

Supporting Information

Hydroboration of Carbon Dioxide with Pinacolborane Catalyzed by Various Aluminum Hydrides: A Comparative Mechanistic Study

Cai-Qin Li,^a Geng Leng^b and Weiyi Li*^c*

^a College of Chemistry and Chemical Engineering, Shanxi Datong University, Datong,
Shanxi, 037009, P. R China.

^b School of Resources and Environment, University of Electronic Science and
Technology of China, Chengdu, Sichuan, 611731, P. R China

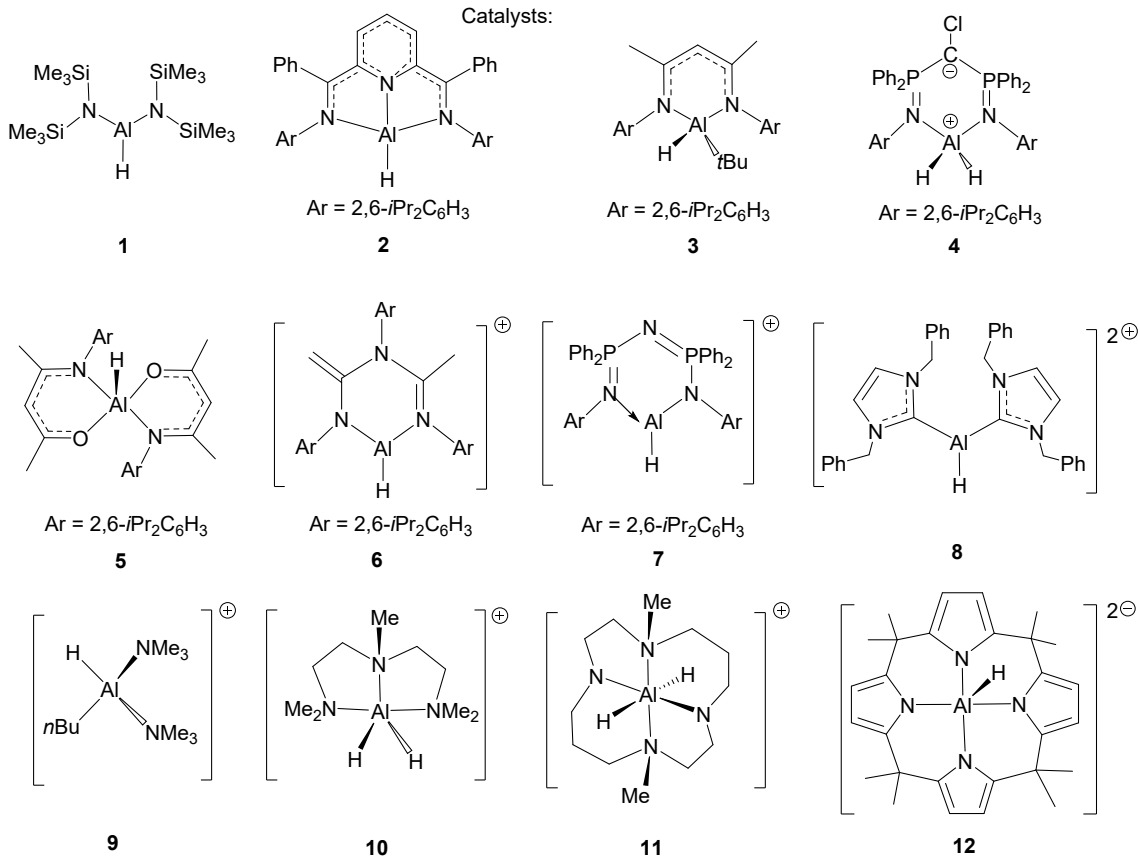
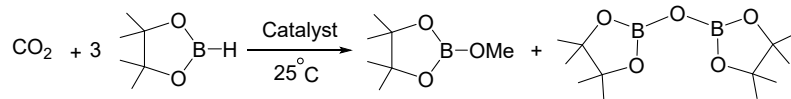
^c School of Science, Research Center for Advanced Computation, Xihua University,
Chengdu, Sichuan, 610039, P. R. China.

Corresponding author's E-mail address: licaiqin19860217@163.com;
weiyili@mail.xhu.edu.cn;

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S1: Computational details.



Optimization and frequency calculation in gas phase: M06-2X/6-31G*, the keyword “Int = ultrafine” was used.

Solvation Method: M06-2X/6-311++G**

For single-point energy calculation, the SCRF = (SMD, ExternalIteration) keyword was used.

S2: Nucleophilicity indices analysis

Table S1 Nucleophilicity indices (η^-) of the AIH active species.

AIH species	ϵ^0_{HOMO} (a.u.)	$\epsilon^{-1}_{\text{HOMO}}$ (a.u.)	ϵ^0_{LUMO} (a.u.)	$\epsilon^{-1}_{\text{LUMO}}$ (a.u.)	$\mu(N)$ (a.u.)	$\mu(N-1)$ (a.u.)	η^- (a.u.)
1	-0.29687	-0.41412	0.00987	-0.32749	-0.144	-0.371	0.227
2	-0.18579	-0.32942	-0.06624	-0.20878	-0.126	-0.269	0.143
3	-0.25686	-0.39560	-0.02040	-0.28239	-0.139	-0.339	0.200
4	-0.24604	-0.36678	-0.02647	-0.25094	-0.136	-0.309	0.173
5	-0.27201	-0.38708	-0.01437	-0.30581	-0.143	-0.346	0.203
6	-0.36834	-0.49372	-0.13200	-0.26404	-0.250	-0.379	0.129
7	-0.37828	-0.48592	-0.11485	-0.20551	-0.247	-0.348	0.099
8	-0.39539	-0.54575	-0.28735	-0.42915	-0.341	-0.487	0.146
9	-0.43234	-0.64339	-0.11586	-0.23450	-0.274	-0.439	0.165
10	-0.44658	-0.64252	-0.11185	-0.23888	-0.279	-0.441	0.161
11	-0.38824	-0.55594	-0.09979	-0.43502	-0.244	-0.495	0.251
12	-0.01232	-0.24018	0.14482	-0.18320	0.066	-0.212	0.278

Table S2 Nucleophilicity indices (η^-) of the AI formate IMs.

AIH species	ϵ^0_{HOMO} (a.u.)	$\epsilon^{-1}_{\text{HOMO}}$ (a.u.)	ϵ^0_{LUMO} (a.u.)	$\epsilon^{-1}_{\text{LUMO}}$ (a.u.)	$\mu(N)$ (a.u.)	$\mu(N-1)$ (a.u.)	η^- (a.u.)
1-IM1	-0.29632	-0.40941	-0.01092	-0.32691	-0.154	-0.368	0.214
2-IM1	-0.17927	-0.32378	-0.06540	-0.20136	-0.122	-0.262	0.140
3-IM1	-0.26626	-0.39561	-0.02158	-0.28416	-0.144	-0.340	0.200
4-IM1	-0.26160	-0.37063	-0.03336	-0.26431	-0.147	-0.317	0.170
5-IM1	-0.28148	-0.38704	-0.02783	-0.31363	-0.155	-0.350	0.195
6-IM1	-0.36485	-0.48747	-0.12978	-0.37676	-0.247	-0.432	0.185
7-IM1	-0.37534	-0.48071	-0.11395	-0.40889	-0.245	-0.445	0.200
8-IM1	-0.38515	-0.56336	-0.28797	-0.43380	-0.337	-0.499	0.163
9-IM1	-0.43172	-0.63780	-0.11669	-0.24781	-0.275	-0.444	0.169
10-IM1	-0.44503	-0.63852	-0.10925	-0.25310	-0.277	-0.446	0.169
11-IM1	-0.40648	-0.56685	-0.10085	-0.45700	-0.254	-0.512	0.258
12-IM1	-0.02193	-0.12018	0.14107	-0.06038	0.060	-0.090	0.150

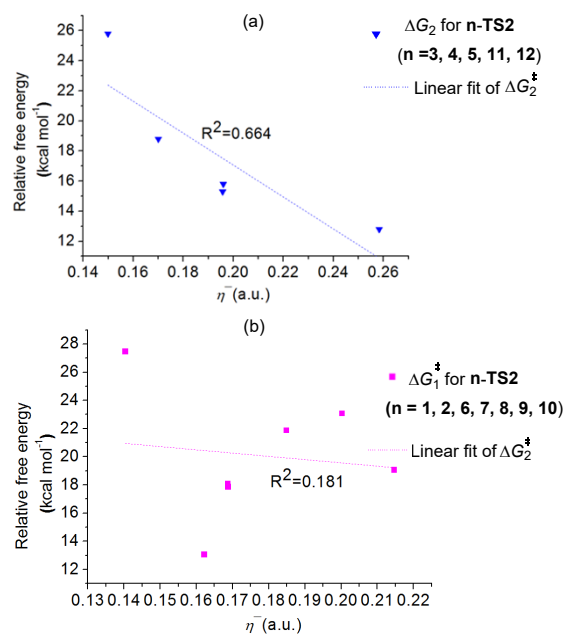


Figure. S1 Relationship between the nucleophilicity indices (η^-) of the Al formate IMs and free energy barrier (ΔG_2^\ddagger) for nucleophilic attack of the Al formate IMs to HBpin.

Table S3. Free energy barrier Overall ΔG_2^\ddagger , activation energies ΔE_2^\ddagger , distortion energies $\Delta E_{\text{dist}}^\ddagger$ and interaction energies $\Delta E_{\text{int}}^\ddagger$ (all in kcal mol⁻¹) for the TSs **n-TS2**. Free Al formate IM **n-IM1** and HBpin is chosen as zero-energy reference.

Transition state	ΔG_2^\ddagger	ΔE_2^\ddagger	$\Delta E_{\text{dist}}^\ddagger$			$\Delta E_{\text{int}}^\ddagger$
			Al-formate	HBpin	total	
1-TS2	19.1	4.4	13.2	4.8	18.2	-13.8
2-TS2	27.5	10.1	17.6	5.2	22.8	-12.8
3-TS2	15.8	2.3	6.3	4.5	10.8	-8.4
4-TS2	18.8	4.5	0.9	7.5	8.4	-3.9
5-TS2	15.3	-2.5	0.9	7.7	8.6	-11.1
6-TS2	21.9	6.1	29.0	7.3	36.4	-30.3
7-TS2	23.1	6.4	26.7	6.7	33.4	-27.0
8-TS2	13.1	-0.8	14.7	6.8	21.5	-22.3
9-TS2	18.1	4.1	9.0	5.5	14.5	-10.4
10-TS2	17.9	5.4	9.3	6.8	16.1	-10.7
11-TS2	12.8	-0.8	1.5	8.3	9.8	-10.6
12-TS2	25.8	11.8	9.1	9.7	18.8	-7.0

S3: Mechanism and energy profile of the reaction mediated by the AlH active species 1, 6 and 8

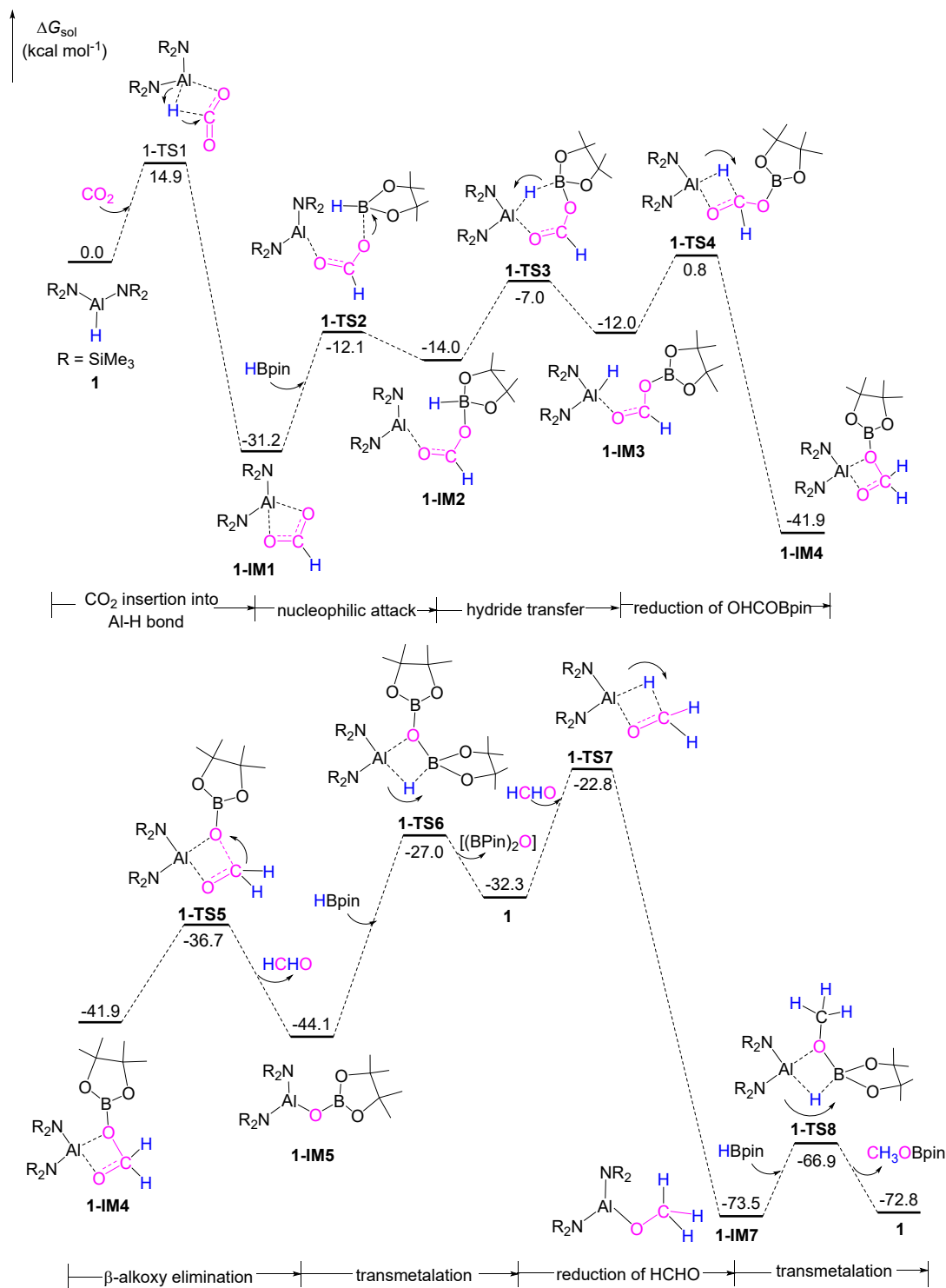


Figure S2. Free energy profile for the hydroboration of CO₂ with HBpin catalyzed by the neutral AlH active species **1**.

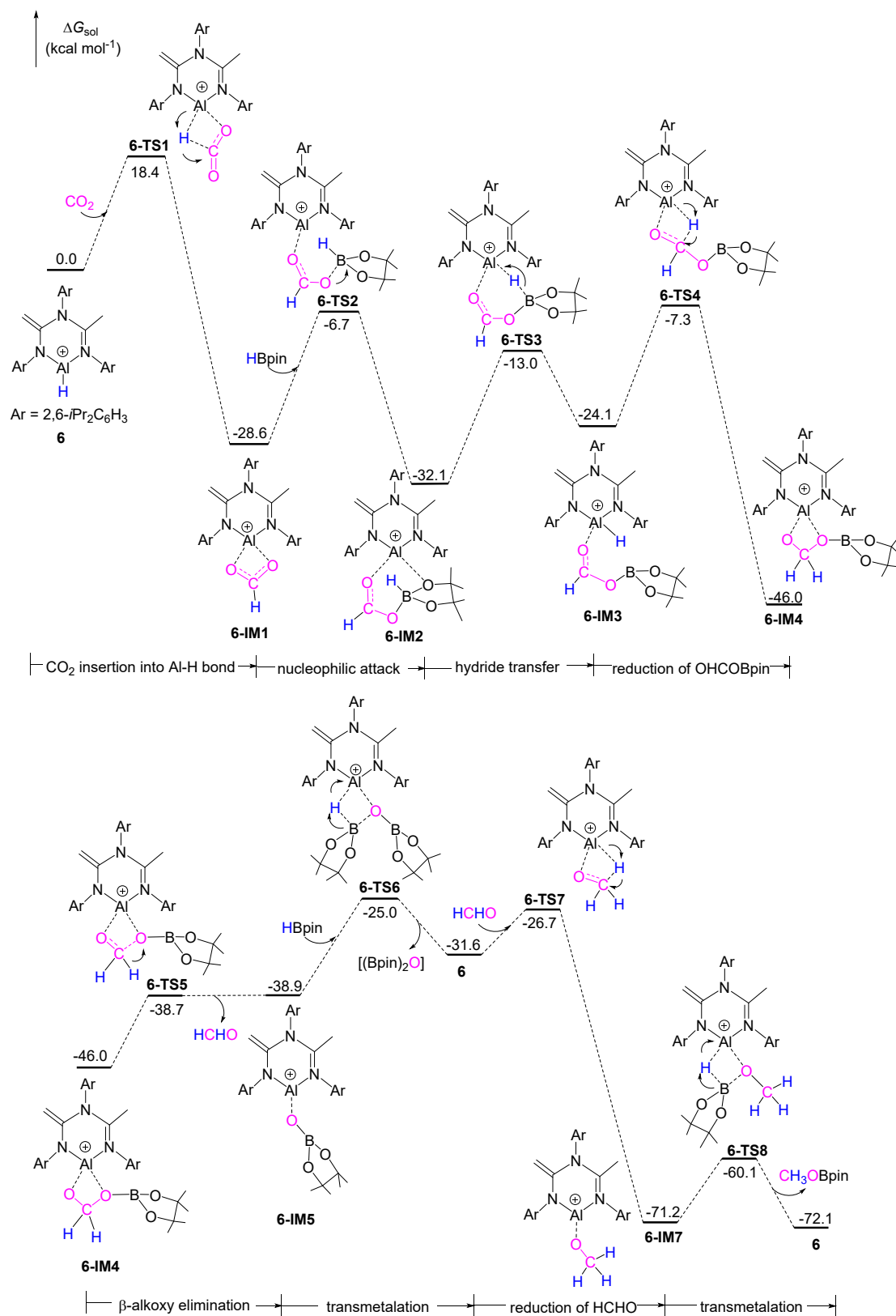


Figure S3. Free energy profile for the hydroboration of CO₂ with HBpin catalyzed by the cationic AlH active species **6**.

