.741160000	-2.300874000	-0.095449000
1	3.296016000	-3.534171000	-1.223657000
1	2.614035000	-2.031768000	-1.841904000
6	2.601591000	3.573589000	-1.187659000
1	3.157481000	3.225955000	-2.063043000
1	1.543025000	3.598770000	-1.462460000
1	2.918598000	4.602814000	-0.992176000
6	2.053116000	3.244996000	1.243462000
1	2.242312000	2.665553000	2.151248000
1	2.352040000	4.278918000	1.444547000
1	0.973920000	3.243349000	1.065460000
6	-4.173513000	0.167813000	-1.847917000
1	-5.235222000	-0.079652000	-1.945248000
1	-3.940395000	0.911707000	-2.616139000
1	-3.607357000	-0.734690000	-2.098307000
6	-4.075479000	-0.483535000	0.576682000
1	-3.477026000	-1.368590000	0.348463000
1	-3.840122000	-0.177647000	1.599275000
1	-5.125542000	-0.794153000	0.559475000
5	0.035211000	-0.360157000	1.647274000
15	2.419334000	0.929495000	-0.337537000
15	-2.130903000	1.354476000	-0.406483000
15	-0.239822000	-2.147204000	-0.958915000
6	-2.405725000	3.042994000	-1.233463000
1	-2.052184000	2.839742000	-2.254298000
6	-1.546149000	4.167583000	-0.663788000
1	-1.546334000	5.010700000	-1.361720000
1	-1.941692000	4.540229000	0.285042000
1	-0.508968000	3.874875000	-0.501058000
6	-3.851048000	3.524960000	-1.318204000
1	-3.875796000	4.477068000	-1.857686000
1	-4.520072000	2.845914000	-1.848398000
1	-4.284838000	3.718845000	-0.331414000
6	3.862543000	0.395867000	-1.434986000
1	4.076940000	-0.622492000	-1.089088000

6	5.147204000	1.210446000	-1.314421000
1	5.930674000	0.738344000	-1.915974000
1	5.032664000	2.229144000	-1.694122000
1	5.533804000	1.284956000	-0.296090000
6	3.430989000	0.327183000	-2.897271000
1	4.228203000	-0.106686000	-3.509277000
1	2.528723000	-0.273638000	-3.046838000
1	3.227490000	1.324784000	-3.300972000
6	-1.453458000	-2.711556000	-2.283181000
1	-2.429362000	-2.501687000	-1.822131000
6	-1.311615000	-1.863063000	-3.542116000
1	-0.293956000	-1.912695000	-3.949902000
1	-1.984668000	-2.226609000	-4.325421000
1	-1.544503000	-0.809482000	-3.372677000
6	-1.398808000	-4.192240000	-2.650887000
1	-0.556953000	-4.411323000	-3.314126000
1	-1.321239000	-4.868864000	-1.797316000
1	-2.304127000	-4.466280000	-3.201579000
7	0.056136000	1.556589000	-3.966332000
7	0.172754000	1.107357000	-2.834684000
1	0.979160000	1.746285000	-4.409277000
1	0.131002000	2.086074000	-0.695003000

TS3_{alt} (Triplet, TE= -3507.073336)

6	-1.561278000	0.620061000	1.917348000
6	-1.654366000	1.303172000	3.143561000
1	-0.747149000	1.482304000	3.718675000
6	-2.864820000	1.760242000	3.651235000
1	-2.889026000	2.284291000	4.604186000
6	-4.040099000	1.555808000	2.937040000
1	-4.991726000	1.913985000	3.321741000
6	-3.983946000	0.903976000	1.712210000
1	-4.902187000	0.770877000	1.145709000
6	-2.766181000	0.443267000	1.200612000
6	0.218810000	-1.464626000	1.833585000
6	-0.371771000	-2.058906000	2.963390000
1	-1.187942000	-1.539440000	3.465163000
6	0.076743000	-3.269043000	3.477307000
1	-0.397188000	-3.693230000	4.359847000
6	1.143442000	-3.930126000	2.874387000
1	1.510126000	-4.869257000	3.281222000
6	1.732222000	-3.385374000	1.739136000
1	2.558079000	-3.912846000	1.266784000
6	1.271623000	-2.177290000	1.207454000
6	1.101908000	1.040147000	1.768616000

6	1.732211000	0.952739000	3.023646000
1	1.424881000	0.167178000	3.714939000
6	2.739478000	1.828208000	3.407592000
1	3.200319000	1.729638000	4.388078000
6	3.170172000	2.819478000	2.530641000
1	3.964858000	3.503908000	2.816790000
6	2.589366000	2.914756000	1.274083000
1	2.951669000	3.670571000	0.582400000
6	1.562996000	2.040479000	0.892856000
23	-0.181727000	-0.185161000	-1.100608000
6	-3.418593000	-1.963216000	-0.394672000
1	-4.465593000	-1.773206000	-0.119258000
6	3.725334000	-1.371183000	-0.226769000
1	4.033399000	-2.396409000	0.029798000
6	-0.147824000	3.596882000	-0.991801000
1	-0.088628000	3.823195000	-2.067322000
6	0.348748000	4.793061000	-0.190821000
1	-0.294003000	5.656879000	-0.388777000
1	0.300949000	4.594146000	0.884018000
1	1.369368000	5.093045000	-0.427474000
6	-1.598189000	3.303984000	-0.643129000
1	-1.716252000	3.010898000	0.405647000
1	-2.220026000	4.190109000	-0.805493000
1	-2.000306000	2.503154000	-1.263430000
6	-3.389028000	-2.648265000	-1.756601000
1	-3.890257000	-2.072385000	-2.537921000
1	-2.369331000	-2.837097000	-2.102366000
1	-3.892324000	-3.618515000	-1.701348000
6	-2.797167000	-2.821355000	0.694959000
1	-2.869529000	-2.350472000	1.678457000
1	-3.311229000	-3.786181000	0.750936000
1	-1.738606000	-3.028907000	0.513522000
6	4.377771000	-0.985577000	-1.547985000
1	5.463897000	-1.098388000	-1.477553000
1	4.043260000	-1.591999000	-2.394198000
1	4.183622000	0.059875000	-1.801034000
6	4.145692000	-0.456187000	0.910169000
1	3.864912000	0.585062000	0.725816000
1	3.703326000	-0.751435000	1.864750000
1	5.233813000	-0.483707000	1.026508000
5	-0.125509000	0.052633000	1.509234000
7	-0.152641000	-1.170440000	-3.976155000
7	-0.243888000	-0.671104000	-2.827665000
1	-1.066287000	-1.216584000	-4.456346000
15	0.887514000	2.051071000	-0.798647000
15	-2.653106000	-0.262746000	-0.474362000

15	1.880149000	-1.537970000	-0.391902000
6	2.384090000	2.280199000	-1.915520000
1	3.188794000	1.811025000	-1.330951000
6	2.788484000	3.719984000	-2.213262000
1	3.644070000	3.719332000	-2.895747000
1	1.992082000	4.282631000	-2.709499000
1	3.093516000	4.282726000	-1.330358000
6	2.218176000	1.506810000	-3.218896000
1	2.072582000	0.435747000	-3.060358000
1	1.367620000	1.872429000	-3.806859000
1	3.108285000	1.627936000	-3.844237000
6	1.687578000	-2.952162000	-1.607180000
1	1.736217000	-2.443177000	-2.580863000
6	0.285301000	-3.525080000	-1.452977000
1	-0.480515000	-2.744307000	-1.351723000
1	0.001763000	-4.123849000	-2.323896000
1	0.202959000	-4.155122000	-0.561614000
6	2.728190000	-4.062418000	-1.590400000
1	2.513993000	-4.772567000	-2.395932000
1	3.747840000	-3.705645000	-1.749401000
1	2.712819000	-4.635550000	-0.659727000
6	-3.873652000	0.710473000	-1.530417000
1	-3.870925000	1.700906000	-1.057682000
6	-5.313397000	0.203833000	-1.520112000
1	-5.949494000	0.924012000	-2.044026000
1	-5.427767000	-0.750252000	-2.040205000
1	-5.731744000	0.082141000	-0.519388000
6	-3.375665000	0.855139000	-2.965028000
1	-2.395185000	1.337329000	-3.024358000
1	-3.293162000	-0.113672000	-3.468189000
1	-4.073190000	1.461178000	-3.551293000
1	-0.298990000	0.527353000	-2.693474000

TS3_{alt} (Quintet, TE= -3507.061569)

6	-1.413468000	0.677822000	1.933855000
6	-1.477271000	1.440917000	3.114398000
1	-0.552875000	1.685727000	3.635628000
6	-2.678908000	1.898183000	3.642334000
1	-2.680418000	2.485515000	4.557905000
6	-3.872429000	1.614778000	2.990042000
1	-4.819387000	1.974152000	3.385244000
6	-3.843858000	0.883273000	1.809563000
1	-4.779365000	0.697402000	1.290262000
6	-2.636595000	0.415329000	1.279938000
6	0.452440000	-1.333770000	1.947085000
6	0.024249000	-1.798104000	3.201985000

1	-0.712259000	-1.216173000	3.756218000
6	0.518674000	-2.969947000	3.763119000
1	0.161853000	-3.298176000	4.736972000
6	1.472160000	-3.718804000	3.081580000
1	1.869308000	-4.633394000	3.514859000
6	1.906566000	-3.294357000	1.831149000
1	2.643890000	-3.890096000	1.298141000
6	1.398860000	-2.125111000	1.257017000
6	1.205388000	1.202857000	1.661742000
6	1.929679000	1.183320000	2.867387000
1	1.731158000	0.391959000	3.590418000
6	2.898423000	2.132757000	3.163288000
1	3.436977000	2.084280000	4.107252000
6	3.190657000	3.134114000	2.242704000
1	3.955437000	3.876574000	2.456967000
6	2.506709000	3.169935000	1.035412000
1	2.759969000	3.940586000	0.313611000
6	1.517810000	2.222481000	0.741587000
23	-0.187305000	-0.197944000	-1.212939000
6	-3.209405000	-2.147820000	-0.056578000
1	-4.234853000	-2.012195000	0.313762000
6	3.667008000	-1.260950000	-0.426419000
1	4.110537000	-2.228473000	-0.150917000
6	-0.443606000	3.587920000	-1.079466000
1	-0.377723000	3.831813000	-2.150284000
6	-0.045383000	4.805900000	-0.258435000
1	-0.744927000	5.626263000	-0.448652000
1	-0.083668000	4.588830000	0.813772000
1	0.955318000	5.177398000	-0.483945000
6	-1.877383000	3.184449000	-0.780416000
1	-2.009528000	2.895712000	0.266827000
1	-2.561512000	4.015874000	-0.979309000
1	-2.185473000	2.343186000	-1.403784000
6	-3.257611000	-2.937128000	-1.359338000
1	-3.883148000	-2.470830000	-2.123866000
1	-2.264673000	-3.065794000	-1.797049000
1	-3.660686000	-3.938981000	-1.180545000
6	-2.415921000	-2.870512000	1.018630000
1	-2.433471000	-2.335372000	1.971343000
1	-2.836722000	-3.866594000	1.190213000
1	-1.366313000	-3.003984000	0.742357000
6	4.147678000	-0.874639000	-1.819432000
1	5.240855000	-0.831784000	-1.848596000
1	3.830914000	-1.570982000	-2.601252000
1	3.782359000	0.117124000	-2.101192000
6	4.093687000	-0.244952000	0.617253000

1	3.709002000	0.756056000	0.402347000
1	3.760702000	-0.517298000	1.621471000
1	5.186161000	-0.174905000	0.638963000
5	0.028806000	0.138577000	1.526462000
7	-0.718149000	-1.557222000	-3.967907000
7	-0.456686000	-1.031285000	-2.912675000
1	-0.704425000	-0.963984000	-4.815929000
15	0.713869000	2.129057000	-0.891007000
15	-2.583151000	-0.412641000	-0.347790000
15	1.837463000	-1.620007000	-0.441064000
6	2.093089000	2.456237000	-2.130387000
1	2.970009000	2.005964000	-1.642555000
6	2.409602000	3.917427000	-2.431634000
1	3.230362000	3.970125000	-3.154089000
1	1.561702000	4.440325000	-2.883611000
1	2.723710000	4.490876000	-1.559277000
6	1.830163000	1.713807000	-3.437528000
1	1.735760000	0.632096000	-3.299661000
1	0.914578000	2.066928000	-3.926386000
1	2.652325000	1.880210000	-4.141107000
6	1.771717000	-3.160118000	-1.525921000
1	1.707064000	-2.726532000	-2.535443000
6	0.487993000	-3.934856000	-1.270340000
1	-0.393314000	-3.291337000	-1.288235000
1	0.343830000	-4.704953000	-2.034323000
1	0.505828000	-4.434350000	-0.296483000
6	2.972485000	-4.099064000	-1.504870000
1	2.807320000	-4.904275000	-2.228252000
1	3.913417000	-3.618980000	-1.779044000
1	3.113511000	-4.581923000	-0.534614000
6	-3.990667000	0.373903000	-1.332623000
1	-4.022641000	1.397663000	-0.937361000
6	-5.374215000	-0.242827000	-1.131783000
1	-6.122850000	0.394736000	-1.612532000
1	-5.461212000	-1.228791000	-1.594604000
1	-5.671853000	-0.349349000	-0.087448000
6	-3.677998000	0.444832000	-2.823676000
1	-2.760639000	1.001515000	-3.033803000
1	-3.565907000	-0.550787000	-3.265593000
1	-4.494099000	0.941312000	-3.358048000
1	-0.746720000	0.549637000	-2.686799000

For catalyst [$4f'_{SB}$]

[$4f'_{SB} - V - H$]⁺ (TE= -3322.247307)

6	1.673732000	-0.944371000	-1.003607000
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6	2.635884000	-0.960215000	-2.022608000
1	2.550592000	-0.258885000	-2.852695000
6	3.676565000	-1.883629000	-2.010466000
1	4.405973000	-1.888455000	-2.816616000
6	3.782536000	-2.808225000	-0.973150000
1	4.594029000	-3.531259000	-0.966416000
6	2.873174000	-2.782736000	0.078080000
1	2.988908000	-3.457393000	0.923520000
6	1.834482000	-1.855054000	0.048859000
6	-0.893855000	-0.944308000	-1.665299000
6	-0.706467000	-1.727545000	-2.817912000
1	0.301555000	-1.852615000	-3.211453000
6	-1.772156000	-2.312210000	-3.489483000
1	-1.594095000	-2.891516000	-4.391789000
6	-3.066583000	-2.162538000	-2.999453000
1	-3.906032000	-2.624947000	-3.512353000
6	-3.282681000	-1.459179000	-1.821068000
1	-4.282557000	-1.407200000	-1.395795000
6	-2.208695000	-0.852531000	-1.171298000
6	0.229763000	1.439761000	-1.137062000
6	-0.566256000	1.927842000	-2.206143000
1	-1.170416000	1.221828000	-2.769152000
6	-0.552828000	3.252597000	-2.608207000
1	-1.151663000	3.564483000	-3.459984000
6	0.215064000	4.179434000	-1.910977000
1	0.223610000	5.225031000	-2.208258000
6	0.947918000	3.770127000	-0.806574000
1	1.494975000	4.497717000	-0.213051000
6	0.977084000	2.426680000	-0.429864000
16	1.729769000	2.078160000	1.158516000
16	0.788637000	-1.583778000	1.465421000
16	-2.461787000	-0.201300000	0.472316000
23	-0.357756000	0.754904000	1.329188000
6	-0.139401000	-3.181568000	1.734900000
1	0.655031000	-3.873945000	2.039111000
6	-3.860292000	1.023315000	0.326724000
1	-4.692872000	0.408296000	-0.035964000
6	3.588740000	1.757786000	0.913636000
1	3.977873000	2.498065000	1.620855000
6	4.012071000	2.120183000	-0.488830000
1	5.098549000	2.012202000	-0.569543000
1	3.560772000	1.454223000	-1.229355000
1	3.763805000	3.149822000	-0.754912000
6	4.019923000	0.376954000	1.343852000
1	3.808869000	-0.370523000	0.580288000
1	5.103730000	0.382708000	1.502093000

1	3.558178000	0.059398000	2.282071000
6	-1.085990000	-2.943888000	2.893693000
1	-0.568752000	-2.606097000	3.794869000
1	-1.849351000	-2.201586000	2.640223000
1	-1.603749000	-3.875629000	3.138277000
6	-0.824560000	-3.688872000	0.487987000
1	-0.147858000	-3.748769000	-0.368647000
1	-1.209307000	-4.696880000	0.674759000
1	-1.673957000	-3.060495000	0.210957000
6	-4.151565000	1.513018000	1.730649000
1	-5.037116000	2.154486000	1.714276000
1	-4.344778000	0.694488000	2.428602000
1	-3.317428000	2.104745000	2.117299000
6	-3.549463000	2.134261000	-0.646023000
1	-2.679551000	2.709678000	-0.314847000
1	-3.356664000	1.758645000	-1.654553000
1	-4.403053000	2.817455000	-0.707221000
5	0.338256000	-0.133128000	-1.124625000
7	-1.270494000	0.562268000	4.186775000
7	-0.810142000	0.651847000	3.073702000
1	-0.658303000	0.980290000	4.919330000
1	-1.080149000	2.276840000	1.432373000

TS3_{alt} (Triplet, TE= -3322.220150)

6	0.017590000	1.382372000	-1.211685000
6	-0.898065000	1.857957000	-2.186759000
1	-1.582897000	1.147766000	-2.643247000
6	-0.911970000	3.168220000	-2.632194000
1	-1.600906000	3.462787000	-3.419832000
6	-0.054965000	4.106795000	-2.062187000
1	-0.068516000	5.141762000	-2.394205000
6	0.802256000	3.718065000	-1.045727000
1	1.440170000	4.449020000	-0.555148000
6	0.864011000	2.380145000	-0.638032000
6	1.396732000	-1.030959000	-1.245974000
6	2.014100000	-1.226456000	-2.490917000
1	1.622172000	-0.713771000	-3.369276000
6	3.126659000	-2.048874000	-2.626727000
1	3.583435000	-2.184215000	-3.604113000
6	3.669531000	-2.685214000	-1.512444000
1	4.547685000	-3.317381000	-1.614472000
6	3.096425000	-2.493899000	-0.261017000
1	3.527164000	-2.961498000	0.622067000
6	1.963981000	-1.686935000	-0.148649000
6	-1.273921000	-0.975871000	-1.452327000

6	-1.310740000	-1.799653000	-2.591020000
1	-0.399138000	-1.943987000	-3.167628000
6	-2.475768000	-2.424887000	-3.015460000
1	-2.465970000	-3.037332000	-3.913656000
6	-3.645983000	-2.290107000	-2.275057000
1	-4.554991000	-2.801744000	-2.580595000
6	-3.635510000	-1.541300000	-1.105442000
1	-4.517872000	-1.514058000	-0.473299000
6	-2.472467000	-0.872271000	-0.720312000
16	-2.397685000	-0.154051000	0.920415000
16	1.875374000	2.032748000	0.796243000
16	1.251684000	-1.385954000	1.466233000
23	-0.108777000	0.683656000	1.256308000
6	3.681430000	1.802887000	0.277085000
1	4.017190000	2.845799000	0.298754000
6	0.389480000	-2.988308000	1.897135000
1	1.230968000	-3.669710000	2.072756000
6	-3.619437000	1.264579000	1.017801000
1	-3.390040000	1.614936000	2.032470000
6	-5.050274000	0.770928000	0.961260000
1	-5.720990000	1.583040000	1.258199000
1	-5.336847000	0.481245000	-0.052895000
1	-5.233796000	-0.072209000	1.630712000
6	-3.338956000	2.354776000	0.010982000
1	-3.451074000	1.987054000	-1.013593000
1	-4.060402000	3.167537000	0.143758000
1	-2.337714000	2.781979000	0.112333000
6	4.342459000	1.018494000	1.388996000
1	4.168234000	1.453252000	2.376316000
1	3.994264000	-0.018556000	1.403753000
1	5.424077000	1.002338000	1.223625000
6	3.895483000	1.218316000	-1.093428000
1	3.241064000	1.654294000	-1.853260000
1	4.926817000	1.424298000	-1.399254000
1	3.764336000	0.137212000	-1.097794000
6	-0.357582000	-2.740265000	3.191408000
1	-0.796189000	-3.676513000	3.547990000
1	0.290402000	-2.353906000	3.982107000
1	-1.179153000	-2.031363000	3.040989000
6	-0.489351000	-3.514371000	0.788085000
1	-1.377201000	-2.892551000	0.649441000
1	0.033219000	-3.582861000	-0.169644000
1	-0.833183000	-4.521061000	1.047140000
5	0.062758000	-0.203846000	-1.114162000
7	-0.189083000	1.047670000	4.271559000
7	-0.272176000	0.910962000	3.037374000

1	-0.819406000	0.407426000	4.776913000
1	-0.688890000	1.906853000	2.385186000

TS3_{alt} (Quintet, TE= -3322.210412)

6	1.308232000	0.094886000	-1.737583000
6	1.798760000	0.841728000	-2.822130000
1	1.180937000	1.635618000	-3.242406000
6	3.043832000	0.581171000	-3.383669000
1	3.388353000	1.166290000	-4.232663000
6	3.855972000	-0.412137000	-2.845085000
1	4.838374000	-0.608305000	-3.266693000
6	3.424432000	-1.128826000	-1.735339000
1	4.075882000	-1.865179000	-1.269808000
6	2.157955000	-0.885282000	-1.203213000
6	-1.288197000	-0.667636000	-1.659417000
6	-1.392341000	-1.062730000	-3.003067000
1	-0.621046000	-0.752548000	-3.708349000
6	-2.463601000	-1.822795000	-3.458076000
1	-2.524953000	-2.100440000	-4.507338000
6	-3.445547000	-2.243757000	-2.566273000
1	-4.276288000	-2.854059000	-2.911068000
6	-3.342553000	-1.916345000	-1.219235000
1	-4.074284000	-2.292466000	-0.507483000
6	-2.282319000	-1.123471000	-0.781086000
6	-0.605870000	1.834301000	-0.964310000
6	-1.456643000	2.478187000	-1.875825000
1	-1.858044000	1.912505000	-2.716792000
6	-1.806402000	3.816722000	-1.729622000
1	-2.462949000	4.287705000	-2.457086000
6	-1.338673000	4.541748000	-0.639684000
1	-1.625006000	5.581686000	-0.505676000
6	-0.516229000	3.924263000	0.297724000
1	-0.170064000	4.469996000	1.172478000
6	-0.140354000	2.593435000	0.120299000
16	0.828139000	1.831175000	1.424376000
16	1.724483000	-1.703022000	0.325432000
16	-2.087346000	-0.860565000	0.977234000
23	0.173855000	-0.531489000	1.931976000
6	1.363608000	-3.482418000	-0.129937000
1	2.354730000	-3.877914000	-0.381597000
6	-3.512108000	0.248662000	1.476804000
1	-4.381113000	-0.414990000	1.399081000
6	2.606087000	2.032251000	0.862837000
1	2.683205000	1.493917000	-0.085892000
6	3.474397000	1.372077000	1.914229000

1	4.525687000	1.453820000	1.622618000
1	3.367879000	1.855097000	2.890545000
1	3.253304000	0.306807000	2.033181000
6	2.916049000	3.497490000	0.658941000
1	2.795488000	4.070238000	1.583496000
1	3.955143000	3.608077000	0.333175000
1	2.285051000	3.951290000	-0.109188000
6	0.839441000	-4.150953000	1.124234000
1	1.511626000	-4.037267000	1.978296000
1	-0.142066000	-3.752552000	1.405961000
1	0.714221000	-5.222070000	0.941684000
6	0.429469000	-3.613430000	-1.307899000
1	0.767241000	-3.044694000	-2.178223000
1	0.371047000	-4.665635000	-1.605616000
1	-0.581758000	-3.284291000	-1.056120000
6	-3.279057000	0.629878000	2.923278000
1	-4.147395000	1.176381000	3.302150000
1	-3.125928000	-0.238755000	3.569477000
1	-2.406974000	1.285164000	3.023168000
6	-3.676655000	1.442575000	0.568166000
1	-2.844303000	2.143539000	0.672030000
1	-3.757620000	1.161164000	-0.484884000
1	-4.594443000	1.976076000	0.837224000
5	-0.170727000	0.366071000	-1.295895000
7	0.806071000	-2.110071000	4.536590000
7	0.600599000	-1.491008000	3.517869000
1	1.104532000	-1.590107000	5.376633000
1	-0.046301000	-0.039413000	3.631184000

Cartesian coordinates of intermediates and TSs involved in the conversion of [4]→[5]_{dis} for the catalysts [**1c''_{PB}**] and [**1f''_{SB}**], along with their total energies (in hartree) including zero point vibrational correction at M06-L-D3(heptane)/6-311+G* level of theory.