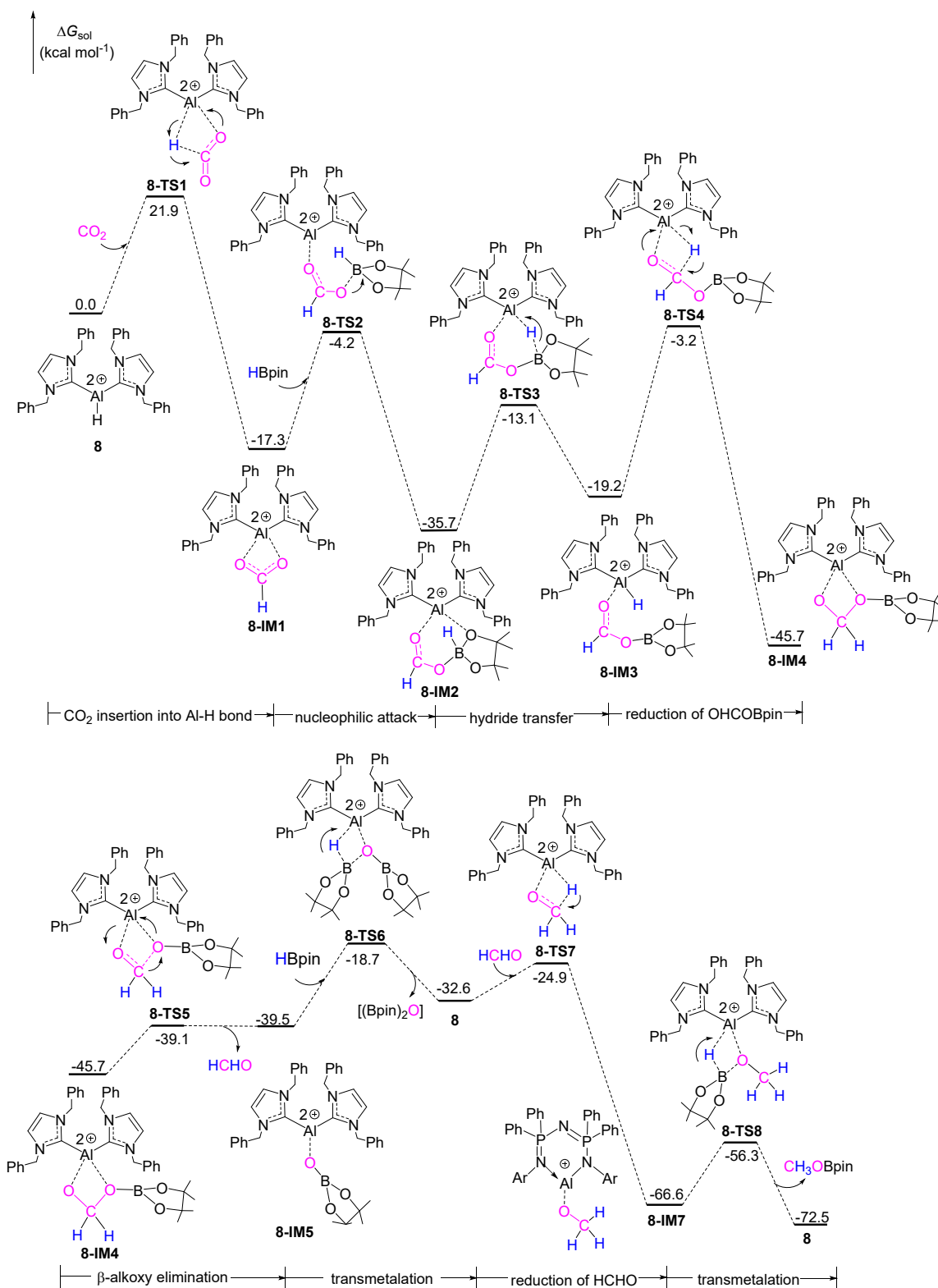


Figure S4. Free energy profile for the hydroboration of CO₂ with HBpin catalyzed by the cationic AlH active species **8**.

S4: Possible competing reactions for the Al acetal intermediates

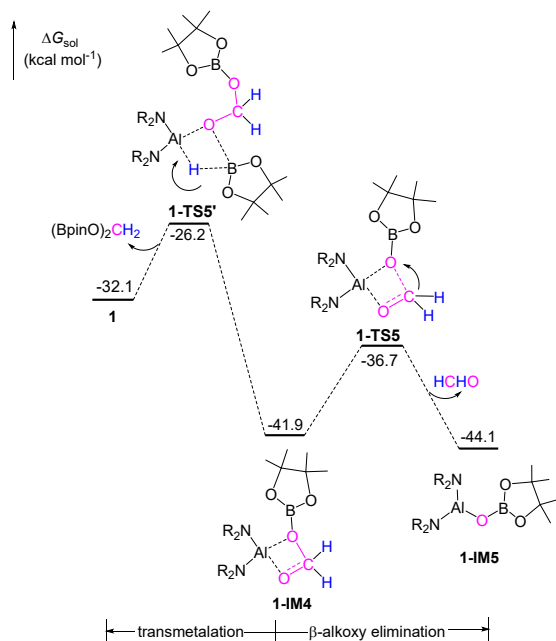


Figure S5. Free energy profile of the possible competing reactions for the Al acetal IM 1-IM4, including β -alkoxy elimination and transmetalation with HBpin.

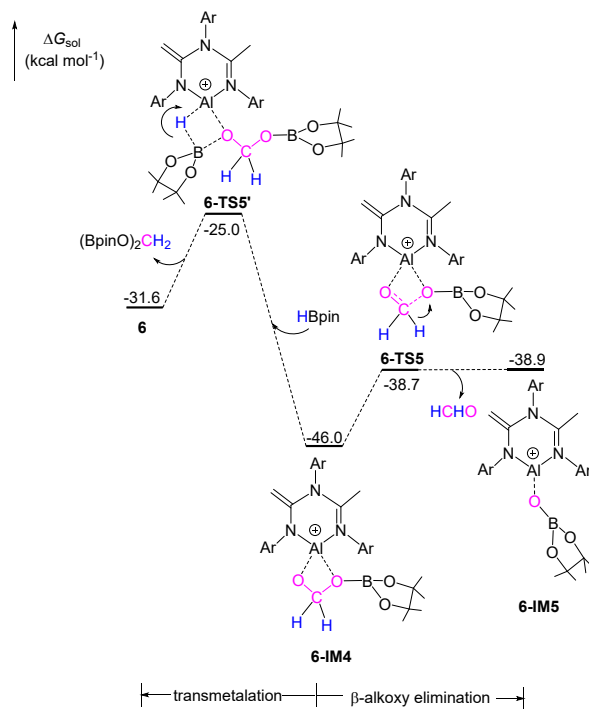


Figure S6. Free energy profile of the possible competing reactions for the Al acetal IM 6-IM4, including β -alkoxy elimination and transmetalation with HBpin.

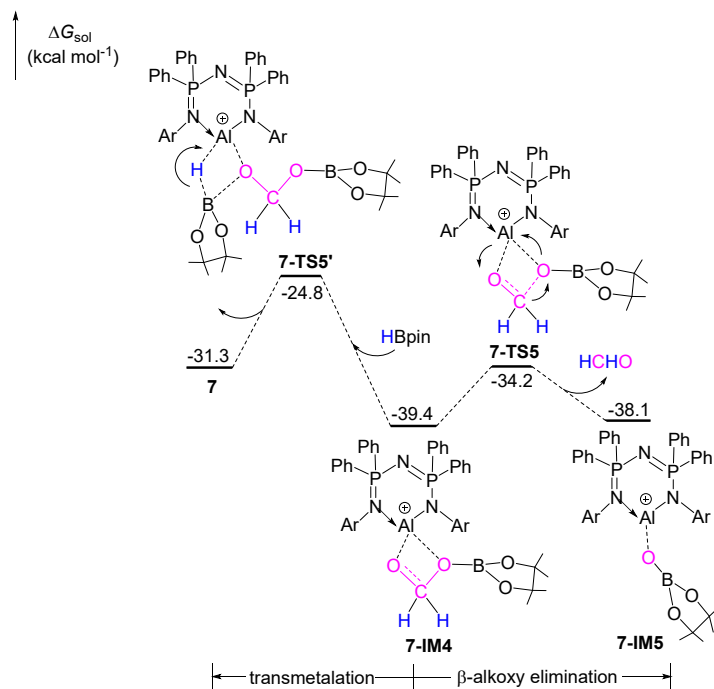


Figure S7. Free energy profile of the possible competing reactions for the Al acetal IM 7-IM4, including β -alkoxy elimination and transmetalation with HBpin.

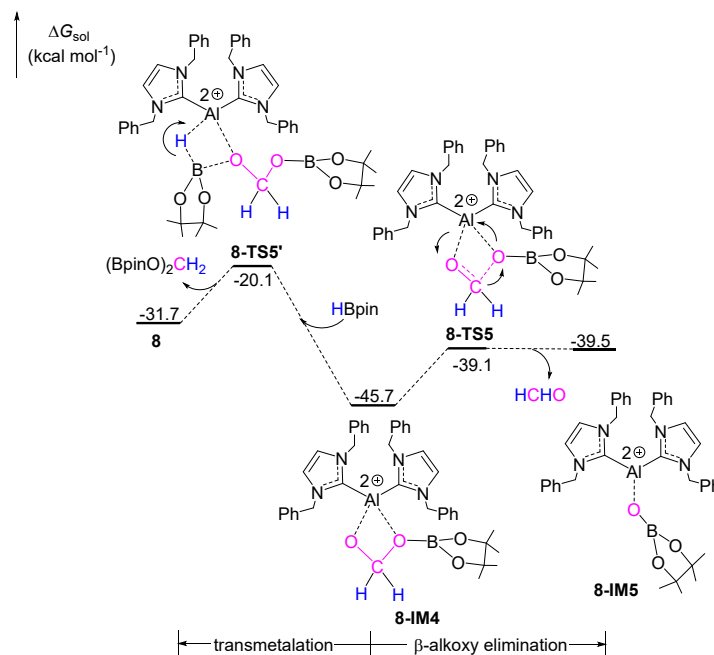


Figure S8. Free energy profile of the possible competing reactions for the Al acetal IM 8-IM4, including β -alkoxy elimination and transmetalation with HBpin.

S5: Comparison of geometric optimization in gas phase and solution phase

To probe the acceptability of the geometric optimization of all stationary points in gas phase, the geometries of all reactants, intermediates, transition states and products in the neutral, cationic and anionic systems were re-optimized with SMD model in the corresponding solvent at the M06-2X/6-31G* level of theory. Then, the single-point energy calculations were also carried out with SMD model at the M06-2X/6-311++G** level. The computed results from the two approaches are presented in Figure S9-11.

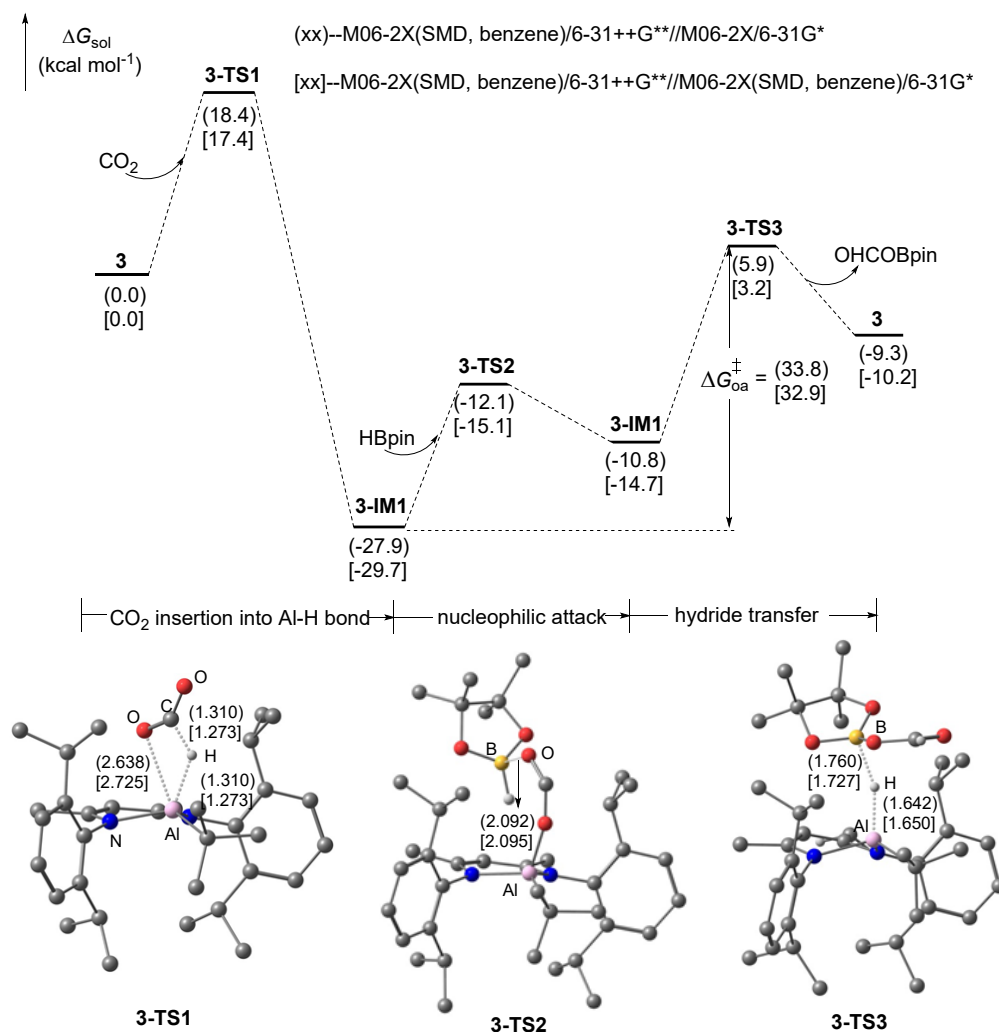


Figure S9. Free energy profile of hydroboration of CO₂ with HBpin to boryl formate using neutral AlH hydride **3**. The bond lengths of the critical TSs and relative Gibbs free energies of all stationary points obtained via geometric optimization in gas and solution phase are given in parenthesis and square brackets, respectively.

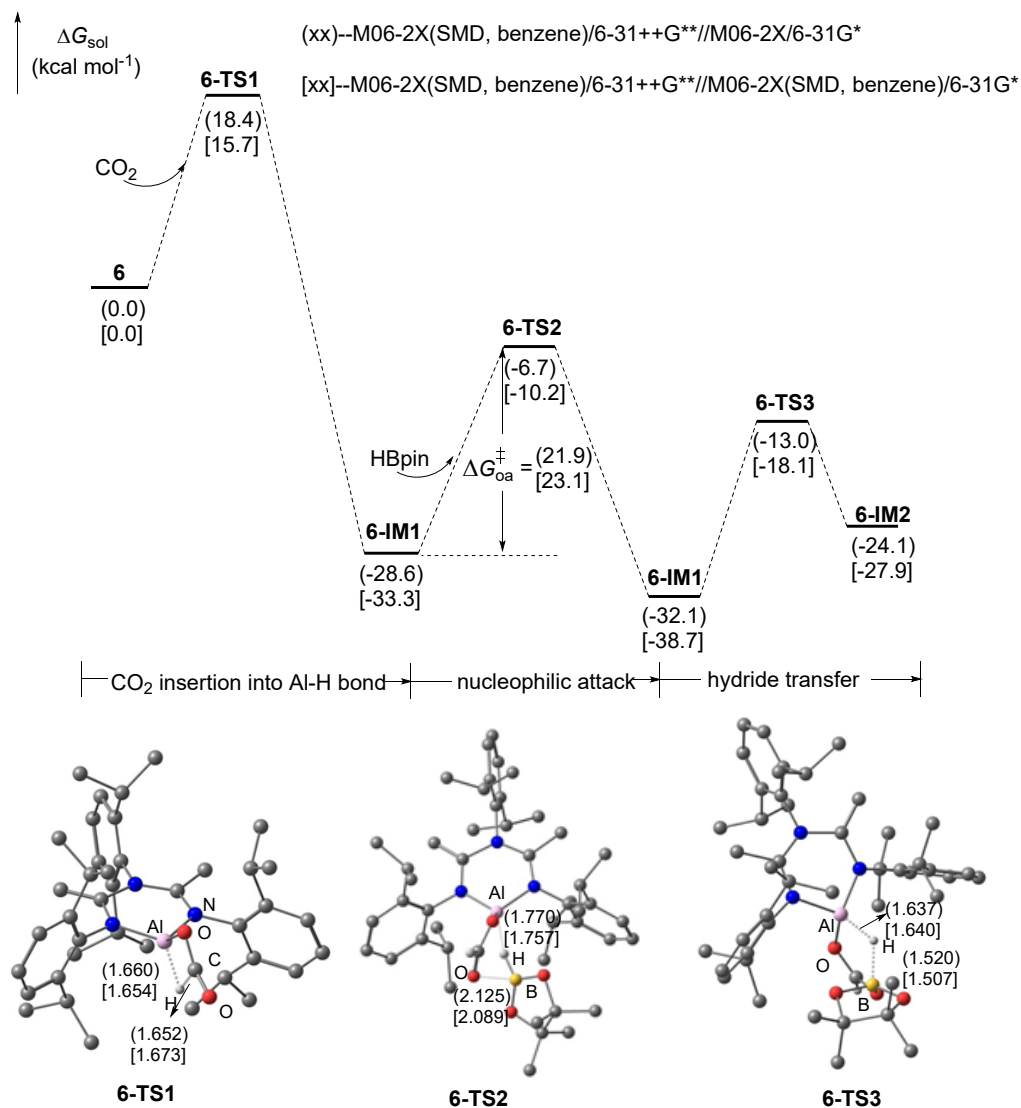


Figure S10. Free energy profile of hydroboration of CO₂ with HBpin to boryl formate using cationic AlH hydride **6**. The bond lengths of the critical TSs and relative Gibbs free energies of all stationary points obtained via geometric optimization in gas and solution phase are given in parenthesis and square brackets, respectively.

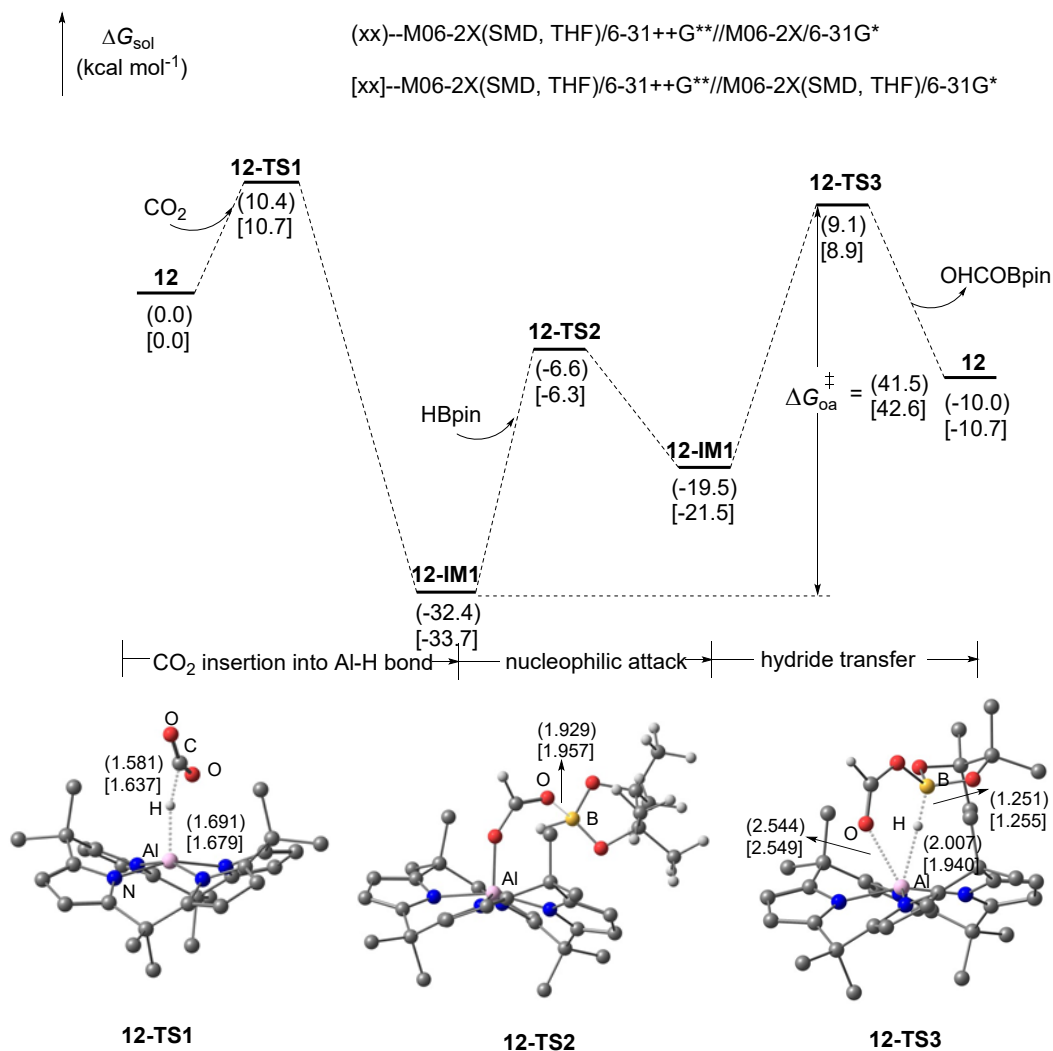


Figure S11. Free energy profile of hydroboration of CO₂ with HBpin to boryl formate using anionic AlH hydride **12**. The bond lengths of the critical TSs and relative Gibbs free energies of all stationary points obtained via geometric optimization in gas and solution phase are given in parenthesis and square brackets, respectively.

S6: Energy summary

Table S4 Energies of the stationary points involved in the hydroboration of CO₂ with HBpin using ALH active species **1**.

Species	H_c^a	G_c^b	E_{sol}^c (in benzene)	ΔH_{sol}^d	ΔG_{sol}^e
CO ₂	0.01547	-0.00879	-188.57497	-	-
HBpin	0.20389	0.16081	-411.81383	-	-
OHCOBpin	0.22306	0.17090	-600.42246	-	-
HCHO	0.03112	0.00566	-114.48955	-	-
[(BpinO) ₂ CH ₂]	0.43274	0.35975	-1012.30076	-	-
[(Bpin) ₂ O]	0.39589	0.32626	-897.78368	-	-
MeOBpin	0.24148	0.18899	-526.39048	-	-
1	0.50905	0.40943	-1989.62025	-	-
1-TS1	0.52521	0.42026	-2178.19112	3.0	14.9
1-IM1	0.53080	0.42691	-2178.27121	-43.8	-31.2
1-TS2	0.73566	0.61115	-2590.07801	-38.7	-12.1
1-IM2	0.73666	0.61368	-2590.08356	-41.6	-14.0
1-TS3	0.73433	0.61191	-2590.07069	-35.0	-7.0
1-IM3	0.73538	0.60929	-2590.07595	-37.6	-12.0
1-TS4	0.73387	0.61061	-2590.05688	-26.6	0.8
1-IM4	0.73936	0.61576	-2590.13019	-69.1	-41.9
1-TS5	0.73649	0.61083	-2590.11695	-62.6	-62.6
1-IM5	0.70288	0.57823	-2475.61223	-	-
1-TS5'	0.90624	0.76719	-2887.42694	-55.6	-27.0
1-TS6	0.90624	0.76719	-2887.42694	-55.6	-27.0
1-TS7	0.54220	0.44034	-2104.11992	-47.0	-22.8
1-IM7	0.54824	0.44201	-2104.20228	-94.9	-73.5
1-TS8	0.75202	0.62865	-2515.27947	-104.6	-66.9

a: H_c is the enthalpy correction calculated at the M06-2X/6-31G* level in gas phase at 298 K;

b: G_c is the Gibbs free energy correction calculated at the M06-2X/6-31G* level in gas phase at 298 K;

c: E_{sol} is the electron energy in the solvent after PCM correction calculated at the M06-2X/(SMD, benzene)//6-311++G(d, p) level;

d: ΔH_{sol} is the relative enthalpy energy in the solvent at 298 K $H_{sol} = H_c + E_{sol}$.

e: ΔG_{sol} is the relative Gibbs free energy in the solvent at 298 K. $G_{sol} = G_c + E_{sol}$.

Table S5 Energies of the stationary points involved in the hydroboration of CO₂ with HBpin using AIH active species **2**.

Species	H_c	G_c	E_{sol} (in benzene)	ΔH_{sol}	ΔG_{sol}
CO ₂	0.01547	-0.00879	-188.57621	-	-
HBpin	0.20389	0.16081	-411.81505	-	-
2	0.85863	0.73552	-2073.97200	-	-
2-TS1	0.87429	0.74760	-2262.53863	6.1	19.1
2-IM1	0.88014	0.75337	-2262.61698	-39.4	-26.4
2-TS2	1.08492	0.94198	-2674.41601	-28.8	1.1
2-IM2	1.08598	0.94457	-2674.42029	-30.8	0.0
2-TS3	1.08358	0.94301	-2674.40828	-24.7	6.6
2-IM3	1.08529	0.94319	-2674.41412	-27.3	3.0

Table S6 Energies of the stationary points involved in the hydroboration of CO₂ with HBpin using AIH active species **3**.

Species	H_c	G_c	E_{sol} (in THF)	ΔH_{sol}	ΔG_{sol}
CO ₂	0.01547	-0.00879	-188.57497	-	-
HBpin	0.20389	0.16081	-411.81383	-	-
3	0.81963	0.70991	-1640.00869	-	-
3-TS1	0.83664	0.72082	-1828.57403	7.0	18.4
3-IM1	0.84111	0.72500	-1828.65209	-39.2	-27.9
3-TS2	1.04608	0.90737	-2240.46218	-36.1	-12.1
3-IM2	1.04747	0.91029	-2240.46302	-35.8	-10.8
3-TS3	1.04370	0.90824	-2240.43446	-20.2	5.9

Table S7 Energies of the stationary points involved in the hydroboration of CO₂ with HBpin using AIH active species **4**.

Species	H_c	G_c	E_{sol} (in benzene)	ΔH_{sol}	ΔG_{sol}
CO ₂	0.01547	-0.00879	-188.57621	-	-
HBpin	0.20389	0.16081	-411.81505	-	-
4	0.99042	0.84926	-3395.51212	-	-
4-TS1	1.00701	0.86196	-3584.07184	10.3	23.1
4-IM1	1.01247	0.86992	-3584.14706	-33.5	-19.1
4-TS2	1.21740	1.05357	-3995.95373	-28.3	-0.3
4-IM2	1.21847	1.05420	-3995.95386	-28.3	0.0
4-TS3	1.21538	1.05336	-3995.93537	-18.1	11.1

Table S8 Energies of the stationary points involved in the hydroboration of CO₂ with HBpin using AIH active species **5**.

Species	H_c	G_c	E_{sol} (in CH ₂ Cl ₂)	ΔH_{sol}	ΔG_{sol}
CO ₂	0.01547	-0.00879	-188.57421	-	-
HBpin	0.20389	0.16081	-411.81623	-	-
5	0.81408	0.69404	-1827.44786	-	-
5-TS1	0.83032	0.70645	-2016.01150	7.1	19.9
5-IM1	0.83524	0.70942	-2016.09076	-39.5	-27.9
5-TS2	1.04043	0.89855	-2427.91091	-41.2	-12.6
5-IM2	1.04217	0.90176	-2427.91177	-40.6	-11.1
5-TS3	1.03873	0.89959	-2427.88777	-27.7	2.6

Table S9 Energies of the stationary points involved in the hydroboration of CO₂ with HBpin using AIH active species **6**.

Species	H_c	G_c	E_{sol} (in benzene)	ΔH_{sol}	ΔG_{sol}
CO ₂	0.01547	-0.00879	-188.57497	-	-
HBpin	0.20389	0.16081	-411.81383	-	-
OHCOBpin	0.22306	0.17090	-600.42246	-	-
HCHO	0.03112	0.00566	-114.48955	-	-
[(BpinO) ₂ CH ₂]	0.43274	0.35975	-1012.30076	-	-
[(Bpin) ₂ O]	0.39589	0.32626	-897.78368	-	-
MeOBpin	0.24148	0.18899	-526.39048	-	-
6	0.94432	0.81604	-1964.89718	-	-
6-TS1	0.96071	0.82560	-2153.46118	7.5	18.4
6-IM1	0.96613	0.83156	-2153.54209	-39.9	-28.6
6-TS2	1.17101	1.01768	-2565.34625	-33.2	-6.7
6-IM2	1.17364	1.02910	-2565.39815	-64.1	-32.1
6-TS3	1.17045	1.02072	-2565.35931	-41.8	-13.0
6-IM3	1.17079	1.01557	-2565.37188	-49.4	-24.1
6-TS4	1.16942	1.01259	-2565.34220	-31.7	-7.3
6-IM4	1.17504	1.02044	-2565.41165	-71.7	-46.0
6-TS5	1.17197	1.01747	-2565.39710	-64.5	-38.7
6-IM5	1.13841	0.98586	-2450.88190	-46.0	-46.0
6-TS5'	1.38004	1.20565	-2977.21563	-64.1	-23.7
6-TS6	1.34311	1.17460	-2862.70268	-53.0	-25.0
6-TS7	0.97740	0.84403	-2079.40137	-49.1	-26.7
6-IM7	0.98397	0.84831	-2079.47648	-92.1	-71.2
6-TS8	1.18910	1.03633	-2491.29983	-97.3	-60.1

Table S10 Energies of the stationary points involved in the hydroboration of CO₂ with HBpin using AlH active species **7**.

Species	H_c	G_c	E_{sol} (in toluene)	ΔH_{sol}	ΔG_{sol}
CO ₂	0.01547	-0.00879	-188.57490	-	-
HBpin	0.20389	0.16081	-411.81365	-	-
OHCOBpin	0.22306	0.17090	-600.42233	-	-
HCHO	0.03112	0.00566	-114.49104	-	-
[(BpinO) ₂ CH ₂]	0.43274	0.35975	-1012.30047	-	-
[(Bpin) ₂ O]	0.39589	0.32626	-897.78337	-	-
MeOBpin	0.24148	0.18899	-526.39206	-	-
7	0.98016	0.84125	-2951.28156	-	-
7-TS1	0.99648	0.85375	-3139.84632	6.9	19.7
7-IM1	1.00185	0.85912	-3139.92685	-40.3	-27.4
7-TS2	1.20707	1.04653	-3551.73028	-33.0	-4.3
7-IM2	1.20986	1.05440	-3551.75862	-49.1	-17.2
7-TS3	1.20580	1.04724	-3551.74026	-40.1	-10.2
7-IM3	1.20692	1.04613	-3551.75125	-46.3	-17.7
7-TS4	1.20494	1.03906	-3551.72161	-28.9	-3.6
7-IM4	1.21025	1.04762	-3551.78725	-66.8	-39.4
7-TS5	1.20796	1.04708	-3551.77841	-62.7	-34.2
7-IM5	1.17404	1.01412	-3437.26777	-	-
7-TS5'	1.41480	1.23420	-3963.60477	-67.9	-24.8
7-TS6	1.37760	1.20253	-3849.08099	-51.2	-20.6
7-TS7	1.01331	0.87260	-3065.78148	-46.4	-21.9
7-IM7	1.01963	0.87433	-3065.86336	-93.8	-72.2
7-TS8	1.22390	1.06437	-3477.69370	-104.0	-64.3

Table S11 Energies of the stationary points involved in the hydroboration of CO₂ with HBpin using AIH active species **8**.

Species	H_c	G_c	E_{sol} (in bromobenzene)	ΔH_{sol}^d	ΔG_{sol}
CO ₂	0.01547	-0.00879	-188.57502	-	-
HBpin	0.20389	0.16081	-411.81492	-	-
OHCOBpin	0.22306	0.17090	-600.42492	-	-
HCHO	0.03112	0.00566	-114.49104	-	-
[(BpinO) ₂ CH ₂]	0.43274	0.35975	-1012.30369	-	-
[(Bpin) ₂ O]	0.39589	0.32626	-897.78625	-	-
MeOBpin	0.24148	0.18899	-526.39206	-	-
8	0.67062	0.55877	-1853.65542	-	-
8-TS1	0.68561	0.56680	-2042.21357	11.0	21.9
8-IM1	0.69168	0.57369	-2042.28296	-28.7	-17.3
8-TS2	0.89652	0.75651	-2454.09910	-28.8	-4.2
8-IM2	0.89720	0.76426	-2454.15705	-64.7	-35.7
8-TS3	0.89514	0.76236	-2454.11906	-42.2	-13.1
8-IM3	0.89606	0.75789	-2454.12438	-44.9	-19.2
8-TS4	0.89415	0.75913	-2454.10010	-30.9	-3.2
8-IM4	0.89944	0.76537	-2454.17416	-74.1	-45.7
8-TS5	0.89663	0.76341	-2454.16158	-67.9	-39.1
8-IM5	0.86326	0.73600	-2339.64939	-	-
8-TS5'	1.10432	0.95162	-2865.97372	-63.8	-20.1
8-TS6	1.06869	0.91451	-2751.44896	-45.5	-18.7
8-TS7	0.70222	0.59139	-1968.16115	-51.2	-24.9
8-IM7	0.70970	0.59303	-1968.22913	-89.1	-66.6
8-TS8	0.91428	0.77601	-2380.04987	-92.4	-56.3

Table S12 Energies of the stationary points involved in the hydroboration of CO₂ with HBpin using AlH active species **9**.