For catalyst [**1c''_{PB}**]

[**4c''_{PB}** -V-H]⁺ (TE= -3507.088650)

6	1.567069000	-0.653872000	1.844241000
6	1.848572000	-1.579368000	2.866937000
1	1.023541000	-2.119171000	3.330452000
6	3.141170000	-1.809021000	3.324580000
1	3.316074000	-2.522805000	4.125823000
6	4.203390000	-1.129002000	2.744624000
1	5.220822000	-1.297200000	3.089153000
6	3.963603000	-0.250426000	1.692119000
1	4.811676000	0.233638000	1.215202000
6	2.669712000	-0.004616000	1.228848000

6	-0.576924000	1.060156000	1.918802000
6	-0.131889000	1.541101000	3.166861000
1	0.763534000	1.112153000	3.614003000
6	-0.834588000	2.512723000	3.873995000
1	-0.473760000	2.840141000	4.845920000
6	-1.988618000	3.059743000	3.332597000
1	-2.549449000	3.814146000	3.878767000
6	-2.410833000	2.658485000	2.066212000
1	-3.289987000	3.128605000	1.628802000
6	-1.725689000	1.679787000	1.351369000
6	-0.976574000	-1.561202000	1.655962000
6	-1.741231000	-1.740741000	2.820049000
1	-1.659614000	-1.014173000	3.629224000
6	-2.604487000	-2.819652000	2.962709000
1	-3.180294000	-2.939246000	3.877402000
6	-2.749559000	-3.728047000	1.919849000
1	-3.439654000	-4.563256000	2.010443000
6	-2.024114000	-3.553966000	0.747387000
1	-2.181472000	-4.250029000	-0.072104000
6	-1.126301000	-2.490326000	0.609116000
23	0.091819000	0.499402000	-1.169572000
6	2.821207000	2.708411000	0.048189000
1	3.890290000	2.707809000	0.301538000
6	-3.851486000	0.629362000	-0.430268000
1	-4.515629000	1.460855000	-0.163390000
6	1.146124000	-3.426724000	-1.059748000
1	1.004479000	-3.888123000	-2.044349000
6	1.049743000	-4.512202000	0.002343000
1	1.854317000	-5.241244000	-0.138893000
1	1.157092000	-4.097935000	1.010533000
1	0.105653000	-5.060828000	-0.022446000
6	2.519759000	-2.780745000	-1.053344000
1	2.741160000	-2.300874000	-0.095449000
1	3.296016000	-3.534171000	-1.223657000
1	2.614035000	-2.031768000	-1.841904000
6	2.601591000	3.573589000	-1.187659000
1	3.157481000	3.225955000	-2.063043000
1	1.543025000	3.598770000	-1.462460000
1	2.918598000	4.602814000	-0.992176000
6	2.053116000	3.244996000	1.243462000
1	2.242312000	2.665553000	2.151248000
1	2.352040000	4.278918000	1.444547000
1	0.973920000	3.243349000	1.065460000
6	-4.173513000	0.167813000	-1.847917000
1	-5.235222000	-0.079652000	-1.945248000
1	-3.940395000	0.911707000	-2.616139000

1	-3.607357000	-0.734690000	-2.098307000
6	-4.075479000	-0.483535000	0.576682000
1	-3.477026000	-1.368590000	0.348463000
1	-3.840122000	-0.177647000	1.599275000
1	-5.125542000	-0.794153000	0.559475000
5	0.035211000	-0.360157000	1.647274000
15	2.419334000	0.929495000	-0.337537000
15	-2.130903000	1.354476000	-0.406483000
15	-0.239822000	-2.147204000	-0.958915000
6	-2.405725000	3.042994000	-1.233463000
1	-2.052184000	2.839742000	-2.254298000
6	-1.546149000	4.167583000	-0.663788000
1	-1.546334000	5.010700000	-1.361720000
1	-1.941692000	4.540229000	0.285042000
1	-0.508968000	3.874875000	-0.501058000
6	-3.851048000	3.524960000	-1.318204000
1	-3.875796000	4.477068000	-1.857686000
1	-4.520072000	2.845914000	-1.848398000
1	-4.284838000	3.718845000	-0.331414000
6	3.862543000	0.395867000	-1.434986000
1	4.076940000	-0.622492000	-1.089088000
6	5.147204000	1.210446000	-1.314421000
1	5.930674000	0.738344000	-1.915974000
1	5.032664000	2.229144000	-1.694122000
1	5.533804000	1.284956000	-0.296090000
6	3.430989000	0.327183000	-2.897271000
1	4.228203000	-0.106686000	-3.509277000
1	2.528723000	-0.273638000	-3.046838000
1	3.227490000	1.324784000	-3.300972000
6	-1.453458000	-2.711556000	-2.283181000
1	-2.429362000	-2.501687000	-1.822131000
6	-1.311615000	-1.863063000	-3.542116000
1	-0.293956000	-1.912695000	-3.949902000
1	-1.984668000	-2.226609000	-4.325421000
1	-1.544503000	-0.809482000	-3.372677000
6	-1.398808000	-4.192240000	-2.650887000
1	-0.556953000	-4.411323000	-3.314126000
1	-1.321239000	-4.868864000	-1.797316000
1	-2.304127000	-4.466280000	-3.201579000
7	0.056136000	1.556589000	-3.966332000
7	0.172754000	1.107357000	-2.834684000
1	0.979160000	1.746285000	-4.409277000
1	0.131002000	2.086074000	-0.695003000

TS4'_{dis} (TE= -3507.062932)

6	-1.434249000	0.766987000	1.905348000
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6	-1.562983000	1.603913000	3.030452000
1	-0.665377000	1.923850000	3.558362000
6	-2.799001000	2.031561000	3.499433000
1	-2.856208000	2.670692000	4.377330000
6	-3.952364000	1.654659000	2.825598000
1	-4.928140000	1.990531000	3.167891000
6	-3.851958000	0.862541000	1.687810000
1	-4.762865000	0.614593000	1.153348000
6	-2.615443000	0.407251000	1.219106000
6	0.465045000	-1.201447000	2.051936000
6	0.042711000	-1.625471000	3.323036000
1	-0.685334000	-1.024100000	3.867273000
6	0.530554000	-2.787477000	3.910670000
1	0.180823000	-3.085257000	4.896378000
6	1.457736000	-3.567699000	3.231579000
1	1.845092000	-4.479518000	3.679140000
6	1.879867000	-3.182148000	1.963600000
1	2.595591000	-3.806666000	1.436050000
6	1.393623000	-2.016688000	1.365615000
6	1.177499000	1.352270000	1.681001000
6	1.925523000	1.437625000	2.868064000
1	1.764752000	0.698035000	3.653066000
6	2.872708000	2.434216000	3.065779000
1	3.431225000	2.475654000	3.998044000
6	3.122127000	3.360486000	2.058699000
1	3.875336000	4.132696000	2.194461000
6	2.414112000	3.282732000	0.866108000
1	2.638655000	3.992770000	0.073924000
6	1.435179000	2.300973000	0.673696000
23	-0.175058000	-0.236180000	-1.457444000
6	-3.113939000	-2.226168000	0.045664000
1	-4.131954000	-2.060020000	0.422152000
6	3.676635000	-1.196259000	-0.280997000
1	4.107668000	-2.150443000	0.054071000
6	-0.550050000	3.528817000	-1.180200000
1	-0.594017000	3.624956000	-2.275190000
6	-0.070181000	4.835892000	-0.565790000
1	-0.788882000	5.630716000	-0.789391000
1	-0.004401000	4.760414000	0.524101000
1	0.900001000	5.169150000	-0.934891000
6	-1.946035000	3.197798000	-0.679462000
1	-1.969689000	3.083017000	0.408448000
1	-2.642181000	4.002335000	-0.937416000
1	-2.317799000	2.277201000	-1.130178000
6	-3.195346000	-3.106583000	-1.195903000
1	-2.205946000	-3.384977000	-1.563242000

1	-3.724777000	-4.036106000	-0.962853000
1	-3.715651000	-2.634053000	-2.031500000
6	-2.315479000	-2.885970000	1.156418000
1	-2.334524000	-2.300871000	2.079255000
1	-2.732980000	-3.872605000	1.383523000
1	-1.265768000	-3.033534000	0.886091000
6	4.222226000	-0.865249000	-1.664602000
1	5.316452000	-0.881619000	-1.654224000
1	3.896146000	-1.557137000	-2.446715000
1	3.923762000	0.139551000	-1.975507000
6	4.061397000	-0.139259000	0.737883000
1	3.680264000	0.850930000	0.472378000
1	3.698150000	-0.377378000	1.740283000
1	5.152106000	-0.061655000	0.792803000
5	0.037107000	0.263787000	1.665578000
7	0.072545000	-1.491958000	-3.744583000
7	-0.884938000	-1.231995000	-3.035131000
1	-0.117955000	-2.282651000	-4.406154000
15	0.604129000	2.082653000	-0.941336000
15	-2.506448000	-0.506300000	-0.372651000
15	1.848688000	-1.571846000	-0.349982000
6	2.000679000	2.298907000	-2.184561000
1	2.885340000	1.993564000	-1.606374000
6	2.244043000	3.698518000	-2.731914000
1	3.035736000	3.661800000	-3.487445000
1	1.359571000	4.113386000	-3.224132000
1	2.568134000	4.411760000	-1.972386000
6	1.812204000	1.308432000	-3.327395000
1	1.731401000	0.266812000	-2.982787000
1	0.921514000	1.526028000	-3.923324000
1	2.674279000	1.322795000	-4.003229000
6	1.856624000	-3.159551000	-1.371686000
1	1.840508000	-2.753189000	-2.394639000
6	0.563669000	-3.929118000	-1.158018000
1	-0.319608000	-3.294810000	-1.266179000
1	0.470248000	-4.742310000	-1.884628000
1	0.516301000	-4.375455000	-0.159671000
6	3.061980000	-4.087731000	-1.274761000
1	2.937907000	-4.902619000	-1.995659000
1	4.009760000	-3.602113000	-1.512312000
1	3.162856000	-4.559536000	-0.294437000
6	-3.967780000	0.185619000	-1.369856000
1	-4.038615000	1.216025000	-0.998164000
6	-5.324395000	-0.479646000	-1.132994000
1	-6.099261000	0.122442000	-1.618115000
1	-5.381924000	-1.475552000	-1.578567000

1	-5.612151000	-0.578970000	-0.085126000
6	-3.696568000	0.244003000	-2.868115000
1	-2.788927000	0.800293000	-3.105149000
1	-3.586536000	-0.753871000	-3.302410000
1	-4.537756000	0.728065000	-3.375067000
1	-0.900556000	0.959813000	-2.417904000

$\eta_{NN}^2 - [4c''_{PB} - V - H]^+$ (TE= -3507.087648)

6	-1.363126000	0.819160000	1.903240000
6	-1.487848000	1.684267000	3.007056000
1	-0.585113000	2.059661000	3.487458000
6	-2.721378000	2.075469000	3.511892000
1	-2.772668000	2.738902000	4.371906000
6	-3.880805000	1.630121000	2.893740000
1	-4.857540000	1.934666000	3.261556000
6	-3.787926000	0.806051000	1.778339000
1	-4.708366000	0.503363000	1.291820000
6	-2.551936000	0.384788000	1.275458000
6	0.621777000	-1.054979000	2.045137000
6	0.301602000	-1.418086000	3.364399000
1	-0.423078000	-0.821439000	3.918638000
6	0.891362000	-2.511674000	3.987943000
1	0.621900000	-2.764842000	5.010654000
6	1.820951000	-3.278465000	3.297008000
1	2.293514000	-4.134242000	3.772677000
6	2.133625000	-2.955227000	1.981164000
1	2.846823000	-3.575396000	1.446042000
6	1.542100000	-1.861120000	1.343070000
6	1.228320000	1.498264000	1.610489000
6	2.019416000	1.665664000	2.758192000
1	1.903626000	0.974338000	3.593571000
6	2.959480000	2.684728000	2.847863000
1	3.558970000	2.792922000	3.748832000
6	3.150934000	3.550181000	1.774742000
1	3.899442000	4.336813000	1.829960000
6	2.391604000	3.393219000	0.622071000
1	2.565321000	4.056587000	-0.222066000
6	1.427343000	2.383093000	0.538061000
23	-0.334166000	-0.289653000	-1.613944000
6	-2.989083000	-2.328744000	0.246903000
1	-4.007744000	-2.214837000	0.639281000
6	3.668791000	-1.057235000	-0.478836000
1	4.153178000	-1.968633000	-0.102190000
6	-0.688851000	3.462907000	-1.222902000
1	-0.852317000	3.457350000	-2.310831000
6	-0.144154000	4.817358000	-0.791494000

1	-0.878672000	5.595791000	-1.022212000
1	0.027142000	4.851043000	0.288709000
1	0.786174000	5.100831000	-1.283812000
6	-2.025499000	3.210206000	-0.542837000
1	-1.930967000	3.208363000	0.547491000
1	-2.736938000	3.999602000	-0.805769000
1	-2.458041000	2.255934000	-0.846197000
6	-3.031773000	-3.257952000	-0.960509000
1	-2.036329000	-3.432731000	-1.377074000
1	-3.434434000	-4.235240000	-0.676296000
1	-3.656412000	-2.877490000	-1.773567000
6	-2.125175000	-2.882409000	1.366486000
1	-2.152429000	-2.248274000	2.256339000
1	-2.482427000	-3.875571000	1.658280000
1	-1.077438000	-2.988762000	1.074639000
6	4.139962000	-0.810755000	-1.907722000
1	5.233067000	-0.836424000	-1.958828000
1	3.766872000	-1.544527000	-2.628365000
1	3.833474000	0.177031000	-2.262364000
6	4.072302000	0.076458000	0.444744000
1	3.657145000	1.037809000	0.132173000
1	3.761595000	-0.098499000	1.477400000
1	5.162356000	0.182286000	0.442923000
5	0.121412000	0.375545000	1.638018000
7	-0.280011000	-2.006054000	-2.791258000
7	-1.074788000	-1.183402000	-3.210265000
15	0.477801000	2.021150000	-0.977492000
15	-2.496817000	-0.603338000	-0.278875000
15	1.855157000	-1.525807000	-0.432262000
6	1.758552000	2.136092000	-2.356317000
1	2.687300000	1.857951000	-1.838450000
6	1.967488000	3.487398000	-3.023850000
1	2.682387000	3.384889000	-3.847090000
1	1.044581000	3.887458000	-3.454112000
1	2.374677000	4.239834000	-2.347037000
6	1.466230000	1.069625000	-3.408763000
1	1.470075000	0.046956000	-2.988111000
1	0.517933000	1.243229000	-3.924426000
1	2.251030000	1.041893000	-4.172294000
6	1.946043000	-3.217400000	-1.269681000
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6	0.783420000	-4.093731000	-0.830460000
1	-0.160065000	-3.547766000	-0.821422000
1	0.663858000	-4.941074000	-1.512624000
1	0.933809000	-4.497716000	0.175434000
6	3.254548000	-4.001258000	-1.216253000

1	3.128717000	-4.924231000	-1.792287000
1	4.103439000	-3.474664000	-1.655059000
1	3.541782000	-4.308582000	-0.207689000
6	-4.050189000	-0.015826000	-1.203819000
1	-4.139941000	1.027298000	-0.873227000
6	-5.354887000	-0.734023000	-0.856745000
1	-6.189507000	-0.193923000	-1.314661000
1	-5.384177000	-1.749383000	-1.260901000
1	-5.572852000	-0.807776000	0.209469000
6	-3.891113000	-0.005312000	-2.718807000
1	-3.020941000	0.567718000	-3.041019000
1	-3.809768000	-1.021128000	-3.122129000
1	-4.779353000	0.438774000	-3.179408000
1	-1.177216000	1.029653000	-2.222520000
1	-1.650246000	-1.364137000	-4.053257000

TS4''_{dis} (TE= -3507.050379)

6	0.954445000	-1.588234000	1.669784000
6	0.670862000	-2.531015000	2.671848000
1	-0.290041000	-2.488785000	3.183540000
6	1.598976000	-3.495055000	3.051970000
1	1.353173000	-4.207567000	3.835991000
6	2.844106000	-3.537703000	2.435636000
1	3.582636000	-4.276745000	2.736473000
6	3.134250000	-2.644138000	1.408653000
1	4.100914000	-2.707547000	0.915282000
6	2.197640000	-1.690207000	1.007544000
6	0.557610000	1.063308000	1.933462000
6	1.277507000	1.098424000	3.140778000
1	1.574303000	0.159232000	3.607871000
6	1.608407000	2.295098000	3.766498000
1	2.162642000	2.283773000	4.702316000
6	1.229971000	3.502710000	3.192428000
1	1.477620000	4.445083000	3.674754000
6	0.543767000	3.499615000	1.982944000
1	0.270182000	4.449695000	1.530075000
6	0.213745000	2.300500000	1.345636000
6	-1.553422000	-0.568043000	1.782941000
6	-1.998274000	-0.291247000	3.087966000
1	-1.294442000	0.120114000	3.811885000
6	-3.311974000	-0.512318000	3.478855000
1	-3.622727000	-0.286083000	4.496251000
6	-4.231942000	-0.999017000	2.556471000
1	-5.268974000	-1.157350000	2.841959000
6	-3.822367000	-1.267043000	1.257365000
1	-4.561269000	-1.618615000	0.543383000

6	-2.492338000	-1.068985000	0.865274000
23	0.139316000	0.105417000	-1.476528000
6	3.987086000	0.253008000	-0.307079000
1	4.745545000	-0.522149000	-0.119996000
6	-2.283548000	2.981380000	-0.037760000
1	-2.078523000	4.025042000	0.235186000
6	-1.720788000	-3.203358000	-1.047079000
1	-2.247917000	-3.444560000	-1.978901000
6	-2.341480000	-3.998088000	0.093601000
1	-2.249409000	-5.070088000	-0.108931000
1	-1.828386000	-3.798466000	1.040180000
1	-3.400550000	-3.785466000	0.251156000
6	-0.261536000	-3.591263000	-1.225178000
1	0.339665000	-3.317437000	-0.351786000
1	-0.167661000	-4.674525000	-1.353418000
1	0.182014000	-3.125477000	-2.109318000
6	4.366383000	1.005789000	-1.577356000
1	3.635722000	1.773200000	-1.835543000
1	5.331555000	1.503770000	-1.441018000
1	4.459809000	0.355807000	-2.449949000
6	3.934063000	1.163828000	0.910553000
1	3.741862000	0.607284000	1.831661000
1	4.889904000	1.683694000	1.031004000
1	3.155271000	1.927684000	0.823732000
6	-3.064945000	2.955987000	-1.344291000
1	-3.969496000	3.567510000	-1.267250000
1	-2.493322000	3.325283000	-2.201915000
1	-3.385685000	1.937800000	-1.584152000
6	-3.073506000	2.367481000	1.103013000
1	-3.394639000	1.347340000	0.883630000
1	-2.508206000	2.345420000	2.038174000
1	-3.978444000	2.958332000	1.279875000
5	-0.010388000	-0.354834000	1.533167000
7	-0.040121000	0.999803000	-3.353619000
7	1.100441000	1.176084000	-2.810599000
1	-0.060810000	0.806097000	-4.367347000
15	-1.944280000	-1.336627000	-0.862067000
15	2.405336000	-0.703191000	-0.518087000
15	-0.569214000	2.287893000	-0.304531000
6	-3.507771000	-0.966104000	-1.855429000
1	-4.006419000	-0.204957000	-1.237837000
6	-4.463227000	-2.144524000	-2.036426000
1	-5.429663000	-1.779609000	-2.397588000
1	-4.096178000	-2.846003000	-2.791263000
1	-4.654257000	-2.719188000	-1.129275000
6	-3.215638000	-0.354900000	-3.219394000

1	-2.644294000	0.573823000	-3.156637000
1	-2.661478000	-1.050053000	-3.861383000
1	-4.154100000	-0.128864000	-3.736579000
6	0.232676000	3.682503000	-1.288783000
1	0.056026000	3.358477000	-2.321541000
6	1.737870000	3.689446000	-1.059430000
1	2.143202000	2.678514000	-1.016283000
1	2.248278000	4.214423000	-1.872858000
1	2.004704000	4.191580000	-0.125027000
6	-0.341921000	5.087801000	-1.150120000
1	0.231148000	5.766601000	-1.790653000
1	-1.384968000	5.167339000	-1.463026000
1	-0.267902000	5.487312000	-0.134611000
6	2.851089000	-2.031819000	-1.790851000
1	2.300501000	-2.904357000	-1.419757000
6	4.319426000	-2.427504000	-1.893482000
1	4.416381000	-3.278259000	-2.576015000
1	4.945742000	-1.629116000	-2.297463000
1	4.755130000	-2.738959000	-0.943203000
6	2.302100000	-1.675974000	-3.168115000
1	1.212544000	-1.516650000	-3.170166000
1	2.753874000	-0.769386000	-3.579139000
1	2.483192000	-2.491881000	-3.876140000
1	-0.669751000	-0.286877000	-2.968976000

For catalyst [**1f'**_{SB}]

[**4f'**_{SB} -**V-H**]⁺ (TE= -3322.247307)

6	1.673732000	-0.944371000	-1.003607000
6	2.635884000	-0.960215000	-2.022608000
1	2.550592000	-0.258885000	-2.852695000
6	3.676565000	-1.883629000	-2.010466000
1	4.405973000	-1.888455000	-2.816616000
6	3.782536000	-2.808225000	-0.973150000
1	4.594029000	-3.531259000	-0.966416000
6	2.873174000	-2.782736000	0.078080000
1	2.988908000	-3.457393000	0.923520000
6	1.834482000	-1.855054000	0.048859000
6	-0.893855000	-0.944308000	-1.665299000
6	-0.706467000	-1.727545000	-2.817912000
1	0.301555000	-1.852615000	-3.211453000
6	-1.772156000	-2.312210000	-3.489483000
1	-1.594095000	-2.891516000	-4.391789000
6	-3.066583000	-2.162538000	-2.999453000
1	-3.906032000	-2.624947000	-3.512353000
6	-3.282681000	-1.459179000	-1.821068000

1	-4.282557000	-1.407200000	-1.395795000
6	-2.208695000	-0.852531000	-1.171298000
6	0.229763000	1.439761000	-1.137062000
6	-0.566256000	1.927842000	-2.206143000
1	-1.170416000	1.221828000	-2.769152000
6	-0.552828000	3.252597000	-2.608207000
1	-1.151663000	3.564483000	-3.459984000
6	0.215064000	4.179434000	-1.910977000
1	0.223610000	5.225031000	-2.208258000
6	0.947918000	3.770127000	-0.806574000
1	1.494975000	4.497717000	-0.213051000
6	0.977084000	2.426680000	-0.429864000
16	1.729769000	2.078160000	1.158516000
16	0.788637000	-1.583778000	1.465421000
16	-2.461787000	-0.201300000	0.472316000
23	-0.357756000	0.754904000	1.329188000
6	-0.139401000	-3.181568000	1.734900000
1	0.655031000	-3.873945000	2.039111000
6	-3.860292000	1.023315000	0.326724000
1	-4.692872000	0.408296000	-0.035964000
6	3.588740000	1.757786000	0.913636000
1	3.977873000	2.498065000	1.620855000
6	4.012071000	2.120183000	-0.488830000
1	5.098549000	2.012202000	-0.569543000
1	3.560772000	1.454223000	-1.229355000
1	3.763805000	3.149822000	-0.754912000
6	4.019923000	0.376954000	1.343852000
1	3.808869000	-0.370523000	0.580288000
1	5.103730000	0.382708000	1.502093000
1	3.558178000	0.059398000	2.282071000
6	-1.085990000	-2.943888000	2.893693000
1	-0.568752000	-2.606097000	3.794869000
1	-1.849351000	-2.201586000	2.640223000
1	-1.603749000	-3.875629000	3.138277000
6	-0.824560000	-3.688872000	0.487987000
1	-0.147858000	-3.748769000	-0.368647000
1	-1.209307000	-4.696880000	0.674759000
1	-1.673957000	-3.060495000	0.210957000
6	-4.151565000	1.513018000	1.730649000
1	-5.037116000	2.154486000	1.714276000
1	-4.344778000	0.694488000	2.428602000
1	-3.317428000	2.104745000	2.117299000
6	-3.549463000	2.134261000	-0.646023000
1	-2.679551000	2.709678000	-0.314847000
1	-3.356664000	1.758645000	-1.654553000
1	-4.403053000	2.817455000	-0.707221000

5	0.338256000	-0.133128000	-1.124625000
7	-1.270494000	0.562268000	4.186775000
7	-0.810142000	0.651847000	3.073702000
1	-0.658303000	0.980290000	4.919330000
1	-1.080149000	2.276840000	1.432373000

TS4'_{dis} (TE= -3322.229207)

6	-1.061574000	-1.074430000	-1.710041000
6	-0.912148000	-1.540476000	-3.025879000
1	-0.297176000	-0.971781000	-3.722619000
6	-1.544223000	-2.699408000	-3.462968000
1	-1.427750000	-3.024895000	-4.493609000
6	-2.303005000	-3.454514000	-2.575214000
1	-2.781918000	-4.373027000	-2.904493000
6	-2.424502000	-3.049708000	-1.249772000
1	-2.974073000	-3.658381000	-0.535848000
6	-1.825672000	-1.862603000	-0.834608000
6	-1.302216000	1.491466000	-0.829330000
6	-2.471193000	1.765088000	-1.558860000
1	-2.770046000	1.076025000	-2.348320000
6	-3.241176000	2.899114000	-1.320044000
1	-4.130994000	3.086701000	-1.915768000
6	-2.879440000	3.779842000	-0.308418000
1	-3.482259000	4.660506000	-0.102862000
6	-1.752340000	3.519221000	0.466775000
1	-1.489866000	4.176345000	1.292054000
6	-0.964588000	2.402097000	0.197390000
6	1.065190000	0.561341000	-1.705279000
6	1.356983000	1.591342000	-2.611232000
1	0.540458000	2.203832000	-2.993038000
6	2.657585000	1.850155000	-3.029456000
1	2.855906000	2.643732000	-3.744844000
6	3.701705000	1.098083000	-2.505353000
1	4.727125000	1.297944000	-2.806209000
6	3.451602000	0.086422000	-1.581259000
1	4.291658000	-0.466973000	-1.176000000
6	2.141216000	-0.190605000	-1.195533000
16	1.720554000	-1.426827000	0.031636000
16	-1.920346000	-1.458229000	0.909271000
16	0.353640000	2.058782000	1.372001000
23	0.073757000	-0.334830000	1.832924000
5	-0.423679000	0.299243000	-1.327646000
7	0.486833000	-2.033271000	3.644050000
7	0.953330000	-0.930638000	3.370681000
1	-1.196632000	0.374046000	2.672606000
1	0.854674000	-2.433545000	4.532235000

6	-3.461659000	-0.387793000	1.124188000
1	-3.094371000	0.637491000	1.012994000
6	-4.490633000	-0.713690000	0.068886000
1	-5.368437000	-0.078899000	0.225614000
1	-4.131058000	-0.532815000	-0.946192000
1	-4.824873000	-1.754139000	0.129445000
6	-3.954203000	-0.622184000	2.535057000
1	-4.318236000	-1.644680000	2.669619000
1	-3.174373000	-0.429124000	3.274851000
1	-4.784361000	0.059132000	2.745512000
6	3.344768000	-2.205963000	0.485685000
1	4.051961000	-1.375292000	0.586177000
6	3.764247000	-3.153374000	-0.621903000
1	4.763855000	-3.547637000	-0.412903000
1	3.079898000	-4.003119000	-0.689495000
1	3.795183000	-2.674765000	-1.603154000
6	3.204339000	-2.894204000	1.827201000
1	3.056252000	-2.181424000	2.639154000
1	2.379226000	-3.613027000	1.840325000
1	4.121287000	-3.451676000	2.038449000
6	1.960198000	2.704336000	0.664955000
1	2.085802000	2.253201000	-0.317025000
6	1.879780000	4.208958000	0.542887000
1	2.821759000	4.594368000	0.139596000
1	1.083895000	4.521934000	-0.138930000
1	1.710455000	4.691104000	1.510224000
6	3.039344000	2.210023000	1.607306000
1	2.920239000	2.610230000	2.618743000
1	3.055518000	1.116191000	1.676111000
1	4.019358000	2.529528000	1.240162000

$\eta_{NN}^2 - [4f''_{SB} - V - H]^+$ (TE= -3322.245344)

6	-1.298698000	-1.341373000	-1.461178000
6	-1.394842000	-2.002311000	-2.693347000
1	-0.930668000	-1.560169000	-3.574598000
6	-2.078683000	-3.207956000	-2.814587000
1	-2.153680000	-3.693276000	-3.784523000
6	-2.641747000	-3.804780000	-1.691676000
1	-3.157980000	-4.757570000	-1.776866000
6	-2.519560000	-3.194058000	-0.447235000
1	-2.918361000	-3.673422000	0.443801000
6	-1.873048000	-1.965122000	-0.343957000
6	-1.448831000	1.316231000	-1.012457000
6	-2.663143000	1.505530000	-1.691124000
1	-2.999371000	0.739496000	-2.389706000
6	-3.441072000	2.644241000	-1.506729000

1	-4.369414000	2.763082000	-2.059844000
6	-3.039499000	3.614750000	-0.597501000
1	-3.648474000	4.499282000	-0.429748000
6	-1.861767000	3.440517000	0.123735000
1	-1.560287000	4.173775000	0.867648000
6	-1.067145000	2.316268000	-0.095676000
6	0.879499000	0.225240000	-1.836514000
6	1.201730000	1.153009000	-2.836391000
1	0.401577000	1.737403000	-3.290454000
6	2.514784000	1.354540000	-3.250852000
1	2.735919000	2.065273000	-4.042722000
6	3.544065000	0.674558000	-2.610854000
1	4.578832000	0.854904000	-2.891540000
6	3.264265000	-0.241179000	-1.597830000
1	4.084657000	-0.743250000	-1.094885000
6	1.940413000	-0.495497000	-1.249989000
16	1.463410000	-1.685537000	0.000393000
16	-1.644605000	-1.268249000	1.296461000
16	0.352486000	2.143046000	0.996093000
23	0.551686000	-0.148617000	1.921090000
5	-0.602697000	0.055628000	-1.377455000
7	1.727986000	0.439824000	3.393024000
7	2.484413000	-0.056832000	2.572897000
1	-0.685085000	0.388063000	2.922213000
1	2.075190000	0.861989000	4.271441000
6	-3.158281000	-0.183106000	1.601555000
1	-2.819747000	0.826037000	1.343407000
6	-4.313586000	-0.597789000	0.720847000
1	-5.161750000	0.064347000	0.921870000
1	-4.085734000	-0.527003000	-0.344339000
1	-4.640788000	-1.620813000	0.931095000
6	-3.489005000	-0.269449000	3.075520000
1	-3.832049000	-1.271221000	3.349703000
1	-2.634242000	-0.010746000	3.703262000
1	-4.294736000	0.434246000	3.306977000
6	3.022658000	-2.481618000	0.592532000
1	3.715949000	-1.669405000	0.837390000
6	3.577454000	-3.403530000	-0.477367000
1	4.529125000	-3.825942000	-0.140161000
1	2.895145000	-4.236637000	-0.666599000
1	3.758139000	-2.902617000	-1.429957000
6	2.660477000	-3.245427000	1.854065000
1	2.317673000	-2.594891000	2.663247000
1	1.887449000	-3.995989000	1.662577000
1	3.541746000	-3.776444000	2.223910000
6	1.819332000	2.838056000	0.054191000