Species	H_c	G_c	E_{sol} (in toluene)	ΔH_{sol}	ΔG_{sol}
CO ₂	0.01547	-0.00879	-188.57490	-	-
HBpin	0.20389	0.16081	-411.81365	-	-
9	0.40351	0.33719	-749.62484	-	-
9-TS1	0.41947	0.34719	-938.17537	15.6	27.1
9-IM1	0.42520	0.35403	-938.25620	-31.5	-19.3
9-TS2	0.63025	0.53739	-1350.06327	-26.7	-1.1
9-IM2	0.63119	0.53944	-1350.06620	-27.9	-1.6
9-TS3	0.62864	0.53737	-1350.04126	-13.9	12.7

Table S13 Energies of the stationary points involved in the hydroboration of CO₂ with HBpin using AlH active species **10**.

Species	H_c	G_c	E_{sol} (in THF)	ΔH_{sol}	ΔG_{sol}
CO ₂	0.01547	-0.00879	-188.57497	-	-
HBpin	0.20389	0.16081	-411.81383	-	-
10	0.36894	0.31236	-764.49094	-	-
10-TS1	0.38543	0.32354	-953.05199	10.2	22.0
10-IM1	0.39120	0.33092	-953.13173	-36.3	-23.4
10-TS2	0.59634	0.51092	-1364.94094	-31.8	-7.7
10-IM2	0.59768	0.51678	-1364.94688	-34.7	-7.7
10-TS3	0.59385	0.51064	-1364.92134	-21.1	4.5

Table S14 Energies of the stationary points involved in the hydroboration of CO₂ with HBpin using AlH active species **11**.

Species	H_c	G_c	E_{sol} (in THF)	ΔH_{sol}	ΔG_{sol}
CO ₂	0.01547	-0.00879	-188.57497	-	-
HBpin	0.20389	0.16081	-411.81383	-	-
11	0.51824	0.45526	-1015.16236	-	-
11-TS1	0.53847	0.47151	-1203.74205	0.8	13.5
11-IM1	0.54024	0.47239	-1203.80134	-35.3	-23.1
11-TS2	0.74466	0.65485	-1615.61759	-35.7	-10.3
11-IM2	0.74567	0.65506	-1615.61894	-35.9	-11.0
11-TS3	0.74212	0.65278	-1615.58207	-15.0	10.7

Table S15 Energies of the stationary points involved in the hydroboration of CO₂ with HBpin using AlH active species **12**.

Species	H_c	G_c	E_{sol} (in THF)	ΔH_{sol}	ΔG_{sol}
CO ₂	0.01547	-0.00879	-188.57497	-	-
HBpin	0.20389	0.16081	-411.81383	-	-
12	0.58735	0.50268	-1548.46655	-	-
12-TS1	0.60313	0.50901	-1737.04134	1.1	10.4
12-IM1	0.60863	0.51561	-1737.11605	-42.4	-32.4
12-TS2	0.81309	0.69860	-2148.91225	-30.2	-6.6
12-IM2	0.81450	0.69959	-2148.93374	-42.8	-19.5
12-TS3	0.81240	0.70064	-2148.88928	-16.2	9.1

Table S16 Energies of the stationary points (optimized in benzene solvent) involved in the hydroboration of CO₂ with HBpin using AlH active species **3**.

Species	H_c^a	G_c^b	E_{sol}^c (in benzene)	ΔH_{sol}^d	ΔG_{sol}^e
CO ₂	0.01540	-0.00889	-188.57499 7	-	-
HBpin	0.20343	0.16014	-411.81385	-	-
OHCOPin	0.22285	0.17173	-600.42256	-20.5	-10.2
3	0.81864	0.70874	-1640.00894	-	-
3-TS1	0.83637	0.72165	-1828.57497	5.2	17.4
3-IM1	0.84023	0.72397	-1828.65238	-41.0	-29.7
3-TS2	1.04506	0.90677	-2240.46262	-39.7	-15.1
3-IM2	1.04656	0.90860	-2240.46373	-39.5	-14.7
3-TS3	1.04272	0.90771	-2240.43439	-23.5	3.2

a: H_c is the enthalpy correction calculated at the M06-2X/6-31G* level in benzene solvent at 298 K;

b: G_c is the Gibbs free energy correction calculated at the M06-2X/6-31G* level in benzene solvent at 298 K;

c: E_{sol} is the electron energy in the solvent after PCM correction calculated at the M06-2X/(SMD, benzene)//6-311++G(d, p) level;

d: ΔH_{sol} is the relative enthalpy energy in the solvent at 298 K $H_{sol} = H_c + E_{sol} + RT\ln(24.5)/2625460$.

e: ΔG_{sol} is the relative Gibbs free energy in the solvent at 298 K. $G_{sol} = G_c + E_{sol} + RT\ln(24.5)/2625460$.

Table S17 Energies of the stationary points (optimized in benzene solvent) involved in the hydroboration of CO₂ with HBpin using AIH active species **6**.

Species	H_c	G_c	E_{sol} (in benzene)	ΔH_{sol}	ΔG_{sol}
CO ₂	0.01540	-0.00889	-188.57499 7	-	-
HBpin	0.20343	0.16014	-411.81385	-	-
OHCOBpin	0.22285	0.17173	-600.42256	-20.5	-10.2
6	0.94468	0.82086	-1964.89750	-	-
6-TS1	0.96094	0.82920	-2153.46169	5.4	15.7
6-IM1	0.96613	0.83156	-2153.54220	-41.8	-33.3
6-TS2	1.17068	1.02192	-2565.34634	-36.9	-10.2
6-IM2	1.17310	1.02852	-2565.39841	-68.1	-38.7
6-TS3	1.17013	1.02277	-2565.35978	-45.7	-18.1
6-IM3	1.17114	1.02226	-2565.37494	-54.6	-27.9

Table S18 Energies of the stationary points (optimized in THF solvent) involved in the hydroboration of CO₂ with HBpin using AIH active species **12**.

Species	H_c	G_c	E_{sol} (in THF)	ΔH_{sol}	ΔG_{sol}
CO ₂	0.01536	-0.00894		-	-
HBpin	0.20313	0.15985		-	-
OHCOBpin	0.22261	0.17171		-21.2	-10.7
12	0.58688	0.50105		-	-
12-TS1	0.60316	0.51028	-1737.04177	-0.0	10.7
12-IM1	0.60871	0.51453	-1737.11674	-43.7	-33.7
12-TS2	0.81374	0.70360	-2148.91445	-33.4	-6.3
12-IM2	0.81395	0.69967	-2148.93478	-46.1	-21.5
12-TS3	0.81291	0.70390	-2148.89059	-19.0	8.9

S7: Cartesian coordinates of the optimized structures

CO ₂ (in gas phase)				HBpin (in benzene solvent)			
6	0.000000000	0.000000000	0.000000000	1	-0.000008000	3.121189000	0.000031000
8	0.000000000	0.000000000	1.162730000	5	-0.000010000	1.932997000	0.000006000
8	0.000000000	0.000000000	-1.162730000	8	-1.063721000	1.186344000	0.419999000
CO ₂ (in benzene solvent)				8	1.063716000	1.186359000	-0.419976000
6	0.000000000	0.000000000	0.000000000	6	-0.779911000	-0.186922000	0.054753000
8	0.000000000	0.000000000	1.162475000	6	0.779913000	-0.186916000	-0.054756000
8	0.000000000	0.000000000	-1.162475000	6	1.469923000	-0.434603000	1.284131000
CO ₂ (in THF solvent)				6	1.346002000	-1.108777000	-1.121594000
6	0.000000000	0.000000000	0.000000000	6	-1.345991000	-1.108805000	1.121577000
8	0.000000000	0.000000000	1.162475000	6	-1.469925000	-0.434587000	-1.284137000
8	0.000000000	0.000000000	-1.162475000	1	-2.535737000	-0.212806000	-1.179892000
HBpin (in gas phase)				1	-1.062707000	0.216408000	-2.064508000
1	0.000007000	3.121341000	-0.000034000	1	-1.362744000	-1.475012000	-1.605398000
5	0.000009000	1.933909000	-0.000007000	1	-2.437846000	-1.039695000	1.125070000
8	-1.063184000	1.184376000	0.418976000	1	-0.985420000	-0.841748000	2.117179000
8	1.063188000	1.184362000	-0.419001000	1	-1.072736000	-2.149236000	0.915258000
6	-0.779689000	-0.185497000	0.054626000	1	1.062697000	0.216372000	2.064514000
6	0.779688000	-0.185502000	-0.054623000	1	2.535734000	-0.212812000	1.179895000
6	1.468907000	-0.435530000	1.285483000	1	1.362749000	-1.475036000	1.605371000
6	1.346362000	-1.108167000	-1.121728000	1	1.072749000	-2.149213000	-0.915297000
6	-1.346371000	-1.108137000	1.121748000	1	2.437856000	-1.039664000	-1.125080000
6	-1.468905000	-0.435550000	-1.285477000	1	0.985435000	-0.841701000	-2.117193000
1	-2.534086000	-0.214326000	-1.179544000	HBpin (in THF solvent)			
1	-1.059594000	0.216925000	-2.062915000	1	-0.000002000	3.122926000	0.000007000
1	-1.357067000	-1.475666000	-1.606014000	5	-0.000002000	1.933869000	0.000001000
1	-2.437274000	-1.034483000	1.126066000	8	1.064933000	1.189605000	-0.418739000
1	-0.982336000	-0.839327000	2.115059000	8	-1.064934000	1.189601000	0.418744000
1	-1.073219000	-2.148354000	0.913964000	6	0.779727000	-0.186724000	-0.055116000
1	1.059601000	0.216964000	2.062909000	6	-0.779726000	-0.186726000	0.055115000
1	2.534088000	-0.214313000	1.179543000	6	-1.470552000	-0.437980000	-1.282179000
1	1.357065000	-1.475638000	1.606042000	6	-1.342343000	-1.107861000	1.123850000
1	1.073199000	-2.148378000	-0.913926000	6	1.342346000	-1.107855000	-1.123854000
1	2.437266000	-1.034525000	-1.126048000	6	1.470552000	-0.437984000	1.282178000
1	0.982330000	-0.839370000	-2.1150440	1	2.537748000	-0.222926000	1.176012000
				1	1.066983000	0.213062000	2.064589000
				1	1.357370000	-1.478725000	1.599913000

1	2.434703000	-1.043923000	-1.126251000	8	-0.483844000	0.866387000	-0.040920000
1	0.980932000	-0.838627000	-2.118758000	6	1.264272000	-0.691001000	0.153283000
1	1.063292000	-2.146428000	-0.916717000	6	0.965879000	0.827422000	-0.086368000
1	-1.066985000	0.213070000	-2.064587000	6	1.514200000	1.760413000	0.978853000
1	-2.537748000	-0.222925000	-1.176011000	6	1.376930000	1.299127000	-1.478142000
1	-1.357369000	-1.478719000	-1.599919000	6	1.296316000	-1.060978000	1.633502000
1	-1.063287000	-2.146433000	0.916709000	6	2.497647000	-1.218264000	-0.557948000
1	-2.434701000	-1.043931000	1.126248000	1	2.622698000	-2.282235000	-0.336986000
1	-0.980929000	-0.838638000	2.118754000	1	2.417507000	-1.102148000	-1.640772000
OHCOPin (in gas phase)							
5	-0.897412000	-0.427223000	-0.317653000	1	1.293013000	-2.150478000	1.726427000
8	0.111322000	-1.343183000	-0.379551000	1	0.417525000	-0.670721000	2.157353000
8	-0.498579000	0.840051000	-0.017326000	1	2.194719000	-0.674182000	2.123458000
6	1.281950000	-0.679292000	0.150446000	1	1.099006000	1.533335000	1.962760000
6	0.946234000	0.830514000	-0.093240000	1	1.255284000	2.793705000	0.730414000
6	1.497948000	1.784414000	0.952773000	1	2.605768000	1.685492000	1.028801000
6	1.318818000	1.300098000	-1.497579000	1	2.464966000	1.361955000	-1.573260000
6	1.357651000	-1.034931000	1.633489000	1	0.956477000	2.293026000	-1.654516000
6	2.511111000	-1.186859000	-0.584447000	1	0.997668000	0.625209000	-2.253407000
1	2.662410000	-2.245240000	-0.355797000	8	-3.260257000	0.569796000	0.821107000
1	2.399931000	-1.083198000	-1.665331000	6	-3.275345000	-0.134449000	-0.146766000
1	3.401933000	-0.635621000	-0.265073000	8	-2.204346000	-0.742025000	-0.689060000
1	1.379809000	-2.123129000	1.733764000	1	-4.182421000	-0.401918000	-0.705820000
1	0.482225000	-0.657754000	2.171461000	HCHO (in gas phase)			
1	2.257986000	-0.621798000	2.097526000	6	-0.000006000	0.527264000	0.000000000
1	1.105047000	1.556082000	1.944999000	1	0.937713000	1.115042000	0.000000000
1	1.211544000	2.808701000	0.699805000	1	-0.937632000	1.115205000	0.000000000
1	2.591477000	1.729602000	0.981201000	8	-0.000006000	-0.674229000	0.000000000
1	2.403090000	1.383924000	-1.615835000	[(BpinO) ₂ CH ₂] (in gas phase)			
1	0.870876000	2.282006000	-1.670369000	1	-0.192758000	2.242320000	1.295205000
1	0.936942000	0.609720000	-2.256400000	5	1.926071000	1.286189000	0.003717000
8	-3.274754000	0.617317000	0.767411000	1	-0.134866000	3.780576000	0.362790000
6	-3.275873000	-0.155628000	-0.143685000	6	0.044225000	2.704655000	0.331352000
8	-2.196873000	-0.808334000	-0.622926000	8	1.402861000	2.539207000	0.027904000
1	-4.172182000	-0.463876000	-0.699089000	8	-0.750072000	2.153298000	-0.683413000
OHCOPin (in benzene solvent)							
5	-0.899335000	-0.390227000	-0.356623000	8	3.266461000	1.072455000	-0.186557000
8	0.088685000	-1.326932000	-0.409599000	8	1.205565000	0.124659000	0.204645000

6	3.435660000	-0.350402000	-0.323940000	[(Bpin) ₂ O] (in gas phase)			
6	2.191467000	-0.906617000	0.441923000	5	-1.221991000	-0.742291000	-0.182403000
6	3.394178000	-0.668865000	-1.817494000	8	-1.461712000	0.291589000	0.688917000
6	4.776595000	-0.748102000	0.271052000	8	-2.337617000	-1.154252000	-0.863717000
6	1.680315000	-2.239644000	-0.077187000	6	-2.784029000	0.776829000	0.383959000
6	2.408189000	-0.972028000	1.952600000	6	-3.458326000	-0.484053000	-0.253138000
1	2.419421000	-0.411163000	-2.243595000	6	-3.437501000	1.273405000	1.663178000
1	4.157477000	-0.072452000	-2.323732000	6	-2.617707000	1.923238000	-0.611961000
1	3.592876000	-1.727631000	-2.008996000	6	-4.495178000	-0.180551000	-1.322285000
1	4.880625000	-0.381744000	1.294138000	6	-4.033314000	-1.436039000	0.793905000
1	5.583529000	-0.318650000	-0.328898000	1	-3.417504000	0.508797000	2.442070000
1	4.890638000	-1.837515000	0.270217000	1	-2.899182000	2.151099000	2.031362000
1	3.086491000	-1.785656000	2.226281000	1	-4.477494000	1.561781000	1.476142000
1	2.822042000	-0.030978000	2.328679000	1	-1.950469000	2.671125000	-0.176023000
1	1.344468000	-2.162927000	-1.113450000	1	-3.576431000	2.396692000	-0.844005000
1	0.840496000	-2.582045000	0.535129000	1	-2.167294000	1.566996000	-1.543792000
1	2.471254000	-2.995350000	-0.018112000	1	-5.316497000	0.410995000	-0.903640000
1	1.442425000	-1.140550000	2.436923000	1	-4.908246000	-1.116888000	-1.707400000
5	-1.592061000	1.124201000	-0.399410000	1	-4.055107000	0.367303000	-2.157642000
8	-2.331282000	0.507294000	-1.376815000	1	-4.289587000	-2.380485000	0.306952000
8	-1.830657000	0.634750000	0.864528000	1	-4.934418000	-1.024718000	1.258592000
6	-2.894090000	-0.668592000	-0.764569000	1	-3.298098000	-1.643116000	1.577856000
6	-2.950006000	-0.264859000	0.747244000	5	1.209134000	-0.749835000	-0.189865000
6	-4.206210000	0.530067000	1.097617000	8	-0.008553000	-1.338535000	-0.343962000
6	-4.243664000	-0.962344000	-1.397792000	8	2.350311000	-1.480249000	0.018061000
6	-1.911768000	-1.808046000	-1.023919000	8	1.429618000	0.604092000	-0.265075000
1	-1.766763000	-1.908630000	-2.103038000	6	3.385961000	-0.531521000	0.340582000
1	-0.944829000	-1.575295000	-0.567984000	6	2.858992000	0.779181000	-0.333914000
1	-2.276131000	-2.760652000	-0.627157000	6	3.437536000	-0.427991000	1.863980000
1	-4.901546000	-0.092351000	-1.353103000	6	4.710886000	-1.040466000	-0.202960000
1	-4.731164000	-1.802551000	-0.891525000	6	3.235319000	2.063629000	0.386449000
1	-4.102769000	-1.230060000	-2.448530000	6	3.227913000	0.868721000	-1.813658000
1	-5.096764000	-0.105582000	1.097092000	1	2.492535000	-0.043254000	2.260418000
1	-4.359401000	1.347766000	0.386358000	1	3.602070000	-1.426101000	2.278196000
1	-4.084433000	0.960241000	2.095296000	1	4.248829000	0.227319000	2.194741000
6	-2.755663000	-1.414979000	1.722259000	1	4.641023000	-1.270627000	-1.267711000
1	-2.819170000	-1.040889000	2.747967000	1	4.995877000	-1.954180000	0.325787000
1	-3.532854000	-2.174429000	1.584770000	1	5.499652000	-0.295662000	-0.051687000
1	-1.776718000	-1.880521000	1.588529000	1	4.294791000	1.069183000	-1.950166000

1	2.976870000	-0.060297000	-2.335265000	14	-1.572031000	-1.351628000	0.961577000
1	2.834771000	2.080487000	1.401684000	14	-3.080288000	0.775666000	-0.668173000
1	2.826492000	2.920389000	-0.156340000	14	2.046310000	1.547884000	0.737481000
1	4.324165000	2.173737000	0.431931000	14	2.635023000	-1.040024000	-0.817141000
1	2.657849000	1.682610000	-2.269351000	6	-2.695621000	2.271937000	-1.752742000
				1	-3.623856000	2.831557000	-1.917466000
				1	-1.986865000	2.961909000	-1.278004000
				1	-2.293071000	1.998471000	-2.731409000
				6	-4.176888000	-0.380813000	-1.672629000
				1	-4.428700000	-1.295980000	-1.126632000
				1	-5.116035000	0.108625000	-1.953886000
				1	-3.663237000	-0.676396000	-2.594304000
				6	-4.028515000	1.439552000	0.822320000
				1	-4.678422000	2.262291000	0.503413000
				1	-4.660204000	0.687285000	1.301198000
				1	-3.339721000	1.835414000	1.577301000
				6	-1.157909000	-2.943675000	0.038030000
				1	-0.178418000	-2.891013000	-0.451906000
				1	-1.137074000	-3.807550000	0.712059000
				1	-1.905084000	-3.138840000	-0.739731000
				6	-3.230335000	-1.613521000	1.818980000
				1	-3.448332000	-0.814162000	2.533469000
				1	-4.078613000	-1.699633000	1.133051000
				1	-3.169869000	-2.551458000	2.383687000
				6	-0.300848000	-1.091637000	2.323037000
				1	-0.524551000	-0.192407000	2.908399000
				1	-0.301931000	-1.946271000	3.009763000
				1	0.705040000	-0.987229000	1.907813000
				6	0.485832000	2.503020000	1.212964000
				1	0.018144000	2.983106000	0.340899000
				1	-0.268709000	1.865231000	1.684411000
				1	0.736718000	3.309578000	1.910966000
				6	3.176204000	2.765812000	-0.152611000
				1	3.330255000	3.663910000	0.456693000
				1	4.159829000	2.338514000	-0.369583000
				1	2.731738000	3.077787000	-1.104390000
				6	2.934706000	0.945173000	2.283797000
				1	3.243511000	1.799525000	2.896738000
				1	2.300790000	0.299219000	2.898775000
				1	3.841142000	0.384147000	2.028116000
MeOBpin (in gas phase)							
5	-1.171771000	-0.412281000	-0.121886000				
8	-0.710401000	0.807738000	0.326505000				
8	-0.167825000	-1.278521000	-0.480567000				
6	0.701461000	0.835446000	0.034639000				
6	1.059161000	-0.688034000	-0.013296000				
6	2.179507000	-1.048457000	-0.975496000				
6	1.339734000	-1.267932000	1.372269000				
6	0.865235000	1.519263000	-1.321559000				
6	1.416508000	1.625770000	1.118283000				
1	1.106767000	2.673608000	1.072704000				
1	1.178148000	1.242115000	2.112083000				
1	2.501225000	1.582314000	0.972699000				
1	0.402147000	2.508524000	-1.275609000				
1	0.369859000	0.943353000	-2.109657000				
1	1.920036000	1.638491000	-1.586412000				
1	1.921761000	-0.781198000	-2.002019000				
1	2.359381000	-2.126385000	-0.938713000				
1	3.106464000	-0.535659000	-0.696804000				
1	2.298030000	-0.918986000	1.768608000				
1	1.367175000	-2.358015000	1.296844000				
1	0.548565000	-0.993467000	2.077289000				
8	-2.481401000	-0.738743000	-0.204511000				
6	-3.437316000	0.249862000	0.137265000				
1	-3.375899000	1.107298000	-0.540282000				
1	-4.425045000	-0.205985000	0.053370000				
1	-3.288480000	0.606099000	1.161283000				
I (in gas phase)							
7	-1.589779000	-0.022233000	-0.188212000				
13	-0.071938000	0.385015000	-1.083093000				
1	-0.165457000	0.876938000	-2.577072000				
7	1.559697000	0.234200000	-0.307336000				

6	4.368222000	-0.403488000	-1.187476000	1	4.365571000	-0.867535000	1.666020000
1	4.859040000	-0.004310000	-0.292658000	1	3.576667000	-0.941803000	3.243379000
1	4.995268000	-1.217849000	-1.567756000	6	0.586123000	-0.021573000	2.733917000
1	4.347633000	0.389199000	-1.942466000	1	0.255940000	-1.066380000	2.717700000
6	2.784629000	-2.385383000	0.493898000	1	0.830176000	0.233156000	3.771482000
1	3.479511000	-3.167939000	0.168140000	1	-0.269955000	0.597556000	2.439700000
1	3.163869000	-1.974408000	1.436428000	6	-0.049829000	-2.823339000	0.047160000
1	1.821298000	-2.859903000	0.708679000	1	0.447017000	-2.735401000	-0.925850000
6	1.936701000	-1.791973000	-2.403751000	1	0.636854000	-2.432980000	0.802412000
1	0.900621000	-2.144111000	-2.308040000	1	-0.202885000	-3.892474000	0.237872000
1	1.964067000	-1.067909000	-3.225443000	6	-2.689648000	-2.855065000	-1.341710000
1	2.532177000	-2.660875000	-2.705507000	1	-2.542436000	-3.938439000	-1.261823000
				1	-3.765264000	-2.665153000	-1.323547000
				1	-2.309712000	-2.540675000	-2.320459000
1-TSI (in gas phase)							
7	1.626554000	-0.007010000	-0.036067000	6	-2.564960000	-2.334453000	1.694994000
13	-0.020741000	0.558532000	-0.520566000	1	-2.604402000	-3.413970000	1.879716000
1	0.032197000	1.635763000	-1.767549000	1	-2.000765000	-1.873232000	2.512954000
7	-1.609437000	-0.255841000	-0.246003000	1	-3.590680000	-1.954695000	1.746392000
14	2.101110000	0.214446000	1.632838000	6	-4.620976000	-0.186195000	-0.575002000
14	2.725827000	-0.533297000	-1.289421000	1	-4.815538000	-1.083208000	0.019581000
14	-1.737308000	-1.986425000	0.036146000	1	-5.472737000	0.489779000	-0.434798000
14	-3.052778000	0.737540000	-0.084285000	1	-4.597755000	-0.476167000	-1.630537000
6	1.763528000	-0.624194000	-2.914839000	6	-3.238277000	1.336812000	1.691681000
1	2.374394000	-1.117074000	-3.679415000	1	-4.157346000	1.920396000	1.817916000
1	0.837273000	-1.209062000	-2.826656000	1	-3.271459000	0.497986000	2.395001000
1	1.496443000	0.366973000	-3.294472000	1	-2.395101000	1.976508000	1.975574000
6	4.142177000	0.692323000	-1.492882000	6	-2.995654000	2.257164000	-1.212843000
1	4.756117000	0.741389000	-0.585732000	1	-2.538619000	3.134580000	-0.743254000
1	4.801040000	0.407134000	-2.320558000	1	-2.480890000	2.063866000	-2.159660000
1	3.761948000	1.700250000	-1.692856000	1	-4.025540000	2.543236000	-1.455247000
6	3.481032000	-2.234534000	-0.982554000	6	-0.016639000	3.023985000	-0.570669000
1	3.917067000	-2.605227000	-1.917815000	8	0.115822000	3.966732000	-1.228524000
1	4.281651000	-2.206160000	-0.238163000	8	-0.177079000	2.358383000	0.428971000
1	2.737444000	-2.964162000	-0.648094000				
6	2.811015000	1.935419000	1.932722000	1-IMI (in gas phase)			
1	2.050440000	2.712526000	1.807060000	7	-1.636732000	-0.041530000	0.009876000
1	3.207405000	2.020930000	2.950887000	13	0.020917000	-0.627542000	-0.381539000
1	3.629114000	2.149995000	1.236481000	1	-0.111225000	-3.830390000	-1.370995000
6	3.404869000	-1.035721000	2.164940000	7	1.609248000	0.194629000	-0.185792000
1	3.093708000	-2.065583000	1.961243000	14	-2.219910000	-0.444128000	1.606844000

14	-2.617869000	0.618322000	-1.274387000	1	4.803610000	1.019445000	0.182533000
14	1.743236000	1.896527000	0.238488000	1	5.480215000	-0.514213000	-0.367875000
14	3.056922000	-0.807926000	-0.094989000	1	4.624106000	0.528625000	-1.510090000
6	-1.502411000	0.872451000	-2.779821000	6	3.204080000	-1.572126000	1.619127000
1	-2.017997000	1.480430000	-3.531475000	1	4.119341000	-2.167359000	1.713790000
1	-0.569810000	1.398606000	-2.533596000	1	3.216479000	-0.804864000	2.400347000
1	-1.235198000	-0.078675000	-3.251107000	1	2.352246000	-2.234209000	1.811891000
6	-3.998094000	-0.576807000	-1.740970000	6	3.036975000	-2.212327000	-1.362461000
1	-4.696708000	-0.718202000	-0.907806000	1	2.521795000	-3.103999000	-0.991889000
1	-4.575771000	-0.208551000	-2.596084000	1	2.585715000	-1.913933000	-2.313640000
1	-3.588453000	-1.558208000	-2.004262000	1	4.072601000	-2.507921000	-1.565121000
6	-3.421347000	2.269655000	-0.843074000	6	-0.028613000	-2.787616000	-1.051339000
1	-3.795427000	2.739365000	-1.760462000	8	0.147457000	-2.488998000	0.167282000
1	-4.273567000	2.148154000	-0.168092000	8	-0.111199000	-1.841172000	-1.887065000
1	-2.718625000	2.964124000	-0.373258000				
6	-2.980455000	-2.166711000	1.658069000		1-TS2 (in gas phase)		
1	-2.231401000	-2.925285000	1.408175000	7	0.205254000	1.594250000	0.148411000
1	-3.374649000	-2.397436000	2.654199000	13	0.829599000	-0.015385000	0.637398000
1	-3.804541000	-2.257001000	0.941986000	1	-0.740351000	-0.994088000	3.856521000
6	-3.508591000	0.787094000	2.212910000	7	2.287641000	-0.862607000	0.015553000
1	-3.157982000	1.820817000	2.126422000	14	-0.336101000	2.765172000	1.339239000
1	-4.448101000	0.701410000	1.655924000	14	0.003431000	1.943541000	-1.564323000
1	-3.735515000	0.593015000	3.267371000	14	3.702849000	0.070173000	-0.448354000
6	-0.743379000	-0.402883000	2.783859000	14	2.389581000	-2.616306000	0.107271000
1	-0.315952000	0.604657000	2.844977000	6	0.050166000	0.341794000	-2.566404000
1	-1.050232000	-0.694807000	3.794503000	1	0.197039000	0.584520000	-3.625554000
1	0.059157000	-1.089196000	2.484298000	1	0.856345000	-0.341129000	-2.274027000
6	0.063370000	2.738570000	0.362013000	1	-0.901598000	-0.191244000	-2.478665000
1	-0.446482000	2.768700000	-0.606807000	6	-1.644521000	2.782234000	-1.927471000
1	-0.616803000	2.269899000	1.078119000	1	-1.714300000	3.796379000	-1.520973000
1	0.231301000	3.776712000	0.673839000	1	-1.782671000	2.853320000	-3.013211000
6	2.678633000	2.873529000	-1.075488000	1	-2.459419000	2.184423000	-1.510402000
1	2.549638000	3.947086000	-0.895130000	6	1.360240000	3.080521000	-2.222418000
1	3.751159000	2.667865000	-1.100325000	1	2.358905000	2.640607000	-2.143500000
1	2.271266000	2.653294000	-2.068788000	1	1.173866000	3.291410000	-3.282525000
6	2.580652000	2.099265000	1.917193000	1	1.378723000	4.038865000	-1.693606000
1	2.647620000	3.160861000	2.181002000	6	-2.199497000	2.710208000	1.589052000
1	1.995366000	1.597302000	2.696029000	1	-2.496725000	3.363654000	2.417628000
1	3.593767000	1.686488000	1.949832000	1	-2.740192000	3.029165000	0.692661000
6	4.626873000	0.165567000	-0.477038000	1	-2.516104000	1.687067000	1.817714000

1	-0.737226000	1.941982000	3.532976000	8	-2.783875000	0.201298000	0.011352000
1	-1.323593000	3.520306000	3.015468000	8	-2.565339000	-2.103654000	-0.018272000
1	-1.759760000	2.081019000	2.082928000	6	-3.881577000	-0.324047000	-0.756668000
6	0.745810000	4.599650000	1.115706000	6	-3.948993000	-1.806632000	-0.266400000
1	1.631244000	4.787232000	0.500082000	6	-4.717118000	-1.949858000	1.049454000
1	-0.125524000	4.998316000	0.586773000	6	-4.482487000	-2.795559000	-1.291353000
1	0.856132000	5.173341000	2.043545000	6	-5.121879000	0.505228000	-0.458337000
6	2.131966000	2.320378000	2.532686000	6	-3.526848000	-0.225247000	-2.239484000
1	3.034249000	2.579592000	1.967846000	1	-3.246162000	0.806592000	-2.472417000
1	2.163283000	2.879276000	3.475385000	1	-2.681595000	-0.876302000	-2.481751000
1	2.183825000	1.254987000	2.782282000	1	-4.374854000	-0.507749000	-2.871580000
6	3.458107000	1.336310000	-1.292532000	1	-4.988940000	1.518207000	-0.850697000
1	2.714366000	1.668293000	-2.022123000	1	-5.299920000	0.575792000	0.616476000
1	3.273183000	1.878995000	-0.360661000	1	-6.004444000	0.066701000	-0.937037000
1	4.443215000	1.632326000	-1.672968000	1	-4.381189000	-1.213698000	1.785114000
6	3.528951000	-1.256699000	-2.822123000	1	-4.531072000	-2.948457000	1.454372000
1	4.286180000	-0.725015000	-3.410057000	1	-5.794456000	-1.828807000	0.898419000
1	3.783876000	-2.319541000	-2.835105000	1	-5.503890000	-2.532357000	-1.587513000
1	2.566805000	-1.138726000	-3.332923000	1	-4.500221000	-3.798541000	-0.855508000
6	5.028602000	-0.966958000	-0.145870000	1	-3.851295000	-2.822522000	-2.181551000
1	5.898877000	-0.592483000	-0.697046000				
1	5.027817000	-0.489362000	0.840613000		1-TS3 (in gas phase)		
1	5.172166000	-2.041373000	0.003630000	7	0.713442000	1.683184000	0.083218000
6	2.901903000	-3.936038000	-0.761624000	13	0.535049000	-0.140556000	-0.010721000
1	3.955527000	-3.703293000	-0.940129000	1	-0.710609000	-0.901098000	3.623793000
1	2.857583000	-4.943042000	-0.330558000	7	1.959963000	-1.234840000	-0.358371000
1	2.392478000	-3.967521000	-1.730468000	14	1.221985000	2.370482000	1.600880000
6	2.886438000	-2.813694000	2.098253000	14	0.054211000	2.639465000	-1.214381000
1	2.830111000	-3.822060000	2.523953000	14	3.451693000	-0.718258000	-1.109464000
1	3.942286000	-2.532918000	2.036907000	14	1.826666000	-2.876703000	0.228938000
1	2.399833000	-2.123585000	2.796223000	6	-0.144440000	1.546210000	-2.748317000
6	0.293016000	-3.424118000	0.620640000	1	-0.783063000	2.047675000	-3.485704000
1	-0.279092000	-2.985648000	1.444059000	1	0.828326000	1.381608000	-3.226549000
1	-0.315407000	-3.317384000	-0.282861000	1	-0.586015000	0.566098000	-2.547167000
1	0.374283000	-4.496306000	0.837255000	6	-1.602174000	3.382866000	-0.691730000
6	-0.764921000	-0.665708000	2.605093000	1	-1.438590000	4.148285000	0.077665000
8	0.364583000	-0.370091000	2.131275000	1	-2.128200000	3.863524000	-1.525279000
8	-1.818695000	-0.876186000	1.954700000	1	-2.252600000	2.617687000	-0.254232000
1	-0.778414000	-0.840519000	-0.081729000	6	1.153067000	4.065577000	-1.789274000
5	-1.981765000	-0.892634000	0.388841000	1	0.834870000	4.368094000	-2.794504000