1	2.045183000	2.123257000	-0.735530000
6	1.456299000	4.178988000	-0.541152000
1	2.321228000	4.577573000	-1.081113000
1	0.631639000	4.107983000	-1.254632000
1	1.181651000	4.908650000	0.227003000
6	2.976737000	2.902125000	1.027821000
1	2.755966000	3.534378000	1.893690000
1	3.273470000	1.913386000	1.387135000
1	3.846276000	3.332072000	0.521372000

TS4''_{dis} (TE= -3322.211383)

6	1.198152000	-1.380642000	1.490910000
6	1.165633000	-2.052054000	2.722410000
1	0.569415000	-1.640220000	3.536123000
6	1.887255000	-3.223253000	2.930893000
1	1.854665000	-3.714579000	3.900091000
6	2.628514000	-3.777574000	1.893563000
1	3.178051000	-4.703236000	2.043772000
6	2.640462000	-3.162155000	0.645423000
1	3.177028000	-3.612994000	-0.185875000
6	1.945765000	-1.969566000	0.459038000
6	1.320799000	1.296230000	1.082501000
6	2.497324000	1.501518000	1.820286000
1	2.837189000	0.718361000	2.497930000
6	3.229986000	2.681072000	1.721884000
1	4.130665000	2.811644000	2.316692000
6	2.817877000	3.681601000	0.850165000
1	3.391227000	4.600126000	0.755255000
6	1.678321000	3.494576000	0.071730000
1	1.373968000	4.251898000	-0.646846000
6	0.933179000	2.324130000	0.198202000
6	-1.000280000	0.167898000	1.824404000
6	-1.308502000	1.064944000	2.857081000
1	-0.500516000	1.627905000	3.323918000
6	-2.616285000	1.264208000	3.287943000
1	-2.825524000	1.954707000	4.100650000
6	-3.654681000	0.601994000	2.644777000
1	-4.685347000	0.773180000	2.945411000
6	-3.389199000	-0.282714000	1.601289000
1	-4.218834000	-0.767746000	1.097684000
6	-2.071417000	-0.517704000	1.219449000
16	-1.620452000	-1.634062000	-0.109102000
16	1.879907000	-1.302072000	-1.206280000
16	-0.404926000	2.083443000	-0.980481000
23	-0.334853000	-0.233272000	-1.827691000
5	0.486173000	0.005712000	1.370149000
7	-0.454138000	0.144386000	-3.762896000

7	-1.617207000	0.197403000	-3.213174000
1	0.572876000	0.757821000	-3.004245000
1	-0.281196000	0.645647000	-4.641786000
6	3.309404000	-0.086773000	-1.356609000
1	2.918961000	0.862375000	-0.975598000
6	4.490660000	-0.537371000	-0.531346000
1	5.300936000	0.190063000	-0.643113000
1	4.256050000	-0.605840000	0.533165000
1	4.872685000	-1.508900000	-0.859842000
6	3.621379000	0.027368000	-2.833479000
1	4.008187000	-0.911934000	-3.238101000
1	2.745604000	0.315659000	-3.422458000
1	4.382946000	0.797259000	-2.988570000
6	-3.216862000	-2.253784000	-0.827598000
1	-3.858978000	-1.371679000	-0.937633000
6	-3.830754000	-3.288320000	0.097102000
1	-4.805270000	-3.597527000	-0.293798000
1	-3.201026000	-4.180243000	0.153886000
1	-3.982434000	-2.927770000	1.116002000
6	-2.903202000	-2.832783000	-2.194737000
1	-2.515081000	-2.080592000	-2.884903000
1	-2.187893000	-3.658656000	-2.127229000
1	-3.818873000	-3.238702000	-2.633413000
6	-1.975726000	2.680268000	-0.143127000
1	-2.122050000	2.042358000	0.726728000
6	-1.796276000	4.117297000	0.288723000
1	-2.710795000	4.463360000	0.781235000
1	-0.978887000	4.234768000	1.005373000
1	-1.606309000	4.780633000	-0.560645000
6	-3.097263000	2.466511000	-1.134947000
1	-2.958189000	3.050377000	-2.049827000
1	-3.199917000	1.417229000	-1.423065000
1	-4.041196000	2.782948000	-0.680114000

Cartesian coordinates of TS involved in the conversion of $[5]_{\text{alt}} \rightarrow [5]_{\text{dis}}$ for the catalysts $[1c''_{\text{PB}}]$ and $[1f''_{\text{SB}}]$, along with their total energies (in hartree) including zero point vibrational correction at M06-L-D3(heptane)/6-311+G* level of theory.

For catalyst $[1c''_{\text{PB}}]$

TS5 (Triplet, TE= -3507.029777)

6	-0.168545000	-1.266032000	1.543673000
6	-1.165254000	-1.932076000	2.313268000
1	-1.957251000	-1.340074000	2.762326000
6	-1.140557000	-3.286999000	2.584147000
1	-1.901276000	-3.721081000	3.229020000

6	-0.153088000	-4.091956000	2.017629000
1	-0.137260000	-5.163725000	2.199293000
6	0.811978000	-3.508317000	1.220231000
1	1.569160000	-4.142064000	0.771036000
6	0.858521000	-2.116528000	1.005903000
6	0.775680000	1.395504000	1.848564000
6	1.099487000	1.640766000	3.192297000
1	0.664098000	1.012579000	3.970059000
6	1.989790000	2.643309000	3.557384000
1	2.230891000	2.799288000	4.606554000
6	2.582845000	3.439842000	2.581357000
1	3.284083000	4.221870000	2.861636000
6	2.268869000	3.233559000	1.243609000
1	2.724770000	3.866292000	0.485513000
6	1.371778000	2.224504000	0.877175000
6	-1.844772000	0.799024000	1.680594000
6	-2.164118000	1.632150000	2.764083000
1	-1.359782000	2.070582000	3.350579000
6	-3.477396000	1.899821000	3.131857000
1	-3.682623000	2.541733000	3.985627000
6	-4.524005000	1.331566000	2.416671000
1	-5.555961000	1.512016000	2.707455000
6	-4.244222000	0.544786000	1.304700000
1	-5.073080000	0.126353000	0.745334000
6	-2.925836000	0.295705000	0.911110000
23	0.055742000	-0.471787000	-0.859758000
6	3.663582000	-1.312903000	1.236379000
1	3.795603000	-2.378553000	1.472342000
6	-0.330674000	3.278693000	-1.279412000
1	0.288187000	4.185513000	-1.238278000
6	-3.247182000	-2.225649000	-0.804620000
1	-3.860053000	-2.182574000	-1.715153000
6	-4.154096000	-2.611419000	0.354378000
1	-4.479936000	-3.650634000	0.241344000
1	-3.646286000	-2.532928000	1.319356000
1	-5.055020000	-1.996958000	0.407919000
6	-2.155517000	-3.264918000	-1.034209000
1	-1.471665000	-3.330804000	-0.183705000
1	-2.593257000	-4.258710000	-1.173651000
1	-1.555963000	-3.048639000	-1.924898000
6	4.943040000	-0.788647000	0.598111000
1	5.159256000	-1.215915000	-0.383528000
1	4.913462000	0.297653000	0.487563000
1	5.794997000	-1.021208000	1.245007000
6	3.368749000	-0.572215000	2.523941000
1	2.427185000	-0.876327000	2.988792000

1	4.169441000	-0.764638000	3.245712000
1	3.334472000	0.506572000	2.361288000
6	-0.832200000	3.074825000	-2.704855000
1	-1.540665000	3.861523000	-2.982810000
1	-0.030963000	3.084637000	-3.448433000
1	-1.351826000	2.117503000	-2.809795000
6	-1.471701000	3.453737000	-0.292462000
1	-2.163153000	2.607648000	-0.303162000
1	-1.119409000	3.569855000	0.736255000
1	-2.049600000	4.347942000	-0.546872000
5	-0.341634000	0.329566000	1.486377000
7	0.564353000	-0.680906000	-3.967039000
7	0.282301000	-0.685367000	-2.594307000
15	-2.494327000	-0.503318000	-0.679707000
15	2.225878000	-1.393221000	0.029941000
15	0.830082000	1.893146000	-0.828813000
6	-3.449826000	0.427339000	-1.999660000
1	-3.128880000	1.470312000	-1.884735000
6	-4.970060000	0.387944000	-1.884630000
1	-5.414834000	0.791716000	-2.799595000
1	-5.364238000	-0.627530000	-1.771083000
1	-5.347063000	0.993703000	-1.061461000
6	-3.002288000	-0.063647000	-3.372459000
1	-1.935624000	0.088969000	-3.540243000
1	-3.212504000	-1.128752000	-3.523803000
1	-3.537337000	0.474611000	-4.160469000
6	2.247417000	2.189944000	-2.029232000
1	1.905619000	1.667539000	-2.935825000
6	3.538151000	1.528962000	-1.573765000
1	3.417336000	0.461672000	-1.398231000
1	4.312624000	1.646411000	-2.338099000
1	3.918759000	1.980766000	-0.652301000
6	2.520833000	3.648189000	-2.394790000
1	3.343245000	3.685158000	-3.116025000
1	1.675830000	4.158920000	-2.857254000
1	2.835770000	4.244355000	-1.533918000
6	2.764245000	-2.733921000	-1.173047000
1	1.810607000	-3.222346000	-1.426836000
6	3.737943000	-3.787471000	-0.649894000
1	3.853161000	-4.576578000	-1.399460000
1	4.734988000	-3.370650000	-0.482781000
1	3.434258000	-4.272043000	0.280212000
6	3.323258000	-2.111648000	-2.452107000
1	2.653912000	-1.374241000	-2.895849000
1	4.292920000	-1.633713000	-2.280214000
1	3.489844000	-2.892097000	-3.201377000

1	-0.280156000	-1.423643000	-3.258073000
1	0.177245000	0.195886000	-4.353163000

TS5 (Quintet, TE= -3506.997164)

6	0.069965000	1.228242000	1.591201000
6	1.018399000	1.907469000	2.411520000
1	1.842594000	1.338786000	2.831917000
6	0.902178000	3.236593000	2.768245000
1	1.624584000	3.676550000	3.451899000
6	-0.126161000	4.012597000	2.232290000
1	-0.212854000	5.067837000	2.479091000
6	-1.037827000	3.422284000	1.378812000
1	-1.826346000	4.035482000	0.955061000
6	-0.999103000	2.045012000	1.083083000
6	-0.759322000	-1.465571000	1.761818000
6	-1.116281000	-1.761910000	3.087109000
1	-0.727050000	-1.142311000	3.895765000
6	-1.979365000	-2.806319000	3.395666000
1	-2.245534000	-3.002911000	4.431942000
6	-2.513012000	-3.593343000	2.378537000
1	-3.192687000	-4.408719000	2.613642000
6	-2.163962000	-3.336782000	1.058080000
1	-2.566655000	-3.968576000	0.269299000
6	-1.294177000	-2.285640000	0.748537000
6	1.843320000	-0.763195000	1.689589000
6	2.170579000	-1.615419000	2.756185000
1	1.368942000	-2.073363000	3.331898000
6	3.484885000	-1.888371000	3.113328000
1	3.695424000	-2.547470000	3.952682000
6	4.526716000	-1.309555000	2.399241000
1	5.561021000	-1.501849000	2.673825000
6	4.238733000	-0.493822000	1.311160000
1	5.065674000	-0.067583000	0.755378000
6	2.918313000	-0.225510000	0.934758000
23	-0.062319000	0.526396000	-0.811558000
6	-3.785394000	1.127325000	1.204787000
1	-3.996025000	2.175256000	1.463574000
6	0.504405000	-3.350260000	-1.252377000
1	-0.148938000	-4.233149000	-1.215735000
6	3.164163000	2.359582000	-0.725179000
1	3.630492000	2.394350000	-1.720062000
6	4.228221000	2.661889000	0.318911000
1	4.564967000	3.699379000	0.222766000
1	3.841914000	2.538207000	1.336308000
1	5.111497000	2.026170000	0.222769000

6	2.053531000	3.402995000	-0.709397000
1	1.514822000	3.409692000	0.239431000
1	2.478206000	4.403669000	-0.842589000
1	1.324640000	3.243412000	-1.507930000
6	-4.998912000	0.534516000	0.501662000
1	-5.228819000	1.004673000	-0.457420000
1	-4.867167000	-0.535956000	0.323433000
1	-5.884215000	0.647371000	1.135453000
6	-3.485007000	0.368444000	2.480985000
1	-2.580953000	0.719576000	2.985782000
1	-4.319406000	0.485228000	3.180399000
1	-3.371695000	-0.700082000	2.289211000
6	1.127398000	-3.244056000	-2.638217000
1	1.621906000	-4.181972000	-2.909758000
1	0.408972000	-3.015861000	-3.430835000
1	1.890777000	-2.463584000	-2.661921000
6	1.569401000	-3.518303000	-0.182554000
1	2.279932000	-2.686919000	-0.175837000
1	1.147361000	-3.595273000	0.822985000
1	2.142996000	-4.431738000	-0.370723000
5	0.328685000	-0.347494000	1.473572000
7	-0.500501000	1.538342000	-3.840664000
7	-0.008303000	1.358212000	-2.607107000
15	2.480092000	0.610890000	-0.638384000
15	-2.318610000	1.306714000	0.048800000
15	-0.667278000	-1.933236000	-0.927731000
6	3.489382000	-0.285480000	-1.944914000
1	3.368466000	-1.345170000	-1.679800000
6	4.980964000	0.027366000	-1.994737000
1	5.445678000	-0.546658000	-2.802997000
1	5.177588000	1.081501000	-2.211677000
1	5.515322000	-0.233270000	-1.082142000
6	2.873023000	-0.052788000	-3.320514000
1	1.830612000	-0.377913000	-3.368584000
1	2.915293000	1.006447000	-3.604441000
1	3.426262000	-0.604520000	-4.087319000
6	-2.026117000	-2.279985000	-2.190164000
1	-1.674470000	-1.723308000	-3.073382000
6	-3.364331000	-1.692012000	-1.766551000
1	-3.290538000	-0.643413000	-1.483107000
1	-4.087594000	-1.764159000	-2.585217000
1	-3.785144000	-2.233537000	-0.913931000
6	-2.219513000	-3.737617000	-2.604009000
1	-3.012611000	-3.792538000	-3.356629000
1	-1.334369000	-4.197372000	-3.044437000
1	-2.539165000	-4.368773000	-1.770143000

6	-2.875899000	2.663483000	-1.126149000
1	-1.935541000	3.189634000	-1.350877000
6	-3.906250000	3.669888000	-0.623439000
1	-4.055486000	4.448629000	-1.378146000
1	-4.882080000	3.203808000	-0.459832000
1	-3.632087000	4.174557000	0.304829000
6	-3.380055000	2.028633000	-2.422737000
1	-2.747812000	1.201579000	-2.753554000
1	-4.391166000	1.624825000	-2.310562000
1	-3.418958000	2.768327000	-3.228214000
1	0.647393000	1.487416000	-3.682467000
1	-1.346817000	0.982252000	-4.084374000

For catalyst [**1f'**_{SB}]

TS5 (Triplet, TE= -3322.186086)

6	1.568726000	1.234116000	0.932961000
6	2.356743000	1.609959000	2.032194000
1	2.065333000	1.291715000	3.032918000
6	3.509475000	2.371593000	1.871344000
1	4.099777000	2.649559000	2.741176000
6	3.915696000	2.771791000	0.600387000
1	4.820726000	3.359819000	0.472506000
6	3.172538000	2.395494000	-0.511532000
1	3.500953000	2.667777000	-1.512568000
6	2.011161000	1.645515000	-0.330039000
6	-1.056765000	1.398705000	1.386415000
6	-0.973585000	2.386844000	2.382816000
1	-0.016692000	2.562685000	2.871848000
6	-2.078914000	3.125453000	2.784962000
1	-1.979058000	3.864974000	3.575575000
6	-3.311166000	2.925580000	2.168620000
1	-4.179075000	3.507207000	2.468379000
6	-3.419849000	2.008407000	1.131537000
1	-4.362717000	1.900780000	0.599864000
6	-2.307537000	1.254301000	0.760139000
6	0.011784000	-1.056073000	1.449505000
6	-0.946479000	-1.343761000	2.459785000
1	-1.478703000	-0.510281000	2.912052000
6	-1.193893000	-2.618550000	2.930498000
1	-1.906834000	-2.765513000	3.738203000
6	-0.548489000	-3.715090000	2.355909000
1	-0.753457000	-4.723874000	2.704713000
6	0.361885000	-3.509724000	1.337104000
1	0.873003000	-4.350115000	0.875260000
6	0.669088000	-2.208002000	0.898990000
16	1.853104000	-2.104822000	-0.442994000

16	1.109894000	1.045891000	-1.756420000
16	-2.398596000	0.269774000	-0.733946000
23	-0.224834000	-0.891529000	-0.966281000
6	0.299580000	2.571463000	-2.472543000
1	1.162771000	3.131469000	-2.853166000
6	-3.901250000	-0.812276000	-0.509047000
1	-4.721553000	-0.088563000	-0.438275000
6	3.431503000	-1.419064000	0.299260000
1	3.160056000	-0.512033000	0.837847000
6	4.339524000	-1.097932000	-0.869693000
1	5.279087000	-0.680323000	-0.495502000
1	4.587939000	-1.992029000	-1.449710000
1	3.898727000	-0.362810000	-1.548051000
6	3.996453000	-2.452609000	1.248174000
1	4.234111000	-3.390116000	0.737103000
1	4.924048000	-2.072585000	1.688542000
1	3.312572000	-2.676671000	2.071175000
6	-0.562073000	2.106664000	-3.628842000
1	0.000058000	1.515166000	-4.356379000
1	-1.408810000	1.508184000	-3.277805000
1	-0.971390000	2.973905000	-4.154541000
6	-0.444633000	3.394998000	-1.448671000
1	0.164368000	3.622011000	-0.569551000
1	-0.739361000	4.348812000	-1.898352000
1	-1.356862000	2.896670000	-1.113578000
6	-4.063413000	-1.638896000	-1.768211000
1	-5.033840000	-2.142326000	-1.755026000
1	-4.018913000	-1.038570000	-2.680943000
1	-3.305707000	-2.428044000	-1.820522000
6	-3.823536000	-1.655697000	0.739453000
1	-2.996499000	-2.370629000	0.681134000
1	-3.691236000	-1.052634000	1.641155000
1	-4.749495000	-2.228166000	0.856574000
5	0.196646000	0.478039000	1.103260000
7	-0.541175000	-2.481257000	-3.670072000
7	-0.522131000	-1.775124000	-2.476751000
1	-0.350141000	-1.801303000	-4.424342000
1	-1.537976000	-2.117235000	-2.876866000

TS5 (Quintet, TE= -3322.165373)

6	-1.438068000	1.320105000	-0.974874000
6	-2.173462000	1.723486000	-2.101060000
1	-1.853701000	1.397954000	-3.090727000
6	-3.308535000	2.519206000	-1.984048000
1	-3.855698000	2.815312000	-2.875909000
6	-3.752250000	2.930208000	-0.729313000

1	-4.642951000	3.545856000	-0.635030000
6	-3.063020000	2.530537000	0.408851000
1	-3.418791000	2.812868000	1.397726000
6	-1.919654000	1.744200000	0.271023000
6	1.220034000	1.331071000	-1.385355000
6	1.229949000	2.295421000	-2.407625000
1	0.300410000	2.517340000	-2.930185000
6	2.390683000	2.953348000	-2.794445000
1	2.360276000	3.677425000	-3.604969000
6	3.589846000	2.691414000	-2.137821000
1	4.501501000	3.208631000	-2.425732000
6	3.609508000	1.796855000	-1.075612000
1	4.527594000	1.645823000	-0.511811000
6	2.442078000	1.123461000	-0.717434000
6	-0.006448000	-1.047374000	-1.460018000
6	0.952929000	-1.395866000	-2.451746000
1	1.542702000	-0.595368000	-2.892152000
6	1.133356000	-2.681631000	-2.920641000
1	1.851987000	-2.868815000	-3.714822000
6	0.409607000	-3.739325000	-2.365396000
1	0.558438000	-4.757601000	-2.714914000
6	-0.505474000	-3.480501000	-1.364570000
1	-1.077194000	-4.289354000	-0.917545000
6	-0.739887000	-2.162821000	-0.925168000
16	-1.935366000	-2.009394000	0.404474000
16	-1.098563000	1.124812000	1.738329000
16	2.437230000	0.179908000	0.809082000
23	0.171268000	-0.839823000	0.911183000
6	-0.224176000	2.614381000	2.454217000
1	-1.062327000	3.231947000	2.800091000
6	3.832497000	-1.045220000	0.660226000
1	4.699028000	-0.422275000	0.409158000
6	-3.480100000	-1.240831000	-0.326309000
1	-3.157168000	-0.343043000	-0.853371000
6	-4.368425000	-0.883187000	0.846871000
1	-5.283354000	-0.409721000	0.478269000
1	-4.667255000	-1.768785000	1.416392000
1	-3.887174000	-0.179747000	1.531952000
6	-4.097553000	-2.230519000	-1.288249000
1	-4.388248000	-3.159379000	-0.788946000
1	-5.000668000	-1.794853000	-1.727792000
1	-3.423077000	-2.481810000	-2.111058000
6	0.575302000	2.115766000	3.640959000
1	-0.043499000	1.577918000	4.364417000
1	1.388856000	1.455616000	3.322864000
1	1.029607000	2.963091000	4.162137000

6	0.597446000	3.370727000	1.437883000
1	0.028024000	3.618966000	0.538252000
1	0.939968000	4.312296000	1.879408000
1	1.485083000	2.809982000	1.136817000
6	4.019493000	-1.665736000	2.030081000
1	4.875773000	-2.345636000	2.008314000
1	4.208400000	-0.916965000	2.803053000
1	3.141825000	-2.247482000	2.325269000
6	3.578438000	-2.061753000	-0.426152000
1	2.675952000	-2.648362000	-0.216450000
1	3.462652000	-1.595510000	-1.406886000
1	4.419031000	-2.760922000	-0.487169000
5	-0.096743000	0.497830000	-1.111574000
7	-0.298854000	-2.446567000	3.459931000
7	0.510447000	-1.872185000	2.557595000
1	-1.319785000	-2.326405000	3.285905000
1	0.669671000	-1.898713000	3.807618000

Cartesian coordinates of TS involved in the conversion of $[6]_{\text{alt}} \rightarrow [6]_{\text{dis}}$ for the catalysts $[1c''_{\text{PB}}]$ and $[1f''_{\text{SB}}]$, along with their total energies (in hartree) including zero point vibrational correction at M06-L-D3(heptane)/6-311+G* level of theory.

For catalyst $[1c''_{\text{PB}}]$

TS6 (Quartet, TE= -3507.183455)

6	-1.472949000	0.548093000	1.899473000
6	-1.647374000	1.338545000	3.050729000
1	-0.763242000	1.707987000	3.570909000
6	-2.902463000	1.672164000	3.547420000
1	-2.988255000	2.291014000	4.438946000
6	-4.045628000	1.216784000	2.899774000
1	-5.034570000	1.471573000	3.274977000
6	-3.911821000	0.446157000	1.750866000
1	-4.810067000	0.117753000	1.233871000
6	-2.649755000	0.119983000	1.242467000
6	0.605727000	-1.235144000	1.987996000
6	0.228287000	-1.719090000	3.251938000
1	-0.564049000	-1.203628000	3.796663000
6	0.833169000	-2.828879000	3.832428000
1	0.506586000	-3.177609000	4.810854000
6	1.861501000	-3.488038000	3.166055000
1	2.346525000	-4.352560000	3.614458000
6	2.255239000	-3.038633000	1.909521000
1	3.048806000	-3.565840000	1.382978000
6	1.629840000	-1.941199000	1.310797000
6	1.082742000	1.351377000	1.634825000

6	1.839597000	1.423274000	2.818803000
1	1.718046000	0.638951000	3.567053000
6	2.753445000	2.441698000	3.058047000
1	3.322957000	2.456658000	3.985826000
6	2.955754000	3.428316000	2.097751000
1	3.685475000	4.218731000	2.260770000
6	2.224845000	3.387000000	0.917553000
1	2.408702000	4.148209000	0.163144000
6	1.289128000	2.371753000	0.683806000
23	-0.123313000	-0.262160000	-1.182489000
6	-2.975071000	-2.492644000	-0.031118000
1	-4.021661000	-2.430397000	0.300696000
6	3.739765000	-0.879350000	-0.482315000
1	4.328091000	-1.777490000	-0.249033000
6	-0.928057000	3.578970000	-0.886927000
1	-0.768269000	4.117559000	-1.829276000
6	-0.778962000	4.561565000	0.265334000
1	-1.549310000	5.338393000	0.200625000
1	-0.898382000	4.061602000	1.232785000
1	0.191882000	5.062645000	0.281929000
6	-2.332640000	3.002289000	-0.922424000
1	-2.560824000	2.439796000	-0.011560000
1	-3.076532000	3.803118000	-1.006151000
1	-2.471193000	2.331649000	-1.774145000
6	-2.911164000	-3.328801000	-1.303395000
1	-3.541394000	-2.939330000	-2.106865000
1	-1.892382000	-3.388063000	-1.696930000
1	-3.235634000	-4.356812000	-1.108513000
6	-2.158687000	-3.111971000	1.092229000
1	-2.245768000	-2.544948000	2.023066000
1	-2.497959000	-4.134607000	1.291624000
1	-1.093451000	-3.162162000	0.848602000
6	4.064616000	-0.419980000	-1.898884000
1	5.135420000	-0.216451000	-2.009664000
1	3.786884000	-1.148474000	-2.667263000
1	3.531717000	0.507847000	-2.133843000
6	4.093713000	0.186119000	0.538013000
1	3.568636000	1.125296000	0.344761000
1	3.851624000	-0.119361000	1.559220000
1	5.167961000	0.400784000	0.500857000
5	0.022436000	0.162523000	1.486514000
7	0.093189000	-1.744140000	-3.996088000
7	-0.077621000	-0.963829000	-2.804470000
15	0.383167000	2.212942000	-0.898089000
15	-2.453016000	-0.727761000	-0.369169000
15	1.958074000	-1.438717000	-0.419661000

6	1.618679000	2.828931000	-2.181885000
1	2.583413000	2.516937000	-1.754301000
6	1.664241000	4.334894000	-2.427528000
1	2.575591000	4.597640000	-2.975578000
1	0.825829000	4.666022000	-3.048271000
1	1.647416000	4.939731000	-1.517849000
6	1.414709000	2.098275000	-3.505044000
1	1.508426000	1.014373000	-3.402486000
1	0.416413000	2.293743000	-3.917587000
1	2.143224000	2.437048000	-4.250488000
6	2.062338000	-3.013745000	-1.447866000
1	1.882525000	-2.628324000	-2.461497000
6	0.902019000	-3.938746000	-1.118833000
1	-0.044360000	-3.396099000	-1.109375000
1	0.818385000	-4.734219000	-1.866881000
1	1.017948000	-4.412934000	-0.138026000
6	3.375426000	-3.787172000	-1.458510000
1	3.277186000	-4.653358000	-2.122716000
1	4.222191000	-3.204851000	-1.828837000
1	3.649077000	-4.180859000	-0.474625000
6	-3.885310000	-0.086741000	-1.426611000
1	-4.010630000	0.940860000	-1.062774000
6	-5.233336000	-0.789554000	-1.290835000
1	-5.994146000	-0.234744000	-1.851295000
1	-5.220007000	-1.801610000	-1.704150000
1	-5.591913000	-0.867459000	-0.262427000
6	-3.478871000	-0.023715000	-2.896592000
1	-2.530534000	0.501155000	-3.048492000
1	-3.357591000	-1.024587000	-3.327328000
1	-4.248154000	0.484028000	-3.489214000
1	-0.892099000	-1.697333000	-3.099760000
1	-0.069036000	-1.077825000	-4.767380000

TS6 (Sextet, TE= -3507.149524)

6	-1.442640000	0.286110000	1.985900000
6	-1.607315000	0.914555000	3.235184000
1	-0.721316000	1.267248000	3.763831000
6	-2.852853000	1.109470000	3.820312000
1	-2.929046000	1.602971000	4.787804000
6	-4.000334000	0.676947000	3.163401000
1	-4.983007000	0.824062000	3.606812000
6	-3.877663000	0.065695000	1.922028000
1	-4.779764000	-0.252922000	1.403229000
6	-2.623829000	-0.124357000	1.329043000
6	0.796718000	-1.285181000	1.885210000
6	0.496880000	-1.879096000	3.124117000

1	-0.360664000	-1.509757000	3.687717000
6	1.267914000	-2.901596000	3.666260000
1	0.999838000	-3.333163000	4.629426000
6	2.395769000	-3.355056000	2.989022000
1	3.021138000	-4.136958000	3.414874000
6	2.705406000	-2.808593000	1.747953000
1	3.578344000	-3.176368000	1.212766000
6	1.906992000	-1.811958000	1.178363000
6	1.009252000	1.340518000	1.638525000
6	1.795023000	1.421770000	2.804057000
1	1.778587000	0.586975000	3.505952000
6	2.606679000	2.513658000	3.083749000
1	3.202353000	2.530607000	3.995103000
6	2.667601000	3.578213000	2.189529000
1	3.307977000	4.434816000	2.389512000
6	1.909091000	3.530467000	1.027452000
1	1.972773000	4.357922000	0.326365000
6	1.087285000	2.431590000	0.745252000
23	-0.155912000	-0.252583000	-1.151833000
6	-2.866724000	-2.630337000	-0.120628000
1	-3.906838000	-2.678156000	0.231198000
6	3.863764000	-0.566684000	-0.663676000
1	4.535632000	-1.388564000	-0.377372000
6	-1.164682000	3.548381000	-0.824031000
1	-1.344422000	3.747690000	-1.892635000
6	-0.819258000	4.853755000	-0.118761000
1	-1.659001000	5.553281000	-0.201412000
1	-0.645115000	4.685790000	0.948582000
1	0.060284000	5.358075000	-0.519253000
6	-2.436977000	2.974209000	-0.221812000
1	-2.307392000	2.734246000	0.838894000
1	-3.261851000	3.691781000	-0.296676000
1	-2.741303000	2.058326000	-0.726482000
6	-2.751776000	-3.379532000	-1.441434000
1	-3.382100000	-2.957677000	-2.231232000
1	-1.721727000	-3.368150000	-1.811414000
1	-3.041496000	-4.429697000	-1.324481000
6	-1.974485000	-3.248324000	0.945396000
1	-2.094619000	-2.760350000	1.916413000
1	-2.211636000	-4.310463000	1.073932000
1	-0.913942000	-3.178714000	0.684076000
6	4.152351000	-0.162435000	-2.104733000
1	5.179422000	0.204079000	-2.209758000
1	4.023206000	-0.982080000	-2.817623000
1	3.484372000	0.644391000	-2.426407000
6	4.101959000	0.587199000	0.293699000

1	3.466122000	1.447486000	0.064101000
1	3.905754000	0.309905000	1.332435000
1	5.142522000	0.925253000	0.229468000
5	0.054496000	0.062464000	1.463799000
7	-0.910262000	-1.605597000	-3.921490000
7	-0.044298000	-1.131671000	-2.941720000
15	0.192981000	2.248096000	-0.837511000
15	-2.479709000	-0.814348000	-0.362721000
15	2.133506000	-1.261589000	-0.555308000
6	1.375317000	2.837977000	-2.180078000
1	2.345961000	2.446317000	-1.839996000
6	1.517148000	4.335689000	-2.421936000
1	2.220022000	4.508526000	-3.244721000
1	0.568518000	4.793137000	-2.721226000
1	1.898183000	4.889716000	-1.562646000
6	1.007045000	2.146838000	-3.491246000
1	1.022475000	1.056117000	-3.416412000
1	0.001626000	2.431442000	-3.826802000
1	1.700872000	2.437707000	-4.288040000
6	2.336806000	-2.847073000	-1.560419000
1	2.157741000	-2.473279000	-2.578621000
6	1.223700000	-3.830721000	-1.228531000
1	0.240981000	-3.354275000	-1.256152000
1	1.211240000	-4.662229000	-1.942461000
1	1.348329000	-4.259333000	-0.228117000
6	3.686194000	-3.555200000	-1.555291000
1	3.659917000	-4.391262000	-2.263971000
1	4.518882000	-2.916130000	-1.856700000
1	3.933177000	-3.986714000	-0.581475000
6	-4.035736000	-0.157915000	-1.231944000
1	-4.254620000	0.760136000	-0.672277000
6	-5.288773000	-1.024729000	-1.182254000
1	-6.126431000	-0.492001000	-1.646603000
1	-5.171926000	-1.962199000	-1.733469000
1	-5.600598000	-1.283468000	-0.167412000
6	-3.719969000	0.234042000	-2.671265000
1	-2.795677000	0.818747000	-2.755400000
1	-3.598035000	-0.648452000	-3.310325000
1	-4.534413000	0.824725000	-3.105294000
1	0.092120000	-2.148681000	-3.647130000
1	-1.872969000	-1.724645000	-3.552247000

For catalyst [**1f'**_{SB}]

TS6 (Quartet, TE= -3322.331928)

6	-1.167712000	1.273671000	-1.094423000
6	-1.989217000	1.378595000	-2.232413000

1	-1.885671000	0.631788000	-3.020693000
6	-2.930478000	2.391016000	-2.382735000
1	-3.542877000	2.434280000	-3.281415000
6	-3.101142000	3.339756000	-1.377742000
1	-3.845109000	4.126564000	-1.479545000
6	-2.331894000	3.254158000	-0.223794000
1	-2.482895000	3.959989000	0.591193000
6	-1.379703000	2.240895000	-0.096967000
6	1.380502000	0.534339000	-1.572399000
6	1.483785000	1.168834000	-2.823887000
1	0.567111000	1.418236000	-3.359678000
6	2.706108000	1.489471000	-3.402383000
1	2.735491000	1.978357000	-4.374324000
6	3.891933000	1.193455000	-2.735277000
1	4.853818000	1.448156000	-3.174294000
6	3.834228000	0.597312000	-1.482555000
1	4.748096000	0.402381000	-0.924102000
6	2.596657000	0.275458000	-0.921089000
6	-0.582663000	-1.319827000	-1.486178000
6	-0.219629000	-1.866414000	-2.728926000
1	0.464632000	-1.306239000	-3.366973000
6	-0.687776000	-3.101996000	-3.165963000
1	-0.373108000	-3.489618000	-4.133286000
6	-1.545023000	-3.847813000	-2.364106000
1	-1.903102000	-4.821664000	-2.690051000
6	-1.925141000	-3.345201000	-1.123102000
1	-2.568680000	-3.926157000	-0.465529000
6	-1.454854000	-2.101780000	-0.703157000
16	-1.847972000	-1.573215000	0.969264000
16	-0.526685000	2.066403000	1.468032000
16	2.591651000	-0.341414000	0.765498000
23	0.243762000	-0.308419000	1.528259000
6	0.723833000	3.458068000	1.456411000
1	0.104209000	4.359167000	1.546304000
6	3.171095000	-2.111637000	0.552563000
1	4.171236000	-1.994338000	0.115672000
6	-3.409550000	-0.566617000	0.742024000
1	-3.166423000	0.205193000	0.006848000
6	-3.723115000	0.067387000	2.081631000
1	-4.612408000	0.700264000	1.995190000
1	-3.929771000	-0.688392000	2.846580000
1	-2.903949000	0.695703000	2.443450000
6	-4.525386000	-1.445736000	0.222358000
1	-4.755956000	-2.258733000	0.918686000
1	-5.436945000	-0.852575000	0.089716000
1	-4.281083000	-1.888484000	-0.746841000

6	1.568563000	3.282788000	2.701820000
1	0.966800000	3.257156000	3.614226000
1	2.147749000	2.353580000	2.654464000
1	2.280215000	4.109200000	2.793088000
6	1.544419000	3.513489000	0.189910000
1	0.924599000	3.528380000	-0.710783000
1	2.156342000	4.422574000	0.187030000
1	2.222272000	2.659771000	0.114726000
6	3.268159000	-2.727020000	1.932748000
1	3.718123000	-3.722301000	1.862422000
1	3.885757000	-2.133295000	2.613189000
1	2.279296000	-2.847363000	2.385527000
6	2.277311000	-2.894446000	-0.379125000
1	1.267968000	-2.998269000	0.034063000
1	2.189720000	-2.424850000	-1.361932000
1	2.682941000	-3.902037000	-0.524432000
5	-0.066799000	0.117116000	-1.042302000
7	0.499195000	-1.991211000	4.225564000
7	0.390635000	-1.088218000	3.117176000
1	0.137196000	-1.453596000	5.029293000
1	1.371263000	-1.128359000	3.690412000

TS6 (Sextet, TE= -3322.304097)

6	-1.377845000	1.168898000	-0.952573000
6	-2.219656000	1.292568000	-2.072820000
1	-2.031434000	0.660931000	-2.942008000
6	-3.293745000	2.175935000	-2.101994000
1	-3.922429000	2.238577000	-2.988198000
6	-3.575957000	2.967593000	-0.991233000
1	-4.422210000	3.650886000	-0.999731000
6	-2.783350000	2.855883000	0.144714000
1	-3.017173000	3.434603000	1.037019000
6	-1.700015000	1.975516000	0.149850000
6	1.205713000	0.837031000	-1.584994000
6	1.161520000	1.448384000	-2.852397000
1	0.209121000	1.480427000	-3.382116000
6	2.280111000	2.005120000	-3.459009000
1	2.195076000	2.459645000	-4.444187000
6	3.507303000	1.989347000	-2.800685000
1	4.388721000	2.432912000	-3.258233000
6	3.588652000	1.427976000	-1.534469000
1	4.528559000	1.451372000	-0.985297000
6	2.456216000	0.855911000	-0.948267000
6	-0.404071000	-1.340479000	-1.365421000
6	0.219068000	-1.925952000	-2.487783000
1	0.910398000	-1.318307000	-3.071547000

6	-0.013360000	-3.239076000	-2.879143000
1	0.493163000	-3.639962000	-3.755484000
6	-0.888107000	-4.041050000	-2.153271000
1	-1.071107000	-5.072358000	-2.446035000
6	-1.513271000	-3.513129000	-1.026752000
1	-2.170248000	-4.134216000	-0.421069000
6	-1.282558000	-2.192459000	-0.644931000
16	-1.944674000	-1.673124000	0.944051000
16	-0.789407000	1.734462000	1.677826000
16	2.627906000	0.278057000	0.750850000
23	0.351406000	-0.467162000	1.351506000
6	0.177945000	3.321727000	1.856316000
1	-0.592230000	4.074166000	2.068068000
6	3.750466000	-1.196072000	0.515957000
1	4.587111000	-0.791468000	-0.067613000
6	-3.574843000	-0.868696000	0.537651000
1	-3.364713000	-0.089062000	-0.197276000
6	-4.086776000	-0.246808000	1.821430000
1	-5.037371000	0.263491000	1.634686000
1	-4.265454000	-1.002608000	2.593642000
1	-3.388395000	0.491091000	2.226309000
6	-4.523476000	-1.890199000	-0.051429000
1	-4.731340000	-2.702509000	0.652785000
1	-5.477894000	-1.413520000	-0.301959000
1	-4.128113000	-2.332506000	-0.969952000
6	1.075587000	3.147057000	3.064416000
1	0.513868000	2.894191000	3.967500000
1	1.813632000	2.355943000	2.893385000
1	1.625414000	4.072811000	3.260885000
6	0.936075000	3.693548000	0.603102000
1	0.293547000	3.725972000	-0.281024000
1	1.384738000	4.685929000	0.724004000
1	1.746039000	2.988612000	0.402298000
6	4.238047000	-1.621919000	1.885026000
1	4.904381000	-2.485525000	1.790839000
1	4.794679000	-0.824688000	2.384492000
1	3.413876000	-1.918714000	2.540078000
6	3.055124000	-2.287191000	-0.267429000
1	2.138340000	-2.618846000	0.233318000
1	2.767163000	-1.945557000	-1.265399000
1	3.717584000	-3.151820000	-0.388138000
5	-0.130879000	0.176742000	-1.009165000
7	1.451104000	-3.203538000	2.846957000
7	0.664901000	-2.144741000	2.346753000
1	1.900424000	-3.689228000	2.049211000
1	0.264297000	-3.158802000	2.925152000

Cartesian coordinates of TS involved in the conversion of [7]_{alt}→[7]_{dis} for the catalysts [1c''_{PB}] and [1f''_{SB}], along with their total energies (in hartree) including zero point vibrational correction at M06-L-D3(heptane)/6-311+G* level of theory.

For catalyst [1c''_{PB}]

TS7 (Quartet, TE= -3507.617766)

6	-1.314168000	0.871666000	1.912904000
6	-1.349449000	1.756335000	3.005667000
1	-0.411236000	2.064046000	3.466464000
6	-2.542556000	2.249713000	3.521304000
1	-2.527106000	2.933339000	4.367315000
6	-3.751258000	1.872773000	2.948347000
1	-4.691662000	2.253035000	3.339833000
6	-3.748472000	1.021976000	1.849301000
1	-4.697381000	0.763281000	1.387971000
6	-2.550224000	0.527594000	1.325158000
6	0.457137000	-1.200490000	2.046462000
6	0.033643000	-1.563514000	3.335205000
1	-0.662646000	-0.913566000	3.865651000
6	0.485198000	-2.721458000	3.959378000
1	0.134987000	-2.971706000	4.958511000
6	1.386516000	-3.555910000	3.307495000
1	1.749058000	-4.460512000	3.789637000
6	1.812829000	-3.231538000	2.023890000
1	2.506959000	-3.895600000	1.513663000
6	1.349602000	-2.076901000	1.387601000
6	1.326748000	1.270312000	1.567735000
6	2.108637000	1.292973000	2.736342000
1	1.899085000	0.571917000	3.526870000
6	3.151430000	2.193978000	2.908629000
1	3.734941000	2.182211000	3.826704000
6	3.463512000	3.091011000	1.892597000
1	4.293643000	3.784559000	2.003551000
6	2.713776000	3.086120000	0.723567000
1	2.985409000	3.773238000	-0.073249000
6	1.642916000	2.199661000	0.559537000
23	-0.179651000	-0.297889000	-1.280331000
6	-3.235261000	-2.085558000	0.153257000
1	-4.254961000	-1.874948000	0.504767000
6	3.573653000	-1.365736000	-0.455474000
1	4.026240000	-2.334907000	-0.206697000
6	-0.441808000	3.626338000	-1.013250000
1	-0.243168000	4.091800000	-1.986355000
6	-0.122464000	4.633444000	0.081819000

1	-0.777839000	5.505718000	-0.011793000
1	-0.285389000	4.206663000	1.077267000
1	0.907835000	4.994561000	0.049977000
6	-1.910247000	3.241935000	-0.981319000
1	-2.183644000	2.768032000	-0.034007000
1	-2.541598000	4.129942000	-1.092921000
1	-2.165345000	2.556000000	-1.792838000
6	-3.319042000	-2.944346000	-1.103006000
1	-3.919557000	-2.491004000	-1.895521000
1	-2.326601000	-3.133794000	-1.519521000
1	-3.765496000	-3.917635000	-0.875503000
6	-2.485987000	-2.786204000	1.275127000
1	-2.481289000	-2.194990000	2.194451000
1	-2.958253000	-3.747630000	1.502241000
1	-1.442173000	-2.987231000	1.016920000
6	3.938064000	-0.997791000	-1.888585000
1	5.024173000	-0.934368000	-2.008734000
1	3.570695000	-1.716385000	-2.628187000
1	3.525770000	-0.019122000	-2.156914000
6	4.104283000	-0.347972000	0.536134000
1	3.750879000	0.662736000	0.319907000
1	3.824242000	-0.585549000	1.565137000
1	5.198209000	-0.324890000	0.489143000
5	0.102513000	0.261560000	1.546110000
7	-0.761557000	-1.962557000	-4.011468000
7	-0.355108000	-1.138417000	-2.841792000
1	-1.062322000	-2.902363000	-3.759879000
15	0.682733000	2.108856000	-0.993143000
15	-2.505431000	-0.413839000	-0.240727000
15	1.738257000	-1.688447000	-0.352325000
6	1.958744000	2.501873000	-2.322495000
1	2.884903000	2.085108000	-1.899935000
6	2.188249000	3.980132000	-2.627116000
1	3.114288000	4.100651000	-3.198289000
1	1.387156000	4.391674000	-3.248210000
1	2.268051000	4.616486000	-1.743454000
6	1.634657000	1.759245000	-3.613592000
1	1.582034000	0.676298000	-3.473356000
1	0.669001000	2.079412000	-4.025291000
1	2.391250000	1.966432000	-4.377919000
6	1.629341000	-3.302658000	-1.328460000
1	1.523633000	-2.925227000	-2.355687000
6	0.353695000	-4.051222000	-0.978424000
1	-0.514472000	-3.391287000	-0.994490000
1	0.172066000	-4.866277000	-1.687702000
1	0.402755000	-4.497812000	0.019638000

6	2.828933000	-4.242824000	-1.301050000
1	2.610982000	-5.121372000	-1.917900000
1	3.741788000	-3.797788000	-1.701505000
1	3.054325000	-4.619232000	-0.299701000
6	-3.864122000	0.382632000	-1.290620000
1	-3.845431000	1.425555000	-0.952196000
6	-5.285032000	-0.140257000	-1.091287000
1	-5.985256000	0.504807000	-1.631827000
1	-5.421418000	-1.149010000	-1.488767000
1	-5.612289000	-0.157383000	-0.050740000
6	-3.516688000	0.361109000	-2.774986000
1	-2.538337000	0.806213000	-2.982695000
1	-3.512064000	-0.660891000	-3.172570000
1	-4.260174000	0.919264000	-3.353144000
1	-1.299942000	-0.968380000	-3.672480000
1	-0.073327000	-1.938875000	-4.759598000

For catalyst [**1f'**_{SB}]

TS7 (Quartet, TE= -3322.770321)

6	1.486192000	-0.963111000	-1.218109000
6	2.342600000	-0.821920000	-2.323945000
1	2.115393000	-0.064691000	-3.074559000
6	3.463205000	-1.627989000	-2.492249000
1	4.098108000	-1.497326000	-3.365355000
6	3.781806000	-2.589034000	-1.537320000
1	4.664865000	-3.211834000	-1.654940000
6	2.984545000	-2.724043000	-0.406916000
1	3.252132000	-3.432804000	0.373998000
6	1.850231000	-1.924601000	-0.264670000
6	-1.174908000	-0.781774000	-1.679472000
6	-1.156389000	-1.489149000	-2.893449000
1	-0.201926000	-1.653721000	-3.393947000
6	-2.321133000	-1.970748000	-3.480051000
1	-2.270185000	-2.506431000	-4.424996000
6	-3.549156000	-1.780068000	-2.853237000
1	-4.461797000	-2.166745000	-3.299380000
6	-3.600196000	-1.125620000	-1.628463000
1	-4.545913000	-1.021632000	-1.100617000
6	-2.425259000	-0.629626000	-1.064659000
6	0.314052000	1.443443000	-1.490405000
6	-0.084889000	1.941338000	-2.740987000
1	-0.577476000	1.269737000	-3.444231000
6	0.128796000	3.266764000	-3.106009000
1	-0.190263000	3.616783000	-4.085009000
6	0.731073000	4.147693000	-2.214391000
1	0.883955000	5.189120000	-2.485762000

6	1.118998000	3.694507000	-0.957422000
1	1.561315000	4.378421000	-0.236568000
6	0.923238000	2.357430000	-0.616776000
16	1.318563000	1.847138000	1.055161000
16	0.952842000	-1.987715000	1.280600000
16	-2.492476000	0.034044000	0.595381000
23	-0.309772000	0.098282000	1.726901000
6	-0.012654000	-3.590690000	1.226130000
1	0.770652000	-4.353580000	1.308677000
6	-3.393684000	1.665835000	0.438057000
1	-4.412910000	1.363681000	0.168964000
6	3.088849000	1.230484000	0.958317000
1	3.065266000	0.369129000	0.284955000
6	3.467381000	0.795998000	2.359087000
1	4.476495000	0.373304000	2.352665000
1	3.469276000	1.639452000	3.056329000
1	2.794464000	0.029859000	2.755945000
6	3.986688000	2.308005000	0.396285000
1	3.986553000	3.205420000	1.022858000
1	5.015672000	1.937347000	0.350315000
1	3.700856000	2.597819000	-0.617879000
6	-0.884872000	-3.604863000	2.464378000
1	-0.309750000	-3.472024000	3.384452000
1	-1.644649000	-2.816005000	2.418294000
1	-1.411581000	-4.560658000	2.536162000
6	-0.792223000	-3.771192000	-0.053628000
1	-0.169577000	-3.654006000	-0.944399000
1	-1.218386000	-4.779677000	-0.080188000
1	-1.620838000	-3.061454000	-0.123986000
6	-3.387262000	2.299974000	1.813793000
1	-3.983092000	3.217115000	1.800103000
1	-3.808301000	1.641329000	2.579188000
1	-2.368158000	2.571856000	2.113935000
6	-2.806722000	2.558439000	-0.626918000
1	-1.797031000	2.884934000	-0.361921000
1	-2.757964000	2.067106000	-1.601646000
1	-3.428118000	3.453382000	-0.737977000
5	0.165003000	-0.099690000	-1.205353000
7	-1.251947000	0.771648000	4.772611000
7	-0.665439000	0.413674000	3.441610000
1	-0.593781000	0.619420000	5.531741000
1	-1.674558000	1.696830000	4.776600000
1	-1.620048000	-0.117104000	4.086575000

Cartesian coordinates of the intermediate and TS involved in the conversion of [6]_{dis}→[7]_{alt} for the catalysts [1c''_{PB}] and [1f''_{SB}], along with their total energies (in hartree) including zero point vibrational correction at M06-L-D3(heptane)/6-311+G* level of theory.

For catalyst [1c''_{PB}]

[6c''_{PB}-V-H]⁺_{dis} (TE = -3507.690919)

6	0.997659000	-1.334711000	1.820066000
6	0.854841000	-2.367037000	2.768532000
1	-0.128138000	-2.555906000	3.198226000
6	1.919829000	-3.158825000	3.178526000
1	1.765169000	-3.938497000	3.920517000
6	3.168024000	-2.965029000	2.605649000
1	4.010831000	-3.591737000	2.887013000
6	3.333789000	-1.974016000	1.645160000
1	4.309360000	-1.873049000	1.184851000
6	2.280544000	-1.141559000	1.252511000
6	-0.533173000	0.942989000	2.162852000
6	-0.260842000	1.092430000	3.532631000
1	0.245533000	0.286430000	4.064806000
6	-0.623859000	2.238525000	4.230577000
1	-0.397143000	2.323764000	5.290746000
6	-1.270387000	3.274167000	3.566957000
1	-1.560590000	4.175336000	4.101338000
6	-1.534990000	3.157460000	2.206969000
1	-2.029831000	3.979262000	1.696222000
6	-1.171291000	2.009897000	1.495948000
6	-1.657451000	-1.352971000	1.434464000
6	-2.548543000	-1.413995000	2.517153000
1	-2.351407000	-0.815392000	3.406723000
6	-3.683446000	-2.214902000	2.478534000
1	-4.355325000	-2.246912000	3.333172000
6	-3.971421000	-2.955685000	1.336527000
1	-4.868353000	-3.568517000	1.290647000
6	-3.115100000	-2.895222000	0.243597000
1	-3.363337000	-3.455082000	-0.654514000
6	-1.957382000	-2.111425000	0.288173000
23	0.465717000	0.384999000	-1.474641000
6	3.386653000	1.517132000	0.761596000
1	4.295606000	1.063979000	1.180782000
6	-3.278687000	1.894736000	-0.512936000
1	-3.563970000	2.862786000	-0.077251000
6	-0.038618000	-3.451855000	-1.566983000
1	0.146454000	-3.358390000	-2.647959000
6	-0.878813000	-4.691900000	-1.295053000
1	-0.326043000	-5.584880000	-1.604290000

1	-1.089672000	-4.800701000	-0.226608000
1	-1.831919000	-4.706283000	-1.824677000
6	1.306240000	-3.573342000	-0.867224000
1	1.192189000	-3.666516000	0.217482000
1	1.832553000	-4.467638000	-1.216356000
1	1.942797000	-2.710443000	-1.067861000
6	3.798811000	2.599099000	-0.228762000
1	4.471262000	2.236806000	-1.008297000
1	2.934783000	3.039521000	-0.730341000
1	4.316708000	3.410250000	0.293133000
6	2.583552000	2.088715000	1.916384000
1	2.334225000	1.327899000	2.659954000
1	3.162268000	2.866974000	2.424888000
1	1.646159000	2.545327000	1.586952000
6	-3.684690000	1.882708000	-1.982728000
1	-4.731863000	2.182322000	-2.090083000
1	-3.091337000	2.552891000	-2.611557000
1	-3.600147000	0.880560000	-2.410114000
6	-3.997622000	0.815435000	0.276082000
1	-3.780086000	-0.189415000	-0.096600000
1	-3.739289000	0.836025000	1.337519000
1	-5.080229000	0.959937000	0.197584000
5	-0.332223000	-0.516397000	1.619259000
7	1.561052000	2.436981000	-3.365168000
7	1.161752000	1.596685000	-2.414381000
1	2.338688000	2.083431000	-3.920637000
15	-0.874672000	-1.833452000	-1.154703000
15	2.534083000	0.089129000	-0.098483000
15	-1.418798000	1.898967000	-0.316235000
6	-2.071439000	-1.493302000	-2.563926000
1	-2.918296000	-1.020437000	-2.047094000
6	-2.594969000	-2.677786000	-3.361791000
1	-3.227749000	-2.319171000	-4.180735000
1	-1.788707000	-3.260067000	-3.817677000
1	-3.205770000	-3.359509000	-2.767697000
6	-1.445384000	-0.460986000	-3.497263000
1	-1.172303000	0.480410000	-2.981181000
1	-0.557454000	-0.842215000	-4.006425000
1	-2.154865000	-0.141093000	-4.268427000
6	-1.009307000	3.601611000	-1.029906000
1	-0.834900000	3.355604000	-2.087190000
6	0.298453000	4.119113000	-0.450860000
1	1.071368000	3.350213000	-0.452203000
1	0.666110000	4.973789000	-1.029399000
1	0.178955000	4.459638000	0.582095000
6	-2.078105000	4.688895000	-0.980809000

1	-1.694080000	5.581476000	-1.485842000
1	-3.007247000	4.420157000	-1.485243000
1	-2.329876000	4.998944000	0.036462000
6	3.950939000	-0.627115000	-1.129312000
1	3.737398000	-1.704783000	-1.113869000
6	5.367828000	-0.410324000	-0.591574000
1	6.059876000	-1.058696000	-1.138195000
1	5.711359000	0.614149000	-0.755531000
1	5.504031000	-0.623169000	0.469154000
6	3.914537000	-0.168582000	-2.584288000
1	2.960740000	-0.387170000	-3.063344000
1	4.102664000	0.906832000	-2.669876000
1	4.706804000	-0.672442000	-3.147544000
1	1.754373000	3.379043000	-3.027661000
1	1.125410000	-0.938010000	-2.282219000