1	1.088979000	4.947083000	-1.146035000	8	-1.997003000	-0.885626000	2.113785000
1	2.204575000	3.766306000	-1.850983000	1	-0.888763000	-0.678014000	-0.508686000
6	-0.194704000	2.349873000	2.877661000	5	-2.709047000	-0.781165000	0.886730000
1	-0.349040000	3.344161000	3.310692000	8	-3.221483000	0.402619000	0.472396000
1	-1.139758000	2.052740000	2.405680000	8	-3.258122000	-1.893915000	0.342101000
1	0.011198000	1.666594000	3.709904000	6	-4.106083000	0.078123000	-0.639244000
6	1.762347000	4.170132000	1.445652000	6	-4.440356000	-1.431243000	-0.364321000
1	2.564679000	4.298190000	0.712222000	6	-5.614592000	-1.614015000	0.594073000
1	0.937770000	4.835746000	1.168353000	6	-4.629566000	-2.281427000	-1.608395000
1	2.139820000	4.505172000	2.419298000	6	-5.296507000	1.020292000	-0.579166000
6	2.700624000	1.418442000	2.294594000	6	-3.333021000	0.278332000	-1.936438000
1	3.623400000	1.720808000	1.786974000	1	-2.944100000	1.299429000	-1.971633000
1	2.829127000	1.631958000	3.362316000	1	-2.488044000	-0.410508000	-2.000101000
1	2.602127000	0.333403000	2.177263000	1	-3.986190000	0.123548000	-2.800657000
6	3.548293000	1.141150000	-1.398712000	1	-4.956975000	2.041326000	-0.775238000
1	2.791795000	1.479554000	-2.113470000	1	-5.777105000	1.000247000	0.400716000
1	3.426065000	1.732631000	-0.488533000	1	-6.033896000	0.750709000	-1.342569000
1	4.532371000	1.363816000	-1.829523000	1	-5.486493000	-1.005270000	1.494830000
6	3.669980000	-1.474946000	-2.826773000	1	-5.665376000	-2.663691000	0.894164000
1	4.535107000	-1.024497000	-3.327449000	1	-6.560888000	-1.339006000	0.119394000
1	3.819662000	-2.557471000	-2.813300000	1	-5.466321000	-1.903135000	-2.204967000
1	2.785603000	-1.267491000	-3.440426000	1	-4.854828000	-3.310044000	-1.314555000
6	4.939047000	-1.176956000	-0.037860000	1	-3.729459000	-2.290175000	-2.225035000
1	5.866084000	-0.825457000	-0.505158000				
1	4.858462000	-0.702015000	0.946778000		1-IM3 (in gas phase)		
1	5.039042000	-2.256096000	0.119707000	7	0.547004000	1.349199000	-0.065684000
6	2.734438000	-4.131029000	-0.850515000	13	1.322354000	-0.140483000	-0.839029000
1	3.811161000	-3.948447000	-0.919674000	1	-1.492903000	-2.438406000	0.665231000
1	2.598088000	-5.130296000	-0.420403000	7	2.989986000	-0.730539000	-0.325872000
1	2.328306000	-4.146908000	-1.867228000	14	0.185540000	1.363145000	1.633138000
6	2.510648000	-3.030551000	1.983144000	14	0.003053000	2.681950000	-1.060255000
1	2.381822000	-4.047659000	2.371164000	14	4.310656000	0.334731000	0.069988000
1	3.578752000	-2.791620000	2.015161000	14	3.265859000	-2.455361000	-0.350804000
1	2.001096000	-2.339033000	2.662695000	6	0.305495000	2.340897000	-2.888276000
6	0.028527000	-3.463802000	0.256794000	1	0.016594000	3.228585000	-3.463391000
1	-0.609306000	-2.966719000	0.994386000	1	1.359061000	2.133363000	-3.108289000
1	-0.452262000	-3.331519000	-0.717879000	1	-0.275612000	1.489662000	-3.252489000
1	0.015716000	-4.534214000	0.494942000	6	-1.848128000	2.998799000	-0.838947000
6	-0.788118000	-0.759371000	2.543084000	1	-2.095416000	3.297026000	0.187046000
8	0.224283000	-0.530217000	1.890651000	1	-2.167406000	3.814234000	-1.498789000

1	-2.443395000	2.113094000	-1.086802000	1	2.487973000	-4.377269000	-1.701106000
6	0.866625000	4.322836000	-0.684312000	6	-0.987465000	-1.663144000	0.079423000
1	0.643374000	5.030589000	-1.491964000	8	0.227268000	-1.564139000	0.088794000
1	0.527020000	4.777369000	0.250438000	8	-1.752050000	-0.861925000	-0.623957000
1	1.953921000	4.216183000	-0.626776000	1	0.905646000	-0.451390000	-2.335734000
6	-1.596375000	0.779965000	2.004508000	5	-3.134580000	-0.862234000	-0.393308000
1	-1.929358000	1.196902000	2.962537000	8	-3.937948000	0.071576000	-0.942032000
1	-2.285422000	1.135902000	1.228480000	8	-3.742054000	-1.792675000	0.389593000
1	-1.700660000	-0.309455000	2.091349000	6	-5.296404000	-0.368941000	-0.666229000
6	0.291785000	3.082347000	2.406501000	6	-5.104279000	-1.306944000	0.578372000
1	1.257454000	3.558264000	2.206691000	6	-5.118779000	-0.554815000	1.904963000
1	-0.494577000	3.757366000	2.052157000	6	-6.042610000	-2.499705000	0.625139000
1	0.180954000	2.990158000	3.493549000	6	-6.156642000	0.855679000	-0.409854000
6	1.363505000	0.265362000	2.610814000	6	-5.770409000	-1.115325000	-1.909356000
1	2.354621000	0.729500000	2.650286000	1	-5.687582000	-0.450032000	-2.772148000
1	1.003843000	0.160761000	3.641360000	1	-5.154421000	-2.000007000	-2.099130000
1	1.492850000	-0.735736000	2.187846000	1	-6.812671000	-1.430704000	-1.808636000
6	3.746817000	2.130829000	0.174109000	1	-6.229701000	1.447141000	-1.326023000
1	3.340881000	2.461804000	-0.789355000	1	-5.727966000	1.486504000	0.370895000
1	2.979160000	2.316821000	0.929549000	1	-7.166642000	0.555712000	-0.111835000
1	4.615065000	2.761870000	0.398627000	1	-4.443591000	0.305866000	1.882955000
6	5.661367000	0.354381000	-1.254591000	1	-4.782968000	-1.229379000	2.697068000
1	6.321360000	1.215712000	-1.096857000	1	-6.126562000	-0.206368000	2.147869000
1	6.284894000	-0.543223000	-1.255055000	1	-7.082039000	-2.159932000	0.678404000
1	5.216819000	0.454250000	-2.251258000	1	-5.832333000	-3.096071000	1.516804000
6	5.123778000	-0.133701000	1.711479000	1	-5.925031000	-3.138171000	-0.252117000
1	5.924984000	0.573929000	1.954379000				
1	4.403840000	-0.125073000	2.536093000		1-TS4 (in gas phase)		
1	5.570081000	-1.133616000	1.677821000	7	-0.504295000	1.535046000	-0.060354000
6	5.041905000	-2.931773000	-0.787776000	13	-0.956773000	-0.228149000	0.018112000
1	5.793000000	-2.541074000	-0.094852000	1	0.958496000	-2.334231000	-1.001256000
1	5.118347000	-4.025628000	-0.770361000	7	-2.601205000	-0.944476000	0.314733000
1	5.305105000	-2.596809000	-1.796360000	14	-0.980152000	2.380833000	-1.517535000
6	2.881924000	-3.224568000	1.331101000	14	0.620304000	2.248781000	1.061687000
1	3.125610000	-4.293141000	1.346541000	14	-3.813182000	-0.119752000	1.269232000
1	3.461685000	-2.734368000	2.121493000	14	-2.982561000	-2.465516000	-0.466293000
1	1.821509000	-3.115197000	1.581195000	6	1.186236000	0.984474000	2.349245000
6	2.218176000	-3.314873000	-1.668568000	1	1.823813000	1.488177000	3.086593000
1	1.140717000	-3.252932000	-1.495254000	1	0.341723000	0.544900000	2.894619000
1	2.418313000	-2.886806000	-2.656376000	1	1.750122000	0.151763000	1.915216000

6	2.159474000	2.895281000	0.175331000	6	-1.469860000	-3.605642000	-0.547670000
1	1.913092000	3.711472000	-0.513591000	1	-0.932608000	-3.488049000	-1.494007000
1	2.882839000	3.287747000	0.900636000	1	-0.776055000	-3.423260000	0.281631000
1	2.655437000	2.111348000	-0.409072000	1	-1.790047000	-4.651255000	-0.482005000
6	-0.105110000	3.694354000	2.034966000	6	0.745676000	-1.294739000	-1.266829000
1	0.605989000	4.009644000	2.808015000	8	-0.369220000	-0.928508000	-1.711193000
1	-0.310155000	4.562677000	1.402416000	8	1.791297000	-0.498390000	-1.417209000
1	-1.039833000	3.416855000	2.532228000	1	0.315078000	-1.082239000	0.623294000
6	0.283606000	2.195210000	-2.902511000	5	2.978349000	-0.741846000	-0.728418000
1	-0.002830000	2.799943000	-3.770866000	8	4.106137000	-0.046543000	-1.007646000
1	1.282481000	2.510889000	-2.584260000	8	3.083071000	-1.673891000	0.255113000
1	0.352227000	1.150506000	-3.219736000	6	5.039485000	-0.370695000	0.057613000
6	-1.236042000	4.224242000	-1.202268000	6	4.500025000	-1.753044000	0.572252000
1	-1.952672000	4.396638000	-0.391901000	6	5.054046000	-2.939725000	-0.210250000
1	-0.306379000	4.744125000	-0.946752000	6	4.645937000	-1.974858000	2.067461000
1	-1.634445000	4.694743000	-2.108682000	6	6.442219000	-0.415680000	-0.523990000
6	-2.629766000	1.691176000	-2.116858000	6	4.925835000	0.741779000	1.095428000
1	-3.422629000	1.904698000	-1.391365000	1	5.135145000	1.698258000	0.609201000
1	-2.910038000	2.161766000	-3.066259000	1	3.916772000	0.792796000	1.517158000
1	-2.611906000	0.607598000	-2.278772000	1	5.641348000	0.596422000	1.909971000
6	-3.184209000	1.557310000	1.855543000	1	6.727051000	0.583894000	-0.862082000
1	-2.296585000	1.442915000	2.490316000	1	6.502164000	-1.095391000	-1.375808000
1	-2.914224000	2.237379000	1.043149000	1	7.159286000	-0.737774000	0.238316000
1	-3.962177000	2.032673000	2.464796000	1	4.950093000	-2.784273000	-1.288849000
6	-4.244246000	-1.055102000	2.853332000	1	4.493274000	-3.836886000	0.064236000
1	-4.786750000	-0.390508000	3.536020000	1	6.110761000	-3.106061000	0.016800000
1	-4.869268000	-1.935358000	2.683467000	1	5.702399000	-1.950748000	2.354410000
1	-3.332354000	-1.383761000	3.364304000	1	4.239869000	-2.954359000	2.333188000
6	-5.399254000	0.145621000	0.280802000	1	4.106102000	-1.214506000	2.635408000
1	-6.137610000	0.690034000	0.880586000				
1	-5.206677000	0.726234000	-0.627164000				
1	-5.858662000	-0.800124000	-0.026260000				
6	-4.299869000	-3.444184000	0.467092000				
1	-5.252112000	-2.917164000	0.577904000				
1	-4.499798000	-4.366898000	-0.090657000				
1	-3.951581000	-3.728520000	1.465473000				
6	-3.594507000	-2.179722000	-2.224135000				
1	-3.906559000	-3.118163000	-2.696753000				
1	-4.447530000	-1.492219000	-2.238977000				
1	-2.799316000	-1.741695000	-2.837400000				
					1-IM4 (in gas phase)		
				7	2.268531000	-0.801958000	0.001531000
				13	0.827507000	0.138692000	-0.580105000
				1	0.183482000	-1.958914000	-2.696610000
				7	0.120055000	1.643244000	0.140945000
				14	3.703499000	-0.344492000	-0.891904000
				14	2.221365000	-2.230949000	0.993655000
				14	0.417118000	2.131751000	1.797939000
				14	-0.759513000	2.751186000	-0.902596000
				6	0.457018000	-2.557819000	1.587382000

1	0.476851000	-3.241627000	2.443611000	1	-0.106418000	4.667412000	-2.368554000
1	-0.079819000	-1.655265000	1.902760000	1	1.052052000	4.472513000	-1.039497000
1	-0.139893000	-3.032546000	0.801058000	1	1.101409000	3.373656000	-2.424088000
6	2.775247000	-3.747685000	0.013040000	6	-1.748203000	1.889868000	-2.263344000
1	3.837961000	-3.692463000	-0.250317000	1	-1.095622000	1.578845000	-3.083313000
1	2.630290000	-4.663756000	0.597262000	1	-2.310038000	1.011449000	-1.923892000
1	2.206596000	-3.844599000	-0.918805000	1	-2.481799000	2.601221000	-2.661521000
6	3.339821000	-2.155242000	2.513904000	6	-0.236376000	-0.985503000	-2.417476000
1	3.150895000	-3.036882000	3.138499000	8	0.669456000	0.023212000	-2.378629000
1	4.399790000	-2.169694000	2.243889000	8	-0.630954000	-1.130497000	-0.974267000
1	3.163396000	-1.266706000	3.126064000	1	-1.149196000	-0.761522000	-2.981071000
6	3.897600000	-1.331921000	-2.483538000	5	-1.943635000	-1.202540000	-0.549172000
1	2.999516000	-1.201927000	-3.097036000	8	-2.977605000	-1.483363000	-1.392465000
1	4.759478000	-0.982792000	-3.063723000	8	-2.291985000	-1.009676000	0.751763000
1	4.031561000	-2.401484000	-2.292941000	6	-4.123874000	-1.727966000	-0.534558000
6	5.268720000	-0.538421000	0.138921000	6	-3.740610000	-0.944217000	0.768400000
1	5.174713000	-0.048472000	1.113768000	6	-4.121973000	0.531774000	0.708150000
1	5.516464000	-1.591367000	0.312279000	6	-4.237776000	-1.571457000	2.059686000
1	6.116342000	-0.086318000	-0.388525000	6	-5.372898000	-1.225127000	-1.236574000
6	3.510953000	1.473099000	-1.373675000	6	-4.192309000	-3.237050000	-0.318101000
1	3.298337000	2.113175000	-0.508766000	1	-4.257129000	-3.731368000	-1.290745000
1	4.431951000	1.839929000	-1.840913000	1	-3.295672000	-3.600876000	0.194328000
1	2.706770000	1.612008000	-2.107348000	1	-5.068967000	-3.514071000	0.274264000
6	1.687686000	1.036316000	2.647301000	1	-5.560135000	-1.829146000	-2.128367000
1	1.313384000	0.017670000	2.791085000	1	-5.262817000	-0.183503000	-1.544345000
1	2.630394000	0.966729000	2.096676000	1	-6.241743000	-1.310056000	-0.575555000
1	1.894273000	1.452705000	3.640934000	1	-3.771474000	0.994297000	-0.220198000
6	-1.147457000	1.975267000	2.842076000	1	-3.648783000	1.052108000	1.545359000
1	-0.920210000	2.129013000	3.903237000	1	-5.205679000	0.664910000	0.778177000
1	-1.934603000	2.680377000	2.560969000	1	-5.331754000	-1.620716000	2.064504000
1	-1.541673000	0.958150000	2.723467000	1	-3.918515000	-0.957803000	2.906575000
6	1.111899000	3.886145000	1.883402000	1	-3.836170000	-2.577280000	2.195368000
1	1.266325000	4.176876000	2.928902000				
1	2.086837000	3.921093000	1.383050000				
1	0.476092000	4.645234000	1.418847000	1-TS5 (in gas phase)			
6	-2.034892000	3.775972000	0.047667000	7	-0.664850000	1.792916000	0.114448000
1	-1.624605000	4.363264000	0.873650000	13	-0.775624000	0.087939000	-0.488047000
1	-2.494680000	4.479494000	-0.656898000	1	0.720724000	-0.347856000	-3.444272000
1	-2.834860000	3.146077000	0.450795000	7	-1.930116000	-1.201539000	0.062355000
6	0.431044000	3.930854000	-1.760493000	14	-0.330499000	3.094256000	-1.011166000
				14	-0.458846000	2.039495000	1.837157000