TS_{hyb} (Doublet, TE = -3507.662111)

6	-0.688929000	-1.683996000	1.723007000
6	-0.912629000	-2.008046000	3.069971000
1	-0.360102000	-1.479913000	3.848170000
6	-1.845930000	-2.971400000	3.434402000
1	-2.014471000	-3.194769000	4.485892000
6	-2.572319000	-3.650390000	2.457041000
1	-3.301135000	-4.405293000	2.742366000
6	-2.367901000	-3.352671000	1.115472000
1	-2.946610000	-3.877796000	0.359128000
6	-1.438278000	-2.370971000	0.758615000
6	1.936485000	-1.066397000	1.407597000
6	2.331963000	-2.080897000	2.293876000
1	1.571368000	-2.714943000	2.747067000
6	3.664740000	-2.276049000	2.643348000
1	3.930123000	-3.065929000	3.342934000
6	4.656684000	-1.448068000	2.125122000
1	5.694955000	-1.578695000	2.420010000
6	4.310051000	-0.472619000	1.196212000
1	5.088907000	0.148253000	0.755803000
6	2.977016000	-0.308491000	0.815254000
6	0.204787000	0.904198000	1.770662000
6	1.091232000	1.284459000	2.814840000
1	1.878638000	0.595974000	3.108413000
6	0.958998000	2.454364000	3.539100000
1	1.619694000	2.645714000	4.381712000
6	-0.004084000	3.390556000	3.170783000
1	-0.098870000	4.332411000	3.706017000
6	-0.854167000	3.101622000	2.120022000
1	-1.597258000	3.839203000	1.836010000

6	-0.805434000	1.865143000	1.449814000
23	-0.029124000	0.488590000	-0.892038000
6	-0.174355000	-3.192713000	-1.736234000
1	-0.933034000	-3.975536000	-1.861041000
6	3.192416000	2.388772000	-0.523248000
1	4.280358000	2.243347000	-0.471996000
6	-3.641205000	1.155719000	1.046104000
1	-3.837888000	2.112578000	1.550270000
6	-3.531249000	0.085331000	2.115321000
1	-4.450728000	0.068530000	2.709510000
1	-3.405409000	-0.911790000	1.687902000
1	-2.698965000	0.262029000	2.801223000
6	-4.784547000	0.876601000	0.078885000
1	-4.684326000	-0.104911000	-0.391612000
1	-5.737640000	0.874177000	0.617003000
1	-4.870050000	1.614308000	-0.722872000
6	0.300318000	-2.777211000	-3.125257000
1	-0.541545000	-2.592727000	-3.800530000
1	0.894000000	-1.858837000	-3.112788000
1	0.913965000	-3.561733000	-3.579849000
6	0.903778000	-3.762298000	-0.820039000
1	0.458773000	-4.305035000	0.018126000
1	1.543257000	-4.462825000	-1.366931000
1	1.549591000	-2.998931000	-0.382483000
6	2.856499000	3.172319000	-1.788061000
1	3.402376000	4.120645000	-1.804881000
1	3.107384000	2.641094000	-2.711149000
1	1.788129000	3.413244000	-1.821654000
6	2.750116000	3.144312000	0.715296000
1	1.660106000	3.254575000	0.754362000
1	3.067760000	2.648299000	1.634153000
1	3.180666000	4.151127000	0.715936000
5	0.406102000	-0.620878000	1.281480000
7	0.064967000	1.121712000	-3.863665000
7	-0.012053000	0.853411000	-2.577432000
1	-0.769417000	1.536194000	-4.274806000
15	-2.038695000	1.525905000	0.151452000
15	-1.070265000	-1.780084000	-0.918171000
15	2.478399000	0.673543000	-0.621021000
6	-2.389099000	3.201210000	-0.642002000
1	-1.412514000	3.700073000	-0.551347000
6	-3.457439000	4.071198000	0.016430000
1	-3.449083000	5.063376000	-0.445683000
1	-4.462568000	3.667333000	-0.132501000
1	-3.326333000	4.219475000	1.089442000
6	-2.707987000	3.065511000	-2.127843000

1	-1.942921000	2.501496000	-2.663061000
1	-3.667879000	2.568654000	-2.300677000
1	-2.776460000	4.054897000	-2.590938000
6	3.446075000	-0.068236000	-2.061339000
1	2.852725000	0.213442000	-2.943846000
6	3.475588000	-1.586381000	-1.972826000
1	2.492360000	-2.013488000	-1.797076000
1	3.859279000	-2.013421000	-2.904839000
1	4.126919000	-1.925968000	-1.161727000
6	4.866187000	0.457262000	-2.241679000
1	5.326097000	-0.042259000	-3.100664000
1	4.928200000	1.530542000	-2.427562000
1	5.497574000	0.228519000	-1.378112000
6	-2.751195000	-1.758304000	-1.776885000
1	-3.420253000	-1.501894000	-0.943416000
6	-3.204540000	-3.097310000	-2.350349000
1	-4.247269000	-3.021105000	-2.675325000
1	-2.621603000	-3.379477000	-3.232466000
1	-3.150867000	-3.926851000	-1.643169000
6	-2.877263000	-0.679097000	-2.843047000
1	-2.672091000	0.317923000	-2.450686000
1	-2.188987000	-0.851961000	-3.677234000
1	-3.892275000	-0.672747000	-3.255256000
1	0.922793000	1.566623000	-4.181058000
1	0.083604000	2.013089000	-1.749165000

TS_{hyb} (Quartet, TE = -3507.668505)

6	-0.717994000	-0.799522000	2.068576000
6	-1.496479000	-0.604695000	3.224694000
1	-1.620420000	0.406671000	3.612517000
6	-2.125157000	-1.656355000	3.881748000
1	-2.719348000	-1.462583000	4.772149000
6	-2.005283000	-2.951243000	3.389075000
1	-2.502568000	-3.780410000	3.886540000
6	-1.249143000	-3.177142000	2.245119000
1	-1.173750000	-4.190838000	1.857248000
6	-0.606309000	-2.122953000	1.587760000
6	1.539602000	0.695047000	1.900759000
6	1.856651000	0.589947000	3.265095000
6	3.113531000	0.921680000	3.754918000
6	4.098364000	1.377748000	2.884205000
6	3.820188000	1.472375000	1.526572000
6	2.559485000	1.121953000	1.030418000
6	-0.850205000	1.817863000	1.438658000
6	-0.554039000	2.843762000	2.350355000
6	-1.386679000	3.944234000	2.520838000

6	-2.561629000	4.040793000	1.786947000
6	-2.876530000	3.050431000	0.860883000
6	-2.023382000	1.961719000	0.660644000
23	0.040004000	-0.157801000	-1.241883000
6	1.920907000	-3.200125000	0.568436000
6	2.266890000	2.822703000	-1.340130000
6	-3.603383000	-0.433990000	0.182900000
6	-3.735922000	-1.795195000	-0.490822000
6	-4.959332000	0.232817000	0.364646000
6	2.819285000	-3.474457000	-0.630715000
6	2.669492000	-2.430274000	1.641881000
6	2.077879000	2.945553000	-2.846293000
6	1.264761000	3.688443000	-0.591930000
5	0.021065000	0.490103000	1.493800000
7	-0.164672000	-0.249556000	-4.303737000
7	-0.074812000	-0.292552000	-3.041218000
1	-1.071181000	-0.209567000	-4.769156000
1	-0.129212000	1.260855000	-2.175931000
1	0.660409000	-0.107642000	-4.885203000
15	-2.287761000	0.650167000	-0.585390000
15	2.180131000	1.057467000	-0.752671000
15	0.319483000	-2.393344000	0.034992000
6	-2.971986000	1.378344000	-2.179980000
6	-3.971152000	2.527506000	-2.135138000
6	-3.500257000	0.244173000	-3.055548000
6	-0.577459000	-3.821831000	-0.819335000
6	-0.106354000	-5.232932000	-0.482387000
6	-0.609734000	-3.609366000	-2.329544000
6	3.673121000	0.220715000	-1.539852000
6	4.879086000	1.117650000	-1.805734000
6	3.308279000	-0.530767000	-2.817278000

For catalyst [**1f'**_{SB}]

[**6f'**_{SB} -V-H]⁺_{dis} (TE = -3322.850968)

6	-1.507398000	-1.123562000	1.184265000
6	-2.361576000	-1.233713000	2.289551000
1	-2.147119000	-0.667931000	3.196231000
6	-3.475963000	-2.066000000	2.249290000
1	-4.123138000	-2.146206000	3.119206000
6	-3.771222000	-2.791000000	1.096155000
1	-4.646596000	-3.434546000	1.064344000
6	-2.966495000	-2.663875000	-0.030304000

1	-3.222683000	-3.179074000	-0.953756000
6	-1.842853000	-1.841195000	0.030374000
6	1.136720000	-1.100302000	1.551358000
6	1.099080000	-1.998666000	2.632465000
1	0.143453000	-2.203471000	3.113694000
6	2.247215000	-2.605241000	3.123823000
1	2.185522000	-3.276667000	3.976376000
6	3.474470000	-2.361836000	2.513350000
1	4.377295000	-2.842628000	2.881227000
6	3.539709000	-1.537897000	1.397086000
1	4.484056000	-1.408119000	0.873275000
6	2.385106000	-0.907822000	0.933234000
6	-0.151612000	1.261720000	1.380753000
6	0.654549000	1.689912000	2.461915000
1	1.336000000	0.976080000	2.918642000
6	0.567814000	2.964973000	3.001777000
1	1.186346000	3.233869000	3.854199000
6	-0.302544000	3.893806000	2.445093000
1	-0.374885000	4.897917000	2.855179000
6	-1.064766000	3.543794000	1.336907000
1	-1.702092000	4.280396000	0.854918000
6	-1.006114000	2.252243000	0.819422000
16	-1.803443000	2.014394000	-0.770239000
16	-0.929296000	-1.419631000	-1.443405000
16	2.465214000	-0.066014000	-0.640591000
23	0.293434000	0.851236000	-1.351755000
6	-0.039437000	-2.982588000	-1.946911000
1	-0.863794000	-3.648581000	-2.230492000
6	3.796214000	1.227831000	-0.438350000
1	4.685813000	0.632492000	-0.199038000
6	-3.431347000	1.146548000	-0.436780000
1	-3.195907000	0.221194000	0.085297000
6	-4.034225000	0.845530000	-1.793075000
1	-4.984188000	0.319442000	-1.658314000
1	-4.244201000	1.757810000	-2.359820000
1	-3.386780000	0.205547000	-2.399041000
6	-4.288667000	2.033162000	0.437795000
1	-4.502293000	2.995468000	-0.037086000
1	-5.246327000	1.537986000	0.628760000
1	-3.823627000	2.226678000	1.408420000
6	0.789252000	-2.635474000	-3.166012000
1	0.192940000	-2.194081000	-3.967537000
1	1.586620000	-1.929117000	-2.913928000
1	1.261119000	-3.541647000	-3.556723000
6	0.765045000	-3.594393000	-0.824189000
1	0.177726000	-3.731657000	0.087855000

1	1.126872000	-4.580370000	-1.134362000
1	1.639846000	-2.986887000	-0.579093000
6	3.963432000	1.886891000	-1.792090000
1	4.790865000	2.600734000	-1.750539000
1	4.188830000	1.162973000	-2.580113000
1	3.059576000	2.437841000	-2.068476000
6	3.488288000	2.201144000	0.672644000
1	2.566968000	2.752597000	0.463845000
1	3.385177000	1.702901000	1.640110000
1	4.305138000	2.925148000	0.761308000
5	-0.172729000	-0.303075000	1.224193000
7	0.801711000	0.888367000	-4.299028000
7	0.544463000	0.872605000	-2.995309000
1	0.130583000	1.441659000	-4.828871000
1	1.753641000	1.183155000	-4.512276000
1	0.895048000	2.405316000	-1.133186000

TS_{hyb} (Doublet, TE = -3322.822926)

6	-1.671543000	-1.174579000	0.863917000
6	-2.495804000	-1.553143000	1.936245000
1	-2.225450000	-1.257024000	2.949568000
6	-3.660324000	-2.286311000	1.731158000
1	-4.280813000	-2.564404000	2.579920000
6	-4.041085000	-2.659496000	0.443453000
1	-4.954726000	-3.226306000	0.283727000
6	-3.260286000	-2.283575000	-0.642695000
1	-3.566213000	-2.533148000	-1.656792000
6	-2.090592000	-1.561078000	-0.412622000
6	0.908767000	-1.473631000	1.415919000
6	0.756964000	-2.463245000	2.400201000
1	-0.219543000	-2.603778000	2.860936000
6	1.820173000	-3.250624000	2.826395000
1	1.666497000	-3.993211000	3.605706000
6	3.079485000	-3.094627000	2.253611000
1	3.913415000	-3.713181000	2.575182000
6	3.258881000	-2.169922000	1.232582000
1	4.222988000	-2.088345000	0.735123000
6	2.183484000	-1.376035000	0.837973000
6	-0.009031000	1.007510000	1.491008000
6	0.985862000	1.244245000	2.492239000
1	1.478757000	0.379102000	2.929567000
6	1.274511000	2.488179000	2.998491000

1	1.987458000	2.586479000	3.813888000
6	0.639905000	3.629642000	2.479019000
1	0.860223000	4.615381000	2.880908000
6	-0.265765000	3.490813000	1.457196000
1	-0.760866000	4.358903000	1.029657000
6	-0.581042000	2.208503000	0.946758000
16	-1.760454000	2.173537000	-0.394479000
16	-1.121406000	-0.916741000	-1.768156000
16	2.329473000	-0.371599000	-0.632145000
23	0.271688000	0.963481000	-0.962013000
6	-0.352083000	-2.425346000	-2.557776000
1	-1.222817000	-2.925389000	-3.000362000
6	3.893883000	0.615344000	-0.416267000
1	4.667610000	-0.160027000	-0.367057000
6	-3.398366000	1.524957000	0.249156000
1	-3.183844000	0.602353000	0.786069000
6	-4.261459000	1.254511000	-0.965185000
1	-5.227721000	0.854900000	-0.642730000
1	-4.460483000	2.167849000	-1.534758000
1	-3.811117000	0.521554000	-1.639607000
6	-3.967419000	2.567016000	1.187355000
1	-4.145116000	3.520620000	0.681203000
1	-4.928551000	2.217450000	1.578282000
1	-3.314094000	2.752439000	2.044002000
6	0.567412000	-1.929958000	-3.654948000
1	0.054825000	-1.275378000	-4.364503000
1	1.419605000	-1.381805000	-3.240870000
1	0.964250000	-2.782090000	-4.214417000
6	0.319555000	-3.340876000	-1.561157000
1	-0.333957000	-3.599024000	-0.723694000
1	0.599299000	-4.274670000	-2.059866000
1	1.232960000	-2.900087000	-1.156364000
6	4.087730000	1.439492000	-1.672963000
1	5.082814000	1.892538000	-1.666718000
1	4.002608000	0.839679000	-2.584149000
1	3.361276000	2.257908000	-1.712188000
6	3.896424000	1.451349000	0.839703000
1	3.124395000	2.225978000	0.799832000
1	3.729268000	0.851684000	1.737762000
1	4.865998000	1.948745000	0.948680000
5	-0.273702000	-0.470083000	1.073484000
7	1.215780000	2.086653000	-3.619965000
7	0.776572000	1.609627000	-2.493048000
1	0.615144000	2.744168000	-4.109713000
1	0.875597000	2.544134000	-1.370470000
1	2.212313000	2.274556000	-3.701906000

TS_{hyb} (Quartet, TE = -3322.822176)

6	-1.455769000	-0.464197000	1.568188000
6	-2.429478000	-0.014599000	2.476540000
1	-2.384037000	1.013454000	2.836132000
6	-3.438736000	-0.851112000	2.940234000
1	-4.167345000	-0.476345000	3.654825000
6	-3.527695000	-2.158666000	2.472849000
1	-4.324712000	-2.813020000	2.816305000
6	-2.615554000	-2.615915000	1.529212000
1	-2.713061000	-3.615923000	1.111966000
6	-1.584854000	-1.779976000	1.097977000
6	1.127707000	0.259124000	1.908888000
6	1.161072000	0.136677000	3.308139000
1	0.221287000	0.076125000	3.857570000
6	2.360259000	0.111000000	4.010189000
1	2.352715000	0.028686000	5.094183000
6	3.569026000	0.172464000	3.323087000
1	4.511500000	0.135380000	3.863264000
6	3.570156000	0.236434000	1.935255000
1	4.510104000	0.216255000	1.387496000
6	2.360220000	0.294439000	1.243210000
6	-0.596630000	1.973591000	0.780014000
6	-0.325692000	3.030773000	1.662927000
1	0.188432000	2.819630000	2.600641000
6	-0.697026000	4.339614000	1.370265000
1	-0.477704000	5.135891000	2.077347000
6	-1.323460000	4.631313000	0.164089000
1	-1.596218000	5.654478000	-0.081507000
6	-1.578197000	3.609662000	-0.745880000
1	-2.031845000	3.829338000	-1.709631000
6	-1.233863000	2.298092000	-0.426892000
16	-1.456511000	1.043777000	-1.690460000
16	-0.551845000	-2.351348000	-0.244138000
16	2.412762000	0.157361000	-0.541817000
23	0.418536000	-0.615797000	-1.811206000
6	0.567920000	-3.646849000	0.503000000
1	-0.123285000	-4.461794000	0.748605000
6	3.198822000	1.755033000	-1.109834000
1	3.994143000	1.906162000	-0.369688000
6	-3.155627000	0.333827000	-1.339316000
1	-3.104035000	-0.084318000	-0.330250000
6	-3.391089000	-0.766897000	-2.352856000
1	-4.371640000	-1.219672000	-2.177755000
1	-3.387316000	-0.381622000	-3.377301000
1	-2.647228000	-1.566157000	-2.285933000

6	-4.192753000	1.432344000	-1.395849000
1	-4.232816000	1.901875000	-2.383480000
1	-5.181562000	1.011030000	-1.188453000
1	-4.010736000	2.213005000	-0.653267000
6	1.513554000	-4.085504000	-0.596646000
1	0.986078000	-4.418700000	-1.494470000
1	2.195160000	-3.276646000	-0.882018000
1	2.126489000	-4.919181000	-0.242154000
6	1.277414000	-3.167716000	1.746334000
1	0.586731000	-2.769339000	2.494248000
1	1.811645000	-4.006308000	2.205386000
1	2.012951000	-2.392579000	1.516311000
6	3.798647000	1.509079000	-2.478127000
1	4.309599000	2.412766000	-2.823011000
1	4.524555000	0.692872000	-2.473588000
1	3.022423000	1.273473000	-3.213206000
6	2.222484000	2.907282000	-1.085878000
1	1.394766000	2.735765000	-1.782625000
1	1.803382000	3.075770000	-0.091758000
1	2.728004000	3.828237000	-1.395688000
5	-0.271753000	0.515965000	1.255837000
7	1.008843000	-2.142513000	-4.424561000
7	0.755702000	-1.566156000	-3.325471000
1	0.323457000	-2.160980000	-5.178382000
1	1.017159000	0.102542000	-3.272595000
1	1.957916000	-2.428496000	-4.660804000

Cartesian coordinates of different nitrogenous species involved in the ligand exchange process (dissociation of NH₃ and addition of N₂), along with their total energies (in hartree) including zero point vibrational correction at M06-D3(heptane)/def2-SVP level of theory.

For catalyst [**1c''_{PB}**]

[V]-NH₃ (TE= -3450.307069)

6	1.212614000	-0.947955000	1.847337000
6	1.122794000	-1.688698000	3.041646000
1	0.184673000	-1.659615000	3.609379000
6	2.176406000	-2.457639000	3.529767000
1	2.058157000	-3.020150000	4.461607000
6	3.379623000	-2.503376000	2.830288000
1	4.220874000	-3.096130000	3.202406000
6	3.495660000	-1.796833000	1.635947000
1	4.437589000	-1.858260000	1.081464000
6	2.427726000	-1.044668000	1.128917000
6	0.053065000	1.522729000	1.813657000
6	0.637354000	1.866385000	3.046889000
1	1.116601000	1.076318000	3.639007000

6	0.627958000	3.167257000	3.544763000
1	1.102909000	3.388549000	4.506187000
6	-0.000975000	4.180324000	2.825213000
1	-0.034357000	5.203221000	3.212523000
6	-0.581656000	3.877239000	1.595573000
1	-1.069391000	4.677319000	1.029546000
6	-0.531715000	2.579645000	1.070379000
6	-1.477964000	-0.674220000	1.721161000
6	-2.111795000	-0.344744000	2.933961000
1	-1.605625000	0.345052000	3.621192000
6	-3.364251000	-0.838973000	3.284738000
1	-3.821517000	-0.550846000	4.236880000
6	-4.038369000	-1.687612000	2.409806000
1	-5.031393000	-2.073807000	2.659280000
6	-3.437382000	-2.036496000	1.204330000
1	-3.984468000	-2.692768000	0.521909000
6	-2.170116000	-1.548403000	0.852126000
23	0.106113000	0.067855000	-1.134407000
6	3.845279000	1.015612000	-0.353391000
1	4.763442000	0.485498000	-0.036494000
6	-2.931147000	2.479649000	-0.667528000
1	-3.095788000	3.557684000	-0.479386000
6	-0.811431000	-3.701545000	-0.671405000
1	-1.038862000	-4.111785000	-1.675473000
6	-1.505220000	-4.543213000	0.386486000
1	-1.134460000	-5.582553000	0.346120000
1	-1.284054000	-4.153295000	1.395674000
1	-2.599421000	-4.578811000	0.278755000
6	0.691908000	-3.761484000	-0.475680000
1	0.991724000	-3.312821000	0.488650000
1	1.043546000	-4.808110000	-0.481683000
1	1.218379000	-3.217221000	-1.273432000
6	4.117223000	1.722174000	-1.673337000
1	4.383527000	1.029063000	-2.487867000
1	3.237763000	2.297962000	-2.005168000
1	4.948696000	2.440722000	-1.568551000
6	3.459417000	2.000437000	0.738214000
1	3.400791000	1.515228000	1.725595000
1	4.199918000	2.816560000	0.803718000
1	2.470714000	2.455009000	0.546400000
6	-3.455658000	2.108498000	-2.046427000
1	-4.549534000	2.240888000	-2.107904000
1	-3.004938000	2.703415000	-2.859660000
1	-3.235155000	1.043528000	-2.250969000
6	-3.643676000	1.686619000	0.410669000
1	-3.484796000	0.603045000	0.275246000

1	-3.289360000	1.944277000	1.421487000
1	-4.730332000	1.875738000	0.370751000
5	-0.035164000	-0.034642000	1.435124000
15	2.512674000	-0.298062000	-0.560721000
15	-1.074889000	2.198187000	-0.648134000
15	-1.401174000	-1.900645000	-0.791622000
6	-0.500281000	3.647005000	-1.735364000
1	-0.617622000	3.203375000	-2.746398000
6	0.983136000	3.877116000	-1.513253000
1	1.428534000	4.476575000	-2.326211000
1	1.171442000	4.406416000	-0.563163000
1	1.506268000	2.908902000	-1.451895000
6	-1.273851000	4.956491000	-1.736083000
1	-0.839797000	5.641591000	-2.485697000
1	-2.337997000	4.834782000	-1.990818000
1	-1.217603000	5.477764000	-0.766781000
6	3.426119000	-1.642907000	-1.560740000
1	3.129335000	-2.559712000	-1.019928000
6	4.946632000	-1.618415000	-1.623267000
1	5.311530000	-2.525604000	-2.136178000
1	5.329872000	-0.757673000	-2.195389000
1	5.428620000	-1.595497000	-0.634013000
6	2.837740000	-1.723841000	-2.962562000
1	3.226425000	-2.601731000	-3.507744000
1	1.735677000	-1.802621000	-2.920698000
1	3.093189000	-0.829719000	-3.561936000
6	-2.877821000	-2.041278000	-1.975906000
1	-3.570811000	-1.264912000	-1.593398000
6	-2.396636000	-1.612665000	-3.355468000
1	-1.601903000	-2.288430000	-3.728008000
1	-3.217935000	-1.628995000	-4.093072000
1	-1.978624000	-0.593398000	-3.321486000
6	-3.627970000	-3.361074000	-2.083415000
1	-2.984454000	-4.164067000	-2.481901000
1	-4.047092000	-3.716572000	-1.130821000
1	-4.472193000	-3.256167000	-2.786998000
7	0.352832000	0.528725000	-3.321940000
1	-0.413839000	1.087964000	-3.703059000
1	1.198847000	1.089927000	-3.444707000
1	0.454091000	-0.272637000	-3.948669000

[V] (TE= -3393.825304)

6	1.120257000	-1.136340000	1.738734000
6	0.969903000	-1.836762000	2.950438000
1	0.086376000	-1.635856000	3.568740000
6	1.892479000	-2.782264000	3.391569000

1	1.729973000	-3.304907000	4.339656000
6	3.017814000	-3.060954000	2.620846000
1	3.752324000	-3.801661000	2.951282000
6	3.194930000	-2.390308000	1.413078000
1	4.075645000	-2.624842000	0.805532000
6	2.261514000	-1.448264000	0.961150000
6	0.357796000	1.489569000	1.723081000
6	1.008605000	1.738279000	2.945778000
1	1.340651000	0.882526000	3.547156000
6	1.247462000	3.025170000	3.421381000
1	1.763321000	3.169180000	4.376171000
6	0.816228000	4.124797000	2.684487000
1	0.979809000	5.142642000	3.051199000
6	0.179874000	3.915082000	1.463328000
1	-0.149473000	4.783463000	0.884566000
6	-0.026111000	2.623140000	0.961484000
6	-1.509050000	-0.460748000	1.705270000
6	-2.059600000	-0.045164000	2.931565000
1	-1.445795000	0.567157000	3.604409000
6	-3.362094000	-0.357758000	3.311461000
1	-3.751206000	-0.005595000	4.272226000
6	-4.171727000	-1.106132000	2.460201000
1	-5.201379000	-1.348836000	2.739522000
6	-3.657455000	-1.537918000	1.240990000
1	-4.302100000	-2.114779000	0.570492000
6	-2.345242000	-1.226680000	0.857872000
23	0.096921000	0.026876000	-1.114592000
6	3.984952000	0.342367000	-0.540838000
1	4.795158000	-0.354935000	-0.251924000
6	-2.450494000	2.952660000	-0.673313000
1	-2.406802000	4.031026000	-0.426475000
6	-1.478680000	-3.518200000	-0.819011000
1	-1.465948000	-3.759703000	-1.903020000
6	-2.556445000	-4.334255000	-0.123030000
1	-2.328054000	-5.410615000	-0.213392000
1	-2.583519000	-4.098109000	0.954453000
1	-3.566582000	-4.179086000	-0.527330000
6	-0.120517000	-3.859296000	-0.228341000
1	-0.086482000	-3.614774000	0.849287000
1	0.097898000	-4.935496000	-0.334879000
1	0.683408000	-3.283475000	-0.709135000
6	4.354584000	1.015964000	-1.853901000
1	4.551818000	0.301145000	-2.667641000
1	3.552590000	1.688716000	-2.198831000
1	5.263128000	1.630276000	-1.730003000
6	3.799938000	1.362462000	0.572458000

1	3.653044000	0.882093000	1.553022000
1	4.683512000	2.019658000	0.644670000
1	2.916765000	2.002651000	0.392729000
6	-3.104044000	2.762717000	-2.033545000
1	-4.150281000	3.113356000	-2.020459000
1	-2.585428000	3.297664000	-2.846247000
1	-3.117835000	1.690584000	-2.301208000
6	-3.237288000	2.238382000	0.409011000
1	-3.254890000	1.149187000	0.230383000
1	-2.807671000	2.394201000	1.411474000
1	-4.281323000	2.595529000	0.425144000
5	0.008030000	-0.037718000	1.382567000
15	2.426682000	-0.692846000	-0.717592000
15	-0.672799000	2.356223000	-0.747413000
15	-1.691415000	-1.645940000	-0.809387000
6	0.111898000	3.684158000	-1.850377000
1	-0.089172000	3.251633000	-2.852061000
6	1.616824000	3.682955000	-1.651131000
1	2.130703000	4.205578000	-2.475833000
1	1.900949000	4.180435000	-0.707761000
1	1.993985000	2.648958000	-1.600965000
6	-0.447093000	5.099100000	-1.847631000
1	0.067214000	5.697602000	-2.619888000
1	-1.523920000	5.144975000	-2.071422000
1	-0.280435000	5.617500000	-0.889502000
6	2.955110000	-2.143953000	-1.819182000
1	2.502494000	-3.005475000	-1.294650000
6	4.437563000	-2.439615000	-1.990366000
1	4.567847000	-3.374379000	-2.562928000
1	4.961013000	-1.649487000	-2.552344000
1	4.968698000	-2.572184000	-1.035026000
6	2.259441000	-2.004738000	-3.167767000
1	2.429072000	-2.893246000	-3.800648000
1	1.165929000	-1.887824000	-3.035284000
1	2.625979000	-1.125749000	-3.728512000
6	-3.078189000	-1.298819000	-2.041555000
1	-3.547005000	-0.388454000	-1.616337000
6	-2.403210000	-0.920474000	-3.355906000
1	-1.853884000	-1.778334000	-3.786360000
1	-3.141145000	-0.590476000	-4.108083000
1	-1.682300000	-0.092054000	-3.210073000
6	-4.160418000	-2.336665000	-2.290049000
1	-3.740799000	-3.276543000	-2.688468000
1	-4.746567000	-2.579570000	-1.390909000
1	-4.872765000	-1.961390000	-3.045282000

[V]-N₂ (TE= -3503.242278)

6	1.350043000	-0.804282000	1.910822000
6	1.365225000	-1.553234000	3.102815000
1	0.429480000	-1.677824000	3.660955000
6	2.522642000	-2.146461000	3.599608000
1	2.485761000	-2.723575000	4.528992000
6	3.724465000	-2.001722000	2.911227000
1	4.644078000	-2.457141000	3.290518000
6	3.740216000	-1.282615000	1.719740000
1	4.683619000	-1.192384000	1.172625000
6	2.572016000	-0.703639000	1.206912000
6	-0.204901000	1.441898000	1.920748000
6	0.304733000	1.846330000	3.168208000
1	0.910910000	1.136737000	3.745303000
6	0.069054000	3.113332000	3.695786000
1	0.493517000	3.388649000	4.666552000
6	-0.716947000	4.023303000	2.992874000
1	-0.923081000	5.016476000	3.402777000
6	-1.231149000	3.657583000	1.751353000
1	-1.842457000	4.377164000	1.197564000
6	-0.960818000	2.399059000	1.200229000
6	-1.343729000	-0.979637000	1.728155000
6	-2.024124000	-0.815088000	2.949879000
1	-1.651078000	-0.071304000	3.665129000
6	-3.164998000	-1.540934000	3.274914000
1	-3.664151000	-1.376875000	4.235155000
6	-3.678389000	-2.462794000	2.365081000
1	-4.584204000	-3.031059000	2.596181000
6	-3.031173000	-2.647455000	1.148332000
1	-3.453657000	-3.360649000	0.435629000
6	-1.873289000	-1.925400000	0.822403000
23	0.133900000	0.130694000	-1.145572000
6	3.568571000	1.626431000	-0.269430000
1	4.577929000	1.297334000	0.043659000
6	-3.322200000	1.923013000	-0.517946000
1	-3.644747000	2.959443000	-0.302613000
6	-0.199098000	-3.745704000	-0.828767000
1	-0.311471000	-4.085225000	-1.877703000
6	-0.794701000	-4.783968000	0.107138000
1	-0.255563000	-5.740783000	-0.003225000
1	-0.686916000	-4.464853000	1.158425000
1	-1.860866000	-4.984598000	-0.072902000
6	1.282261000	-3.579563000	-0.547222000
1	1.458426000	-3.172349000	0.464904000
1	1.801641000	-4.551239000	-0.611475000
1	1.746972000	-2.894427000	-1.270379000

6	3.675670000	2.353307000	-1.603188000
1	4.228662000	1.775269000	-2.359908000
1	2.683085000	2.568632000	-2.031936000
1	4.198183000	3.317476000	-1.479992000
6	2.997015000	2.510656000	0.827181000
1	3.036431000	2.016915000	1.811427000
1	3.568103000	3.452324000	0.897023000
1	1.940301000	2.770463000	0.641330000
6	-3.805800000	1.513071000	-1.900736000
1	-4.908090000	1.513757000	-1.948709000
1	-3.437615000	2.170915000	-2.705541000
1	-3.463332000	0.488756000	-2.133220000
6	-3.895361000	1.015460000	0.553055000
1	-3.600152000	-0.034662000	0.390020000
1	-3.560898000	1.298194000	1.563914000
1	-4.997811000	1.059458000	0.534849000
5	-0.025334000	-0.095165000	1.497305000
15	2.546853000	0.067767000	-0.466320000
15	-1.449796000	1.966520000	-0.519812000
15	-1.066960000	-2.067636000	-0.828714000
6	-1.128055000	3.488771000	-1.594032000
1	-1.153940000	3.035617000	-2.605108000
6	0.283877000	3.994397000	-1.360054000
1	0.598547000	4.676767000	-2.167565000
1	0.365805000	4.540640000	-0.404381000
1	0.993264000	3.154326000	-1.319832000
6	-2.129259000	4.634065000	-1.584297000
1	-1.816635000	5.393432000	-2.321904000
1	-3.150417000	4.326481000	-1.856426000
1	-2.177591000	5.146203000	-0.609360000
6	3.679351000	-1.059388000	-1.491739000
1	3.533495000	-2.037386000	-0.998110000
6	5.173569000	-0.766258000	-1.494361000
1	5.702197000	-1.567019000	-2.039745000
1	5.413800000	0.177243000	-2.010286000
1	5.619543000	-0.716274000	-0.489393000
6	3.156455000	-1.165234000	-2.918277000
1	3.724303000	-1.922335000	-3.486116000
1	2.088204000	-1.444695000	-2.944522000
1	3.252532000	-0.207281000	-3.459449000
6	-2.486934000	-2.321998000	-2.051539000
1	-3.287520000	-1.678080000	-1.635123000
6	-2.055589000	-1.750696000	-3.396582000
1	-1.150814000	-2.260876000	-3.778673000
1	-2.849796000	-1.877301000	-4.152251000
1	-1.818165000	-0.677302000	-3.324492000

6	-3.041381000	-3.726651000	-2.244405000
1	-2.282562000	-4.410951000	-2.660707000
1	-3.435002000	-4.185332000	-1.325569000
1	-3.872305000	-3.699064000	-2.969836000
7	0.497010000	1.114694000	-4.064914000
7	0.359274000	0.706241000	-3.018725000

[V]-NH₃⁺ (TE= -3450.183507)

6	-1.557058000	0.311344000	1.907877000
6	-1.691905000	0.834884000	3.207703000
1	-0.792191000	0.987629000	3.814612000
6	-2.925468000	1.176236000	3.753467000
1	-2.979204000	1.582968000	4.767596000
6	-4.087862000	1.003379000	3.005846000
1	-5.063958000	1.267488000	3.421807000
6	-3.991702000	0.500701000	1.713220000
1	-4.907083000	0.382548000	1.124305000
6	-2.747247000	0.166177000	1.161396000
6	0.388549000	-1.612458000	1.659407000
6	-0.142740000	-2.321805000	2.752691000
1	-0.988610000	-1.892235000	3.302550000
6	0.392585000	-3.533414000	3.180675000
1	-0.045658000	-4.050386000	4.039532000
6	1.502808000	-4.072618000	2.533555000
1	1.949537000	-5.008167000	2.881192000
6	2.034231000	-3.412403000	1.429404000
1	2.901569000	-3.845507000	0.920740000
6	1.469330000	-2.216006000	0.969379000
6	1.074408000	0.957619000	1.786477000
6	1.731002000	0.810052000	3.023303000
1	1.471642000	-0.041443000	3.664885000
6	2.710600000	1.697782000	3.454542000
1	3.194811000	1.548686000	4.424176000
6	3.085370000	2.767063000	2.642433000
1	3.861604000	3.466222000	2.965181000
6	2.471158000	2.929451000	1.406309000
1	2.787336000	3.756659000	0.764184000
6	1.473976000	2.040144000	0.976813000
23	-0.143722000	-0.162990000	-1.157192000
6	-3.419291000	-2.072748000	-0.601112000
1	-4.474546000	-1.900862000	-0.318792000
6	3.832259000	-1.220748000	-0.530522000
1	4.241185000	-2.231810000	-0.340126000
6	-0.392016000	3.674999000	-0.646096000
1	-0.524087000	3.928971000	-1.718866000
6	0.141271000	4.881862000	0.110677000

1	-0.596504000	5.699740000	0.055841000
1	0.276981000	4.639726000	1.178009000
1	1.090949000	5.274766000	-0.272992000
6	-1.738903000	3.283441000	-0.062550000
1	-1.646593000	3.013143000	1.004902000
1	-2.451054000	4.122291000	-0.132186000
1	-2.172787000	2.419848000	-0.582080000
6	-3.377087000	-2.694978000	-1.989816000
1	-3.769151000	-2.031678000	-2.778315000
1	-2.349770000	-2.984324000	-2.269979000
1	-3.979099000	-3.618266000	-2.013798000
6	-2.793695000	-2.985691000	0.440524000
1	-2.919401000	-2.594058000	1.461705000
1	-3.267883000	-3.980345000	0.400841000
1	-1.711208000	-3.128580000	0.275171000
6	4.370814000	-0.708810000	-1.857920000
1	5.469659000	-0.630557000	-1.818765000
1	4.120333000	-1.359951000	-2.711410000
1	3.982088000	0.300159000	-2.079637000
6	4.227418000	-0.316933000	0.624098000
1	3.841250000	0.708301000	0.488791000
1	3.849978000	-0.685761000	1.591105000
1	5.325829000	-0.253078000	0.691482000
5	-0.079557000	-0.100278000	1.442465000
15	-2.635814000	-0.371114000	-0.588593000
15	1.987275000	-1.463871000	-0.622043000
15	0.724284000	2.165014000	-0.689369000
6	1.788704000	-2.850175000	-1.881973000
1	1.873581000	-2.298961000	-2.841050000
6	0.372317000	-3.391969000	-1.759116000
1	0.080705000	-3.977752000	-2.648196000
1	0.273546000	-4.048960000	-0.878149000
1	-0.389129000	-2.596992000	-1.629543000
6	2.798428000	-3.984792000	-1.908910000
1	2.586023000	-4.648668000	-2.764131000
1	3.837056000	-3.638153000	-2.020971000
1	2.738342000	-4.607919000	-1.002857000
6	-3.883288000	0.719266000	-1.507726000
1	-3.932414000	1.616306000	-0.865199000
6	-5.299794000	0.181793000	-1.652583000
1	-5.935722000	0.954387000	-2.115848000
1	-5.349840000	-0.704308000	-2.305479000
1	-5.767786000	-0.084304000	-0.692774000
6	-3.328762000	1.142612000	-2.861719000
1	-3.989633000	1.887027000	-3.335802000
1	-2.325522000	1.599156000	-2.773977000

1	-3.264017000	0.286858000	-3.558223000
6	2.148284000	2.591453000	-1.851630000
1	3.000966000	2.059381000	-1.384915000
6	1.876115000	1.957156000	-3.208988000
1	0.946498000	2.352867000	-3.661120000
1	2.697335000	2.170807000	-3.913652000
1	1.785171000	0.861866000	-3.124432000
6	2.528738000	4.052665000	-2.034048000
1	1.702918000	4.639960000	-2.470025000
1	2.845402000	4.546452000	-1.104469000
1	3.375447000	4.122963000	-2.736902000
7	-0.382825000	-0.516652000	-3.367095000
1	0.472015000	-0.631347000	-3.917575000
1	-0.966169000	-1.325009000	-3.602204000
1	-0.865867000	0.286508000	-3.778836000

[V]⁺ (TE= -3393.702712)

6	-1.573054000	0.626759000	1.795473000
6	-1.695954000	1.311052000	3.018099000
1	-0.804891000	1.451957000	3.640573000
6	-2.911049000	1.821616000	3.467024000
1	-2.960787000	2.346634000	4.425322000
6	-4.057932000	1.668164000	2.692862000
1	-5.017165000	2.067402000	3.033354000
6	-3.969454000	1.009919000	1.469982000
1	-4.871466000	0.907903000	0.857247000
6	-2.748109000	0.498626000	1.014552000
6	0.104735000	-1.544562000	1.578618000
6	-0.623019000	-2.179863000	2.605594000
1	-1.401811000	-1.613752000	3.129312000
6	-0.361702000	-3.486037000	3.005198000
1	-0.937937000	-3.932429000	3.820661000
6	0.643311000	-4.217209000	2.376369000
1	0.868980000	-5.238972000	2.693356000
6	1.361513000	-3.635677000	1.335706000
1	2.149177000	-4.218618000	0.849306000
6	1.099040000	-2.323441000	0.918210000
6	1.136532000	0.944806000	1.757131000
6	1.747966000	0.803418000	3.015018000
1	1.362814000	0.050133000	3.714313000
6	2.835355000	1.585391000	3.394033000
1	3.285894000	1.453327000	4.382055000
6	3.357814000	2.525305000	2.507586000
1	4.218003000	3.137314000	2.792159000
6	2.782781000	2.675290000	1.249258000
1	3.209140000	3.405120000	0.555182000

6	1.678895000	1.898687000	0.870817000
23	-0.125858000	-0.292081000	-0.992991000
6	-3.665468000	-1.779348000	-0.622147000
1	-4.693802000	-1.424877000	-0.418753000
6	3.776970000	-1.786158000	-0.256605000
1	3.929368000	-2.844506000	0.031831000
6	0.066101000	3.632714000	-0.921796000
1	-0.115023000	3.744294000	-2.011018000
6	0.852681000	4.828507000	-0.405318000
1	0.259091000	5.745928000	-0.554086000
1	1.034407000	4.735553000	0.678542000
1	1.818992000	4.981579000	-0.903616000
6	-1.270284000	3.559795000	-0.199535000
1	-1.127459000	3.415837000	0.886624000
1	-1.835061000	4.496075000	-0.337821000
1	-1.891030000	2.727755000	-0.557900000
6	-3.643149000	-2.498807000	-1.963577000
1	-3.940223000	-1.860471000	-2.809627000
1	-2.641264000	-2.902977000	-2.185906000
1	-4.335427000	-3.356550000	-1.943413000
6	-3.246798000	-2.711905000	0.501888000
1	-3.301653000	-2.229159000	1.490007000
1	-3.907551000	-3.594223000	0.521635000
1	-2.213419000	-3.081651000	0.368495000
6	4.564564000	-1.497164000	-1.525689000
1	5.644705000	-1.518733000	-1.308311000
1	4.380714000	-2.232710000	-2.324244000
1	4.334779000	-0.493893000	-1.927402000
6	4.204632000	-0.893050000	0.896809000
1	4.069476000	0.174820000	0.649172000
1	3.631991000	-1.094056000	1.816598000
1	5.271477000	-1.052105000	1.122172000
5	-0.131904000	0.028558000	1.452044000
15	-2.616469000	-0.232478000	-0.665243000
15	1.949766000	-1.609977000	-0.550972000
15	0.921619000	1.972372000	-0.797054000
6	1.560629000	-2.753437000	-1.993010000
1	2.213251000	-2.356567000	-2.794724000
6	0.115522000	-2.453321000	-2.385401000
1	-0.269632000	-3.165814000	-3.134055000
1	-0.577299000	-2.554070000	-1.519852000
1	-0.015924000	-1.455260000	-2.869674000
6	1.807817000	-4.242493000	-1.845154000
1	1.659635000	-4.749312000	-2.813322000
1	2.833936000	-4.467955000	-1.512227000
1	1.105946000	-4.698361000	-1.127658000

6	-3.521124000	0.932870000	-1.834638000
1	-3.395490000	1.914864000	-1.344784000
6	-5.012903000	0.705492000	-2.028105000
1	-5.426132000	1.510465000	-2.658158000
1	-5.231900000	-0.243902000	-2.542024000
1	-5.579554000	0.715498000	-1.084652000
6	-2.781540000	0.967237000	-3.167985000
1	-3.235351000	1.707564000	-3.847743000
1	-1.716320000	1.236355000	-3.041056000
1	-2.816688000	-0.010630000	-3.681228000
6	2.325302000	1.963632000	-2.046457000
1	3.027120000	1.241657000	-1.584592000
6	1.797633000	1.364263000	-3.345233000
1	1.022473000	2.006415000	-3.801714000
1	2.607881000	1.256089000	-4.086053000
1	1.354283000	0.362623000	-3.193635000
6	3.071859000	3.255197000	-2.337987000
1	2.415069000	4.009416000	-2.802838000
1	3.539176000	3.704538000	-1.449579000
1	3.882313000	3.053145000	-3.058224000

[V]-N₂¹⁺(TE= -3503.092601)

6	-1.690295000	0.896407000	1.754228000
6	-1.897268000	1.736911000	2.861717000
1	-1.031579000	2.089896000	3.433129000
6	-3.170102000	2.131608000	3.266771000
1	-3.286968000	2.783353000	4.137311000
6	-4.289824000	1.695617000	2.564143000
1	-5.294266000	1.994331000	2.875936000
6	-4.117486000	0.889738000	1.442190000
1	-5.000087000	0.576124000	0.874892000
6	-2.838868000	0.500542000	1.027323000
6	0.064542000	-1.182824000	1.795320000
6	-0.700102000	-1.653517000	2.889646000
1	-1.513053000	-1.029652000	3.274955000
6	-0.434133000	-2.853474000	3.534990000
1	-1.035914000	-3.152195000	4.397819000
6	0.602155000	-3.667148000	3.083716000
1	0.829956000	-4.611237000	3.585773000
6	1.343986000	-3.268698000	1.978707000
1	2.144554000	-3.921238000	1.618741000
6	1.094016000	-2.052437000	1.325714000
6	0.996339000	1.380406000	1.744191000
6	1.511742000	1.488363000	3.047195000
1	1.106420000	0.844777000	3.838518000
6	2.536615000	2.377545000	3.356259000

1	2.918547000	2.437472000	4.379464000
6	3.086339000	3.179689000	2.357249000
1	3.898064000	3.874488000	2.588944000
6	2.603485000	3.083313000	1.056358000
1	3.055254000	3.701821000	0.275113000
6	1.564559000	2.194573000	0.746046000
23	-0.069253000	-0.381547000	-0.884958000
6	-3.460117000	-2.020183000	-0.447635000
1	-4.533352000	-1.787394000	-0.319009000
6	3.786631000	-1.424839000	0.216414000
1	4.096354000	-2.416424000	0.598379000
6	-0.092359000	3.485508000	-1.335331000
1	-0.169652000	3.476367000	-2.442508000
6	0.489666000	4.810126000	-0.864335000
1	-0.197708000	5.625632000	-1.144525000
1	0.577186000	4.826305000	0.235008000
1	1.471018000	5.052976000	-1.289536000
6	-1.479684000	3.320038000	-0.739289000
1	-1.441037000	3.330593000	0.364665000
1	-2.137750000	4.145693000	-1.056221000
1	-1.945761000	2.374161000	-1.040508000
6	-3.267810000	-2.808715000	-1.735898000
1	-3.556082000	-2.252468000	-2.641957000
1	-2.215508000	-3.117963000	-1.856239000
1	-3.871725000	-3.730490000	-1.711119000
6	-2.994192000	-2.822744000	0.753609000
1	-3.170414000	-2.294931000	1.703733000
1	-3.538900000	-3.780386000	0.795208000
1	-1.916755000	-3.060530000	0.693200000
6	4.601020000	-1.089616000	-1.024732000
1	5.675689000	-1.076030000	-0.780321000
1	4.459751000	-1.805363000	-1.850414000
1	4.342404000	-0.088415000	-1.408133000
6	3.993740000	-0.402477000	1.317001000
1	3.704478000	0.609944000	0.989503000
1	3.418219000	-0.640411000	2.225479000
1	5.060247000	-0.368778000	1.593877000
5	-0.205101000	0.369856000	1.498638000
15	-2.602884000	-0.365039000	-0.574440000
15	1.991228000	-1.661408000	-0.231937000
15	0.931158000	1.957159000	-0.958641000
6	2.008124000	-3.252186000	-1.251201000
1	2.160423000	-2.846782000	-2.272621000
6	0.647769000	-3.935593000	-1.218973000
1	0.560977000	-4.657303000	-2.047673000
1	0.497104000	-4.489332000	-0.277579000

1	-0.192085000	-3.226259000	-1.308565000
6	3.117266000	-4.262556000	-0.994194000
1	3.022322000	-5.089603000	-1.717346000
1	4.127594000	-3.846288000	-1.116935000
1	3.055480000	-4.715279000	0.008539000
6	-3.663359000	0.622240000	-1.793216000
1	-3.700047000	1.617101000	-1.314889000
6	-5.099378000	0.151007000	-1.972706000
1	-5.630600000	0.861321000	-2.627617000
1	-5.161912000	-0.836056000	-2.458051000
1	-5.665869000	0.101344000	-1.030519000
6	-2.968785000	0.768174000	-3.140763000
1	-3.532605000	1.464613000	-3.783134000
1	-1.941031000	1.160737000	-3.046734000
1	-2.913746000	-0.192139000	-3.681580000
6	2.439002000	2.017756000	-2.084673000
1	3.222452000	1.568163000	-1.444066000
6	2.207773000	1.106290000	-3.282911000
1	1.320682000	1.418351000	-3.865801000
1	3.073003000	1.139593000	-3.965653000
1	2.066267000	0.056440000	-2.981166000
6	2.926505000	3.378412000	-2.559116000
1	2.173428000	3.888485000	-3.183000000
1	3.213351000	4.056986000	-1.743183000
1	3.820462000	3.240431000	-3.189380000
7	-0.281434000	-1.501570000	-3.851800000
7	-0.203789000	-1.130211000	-2.805197000

[V]-NH₃⁺ (TE= -3450.347845)

6	1.171044000	-0.909631000	1.789093000
6	1.071632000	-1.757017000	2.917990000
1	0.097693000	-1.839548000	3.419654000
6	2.153809000	-2.465396000	3.432962000
1	2.020036000	-3.104267000	4.314506000
6	3.416476000	-2.341858000	2.846686000
1	4.280266000	-2.879486000	3.252641000
6	3.552581000	-1.536866000	1.715879000
1	4.536418000	-1.465899000	1.236492000
6	2.451380000	-0.867449000	1.166770000
6	-0.007064000	1.504369000	1.749863000
6	0.642253000	1.919201000	2.935063000
1	1.255158000	1.184308000	3.475797000
6	0.500888000	3.197642000	3.465314000
1	1.015500000	3.462548000	4.397178000
6	-0.331000000	4.133617000	2.840255000
1	-0.475903000	5.130706000	3.270069000

6	-0.957927000	3.779101000	1.646221000
1	-1.593864000	4.515375000	1.139385000
6	-0.756714000	2.515222000	1.075985000
6	-1.488184000	-0.668011000	1.647903000
6	-2.199216000	-0.289950000	2.808720000
1	-1.760297000	0.480062000	3.458504000
6	-3.424900000	-0.846070000	3.160520000
1	-3.935906000	-0.517998000	4.073874000
6	-4.003765000	-1.824632000	2.349293000
1	-4.973906000	-2.264580000	2.605216000
6	-3.331908000	-2.228830000	1.196907000
1	-3.802627000	-2.983234000	0.557640000
6	-2.099950000	-1.661500000	0.839978000
23	0.100871000	0.063546000	-1.125021000
6	3.769642000	1.298503000	-0.305784000
1	4.719000000	0.817524000	-0.001268000
6	-3.101678000	2.247937000	-0.774956000
1	-3.353530000	3.311063000	-0.597177000
6	-0.481522000	-3.737465000	-0.581050000
1	-0.790076000	-4.249203000	-1.513267000
6	-1.001263000	-4.524453000	0.610220000
1	-0.566454000	-5.541150000	0.622246000
1	-0.713177000	-4.028635000	1.554144000
1	-2.097627000	-4.627899000	0.619982000
6	1.034570000	-3.703057000	-0.562835000
1	1.413416000	-3.175877000	0.330113000
1	1.448629000	-4.728439000	-0.552723000
1	1.432052000	-3.180405000	-1.447114000
6	3.993020000	2.023666000	-1.624684000
1	4.284186000	1.346366000	-2.445045000
1	3.078113000	2.551476000	-1.943560000
1	4.787173000	2.786827000	-1.529631000
6	3.358577000	2.265761000	0.790686000
1	3.311570000	1.770395000	1.773429000
1	4.075866000	3.103976000	0.861857000
1	2.356016000	2.691359000	0.608426000
6	-3.519430000	1.847686000	-2.181845000
1	-4.615869000	1.897037000	-2.310210000
1	-3.064170000	2.477662000	-2.966409000
1	-3.203586000	0.802534000	-2.368702000
6	-3.828374000	1.404545000	0.252939000
1	-3.577635000	0.336175000	0.135074000
1	-3.557017000	1.684445000	1.282950000
1	-4.922520000	1.513164000	0.140962000
5	-0.057876000	-0.024397000	1.268340000
15	2.499284000	-0.092917000	-0.507442000

15	-1.224691000	2.084929000	-0.644994000
15	-1.219373000	-1.980022000	-0.752891000
6	-0.741715000	3.623217000	-1.693707000
1	-0.782821000	3.198528000	-2.719245000
6	0.707051000	3.968657000	-1.404201000
1	1.142381000	4.619432000	-2.184721000
1	0.807605000	4.487082000	-0.434204000
1	1.300356000	3.041851000	-1.332053000
6	-1.611322000	4.870737000	-1.691278000
1	-1.193705000	5.626961000	-2.382204000
1	-2.647925000	4.680672000	-2.012654000
1	-1.650810000	5.343456000	-0.695726000
6	3.558419000	-1.362333000	-1.500540000
1	3.299741000	-2.299962000	-0.976364000
6	5.075348000	-1.246589000	-1.511737000
1	5.519364000	-2.113266000	-2.036062000
1	5.424371000	-0.344775000	-2.043229000
1	5.517571000	-1.224123000	-0.503338000
6	3.023801000	-1.473254000	-2.920755000
1	3.459811000	-2.339822000	-3.451439000
1	1.923492000	-1.590989000	-2.905449000
1	3.262491000	-0.572612000	-3.519014000
6	-2.651498000	-2.354566000	-1.970480000
1	-3.416437000	-1.614574000	-1.657540000
6	-2.168009000	-1.981318000	-3.363959000
1	-1.307479000	-2.612180000	-3.664996000
1	-2.959501000	-2.111246000	-4.125202000
1	-1.824714000	-0.933072000	-3.383407000
6	-3.289521000	-3.736477000	-2.005270000
1	-2.599396000	-4.488842000	-2.425870000
1	-3.608420000	-4.105805000	-1.018569000
1	-4.182469000	-3.734108000	-2.657461000
7	0.334168000	0.568384000	-3.340798000
1	0.557590000	-0.206968000	-3.967108000
1	-0.480672000	1.038116000	-3.738859000
1	1.111886000	1.227509000	-3.406546000

[V]⁻(TE= -3393.874450)