14	-3.633578000	-0.870396000	-0.160566000	1	-2.280745000	-4.823059000	1.534520000
14	-1.361074000	-2.809480000	0.447160000	1	-2.932453000	-3.371540000	2.302947000
6	-0.646215000	0.402586000	2.749060000	6	-0.855942000	-3.758441000	-1.109969000
1	-0.537048000	0.583514000	3.825175000	1	-0.740285000	-4.826823000	-0.894823000
1	-1.606919000	-0.092627000	2.577541000	1	-1.605364000	-3.659419000	-1.904223000
1	0.150528000	-0.291445000	2.457535000	1	0.107678000	-3.396188000	-1.487530000
6	1.292271000	2.611137000	2.255169000	6	0.124605000	-2.834454000	1.609881000
1	1.380325000	2.850837000	3.321232000	1	0.925505000	-2.146229000	1.321987000
1	1.969114000	1.778001000	2.033974000	1	-0.172683000	-2.587061000	2.634066000
1	1.632444000	3.481303000	1.685986000	1	0.542290000	-3.849173000	1.620701000
6	-1.740271000	3.228286000	2.542889000	6	-0.142837000	-0.626199000	-2.828561000
1	-1.681642000	3.231714000	3.637467000	8	-0.940531000	0.249681000	-2.436161000
1	-1.609963000	4.258056000	2.200263000	8	0.772280000	-0.732743000	-0.955342000
1	-2.750018000	2.905140000	2.265283000	1	-0.388279000	-1.689562000	-2.749221000
6	1.364353000	2.788234000	-1.787115000	5	2.064879000	-0.740034000	-0.571521000
1	1.645173000	3.560328000	-2.511455000	8	2.506357000	-0.267735000	0.647588000
1	2.123019000	2.766076000	-0.995747000	8	3.079352000	-1.254294000	-1.348934000
1	1.395395000	1.818162000	-2.298647000	6	3.948802000	-0.286517000	0.599995000
6	-0.302935000	4.793053000	-0.182121000	6	4.225698000	-1.382956000	-0.482663000
1	-1.318118000	5.107008000	0.082930000	6	5.491063000	-1.169374000	-1.296801000
1	0.319044000	4.870643000	0.712924000	6	4.192636000	-2.797632000	0.093575000
1	0.078837000	5.516892000	-0.912287000	6	4.408536000	1.099734000	0.153949000
6	-1.633705000	3.291995000	-2.357517000	6	4.478385000	-0.607184000	1.987717000
1	-2.619069000	3.465871000	-1.911507000	1	4.240264000	0.215571000	2.668189000
1	-1.385178000	4.172615000	-2.962405000	1	4.025143000	-1.518678000	2.382729000
1	-1.708021000	2.431873000	-3.025735000	1	5.566485000	-0.730762000	1.966353000
6	-3.854243000	0.894387000	-0.786835000	1	4.000060000	1.848816000	0.838321000
1	-3.479285000	1.638653000	-0.076036000	1	4.046764000	1.323714000	-0.854744000
1	-3.346548000	1.064094000	-1.743105000	1	5.499882000	1.178964000	0.160768000
1	-4.922148000	1.085173000	-0.946145000	1	5.456445000	-0.226043000	-1.844981000
6	-4.637064000	-1.005786000	1.429485000	1	5.602480000	-1.982139000	-2.019884000
1	-4.165863000	-0.425524000	2.230875000	1	6.371154000	-1.167980000	-0.644900000
1	-5.638878000	-0.591422000	1.266671000	1	5.067664000	-2.997172000	0.719261000
1	-4.756418000	-2.033454000	1.781907000	1	4.182304000	-3.513692000	-0.732439000
6	-4.361499000	-2.011078000	-1.478236000	1	3.290153000	-2.954730000	0.693954000
1	-5.431906000	-1.822308000	-1.617374000				
1	-3.863235000	-1.827356000	-2.437705000				
1	-4.239176000	-3.072880000	-1.240352000				
6	-2.682961000	-3.822461000	1.336603000				
1	-3.611920000	-3.948088000	0.772154000				
					1-IM5 (in gas phase)		
				7	-1.048125000	1.653956000	0.009858000
				13	-0.551654000	-0.025161000	-0.362892000
				7	-1.551536000	-1.496527000	-0.138101000

14	-0.502215000	2.920001000	-1.079777000	6	-1.926028000	-4.041736000	1.404885000
14	-1.864117000	2.017087000	1.517311000	1	-2.716657000	-4.442479000	0.763180000
14	-3.170327000	-1.573284000	-0.796442000	1	-1.379538000	-4.894173000	1.824357000
14	-0.722192000	-2.904009000	0.505602000	1	-2.402594000	-3.511532000	2.236981000
6	-1.710847000	0.544383000	2.684364000	6	0.183539000	-3.836379000	-0.851509000
1	-2.200355000	0.773090000	3.638020000	1	0.720782000	-4.704669000	-0.453832000
1	-2.163040000	-0.368022000	2.281326000	1	-0.507620000	-4.190645000	-1.623595000
1	-0.656189000	0.332517000	2.901986000	1	0.911675000	-3.173792000	-1.333542000
6	-1.042466000	3.475840000	2.384075000	6	0.531168000	-2.341320000	1.801627000
1	-1.078076000	4.403481000	1.804163000	1	1.199755000	-1.536094000	1.470483000
1	-1.537356000	3.668150000	3.342901000	1	0.019665000	-1.996731000	2.706905000
1	0.009612000	3.249259000	2.589156000	1	1.169517000	-3.186521000	2.087150000
6	-3.689594000	2.398226000	1.254430000	8	0.995902000	-0.304737000	-1.071687000
1	-4.179649000	2.611557000	2.211300000	5	2.268198000	-0.248758000	-0.648842000
1	-3.833369000	3.267192000	0.604174000	8	2.633605000	0.257604000	0.591252000
1	-4.210138000	1.550415000	0.795551000	8	3.349028000	-0.722109000	-1.360009000
6	1.154698000	3.603896000	-0.510934000	6	4.073081000	0.273488000	0.634031000
1	1.609251000	4.253293000	-1.267101000	6	4.444581000	-0.810980000	-0.432653000
1	1.061244000	4.176871000	0.417399000	6	5.747255000	-0.555511000	-1.173281000
1	1.838040000	2.769322000	-0.315166000	6	4.426247000	-2.228208000	0.140170000
6	-1.788827000	4.291691000	-1.203004000	6	4.524119000	1.674732000	0.227724000
1	-2.731852000	3.893323000	-1.594079000	6	4.527586000	-0.043493000	2.049765000
1	-2.001236000	4.781262000	-0.247531000	1	4.230429000	0.767719000	2.720308000
1	-1.440860000	5.063902000	-1.898475000	1	4.074526000	-0.968873000	2.411939000
6	-0.310047000	2.200206000	-2.810627000	1	5.617670000	-0.141843000	2.092134000
1	-1.268659000	1.821056000	-3.183691000	1	4.058361000	2.404390000	0.896087000
1	0.021264000	2.981067000	-3.504751000	1	4.213058000	1.901398000	-0.797341000
1	0.424022000	1.388946000	-2.853969000	1	5.610953000	1.781887000	0.295635000
6	-3.470439000	-0.056744000	-1.879237000	1	5.712917000	0.387870000	-1.721451000
1	-3.347638000	0.889747000	-1.342146000	1	5.922744000	-1.361259000	-1.891342000
1	-2.783813000	-0.050842000	-2.735762000	1	6.589678000	-0.529234000	-0.473650000
1	-4.488359000	-0.084636000	-2.284707000	1	5.269023000	-2.403700000	0.815503000
6	-4.479168000	-1.632362000	0.555990000	1	4.484208000	-2.940401000	-0.687160000
1	-5.484853000	-1.587284000	0.122803000	1	3.494748000	-2.415978000	0.685730000
1	-4.410525000	-2.553387000	1.143718000				
1	-4.374177000	-0.788881000	1.247196000				
6	-3.364497000	-3.074711000	-1.920209000	7	1.058841000	-1.927433000	0.289855000
1	-4.374553000	-3.103655000	-2.344638000	13	1.416652000	-0.142190000	0.287918000
1	-2.653493000	-3.017883000	-2.751854000	1	-0.201632000	-0.610658000	-2.442111000
1	-3.196963000	-4.025610000	-1.404600000	7	3.057361000	0.533854000	-0.140537000

1-TS5' (in gas phase)

14	1.639486000	-2.960299000	-0.994949000	6	5.028888000	1.357074000	-2.218461000
14	-0.004762000	-2.599332000	1.516530000	1	4.978645000	0.382184000	-2.716937000
14	4.327518000	0.031725000	0.952974000	1	5.236365000	2.114583000	-2.983089000
14	3.398351000	1.751262000	-1.346820000	1	5.884702000	1.339888000	-1.535028000
6	-1.070111000	-1.291030000	2.365649000	6	2.088549000	1.873469000	-2.705700000
1	-1.826375000	-1.810937000	2.967143000	1	2.517635000	2.452373000	-3.532406000
1	-0.481903000	-0.657389000	3.037467000	1	1.780720000	0.904286000	-3.111609000
1	-1.593169000	-0.639348000	1.659082000	1	1.198923000	2.402577000	-2.352297000
6	-1.161689000	-3.914351000	0.818687000	6	3.511456000	3.488361000	-0.619386000
1	-0.626265000	-4.813188000	0.493808000	1	2.594910000	3.707201000	-0.061739000
1	-1.858074000	-4.216596000	1.609904000	1	4.364183000	3.617575000	0.052750000
1	-1.754485000	-3.535897000	-0.018479000	1	3.604499000	4.227092000	-1.424774000
6	0.976347000	-3.437199000	2.900143000	6	-0.832631000	-0.056096000	-1.744439000
1	0.296601000	-3.999586000	3.551548000	8	0.074928000	0.655533000	-0.898011000
1	1.721956000	-4.138922000	2.511126000	8	-1.588731000	-0.947133000	-1.007898000
1	1.501150000	-2.705385000	3.523058000	1	-1.455424000	0.678532000	-2.262979000
6	0.254853000	-3.634460000	-2.102006000	5	-2.926621000	-0.762493000	-0.793648000
1	-0.158729000	-4.576888000	-1.732410000	8	-3.696883000	0.213209000	-1.373070000
1	-0.577725000	-2.927264000	-2.180370000	8	-3.619152000	-1.634929000	-0.001159000
1	0.646816000	-3.817821000	-3.109310000	6	-5.069103000	-0.159099000	-1.096446000
6	2.588445000	-4.434858000	-0.299254000	6	-4.919628000	-1.040444000	0.188914000
1	3.393122000	-4.110460000	0.370056000	6	-4.828954000	-0.209935000	1.467037000
1	1.929751000	-5.098524000	0.272855000	6	-5.954726000	-2.143237000	0.329629000
1	3.034432000	-5.028192000	-1.105478000	6	-5.897450000	1.099990000	-0.910678000
6	2.771362000	-2.021978000	-2.180495000	6	-5.566044000	-0.955762000	-2.300519000
1	3.098240000	-2.716432000	-2.963896000	1	-5.444592000	-0.348007000	-3.201104000
1	2.248062000	-1.196904000	-2.680043000	1	-4.987808000	-1.876744000	-2.425051000
1	3.654699000	-1.596091000	-1.701205000	1	-6.622774000	-1.218707000	-2.196869000
6	5.503991000	-1.249669000	0.218181000	1	-5.932966000	1.659081000	-1.850082000
1	4.988450000	-2.199294000	0.036519000	1	-5.470748000	1.745241000	-0.141128000
1	5.949721000	-0.925457000	-0.727410000	1	-6.923295000	0.842179000	-0.626456000
1	6.320527000	-1.447668000	0.922853000	1	-4.058166000	0.560349000	1.356750000
6	3.551260000	-0.787231000	2.468075000	1	-4.534662000	-0.865744000	2.290877000
1	4.324187000	-0.966102000	3.224637000	1	-5.783426000	0.264462000	1.715283000
1	2.771260000	-0.173303000	2.936648000	1	-6.962337000	-1.718080000	0.389894000
1	3.112345000	-1.756532000	2.209158000	1	-5.764018000	-2.706144000	1.247190000
6	5.366230000	1.484043000	1.563944000	1	-5.913128000	-2.838209000	-0.511136000
1	6.091215000	1.127718000	2.304933000	1	0.615457000	0.749673000	1.389793000
1	5.929329000	1.974629000	0.763244000	5	-0.422291000	1.640844000	0.014925000
1	4.736421000	2.240364000	2.044020000	8	0.181954000	2.869517000	0.092542000

8	-1.727995000	1.624695000	0.433332000	6	1.869220000	-3.662030000	-1.956034000
6	-0.842842000	3.800353000	0.500254000	1	1.411859000	-4.317948000	-2.706203000
6	-1.910519000	2.865775000	1.165300000	1	2.931890000	-3.916152000	-1.897927000
6	-1.617683000	2.564623000	2.632312000	1	1.416997000	-3.887511000	-0.983019000
6	-3.340064000	3.349956000	0.987057000	6	2.392920000	-1.403662000	-4.012143000
6	-0.232597000	4.828660000	1.437379000	1	3.480763000	-1.496348000	-3.960081000
6	-1.352451000	4.466581000	-0.776942000	1	2.038227000	-2.040895000	-4.830495000
1	-0.502800000	4.918872000	-1.295504000	1	2.159318000	-0.364965000	-4.273367000
1	-1.809689000	3.729208000	-1.445366000	6	-0.313360000	-1.763241000	-2.770246000
1	-2.087553000	5.247634000	-0.561983000	1	-0.927672000	-2.147005000	-1.949959000
1	0.498075000	5.431373000	0.890753000	1	-0.669507000	-0.760070000	-3.018273000
1	0.278075000	4.346237000	2.272843000	1	-0.504878000	-2.404130000	-3.639979000
1	-1.005303000	5.498313000	1.830223000	6	1.932081000	3.424593000	-1.508908000
1	-1.800702000	3.442005000	3.259931000	1	2.618522000	2.647033000	-1.871791000
1	-0.582990000	2.236290000	2.767751000	1	0.990611000	3.318083000	-2.056000000
1	-2.274595000	1.753681000	2.961423000	1	2.372244000	4.390769000	-1.780642000
1	-4.027292000	2.719787000	1.558510000	6	3.290077000	3.977902000	1.138019000
1	-3.634720000	3.324551000	-0.064430000	1	3.592845000	4.902781000	0.632524000
1	-3.439053000	4.374966000	1.360500000	1	3.183395000	4.206306000	2.201999000
				1	4.105401000	3.255573000	1.030274000
				6	0.296904000	4.523285000	0.847508000
1-TS6 (in gas phase)				1	0.242109000	4.659351000	1.934083000
7	2.030159000	-0.795566000	-1.089181000	1	0.428743000	5.513334000	0.396260000
13	0.927763000	0.537891000	-0.546421000	1	-0.660346000	4.105150000	0.517540000
7	1.288984000	1.703512000	0.810566000	6	1.780317000	2.344104000	3.707627000
14	1.531171000	-1.856218000	-2.396486000	1	1.519547000	3.406796000	3.661442000
14	3.568164000	-1.141679000	-0.317278000	1	1.535694000	1.991056000	4.716300000
14	1.688326000	3.343295000	0.364418000	1	2.863827000	2.255689000	3.574664000
14	0.839380000	1.302505000	2.446185000	6	-0.999692000	1.534209000	2.811801000
6	4.267599000	0.362494000	0.575059000	1	-1.187865000	1.387210000	3.882680000
1	5.282372000	0.127142000	0.918189000	1	-1.327396000	2.543594000	2.541274000
1	4.339085000	1.209344000	-0.118213000	1	-1.635719000	0.837092000	2.256151000
1	3.676755000	0.694133000	1.431088000	6	1.280313000	-0.496363000	2.816506000
6	3.426833000	-2.601863000	0.880923000	1	0.862084000	-1.209403000	2.096917000
1	3.707932000	-3.540714000	0.391954000	1	2.366088000	-0.643744000	2.821764000
1	4.084604000	-2.468845000	1.747570000	1	0.906821000	-0.771479000	3.811207000
1	2.400706000	-2.711296000	1.246118000	8	-0.810474000	-0.182960000	-0.020271000
6	4.898980000	-1.580392000	-1.587057000	5	-1.320670000	-1.353503000	0.508464000
1	5.838735000	-1.775633000	-1.056444000	8	-0.548904000	-2.462843000	0.671434000
1	4.670268000	-2.469455000	-2.182570000	8	-2.603377000	-1.468590000	0.950882000
1	5.074654000	-0.747890000	-2.277098000				