6	0.889783000	-1.252040000	1.704476000
6	0.568290000	-2.029044000	2.841407000
1	-0.347800000	-1.782547000	3.394979000
6	1.364743000	-3.076605000	3.298464000
1	1.067240000	-3.641147000	4.190455000
6	2.551150000	-3.395265000	2.635057000
1	3.195117000	-4.206650000	2.991177000
6	2.895408000	-2.668418000	1.495670000

1	3.814350000	-2.934498000	0.958939000
6	2.074789000	-1.640064000	1.014660000
6	0.536457000	1.425441000	1.683777000
6	1.302049000	1.601839000	2.857721000
1	1.597361000	0.706019000	3.421541000
6	1.663869000	2.853923000	3.346162000
1	2.248292000	2.933163000	4.270819000
6	1.252484000	4.011813000	2.680074000
1	1.503391000	5.003707000	3.071256000
6	0.525165000	3.883095000	1.497863000
1	0.218350000	4.789697000	0.962977000
6	0.211204000	2.620939000	0.973935000
6	-1.574620000	-0.192477000	1.648826000
6	-2.109331000	0.386555000	2.820271000
1	-1.440332000	0.984491000	3.454438000
6	-3.440689000	0.236548000	3.198604000
1	-3.806229000	0.708179000	4.118741000
6	-4.311477000	-0.517681000	2.409201000
1	-5.362265000	-0.640460000	2.693108000
6	-3.824370000	-1.107204000	1.243944000
1	-4.513013000	-1.685387000	0.617950000
6	-2.486335000	-0.943793000	0.857526000
23	0.103820000	0.015626000	-1.072395000
6	4.019376000	-0.045623000	-0.489526000
1	4.748874000	-0.825887000	-0.195591000
6	-2.142440000	3.171302000	-0.778969000
1	-2.016493000	4.248940000	-0.556918000
6	-1.807875000	-3.365844000	-0.765085000
1	-1.934855000	-3.622671000	-1.838331000
6	-2.897870000	-4.040748000	0.051403000
1	-2.806192000	-5.140311000	-0.019599000
1	-2.798323000	-3.771825000	1.117471000
1	-3.917803000	-3.774466000	-0.264014000
6	-0.447184000	-3.865115000	-0.313008000
1	-0.279325000	-3.642016000	0.756096000
1	-0.356511000	-4.957517000	-0.451270000
1	0.359792000	-3.362905000	-0.866451000
6	4.456101000	0.568404000	-1.811070000
1	4.535625000	-0.168182000	-2.626578000
1	3.740751000	1.339567000	-2.142112000
1	5.441298000	1.058851000	-1.710533000
6	3.966548000	1.004542000	0.607677000
1	3.746415000	0.560312000	1.591516000
1	4.928481000	1.543562000	0.679989000
1	3.173215000	1.749182000	0.414010000
6	-2.728547000	2.996345000	-2.171644000

1	-3.751120000	3.410208000	-2.232202000
1	-2.127037000	3.476117000	-2.962241000
1	-2.788669000	1.918184000	-2.413290000
6	-3.060222000	2.564116000	0.262987000
1	-3.151114000	1.474061000	0.113827000
1	-2.682554000	2.711747000	1.286974000
1	-4.070857000	3.006169000	0.198832000
5	-0.022944000	-0.012585000	1.242410000
15	2.343625000	-0.903122000	-0.654380000
15	-0.425548000	2.391002000	-0.736826000
15	-1.822335000	-1.467594000	-0.776328000
6	0.504142000	3.656303000	-1.831486000
1	0.282228000	3.245074000	-2.838221000
6	1.996905000	3.507372000	-1.604917000
1	2.581571000	3.978493000	-2.415442000
1	2.308181000	3.966591000	-0.649994000
1	2.259578000	2.438141000	-1.551710000
6	0.093143000	5.120759000	-1.835355000
1	0.695066000	5.678891000	-2.576308000
1	-0.965077000	5.275773000	-2.099364000
1	0.269052000	5.605213000	-0.860304000
6	2.788799000	-2.413070000	-1.738932000
1	2.232515000	-3.218758000	-1.225845000
6	4.235633000	-2.868733000	-1.855576000
1	4.290801000	-3.813278000	-2.427423000
1	4.866649000	-2.139466000	-2.390231000
1	4.707661000	-3.058473000	-0.878606000
6	2.160432000	-2.218716000	-3.113301000
1	2.251841000	-3.128277000	-3.735193000
1	1.083598000	-1.976153000	-3.015315000
1	2.639742000	-1.389728000	-3.666375000
6	-3.188521000	-1.091676000	-2.044301000
1	-3.567149000	-0.113208000	-1.685062000
6	-2.482512000	-0.867707000	-3.377105000
1	-2.029064000	-1.804836000	-3.752139000
1	-3.179823000	-0.503410000	-4.154051000
1	-1.667718000	-0.125190000	-3.269711000
6	-4.367654000	-2.033171000	-2.229543000
1	-4.041250000	-3.036577000	-2.555907000
1	-4.971821000	-2.155709000	-1.317217000
1	-5.044841000	-1.649400000	-3.014794000
[V]-N ₂ ⁺ (TE= -3503.300359)			
6	-1.227428000	0.848789000	1.836367000
6	-1.173093000	1.702676000	2.961043000
1	-0.199158000	1.881004000	3.436295000
6	-2.301533000	2.314955000	3.500115000

1	-2.203222000	2.969457000	4.374291000
6	-3.561066000	2.078424000	2.945518000
1	-4.457840000	2.540582000	3.371608000
6	-3.655027000	1.261418000	1.820349000
1	-4.638546000	1.100075000	1.364504000
6	-2.511111000	0.690112000	1.249130000
6	0.190803000	-1.439859000	1.850189000
6	-0.361517000	-1.847946000	3.083604000
1	-1.015267000	-1.146721000	3.620724000
6	-0.087669000	-3.087125000	3.655374000
1	-0.538774000	-3.356212000	4.617979000
6	0.785706000	-3.977996000	3.024994000
1	1.025353000	-4.944136000	3.481545000
6	1.333738000	-3.622948000	1.793429000
1	2.005567000	-4.325001000	1.285161000
6	1.007440000	-2.401136000	1.192123000
6	1.430682000	0.867229000	1.639143000
6	2.172870000	0.612021000	2.812979000
1	1.828284000	-0.182801000	3.488353000
6	3.324655000	1.317983000	3.145018000
1	3.866267000	1.081279000	4.068515000
6	3.794498000	2.324791000	2.299266000
1	4.708018000	2.878869000	2.539925000
6	3.088426000	2.608740000	1.133452000
1	3.473586000	3.385774000	0.465931000
6	1.928859000	1.894259000	0.800958000
23	-0.126993000	-0.120551000	-1.132827000
6	-3.578916000	-1.654442000	-0.176462000
1	-4.573809000	-1.295204000	0.151407000
6	3.289158000	-1.904536000	-0.699100000
1	3.654060000	-2.936321000	-0.534652000
6	0.104277000	3.744408000	-0.682175000
1	0.358470000	4.241876000	-1.637401000
6	0.550575000	4.630433000	0.468613000
1	0.009232000	5.593643000	0.442539000
1	0.330045000	4.150687000	1.438371000
1	1.629006000	4.852078000	0.453701000
6	-1.400938000	3.559629000	-0.656784000
1	-1.729584000	3.031791000	0.256082000
1	-1.913095000	4.538801000	-0.682498000
1	-1.742986000	2.973726000	-1.524299000
6	-3.735646000	-2.396426000	-1.496872000
1	-4.286992000	-1.812082000	-2.250573000
1	-2.757371000	-2.642913000	-1.942416000
1	-4.281738000	-3.345955000	-1.351921000
6	-3.022658000	-2.550082000	0.917415000

1	-3.009942000	-2.040136000	1.893964000
1	-3.632887000	-3.465807000	1.015691000
1	-1.982675000	-2.855286000	0.711973000
6	3.627901000	-1.459833000	-2.114731000
1	4.720454000	-1.419385000	-2.272795000
1	3.199106000	-2.116007000	-2.891318000
1	3.221894000	-0.445843000	-2.288636000
6	3.951428000	-1.000652000	0.321269000
1	3.614577000	0.043511000	0.207225000
1	3.722373000	-1.302014000	1.355731000
1	5.048605000	-1.018546000	0.192332000
5	0.068971000	0.065716000	1.281226000
15	-2.512342000	-0.118331000	-0.403434000
15	1.415896000	-1.961973000	-0.540942000
15	1.011986000	2.072267000	-0.786433000
6	1.072341000	-3.521034000	-1.577704000
1	1.057870000	-3.093697000	-2.600194000
6	-0.330390000	-4.018051000	-1.282013000
1	-0.681454000	-4.719014000	-2.059852000
1	-0.379887000	-4.537031000	-0.308121000
1	-1.028508000	-3.168404000	-1.236782000
6	2.067910000	-4.670699000	-1.571336000
1	1.718549000	-5.468655000	-2.251736000
1	3.074176000	-4.379313000	-1.911713000
1	2.168935000	-5.129984000	-0.573357000
6	-3.688801000	0.993481000	-1.422588000
1	-3.500169000	1.982060000	-0.966702000
6	-5.188624000	0.741417000	-1.356144000
1	-5.725280000	1.535221000	-1.906969000
1	-5.475183000	-0.214544000	-1.825513000
1	-5.589168000	0.738600000	-0.330449000
6	-3.222086000	1.051249000	-2.870477000
1	-3.788971000	1.810973000	-3.438847000
1	-2.146399000	1.294391000	-2.936872000
1	-3.358494000	0.082847000	-3.385149000
6	2.372340000	2.498159000	-2.050382000
1	3.203092000	1.836369000	-1.730476000
6	1.897134000	2.053027000	-3.426493000
1	0.965638000	2.579688000	-3.712548000
1	2.652678000	2.272816000	-4.202431000
1	1.673103000	0.974668000	-3.453119000
6	2.891025000	3.928183000	-2.133124000
1	2.136816000	4.604091000	-2.572479000
1	3.188955000	4.358618000	-1.165260000
1	3.773297000	3.974065000	-2.796703000
7	-0.365551000	-1.089144000	-4.066725000

7 -0.285781000 -0.681373000 -3.002535000

For catalyst [**I**'_{SB}]

[**V**]-NH₃ (TE= -3265.958642)

6	-0.307507000	1.713584000	1.154431000
6	0.101967000	2.333016000	2.350501000
1	0.655143000	1.736192000	3.086946000
6	-0.151368000	3.673750000	2.631173000
1	0.191085000	4.107373000	3.576228000
6	-0.833456000	4.463332000	1.707212000
1	-1.033733000	5.518868000	1.913765000
6	-1.231167000	3.897623000	0.499469000
1	-1.728346000	4.508563000	-0.262172000
6	-0.968889000	2.550286000	0.233881000
6	-1.193815000	-0.826597000	1.453923000
6	-1.765235000	-0.594406000	2.719747000
1	-1.418926000	0.270032000	3.300164000
6	-2.762461000	-1.402702000	3.260258000
1	-3.173508000	-1.173839000	4.248736000
6	-3.240718000	-2.495948000	2.540677000
1	-4.027833000	-3.135366000	2.951192000
6	-2.722533000	-2.747253000	1.273781000
1	-3.111418000	-3.574632000	0.669859000
6	-1.722185000	-1.925340000	0.745294000
6	1.469078000	-0.347435000	1.307415000
6	1.719632000	-0.812947000	2.612557000
1	0.892191000	-0.819264000	3.333140000
6	2.960410000	-1.296259000	3.020804000
1	3.096552000	-1.652639000	4.046894000
6	4.018700000	-1.344616000	2.116863000
1	4.993314000	-1.741793000	2.415569000
6	3.812011000	-0.905569000	0.812396000
1	4.616109000	-0.981409000	0.073666000
6	2.565240000	-0.403799000	0.420192000
16	2.360339000	-0.026813000	-1.335984000
16	-1.349715000	1.953524000	-1.422919000
16	-1.246804000	-2.222221000	-0.966835000
23	-0.085958000	-0.145367000	-1.509688000
6	-3.217531000	1.737763000	-1.378668000
1	-3.616626000	2.768386000	-1.410069000
6	-0.135168000	-3.737668000	-0.838494000
1	-0.828662000	-4.574729000	-0.636419000
6	3.130645000	1.683767000	-1.503391000
1	2.910225000	1.877290000	-2.570722000
6	4.627142000	1.635107000	-1.289246000
1	5.077961000	2.610562000	-1.541179000

1	4.865684000	1.429380000	-0.231842000
1	5.109921000	0.863254000	-1.909558000
6	2.448694000	2.717684000	-0.643231000
1	2.563960000	2.480174000	0.428984000
1	2.891528000	3.713302000	-0.818218000
1	1.371188000	2.773149000	-0.859815000
6	-3.561217000	0.995432000	-2.651353000
1	-3.219519000	1.533395000	-3.552043000
1	-3.076971000	0.000078000	-2.632264000
1	-4.650246000	0.845911000	-2.735675000
6	-3.700159000	1.015846000	-0.146222000
1	-3.417249000	1.537184000	0.781772000
1	-4.800032000	0.928029000	-0.168313000
1	-3.274396000	-0.001359000	-0.105187000
6	0.492594000	-3.882291000	-2.207157000
1	1.148162000	-4.767812000	-2.246563000
1	-0.263636000	-3.981213000	-3.004596000
1	1.109695000	-2.987321000	-2.418054000
6	0.897537000	-3.619335000	0.252900000
1	1.561660000	-2.759839000	0.057451000
1	0.444107000	-3.475265000	1.246287000
1	1.516661000	-4.532323000	0.287489000
5	-0.017081000	0.147994000	0.947675000
7	-0.184866000	-0.428924000	-3.727296000
1	-0.493041000	0.404427000	-4.233360000
1	0.712476000	-0.692111000	-4.140830000
1	-0.839532000	-1.170687000	-3.988180000

[V] (TE= -3209.473694)

6	0.352700000	-1.658846000	1.073807000
6	-0.042029000	-2.245178000	2.290949000
1	-0.595852000	-1.632254000	3.013348000
6	0.228831000	-3.573911000	2.609101000
1	-0.100708000	-3.982937000	3.569375000
6	0.910355000	-4.383026000	1.702109000
1	1.123046000	-5.429938000	1.937488000
6	1.292704000	-3.849907000	0.474811000
1	1.789389000	-4.478778000	-0.272169000
6	1.016904000	-2.513230000	0.171829000
6	1.204911000	0.911389000	1.261929000
6	1.808842000	0.738637000	2.521889000
1	1.494669000	-0.111035000	3.141082000
6	2.797870000	1.589977000	3.008948000
1	3.234987000	1.408940000	3.995964000
6	3.234887000	2.664427000	2.237162000
1	4.015309000	3.336828000	2.605169000

6	2.684982000	2.854680000	0.973343000
1	3.043362000	3.665526000	0.329767000
6	1.690842000	1.992927000	0.498946000
6	-1.453049000	0.383731000	1.166279000
6	-1.697610000	0.900615000	2.452855000
1	-0.863050000	0.951148000	3.163226000
6	-2.942769000	1.378058000	2.853459000
1	-3.076007000	1.773085000	3.865468000
6	-4.009218000	1.371920000	1.957902000
1	-4.988022000	1.763661000	2.249488000
6	-3.806714000	0.885874000	0.670036000
1	-4.618334000	0.920122000	-0.063253000
6	-2.556137000	0.386278000	0.285985000
16	-2.377328000	-0.054991000	-1.458352000
16	1.390311000	-1.971166000	-1.506283000
16	1.182755000	2.228484000	-1.214386000
23	0.072228000	0.092462000	-1.591640000
6	3.253871000	-1.727565000	-1.469336000
1	3.660027000	-2.754938000	-1.426189000
6	0.051854000	3.729813000	-1.118067000
1	0.739743000	4.575894000	-0.935721000
6	-3.117450000	-1.782821000	-1.558582000
1	-2.928996000	-1.996835000	-2.627705000
6	-4.606762000	-1.754927000	-1.297554000
1	-5.044551000	-2.744996000	-1.511674000
1	-4.817593000	-1.527644000	-0.238733000
1	-5.123547000	-1.009817000	-1.922856000
6	-2.386232000	-2.780410000	-0.696526000
1	-2.472364000	-2.520064000	0.373246000
1	-2.812327000	-3.788860000	-0.834579000
1	-1.315613000	-2.818045000	-0.947775000
6	3.597446000	-1.074345000	-2.789572000
1	3.274015000	-1.679991000	-3.651759000
1	3.102309000	-0.086629000	-2.852269000
1	4.684961000	-0.913902000	-2.871585000
6	3.721032000	-0.918509000	-0.286468000
1	3.430424000	-1.372875000	0.673901000
1	4.820766000	-0.829545000	-0.304481000
1	3.293415000	0.098029000	-0.322881000
6	-0.577731000	3.840361000	-2.488746000
1	-1.245057000	4.716257000	-2.540518000
1	0.175581000	3.935158000	-3.287810000
1	-1.185034000	2.936947000	-2.689113000
6	-0.974120000	3.626845000	-0.018997000
1	-1.638949000	2.763603000	-0.194001000
1	-0.514872000	3.503429000	0.974570000

1	-1.594503000	4.539269000	0.001585000
5	0.038211000	-0.105960000	0.829696000

[V]-N₂ (TE= -3265.958642)

6	-0.327816000	1.785322000	1.131618000
6	0.081173000	2.481609000	2.284390000
1	0.673792000	1.948789000	3.038507000
6	-0.226790000	3.822398000	2.500733000
1	0.113867000	4.318967000	3.414627000
6	-0.959687000	4.533225000	1.551755000
1	-1.201321000	5.588438000	1.708233000
6	-1.352677000	3.891169000	0.382025000
1	-1.886057000	4.441284000	-0.400915000
6	-1.039957000	2.542961000	0.183927000
6	-1.146507000	-0.747837000	1.591475000
6	-1.702049000	-0.453721000	2.851212000
1	-1.379732000	0.458445000	3.368476000
6	-2.656261000	-1.263244000	3.461183000
1	-3.057216000	-0.988293000	4.441699000
6	-3.107717000	-2.415834000	2.820483000
1	-3.862809000	-3.055374000	3.286474000
6	-2.608941000	-2.725958000	1.559807000
1	-2.982911000	-3.599255000	1.014328000
6	-1.647049000	-1.903957000	0.963619000
6	1.496364000	-0.216389000	1.395947000
6	1.764013000	-0.570395000	2.732341000
1	0.939987000	-0.552147000	3.456050000
6	3.022895000	-0.972117000	3.169555000
1	3.174908000	-1.240950000	4.219510000
6	4.080486000	-1.053464000	2.266373000
1	5.069328000	-1.389823000	2.590881000
6	3.854693000	-0.731472000	0.932589000
1	4.657417000	-0.841119000	0.196973000
6	2.589126000	-0.304424000	0.511421000
16	2.365286000	-0.082758000	-1.263884000
16	-1.420254000	1.844945000	-1.428490000
16	-1.200544000	-2.280066000	-0.735973000
23	-0.088698000	-0.228256000	-1.522986000
6	-3.265006000	1.540655000	-1.371984000
1	-3.703866000	2.549977000	-1.477382000
6	-0.041762000	-3.740943000	-0.589606000
1	-0.710663000	-4.590183000	-0.357463000
6	3.054640000	1.622330000	-1.610536000
1	2.861377000	1.677697000	-2.698391000
6	4.544172000	1.669218000	-1.351009000
1	4.952679000	2.632871000	-1.699293000

1	4.759096000	1.594658000	-0.271422000
1	5.082337000	0.861242000	-1.870837000
6	2.300829000	2.717157000	-0.896977000
1	2.365178000	2.599150000	0.199127000
1	2.727510000	3.700699000	-1.156950000
1	1.236596000	2.720631000	-1.175667000
6	-3.581538000	0.702783000	-2.592610000
1	-3.215302000	1.165505000	-3.523800000
1	-3.115857000	-0.295510000	-2.499060000
1	-4.670896000	0.562409000	-2.685990000
6	-3.730698000	0.899169000	-0.088537000
1	-3.457650000	1.490738000	0.799501000
1	-4.829170000	0.797514000	-0.105505000
1	-3.297963000	-0.108707000	0.028872000
6	0.570612000	-3.917092000	-1.962932000
1	1.193635000	-4.826066000	-1.989014000
1	-0.193133000	-4.002280000	-2.753418000
1	1.217141000	-3.053195000	-2.203373000
6	0.995320000	-3.578314000	0.493493000
1	1.658907000	-2.723984000	0.276966000
1	0.545251000	-3.415707000	1.485544000
1	1.617965000	-4.487569000	0.547280000
5	-0.000607000	0.219756000	1.013057000
7	-0.239709000	-0.752687000	-4.577154000
7	-0.176055000	-0.558555000	-3.466583000

[V]-NH₃⁺ (TE= -3265.840275)

6	-0.591456000	1.903632000	0.734049000
6	-0.206632000	2.941773000	1.603452000
1	0.606378000	2.760892000	2.315788000
6	-0.832729000	4.186135000	1.606225000
1	-0.507218000	4.955482000	2.312332000
6	-1.867412000	4.453899000	0.712155000
1	-2.361320000	5.429119000	0.705772000
6	-2.240968000	3.475697000	-0.203449000
1	-3.010935000	3.684797000	-0.953801000
6	-1.612768000	2.227956000	-0.184323000
6	-0.917761000	-0.635979000	1.556800000
6	-1.509962000	-0.323627000	2.794871000
1	-1.334831000	0.668021000	3.230048000
6	-2.321613000	-1.221231000	3.481520000
1	-2.754046000	-0.936993000	4.445116000
6	-2.596789000	-2.475374000	2.936892000
1	-3.241290000	-3.182855000	3.465217000
6	-2.067129000	-2.807025000	1.695182000
1	-2.306331000	-3.768499000	1.228217000

6	-1.237661000	-1.897350000	1.030691000
6	1.592798000	0.356606000	1.372148000
6	1.856175000	0.471537000	2.751041000
1	1.013868000	0.602307000	3.440099000
6	3.139655000	0.405175000	3.283236000
1	3.285458000	0.500207000	4.363057000
6	4.233776000	0.198926000	2.445410000
1	5.245872000	0.131127000	2.852687000
6	4.018366000	0.048703000	1.081991000
1	4.857149000	-0.161144000	0.410828000
6	2.721245000	0.139326000	0.559839000
16	2.583167000	-0.247969000	-1.199539000
16	-2.002437000	1.093998000	-1.521874000
16	-0.680229000	-2.354199000	-0.611958000
23	0.123305000	-0.199782000	-1.498680000
6	-3.732818000	0.440602000	-1.233939000
1	-4.365907000	1.247317000	-1.644006000
6	0.622112000	-3.654891000	-0.295448000
1	0.018958000	-4.526096000	0.018023000
6	2.790805000	1.387866000	-2.082269000
1	2.945870000	1.038242000	-3.120367000
6	4.007593000	2.142396000	-1.604576000
1	4.144666000	3.048185000	-2.217550000
1	3.888259000	2.463870000	-0.556562000
1	4.923525000	1.537407000	-1.681229000
6	1.523269000	2.210893000	-1.997569000
1	1.285928000	2.499062000	-0.959787000
1	1.626174000	3.141995000	-2.579672000
1	0.639476000	1.713228000	-2.461669000
6	-3.855169000	-0.798995000	-2.093866000
1	-3.570127000	-0.609364000	-3.142383000
1	-3.225484000	-1.614817000	-1.697053000
1	-4.899193000	-1.151123000	-2.093093000
6	-4.068166000	0.204023000	0.216209000
1	-3.889071000	1.094072000	0.839260000
1	-5.138592000	-0.049230000	0.294269000
1	-3.489116000	-0.634983000	0.632110000
6	1.278772000	-3.937936000	-1.629630000
1	1.969724000	-4.790677000	-1.534344000
1	0.541353000	-4.191414000	-2.409323000
1	1.871390000	-3.069184000	-1.967043000
6	1.598081000	-3.285525000	0.793938000
1	2.236213000	-2.436941000	0.500185000
1	1.094768000	-3.022650000	1.737443000
1	2.257844000	-4.145964000	0.993828000
5	0.060997000	0.452033000	0.903849000

7	-0.009161000	-0.829293000	-3.633261000
1	-0.358819000	-0.113119000	-4.276328000
1	0.853794000	-1.183229000	-4.055347000
1	-0.680951000	-1.599748000	-3.701039000

[V]⁺ (TE= -3209.351568)

6	-1.946786000	0.366993000	1.385297000
6	-2.588533000	1.241329000	2.279238000
1	-1.978166000	1.784407000	3.009784000
6	-3.966347000	1.434703000	2.266325000
1	-4.430339000	2.119185000	2.981466000
6	-4.749559000	0.753202000	1.338893000
1	-5.834083000	0.889638000	1.320607000
6	-4.149283000	-0.109637000	0.425207000
1	-4.769827000	-0.645242000	-0.297177000
6	-2.764592000	-0.280601000	0.435621000
6	0.205923000	-1.282070000	1.618522000
6	-0.635862000	-2.282070000	2.182203000
1	-1.646435000	-1.990890000	2.487342000
6	-0.217390000	-3.579537000	2.402608000
1	-0.896705000	-4.301216000	2.863265000
6	1.086427000	-3.959938000	2.060008000
1	1.437974000	-4.975596000	2.259097000
6	1.941265000	-3.039890000	1.479688000
1	2.966558000	-3.329240000	1.242194000
6	1.508129000	-1.726974000	1.218589000
6	0.498192000	1.472404000	1.673806000
6	1.076506000	1.791638000	2.909465000
1	0.952487000	1.093911000	3.746516000
6	1.803296000	2.966953000	3.093901000
1	2.246657000	3.191217000	4.067748000
6	1.961090000	3.852339000	2.032744000
1	2.521836000	4.781398000	2.166023000
6	1.408680000	3.558835000	0.785664000
1	1.547440000	4.264006000	-0.037425000
6	0.699478000	2.372140000	0.611755000
23	0.356341000	-0.585112000	-0.591790000
5	-0.384104000	0.177336000	1.497932000
6	3.241537000	-1.516719000	-1.115860000
1	3.624224000	-0.649925000	-1.686485000
6	2.107632000	-2.161207000	-1.894413000
1	2.508412000	-2.668778000	-2.787289000
1	1.573404000	-2.933816000	-1.313212000
1	1.383024000	-1.423826000	-2.320255000
6	4.394512000	-2.461103000	-0.850407000
1	4.896352000	-2.694729000	-1.803631000

1	5.140942000	-2.014992000	-0.177011000
1	4.061437000	-3.419009000	-0.423571000
6	-2.723618000	-0.747750000	-2.418665000
1	-3.007196000	0.300133000	-2.213722000
6	-3.919265000	-1.582295000	-2.827346000
1	-4.329736000	-1.202632000	-3.777426000
1	-3.623594000	-2.633002000	-2.983608000
1	-4.730894000	-1.568859000	-2.086443000
6	-1.626984000	-0.811245000	-3.460354000
1	-2.024958000	-0.514139000	-4.444262000
1	-0.788725000	-0.136407000	-3.221643000
1	-1.236358000	-1.839567000	-3.564537000
6	1.316937000	2.582088000	-2.176038000
1	2.225379000	2.681834000	-1.555547000
6	1.570852000	1.605775000	-3.302911000
1	0.653367000	1.406898000	-3.882866000
1	2.305953000	2.034816000	-4.003149000
1	1.977852000	0.646352000	-2.944601000
6	0.851174000	3.926304000	-2.697846000
1	-0.066346000	3.809580000	-3.297993000
1	0.630559000	4.644870000	-1.894828000
1	1.625394000	4.367428000	-3.347028000
16	2.630597000	-0.570051000	0.391156000
16	0.037686000	1.886679000	-1.006197000
16	-2.011513000	-1.366937000	-0.803269000

[V]-N₂⁺ (TE= -3318.744561)

6	2.070882000	0.785452000	-1.346413000
6	2.732913000	1.827563000	-2.017815000
1	2.133244000	2.613318000	-2.491033000
6	4.119998000	1.889722000	-2.102360000
1	4.599536000	2.712377000	-2.639330000
6	4.893056000	0.901345000	-1.498682000
1	5.983982000	0.933756000	-1.560763000
6	4.273837000	-0.137112000	-0.809043000
1	4.885236000	-0.912238000	-0.339478000
6	2.880986000	-0.179931000	-0.719290000
6	-0.219432000	-0.530221000	-1.928166000
6	0.531938000	-1.391968000	-2.779015000
1	1.567432000	-1.116769000	-3.003574000
6	-0.003178000	-2.521458000	-3.363755000
1	0.606493000	-3.133787000	-4.032409000
6	-1.333534000	-2.873070000	-3.102024000
1	-1.770321000	-3.762885000	-3.562779000
6	-2.106108000	-2.100227000	-2.252935000
1	-3.138533000	-2.391794000	-2.060505000

6	-1.563862000	-0.948729000	-1.652567000
6	-0.233140000	2.110235000	-1.003756000
6	-0.695995000	2.986395000	-1.993295000
1	-0.622940000	2.686394000	-3.045607000
6	-1.259354000	4.219212000	-1.666983000
1	-1.622900000	4.881220000	-2.457423000
6	-1.356834000	4.605113000	-0.333351000
1	-1.787373000	5.574506000	-0.068387000
6	-0.902657000	3.756364000	0.676113000
1	-0.976127000	4.072494000	1.720562000
6	-0.364291000	2.518277000	0.333537000
23	-0.285562000	-0.820223000	0.364743000
5	0.493105000	0.755841000	-1.368593000
6	-4.061609000	-0.766368000	-0.015775000
1	-4.360328000	-0.039669000	0.764353000
6	-3.915604000	-2.123003000	0.636449000
1	-3.317192000	-2.070310000	1.557902000
1	-4.916086000	-2.487792000	0.920609000
1	-3.469985000	-2.881962000	-0.024915000
6	-5.086103000	-0.695645000	-1.132228000
1	-6.074471000	-0.970414000	-0.729866000
1	-5.160519000	0.319591000	-1.548997000
1	-4.869407000	-1.387270000	-1.960193000
6	3.048787000	-1.398776000	1.863378000
1	3.513190000	-0.398121000	1.820070000
6	4.092548000	-2.494603000	1.923793000
1	4.673560000	-2.404185000	2.856274000
1	3.613299000	-3.487616000	1.920864000
1	4.799548000	-2.462813000	1.082184000
6	2.093895000	-1.476288000	3.033119000
1	2.672127000	-1.434005000	3.970635000
1	1.381695000	-0.637710000	3.048612000
1	1.536665000	-2.428221000	3.044825000
6	-1.107187000	1.545189000	2.936936000
1	-1.932569000	2.079380000	2.433771000
6	-1.591229000	0.190791000	3.408664000
1	-0.767411000	-0.426781000	3.807074000
1	-2.317532000	0.325695000	4.226894000
1	-2.093472000	-0.371030000	2.604165000
6	-0.525553000	2.372405000	4.064138000
1	0.323351000	1.847598000	4.534267000
1	-0.162401000	3.353792000	3.723624000
1	-1.288901000	2.540887000	4.841462000
7	-0.883754000	-3.525633000	1.904391000
7	-0.732366000	-2.550794000	1.388527000
16	-2.479646000	0.085592000	-0.501513000

16	2.127693000	-1.524778000	0.226004000
16	0.182911000	1.343016000	1.594165000

[V]-NH₃⁺(TE= -3318.744561)

6	-0.107722000	1.697876000	1.130168000
6	0.498385000	2.315258000	2.252103000
1	1.069433000	1.676141000	2.940140000
6	0.391847000	3.674449000	2.532136000
1	0.877523000	4.087645000	3.424846000
6	-0.346203000	4.514813000	1.692131000
1	-0.439855000	5.584855000	1.905970000
6	-0.928471000	3.966877000	0.549328000
1	-1.457229000	4.609342000	-0.165990000
6	-0.793667000	2.602860000	0.275121000
6	-1.294389000	-0.683005000	1.399258000
6	-1.963135000	-0.317837000	2.592650000
1	-1.577282000	0.548494000	3.148088000
6	-3.064382000	-1.002935000	3.099124000
1	-3.531589000	-0.670591000	4.034338000
6	-3.568964000	-2.121157000	2.428969000
1	-4.433675000	-2.669114000	2.818301000
6	-2.968556000	-2.505654000	1.229729000
1	-3.375890000	-3.343006000	0.649350000
6	-1.874984000	-1.793279000	0.727821000
6	1.379014000	-0.541978000	1.292196000
6	1.537587000	-1.209498000	2.532986000
1	0.673030000	-1.234230000	3.210859000
6	2.718918000	-1.826622000	2.933357000
1	2.772909000	-2.319716000	3.911908000
6	3.837863000	-1.816421000	2.096035000
1	4.770472000	-2.308304000	2.392216000
6	3.729419000	-1.198771000	0.849469000
1	4.566944000	-1.239824000	0.143435000
6	2.534793000	-0.580782000	0.461672000
16	2.375612000	-0.113176000	-1.281172000
16	-1.251359000	2.039527000	-1.377403000
16	-1.371966000	-2.135755000	-0.973654000
23	-0.074787000	-0.116743000	-1.433965000
6	-3.138673000	1.927592000	-1.355295000
1	-3.485521000	2.975860000	-1.430393000
6	-0.368531000	-3.742613000	-0.862307000
1	-1.123089000	-4.539450000	-0.719703000
6	3.267206000	1.550043000	-1.424474000
1	3.031466000	1.791644000	-2.479858000
6	4.760574000	1.375229000	-1.256160000
1	5.294014000	2.317361000	-1.478887000

1	4.999979000	1.100990000	-0.213963000
1	5.159407000	0.587033000	-1.916028000
6	2.700495000	2.611314000	-0.516480000
1	2.850342000	2.340811000	0.543195000
1	3.197598000	3.582165000	-0.694547000
1	1.617343000	2.735094000	-0.670022000
6	-3.499489000	1.156060000	-2.605417000
1	-3.133199000	1.654405000	-3.520460000
1	-3.032307000	0.152830000	-2.544508000
1	-4.591962000	1.028984000	-2.697674000
6	-3.677821000	1.273535000	-0.109533000
1	-3.374788000	1.810546000	0.803096000
1	-4.781763000	1.236615000	-0.141641000
1	-3.295547000	0.241735000	-0.026099000
6	0.303915000	-3.870344000	-2.210499000
1	0.933165000	-4.775553000	-2.262801000
1	-0.426532000	-3.909810000	-3.038083000
1	0.951644000	-2.982322000	-2.360825000
6	0.629487000	-3.730105000	0.265060000
1	1.334448000	-2.891783000	0.129482000
1	0.146195000	-3.599786000	1.246145000
1	1.206258000	-4.672582000	0.283230000
5	-0.012716000	0.121801000	0.854483000
7	-0.175615000	-0.368387000	-3.723011000
1	-0.451577000	0.485841000	-4.210757000
1	0.720128000	-0.651047000	-4.124615000
1	-0.851190000	-1.085444000	-3.997120000

[V]-(TE= -3318.744561)

6	0.129041000	-1.676503000	1.045052000
6	-0.404568000	-2.253175000	2.218600000
1	-0.927085000	-1.592873000	2.924506000
6	-0.290031000	-3.608173000	2.521895000
1	-0.717619000	-3.998679000	3.452977000
6	0.374722000	-4.470555000	1.647036000
1	0.472501000	-5.536872000	1.876773000
6	0.886333000	-3.956158000	0.456998000
1	1.362799000	-4.619877000	-0.274798000
6	0.754396000	-2.594394000	0.166350000
6	1.320642000	0.716356000	1.246620000
6	1.993817000	0.374969000	2.441016000
1	1.607074000	-0.472699000	3.023161000
6	3.112207000	1.057831000	2.913617000
1	3.586066000	0.747587000	3.852499000
6	3.626019000	2.141883000	2.199155000
1	4.503038000	2.689250000	2.560558000

6	3.019355000	2.498065000	0.995585000
1	3.435084000	3.308983000	0.385048000
6	1.902960000	1.794491000	0.529059000
6	-1.366177000	0.580103000	1.152074000
6	-1.513152000	1.259961000	2.383678000
1	-0.647841000	1.281342000	3.060021000
6	-2.686869000	1.897621000	2.776367000
1	-2.738209000	2.397616000	3.750906000
6	-3.797315000	1.901749000	1.930098000
1	-4.724715000	2.407319000	2.219132000
6	-3.695169000	1.274613000	0.689635000
1	-4.529900000	1.322380000	-0.018724000
6	-2.512120000	0.625358000	0.311317000
16	-2.386527000	0.115687000	-1.418856000
16	1.155712000	-2.058422000	-1.508347000
16	1.391242000	2.115105000	-1.172525000
23	0.058183000	0.123782000	-1.495963000
6	3.046384000	-2.015612000	-1.527816000
1	3.352076000	-3.079032000	-1.532997000
6	0.442502000	3.761062000	-1.054424000
1	1.218170000	4.512170000	-0.813878000
6	-3.296416000	-1.547706000	-1.494742000
1	-3.067532000	-1.827760000	-2.541450000
6	-4.786335000	-1.350408000	-1.324884000
1	-5.329989000	-2.292726000	-1.519891000
1	-5.020783000	-1.045597000	-0.290055000
1	-5.179715000	-0.578111000	-2.006131000
6	-2.730033000	-2.575523000	-0.550338000
1	-2.873558000	-2.264473000	0.499314000
1	-3.230274000	-3.550974000	-0.688873000
1	-1.649005000	-2.708134000	-0.707647000
6	3.404614000	-1.346753000	-2.835758000
1	3.015458000	-1.901387000	-3.706174000
1	2.959498000	-0.332112000	-2.849968000
1	4.497900000	-1.247419000	-2.946713000
6	3.625691000	-1.294255000	-0.338443000
1	3.326497000	-1.759532000	0.614102000
1	4.729098000	-1.288102000	-0.392180000
1	3.270308000	-0.249392000	-0.321615000
6	-0.117717000	3.977795000	-2.441000000
1	-0.726371000	4.897024000	-2.488152000
1	0.674065000	4.043129000	-3.206120000
1	-0.769415000	3.117994000	-2.697394000
6	-0.635447000	3.725849000	-0.005254000
1	-1.344820000	2.910112000	-0.233240000
1	-0.230594000	3.537898000	1.001703000

1	-1.193377000	4.679459000	0.015097000
5	0.028427000	-0.100469000	0.738810000

[V]-N₂⁺(TE= -3318.940864)

6	0.764441000	-0.656022000	-1.991020000
6	1.547983000	-0.369325000	-3.124080000
1	1.536927000	0.658098000	-3.511437000
6	2.323887000	-1.335536000	-3.762877000
1	2.921068000	-1.067003000	-4.641703000
6	2.325355000	-2.650747000	-3.296299000
1	2.918382000	-3.421643000	-3.799570000
6	1.571836000	-2.979526000	-2.167287000
1	1.579265000	-4.009569000	-1.794754000
6	0.847119000	-1.982542000	-1.513957000
6	-1.736131000	0.168321000	-1.505155000
6	-2.250683000	-0.469842000	-2.657608000
1	-1.535174000	-0.911846000	-3.363319000
6	-3.609840000	-0.528245000	-2.945769000
1	-3.952796000	-1.032738000	-3.856513000
6	-4.536125000	0.095279000	-2.104295000
1	-5.604285000	0.095501000	-2.344408000
6	-4.077536000	0.713254000	-0.941160000
1	-4.785857000	1.211483000	-0.272212000
6	-2.719739000	0.670613000	-0.616787000
6	0.313476000	1.882931000	-1.154807000
6	-0.393170000	3.006924000	-1.636462000
1	-1.354717000	2.835960000	-2.138147000
6	0.079715000	4.311421000	-1.505301000
1	-0.513468000	5.147384000	-1.893754000
6	1.312023000	4.554856000	-0.900782000
1	1.696275000	5.574696000	-0.795928000
6	2.051778000	3.475919000	-0.402495000
1	3.008200000	3.670946000	0.091651000
6	1.539149000	2.185115000	-0.498930000
23	0.060408000	0.020773000	1.133479000
5	-0.186784000	0.380383000	-1.242610000
6	-3.164809000	0.351154000	2.231263000
1	-2.549670000	0.538446000	3.130813000
6	-3.211050000	-1.136594000	1.963465000
1	-3.793274000	-1.647178000	2.750483000
1	-3.685883000	-1.354163000	0.990702000
1	-2.195914000	-1.568305000	1.943667000
6	-4.538166000	0.953845000	2.455921000
1	-4.971689000	0.558153000	3.391432000
1	-4.495029000	2.051461000	2.537350000
1	-5.236267000	0.693271000	1.643915000

6	0.989586000	-3.554788000	0.865210000
1	1.977118000	-3.486265000	0.373934000
6	0.384693000	-4.931468000	0.676533000
1	0.998479000	-5.706887000	1.169372000
1	-0.625180000	-4.968291000	1.121199000
1	0.283329000	-5.199534000	-0.387355000
6	1.124074000	-3.182551000	2.326259000
1	1.720261000	-3.938289000	2.867155000
1	1.607892000	-2.198146000	2.440970000
1	0.135038000	-3.119628000	2.816784000
6	3.426441000	1.440857000	1.543732000
1	2.910439000	2.342292000	1.923171000
6	3.554719000	0.411578000	2.649568000
1	3.929920000	-0.546879000	2.245804000
1	4.276766000	0.754739000	3.410453000
1	2.592875000	0.218983000	3.147666000
6	4.785124000	1.785056000	0.961017000
1	5.279345000	0.868841000	0.594271000
1	4.720176000	2.481446000	0.111087000
1	5.438320000	2.238696000	1.727780000
7	0.049851000	0.041458000	4.221108000
7	0.082806000	0.031088000	3.072904000
16	-2.132266000	1.277870000	0.977776000
16	-0.056203000	-2.257976000	0.020781000
16	2.323479000	0.728157000	0.236881000

Cartesian coordinates of the species involved during the conversion of $[2c'_{PB} -V-H]^+ \rightarrow [2c'_{PB} -V-H-B]$ along with their total energies (in hartree) including zero point vibrational correction at M06-D3(heptane)/def2-SVP level of theory.

$[2c'_{PB} -V-H]$ (TE= -3049.461825)

6	1.164807000	2.261958000	1.918024000
6	0.998759000	1.041255000	2.823699000
6	-2.425736000	1.353107000	1.778249000
6	-1.692529000	0.495497000	2.807903000
6	1.315014000	-2.068534000	1.822473000
6	0.092453000	-1.536637000	2.564361000
1	-1.888403000	2.291003000	1.591875000
1	-1.677020000	1.053932000	3.758885000
1	1.603543000	-3.077652000	2.138838000
1	0.213027000	-1.764162000	3.640664000
1	1.851844000	3.013819000	2.329938000
1	1.967565000	0.521591000	2.897714000
6	1.949931000	3.283443000	-0.744495000
1	2.987651000	3.604481000	-0.570172000
6	-3.637053000	-0.934215000	0.445563000

1	-2.949443000	-1.656823000	0.912909000
6	2.763339000	-2.254443000	-0.677896000
1	3.336220000	-1.427515000	-0.238114000
23	-0.108017000	0.229925000	-0.525750000
1	0.204135000	2.765601000	1.766957000
1	0.809126000	1.404655000	3.848717000
1	-0.796814000	-2.117814000	2.269010000
1	2.189099000	-1.430791000	2.015323000
1	-2.311092000	-0.391699000	3.018818000
1	-3.436947000	1.632294000	2.108133000
6	3.423586000	-3.560522000	-0.256775000
1	4.464015000	-3.592809000	-0.599471000
1	3.436759000	-3.695252000	0.828821000
1	2.923173000	-4.431117000	-0.693881000
6	2.775105000	-2.084417000	-2.191247000
1	2.159083000	-2.840219000	-2.693600000
1	2.394595000	-1.105593000	-2.497369000
1	3.790339000	-2.187032000	-2.590206000
6	-4.798634000	-0.739952000	1.412678000
1	-5.292270000	-1.700691000	1.602082000
1	-4.477555000	-0.351341000	2.382545000
1	-5.563012000	-0.064745000	1.022420000
6	-4.107381000	-1.526072000	-0.878828000
1	-4.888003000	-0.909353000	-1.336123000
1	-3.295953000	-1.615418000	-1.608103000
1	-4.533311000	-2.525916000	-0.737871000
6	1.767823000	3.004420000	-2.232808000
1	2.389102000	2.177420000	-2.591792000
1	0.725972000	2.742366000	-2.444411000
1	2.018679000	3.889370000	-2.828786000
6	1.024220000	4.405233000	-0.295083000
1	1.220848000	4.729650000	0.730421000
1	1.144285000	5.280134000	-0.944004000
1	-0.023874000	4.092476000	-0.355799000
6	0.223320000	-3.631832000	-0.468387000
1	0.820924000	-3.988151000	-1.320386000
6	-1.198229000	-3.417106000	-0.962752000
1	-1.845310000	-3.050018000	-0.159949000
1	-1.246298000	-2.685603000	-1.774201000
1	-1.634067000	-4.353719000	-1.329136000
6	0.260977000	-4.698247000	0.617684000
1	-0.191947000	-5.627269000	0.253269000
1	1.274299000	-4.939986000	0.947607000
1	-0.307683000	-4.392556000	1.502674000
6	-3.401958000	1.784149000	-0.879887000
1	-2.844911000	2.692518000	-0.605711000

6	-4.866689000	2.002821000	-0.527256000
1	-5.497366000	1.167060000	-0.846180000
1	-5.030158000	2.152160000	0.543760000
1	-5.248463000	2.894007000	-1.038881000
6	-3.209667000	1.578554000	-2.376118000
1	-3.629210000	0.629727000	-2.726682000
1	-3.705236000	2.376047000	-2.941516000
1	-2.150561000	1.593317000	-2.642752000
6	3.501204000	1.216651000	0.578052000
1	3.420926000	0.229764000	1.057729000
6	4.258134000	2.136443000	1.526100000
1	5.308072000	1.831443000	1.605388000
1	4.257454000	3.176411000	1.178758000
1	3.842590000	2.127815000	2.536866000
6	4.256436000	1.047867000	-0.735709000
1	5.223725000	0.558676000	-0.574376000
1	3.703468000	0.450772000	-1.467012000
1	4.466353000	2.016254000	-1.203047000
15	-2.485077000	0.513301000	0.141284000
15	1.718209000	1.710528000	0.248423000
15	1.043161000	-1.997008000	-0.000132000
5	-0.194112000	0.031753000	2.463666000
7	-0.191232000	-0.330416000	-3.626919000
7	-0.153829000	-0.082811000	-2.524400000
1	-0.579396000	1.915184000	-0.546321000

$[2c'_{PB} - V-H-B]$ (TE= -3049.490923)

6	0.520070000	2.300227000	-2.012901000
6	-0.256663000	1.291854000	-2.866128000
6	2.417559000	-0.708742000	-2.029357000
6	1.162840000	-1.099896000	-2.814507000
6	-2.705904000	-0.649530000	-1.752837000
6	-1.579665000	-1.074619000	-2.699440000
1	2.658118000	0.351299000	-2.186365000
1	1.396537000	-1.000121000	-3.887306000
1	-3.674807000	-1.098504000	-2.007917000
1	-1.932348000	-0.918273000	-3.732321000
1	0.441410000	3.329230000	-2.391471000
1	-1.307412000	1.627771000	-2.907035000
6	1.021885000	3.565968000	0.629587000
1	0.403271000	4.474818000	0.652534000
6	2.574231000	-2.748681000	0.038638000
1	1.808410000	-3.170432000	-0.632363000
6	-3.784319000	-0.189286000	0.905823000
1	-3.723624000	0.858247000	0.570901000
23	-0.014744000	-0.129681000	0.582113000

1	1.591965000	2.069454000	-2.017567000
1	0.095025000	1.397166000	-3.905584000
1	-1.436513000	-2.163942000	-2.615431000
1	-2.860553000	0.438177000	-1.815278000
1	0.992581000	-2.181034000	-2.672184000
1	3.310966000	-1.256057000	-2.361468000
6	-5.160344000	-0.729515000	0.542982000
1	-5.945944000	-0.126974000	1.013097000
1	-5.349688000	-0.723477000	-0.534106000
1	-5.296146000	-1.755650000	0.900920000
6	-3.567115000	-0.215108000	2.413510000
1	-3.559345000	-1.239615000	2.804538000
1	-2.618726000	0.246542000	2.701309000
1	-4.369847000	0.316815000	2.935932000
6	3.933821000	-3.272322000	-0.403824000
1	3.931645000	-4.368022000	-0.430325000
1	4.226888000	-2.927304000	-1.399264000
1	4.722258000	-2.978474000	0.296616000
6	2.249363000	-3.215842000	1.453641000
1	3.023971000	-2.922594000	2.168301000
1	1.302462000	-2.808166000	1.816728000
1	2.177299000	-4.308468000	1.493061000
6	1.295662000	3.135090000	2.067228000
1	0.379998000	2.886480000	2.613082000
1	1.930898000	2.241099000	2.095967000
1	1.811587000	3.925285000	2.624453000
6	2.318152000	3.902979000	-0.093787000
1	2.150052000	4.320877000	-1.089532000
1	2.895540000	4.637492000	0.478374000
1	2.959889000	3.022330000	-0.214348000
6	-2.655116000	-2.828612000	0.241756000
1	-3.144643000	-2.906456000	1.225167000
6	-1.335829000	-3.588594000	0.314561000
1	-0.754206000	-3.469387000	-0.608339000
1	-0.706971000	-3.230975000	1.133768000
1	-1.507149000	-4.661515000	0.460650000
6	-3.570491000	-3.450349000	-0.806371000
1	-3.765432000	-4.501141000	-0.563409000
1	-4.538682000	-2.952317000	-0.888930000
1	-3.108916000	-3.433223000	-1.798713000
6	3.736151000	0.033026000	0.449636000
1	3.359289000	1.064824000	0.369912000
6	5.027447000	-0.039999000	-0.356226000
1	5.494717000	-1.026396000	-0.309537000
1	4.880673000	0.204484000	-1.411176000
1	5.757295000	0.675396000	0.040615000

6	3.980820000	-0.244732000	1.927172000
1	4.445585000	-1.224305000	2.079566000
1	4.662619000	0.498137000	2.355596000
1	3.057799000	-0.222650000	2.516067000
6	-1.698362000	3.028678000	-0.273642000
1	-2.324227000	2.251890000	-0.738203000
6	-1.810164000	4.294134000	-1.110576000
1	-2.821818000	4.711153000	-1.050035000
1	-1.125529000	5.078507000	-0.767247000
1	-1.599320000	4.112704000	-2.167624000
6	-2.193784000	3.245229000	1.151020000
1	-3.252339000	3.527721000	1.163199000
1	-2.083260000	2.344135000	1.765451000
1	-1.645831000	4.051952000	1.651404000
15	2.259882000	-0.918906000	-0.194631000
15	0.002833000	2.249976000	-0.240832000
15	-2.338681000	-0.984515000	0.031302000
5	-0.187626000	-0.282285000	-2.429677000
7	0.146730000	-0.502512000	3.683295000
7	0.084150000	-0.363234000	2.556397000
1	-0.136379000	-0.280680000	-1.175520000

TS (TE= -3049.463264)

6	-0.689443000	2.932404000	1.693873000
6	0.119930000	2.059082000	2.647803000
6	-1.679344000	-1.601885000	2.423870000
6	-1.390185000	-0.238530000	3.056450000
6	2.488328000	-0.136555000	1.841265000
6	1.272266000	-0.397072000	2.724909000
1	-2.589686000	-2.063845000	2.829938000
1	-2.272519000	0.409636000	2.948800000
1	3.385393000	-0.671914000	2.182975000
1	1.566028000	-0.173131000	3.768825000
1	-0.628233000	4.004248000	1.926909000
1	1.183372000	2.340745000	2.576164000
6	-1.376782000	3.619990000	-1.079443000
1	-0.974814000	4.643915000	-1.108113000
6	-1.738001000	-3.390554000	0.140059000
1	-0.656453000	-3.583696000	0.208330000
6	3.506204000	0.408698000	-0.801124000
1	3.242021000	1.459717000	-0.620970000
23	-0.239192000	0.127452000	-0.343281000
1	-1.746728000	2.654784000	1.754279000
1	-0.162703000	2.331794000	3.679949000
1	1.063384000	-1.473116000	2.735606000
1	2.751527000	0.931718000	1.859029000

1	-1.286694000	-0.398272000	4.145429000
1	-0.869130000	-2.306750000	2.655345000
6	4.895490000	0.171665000	-0.224046000
1	5.637644000	0.783983000	-0.748832000
1	4.959763000	0.425690000	0.837083000
1	5.216934000	-0.869563000	-0.333727000
6	3.482470000	0.173204000	-2.305434000
1	3.846096000	-0.827880000	-2.561237000
1	2.477656000	0.278007000	-2.728578000
1	4.134615000	0.886477000	-2.821587000
6	-2.420729000	-4.383229000	1.074092000
1	-2.148783000	-5.407992000	0.793981000
1	-2.126476000	-4.250187000	2.118427000
1	-3.510133000	-4.323911000	1.029049000
6	-2.142371000	-3.614760000	-1.312010000
1	-3.224182000	-3.514501000	-1.449653000
1	-1.660046000	-2.906292000	-1.993581000
1	-1.873973000	-4.624142000	-1.643415000
6	-1.461112000	3.083831000	-2.504989000
1	-0.484670000	2.934299000	-2.973307000
1	-1.972524000	2.116167000	-2.521804000
1	-2.033737000	3.767138000	-3.142167000
6	-2.769874000	3.664270000	-0.463626000
1	-2.798857000	4.203742000	0.485952000
1	-3.471557000	4.159556000	-1.143893000
1	-3.155634000	2.652919000	-0.283623000
6	2.601972000	-2.304699000	-0.197080000
1	3.691904000	-2.328691000	-0.342329000
6	1.925926000	-2.845482000	-1.454026000
1	0.837252000	-2.865476000	-1.332979000
1	2.130509000	-2.248144000	-2.346041000
1	2.253871000	-3.870649000	-1.660461000
6	2.263266000	-3.182372000	0.999543000
1	2.525565000	-4.226345000	0.794732000
1	2.789054000	-2.884220000	1.910352000
1	1.189358000	-3.159760000	1.218940000
6	-3.560742000	-0.973934000	0.324643000
1	-3.571419000	-0.093393000	0.986117000
6	-4.663443000	-1.920960000	0.775984000
1	-4.773071000	-2.771986000	0.096107000
1	-4.503637000	-2.318365000	1.782320000
1	-5.629133000	-1.402250000	0.784689000
6	-3.812096000	-0.478971000	-1.094596000
1	-3.761811000	-1.287895000	-1.830816000
1	-4.809424000	-0.031403000	-1.176501000
1	-3.081597000	0.278426000	-1.393204000

6	1.419397000	3.556968000	-0.206123000
1	2.127155000	2.943560000	0.373592000
6	1.421317000	4.957313000	0.389861000
1	2.380054000	5.454951000	0.203251000
1	0.646332000	5.595331000	-0.049576000
1	1.268237000	4.951981000	1.471665000
6	1.882226000	3.572740000	-1.658461000
1	2.925867000	3.897734000	-1.739501000
1	1.804481000	2.587194000	-2.131748000
1	1.285978000	4.270298000	-2.257090000
15	-1.798318000	-1.566241000	0.576097000
15	-0.184043000	2.600066000	-0.049516000
15	2.128403000	-0.508462000	0.069291000
5	-0.063289000	0.469819000	2.509634000
7	-0.631116000	-0.396586000	-3.418857000
7	-0.505818000	-0.181901000	-2.310959000
1	-1.332262000	0.669871000	0.857331000