6	-1.447059000	-3.508588000	1.122873000	1-TS7 (in gas phase)			
6	-2.626809000	-2.684716000	1.744825000	7	-1.632185000	-0.042522000	0.027927000
6	-3.995090000	-3.329667000	1.614014000	13	-0.107193000	0.666764000	-0.661245000
6	-2.357931000	-2.264145000	3.187288000	1	-0.188061000	1.194872000	-2.207038000
6	-1.866695000	-4.296672000	-0.114511000	7	1.572968000	0.161443000	-0.179477000
6	-0.695816000	-4.392312000	2.103207000	14	-1.594354000	-1.683805000	0.655215000
1	0.104254000	-4.920438000	1.576628000	14	-3.176564000	0.697692000	-0.352734000
1	-0.244934000	-3.801082000	2.903296000	14	2.225960000	0.819621000	1.308167000
1	-1.368065000	-5.136140000	2.543685000	14	2.519615000	-0.880449000	-1.211493000
1	-0.970230000	-4.655712000	-0.627750000	6	-2.962637000	2.352952000	-1.240046000
1	-2.428853000	-3.665818000	-0.810605000	1	-3.959948000	2.720256000	-1.508798000
1	-2.485075000	-5.157720000	0.155880000	1	-2.496310000	3.105443000	-0.596148000
1	-4.264266000	-3.484420000	0.567613000	1	-2.386957000	2.264882000	-2.167149000
1	-4.748599000	-2.682422000	2.070813000	6	-4.178139000	-0.391170000	-1.524937000
1	-4.012031000	-4.294563000	2.131500000	1	-4.374200000	-1.390455000	-1.123474000
1	-2.413342000	-3.118307000	3.868384000	1	-5.145967000	0.070436000	-1.751613000
1	-3.108041000	-1.526821000	3.485488000	1	-3.636749000	-0.515229000	-2.470004000
1	-1.369665000	-1.800826000	3.283064000	6	-4.180331000	1.082649000	1.196070000
1	-0.053242000	1.187351000	-1.690723000	1	-4.985754000	1.784106000	0.949271000
5	-1.600483000	0.776017000	-0.764748000	1	-4.637310000	0.199573000	1.649319000
8	-1.925210000	1.991143000	-0.214530000	1	-3.542730000	1.557930000	1.949639000
8	-2.486184000	0.338351000	-1.716563000	6	-1.401135000	-2.902990000	-0.772103000
6	-2.907836000	2.564712000	-1.104995000	1	-0.468694000	-2.722773000	-1.320981000
6	-3.580983000	1.285389000	-1.706372000	1	-1.378294000	-3.939878000	-0.417874000
6	-4.656523000	0.702673000	-0.792366000	1	-2.225246000	-2.805880000	-1.487326000
6	-4.105195000	1.446701000	-3.123010000	6	-3.164666000	-2.124668000	1.604306000
6	-3.833630000	3.449804000	-0.287605000	1	-3.270590000	-1.503169000	2.499499000
6	-2.166272000	3.387801000	-2.157219000	1	-4.086531000	-2.041703000	1.021538000
1	-1.547521000	4.135478000	-1.652312000	1	-3.078269000	-3.166532000	1.934981000
1	-1.510875000	2.754598000	-2.762830000	6	-0.182245000	-1.979021000	1.864612000
1	-2.867374000	3.905621000	-2.818862000	1	-0.278224000	-1.355011000	2.759371000
1	-3.275249000	4.312360000	0.088028000	1	-0.200700000	-3.028040000	2.184206000
1	-4.243317000	2.908641000	0.567455000	1	0.792047000	-1.781226000	1.411309000
1	-4.658998000	3.818171000	-0.906326000	6	0.837715000	1.313697000	2.498542000
1	-4.282484000	0.596290000	0.230283000	1	0.771050000	2.402937000	2.586408000
1	-4.924486000	-0.292611000	-1.157458000	1	-0.146693000	0.952596000	2.180682000
1	-5.554179000	1.328536000	-0.784239000	1	1.029643000	0.905908000	3.497281000
1	-4.873943000	2.226044000	-3.160044000	6	3.257130000	2.364422000	0.958853000
1	-4.553741000	0.506815000	-3.456283000	1	3.717102000	2.736032000	1.881914000
1	-3.303094000	1.707730000	-3.815863000	1	4.059322000	2.169656000	0.239781000

1	-1.834301000	-1.136313000	-3.606233000	6	-1.243269000	3.977993000	1.973425000
1	-0.728099000	-2.524392000	-3.553728000	1	-1.131181000	4.280431000	3.021426000
8	-0.147893000	-0.915064000	-2.429024000	1	-1.054236000	4.860498000	1.355643000
1-TS8 (in gas phase)				1	-2.285505000	3.680724000	1.819973000
7	-1.989618000	-1.061417000	0.083727000	6	1.703503000	3.264949000	1.592032000
13	-0.461388000	-0.075301000	0.138588000	1	1.790665000	4.115274000	0.904857000
7	-0.381350000	1.743703000	0.096003000	1	2.011242000	3.609532000	2.585673000
14	-1.911102000	-2.773702000	0.478150000	1	2.401044000	2.491686000	1.250564000
14	-3.582916000	-0.349729000	-0.135603000	6	-0.727721000	4.333739000	-1.382269000
14	-0.048561000	2.565488000	1.596541000	1	-0.049774000	4.944027000	-0.775352000
14	-0.194070000	2.525891000	-1.448851000	1	-0.725019000	4.752382000	-2.395476000
6	-3.619875000	1.492182000	0.251299000	1	-1.738082000	4.443530000	-0.974118000
1	-4.657879000	1.839723000	0.182454000	6	1.573043000	2.501874000	-2.108956000
1	-3.277028000	1.666455000	1.277725000	1	1.647705000	3.118992000	-3.012379000
1	-3.001755000	2.107354000	-0.404992000	1	2.275830000	2.893752000	-1.366261000
6	-4.222629000	-0.623595000	-1.889014000	1	1.904416000	1.488090000	-2.352480000
1	-4.332765000	-1.688278000	-2.117933000	6	-1.309418000	1.664644000	-2.715353000
1	-5.205027000	-0.152865000	-2.011945000	1	-1.348807000	0.577147000	-2.578446000
1	-3.550297000	-0.188278000	-2.634945000	1	-2.339767000	2.029910000	-2.642340000
6	-4.851442000	-1.077735000	1.064093000	1	-0.961776000	1.855042000	-3.737380000
1	-5.823843000	-0.611325000	0.865742000	8	0.730104000	-0.585558000	-1.300603000
1	-4.987216000	-2.160296000	0.991040000	1	0.767439000	-0.755706000	0.988540000
1	-4.579963000	-0.841979000	2.099177000	5	1.879594000	-0.804137000	-0.457132000
6	-3.076335000	-3.780960000	-0.616491000	8	2.720126000	0.245613000	-0.155283000
1	-2.990816000	-4.842247000	-0.355637000	8	2.501677000	-2.030463000	-0.425747000
1	-4.130551000	-3.503964000	-0.529424000	6	3.864449000	-0.351069000	0.488326000
1	-2.791120000	-3.676645000	-1.670001000	6	3.902763000	-1.767626000	-0.177362000
6	-2.294009000	-3.080214000	2.298365000	6	4.595193000	-1.757224000	-1.538480000
1	-3.317686000	-2.815574000	2.575103000	6	4.462371000	-2.872711000	0.702106000
1	-2.137355000	-4.134944000	2.552145000	6	5.079056000	0.518857000	0.209461000
1	-1.614744000	-2.484228000	2.919646000	6	3.586866000	-0.415091000	1.990124000
6	-0.203686000	-3.515596000	0.189344000	1	2.732288000	-1.062208000	2.208570000
1	0.164767000	-3.395114000	-0.833949000	1	4.459367000	-0.784580000	2.537568000
1	0.561631000	-3.117241000	0.860074000	1	4.960463000	1.481097000	0.716045000
1	-0.278668000	-4.594148000	0.376279000	1	5.193595000	0.708778000	-0.859567000
6	-0.208569000	1.316641000	3.007954000	1	5.989832000	0.041996000	0.587410000
1	-1.155926000	0.761471000	2.959682000	1	4.204486000	-0.949051000	-2.165897000
1	0.606726000	0.585943000	3.007348000	1	4.402664000	-2.709859000	-2.039816000
1	-0.191566000	1.836633000	3.972363000	1	5.677088000	-1.629308000	-1.438289000

1	5.498285000	-2.651981000	0.980974000	1	7.392630000	-2.983818000	0.047318000
1	4.448505000	-3.819823000	0.155724000	6	5.411164000	-3.139552000	0.876436000
1	3.869541000	-2.993569000	1.610696000	1	5.692404000	-3.871137000	1.627679000
6	0.526400000	-1.333542000	-2.506071000	6	4.097314000	-2.685989000	0.814826000
1	0.685551000	-0.665241000	-3.355350000	1	3.366246000	-3.042024000	1.534577000
1	1.230091000	-2.166871000	-2.532567000	6	-2.881323000	1.092350000	0.288669000
1	-0.501717000	-1.704048000	-2.505928000	6	-2.982688000	1.840730000	1.478028000
				6	-3.879005000	2.910585000	1.516279000
				1	-3.967137000	3.495610000	2.428404000
2 (in gas phase)				6	-4.655226000	3.240695000	0.413739000
13	-0.000003000	0.364678000	-0.000077000	1	-5.345774000	4.077093000	0.461545000
7	-1.930189000	0.028008000	0.224270000	6	-4.537795000	2.496566000	-0.752932000
7	0.000005000	-1.480183000	-0.000155000	1	-5.137582000	2.761480000	-1.619816000
7	1.930110000	0.028164000	-0.224208000	6	-3.656559000	1.418109000	-0.840009000
6	-2.308502000	-1.263783000	0.172763000	6	-2.166191000	1.519829000	2.721057000
6	-1.204571000	-2.156510000	0.078498000	1	-1.570788000	0.623699000	2.515533000
6	-1.206536000	-3.546165000	0.110550000	6	-3.062028000	1.209435000	3.927323000
1	-2.143994000	-4.080001000	0.223912000	1	-3.736891000	0.371390000	3.727516000
6	0.000062000	-4.245028000	-0.000525000	1	-3.674115000	2.076044000	4.199160000
1	0.000082000	-5.328705000	-0.000694000	1	-2.448962000	0.949437000	4.796418000
6	1.206609000	-3.546105000	-0.111374000	6	-1.203199000	2.665444000	3.056590000
1	2.144081000	-4.079891000	-0.224876000	1	-0.548346000	2.889182000	2.209597000
6	1.204640000	-2.156430000	-0.078946000	1	-0.583142000	2.403737000	3.921103000
6	2.308511000	-1.263666000	-0.173006000	1	-1.757371000	3.577499000	3.305640000
6	-3.708696000	-1.734544000	0.140843000	6	-3.534204000	0.667957000	-2.155481000
6	-4.681227000	-1.232202000	1.017040000	1	-2.907987000	-0.214325000	-1.997335000
1	-4.403036000	-0.485474000	1.752813000	6	-4.897459000	0.183245000	-2.661674000
6	-5.994599000	-1.681085000	0.948253000	1	-5.428868000	-0.379356000	-1.887308000
1	-6.732737000	-1.281566000	1.636631000	1	-4.769257000	-0.466295000	-3.534148000
6	-6.364960000	-2.638130000	0.004388000	1	-5.529527000	1.024352000	-2.967182000
1	-7.392686000	-2.983632000	-0.047864000	6	-2.831863000	1.544756000	-3.199985000
6	-5.411320000	-3.139084000	-0.877259000	1	-1.844688000	1.859316000	-2.844646000
1	-5.692684000	-3.870290000	-1.628824000	1	-3.416797000	2.448062000	-3.406192000
6	-4.097433000	-2.685629000	-0.815563000	1	-2.705440000	0.999156000	-4.141372000
1	-3.366441000	-3.041363000	-1.535542000	6	2.881151000	1.092594000	-0.288367000
6	3.708703000	-1.734418000	-0.141158000	6	3.656661000	1.417960000	0.840248000
6	4.681369000	-1.231711000	-1.017007000	6	4.537978000	2.496358000	0.753308000
1	4.403336000	-0.484600000	-1.752448000	1	5.138004000	2.760928000	1.620131000
6	5.994712000	-1.680700000	-0.948295000	6	4.655218000	3.240844000	-0.413156000
1	6.732936000	-1.280875000	-1.636405000	1	5.345865000	4.077166000	-0.460871000
6	6.364931000	-2.638227000	-0.004868000				

6	2.567196000	-1.785400000	0.099928000	1	-1.746109000	1.360719000	4.475030000
6	-3.229384000	-3.028924000	0.020552000	1	-3.175556000	2.204243000	3.862879000
6	-4.421925000	-2.670075000	0.667399000	6	-2.822150000	-0.544030000	-2.153157000
1	-4.401138000	-1.917669000	1.446394000	1	-2.087970000	-1.301307000	-1.860742000
6	-5.629759000	-3.261636000	0.317100000	6	-3.970481000	-1.249168000	-2.889112000
1	-6.537858000	-2.965877000	0.833547000	1	-4.557458000	-1.874843000	-2.211075000
6	-5.679403000	-4.230116000	-0.684362000	1	-3.578460000	-1.882450000	-3.692535000
1	-6.624876000	-4.689900000	-0.954857000	1	-4.645811000	-0.516065000	-3.344972000
6	-4.508119000	-4.590278000	-1.344251000	6	-2.121714000	0.443385000	-3.092453000
1	-4.535292000	-5.323717000	-2.144556000	1	-1.318856000	0.988832000	-2.583834000
6	-3.301474000	-3.985786000	-1.006272000	1	-2.830726000	1.184485000	-3.480460000
1	-2.405548000	-4.221814000	-1.571941000	1	-1.691501000	-0.086725000	-3.950166000
6	4.002599000	-2.100491000	-0.077975000	6	2.803601000	0.572414000	-0.314393000
6	4.822305000	-1.511808000	-1.054089000	6	3.745500000	1.161418000	0.550013000
1	4.416006000	-0.781708000	-1.742931000	6	4.513174000	2.223016000	0.065595000
6	6.165477000	-1.856975000	-1.145647000	1	5.249988000	2.680435000	0.720494000
1	6.781484000	-1.391184000	-1.908293000	6	4.348961000	2.705268000	-1.222097000
6	6.722751000	-2.786249000	-0.269311000	1	4.954870000	3.532476000	-1.579096000
1	7.774498000	-3.044421000	-0.343198000	6	3.391756000	2.134246000	-2.051022000
6	5.923244000	-3.372065000	0.707707000	1	3.256030000	2.534360000	-3.048937000
1	6.347629000	-4.084159000	1.408477000	6	2.603195000	1.065142000	-1.624031000
6	4.579078000	-3.029892000	0.805741000	6	3.980111000	0.716640000	1.985036000
1	3.970590000	-3.455564000	1.596560000	1	3.219045000	-0.030029000	2.244124000
6	-2.808170000	-0.134309000	0.384150000	6	3.864527000	1.902472000	2.962201000
6	-3.330545000	0.519257000	1.520638000	1	3.024982000	2.556339000	2.721048000
6	-4.364372000	1.441053000	1.350351000	1	4.773583000	2.512795000	2.928976000
1	-4.775354000	1.941535000	2.224046000	1	3.758489000	1.538628000	3.989932000
6	-4.867516000	1.739106000	0.092156000	6	5.372550000	0.090670000	2.165961000
1	-5.668463000	2.464437000	-0.020646000	1	5.554655000	-0.742494000	1.487281000
6	-4.340074000	1.098892000	-1.021694000	1	5.495169000	-0.265190000	3.194817000
1	-4.736712000	1.324782000	-2.009054000	1	6.144318000	0.846738000	1.981965000
6	-3.321738000	0.151431000	-0.898222000	6	1.598541000	0.431517000	-2.583149000
6	-2.812641000	0.266307000	2.928026000	1	0.685738000	0.210843000	-2.015237000
1	-1.962480000	-0.415239000	2.860362000	6	2.098726000	-0.898208000	-3.169718000
6	-3.871309000	-0.389652000	3.824778000	1	1.349544000	-1.301229000	-3.859791000
1	-4.152220000	-1.384332000	3.466885000	1	2.287402000	-1.657954000	-2.406354000
1	-4.778939000	0.222377000	3.874739000	1	3.024567000	-0.740278000	-3.735823000
1	-3.485229000	-0.500375000	4.843848000	6	1.209509000	1.363975000	-3.732838000
6	-2.327086000	1.573623000	3.570723000	1	0.887805000	2.337674000	-3.354012000
1	-1.716714000	2.151816000	2.871616000	1	0.389731000	0.922603000	-4.305803000

1	2.045459000	1.508011000	-4.426547000	1	2.930064000	-4.477189000	-0.732518000
6	0.738592000	1.518098000	2.413684000	6	1.745751000	-2.799060000	-0.121865000
8	0.295054000	0.311453000	2.294143000	6	2.675030000	-1.715136000	-0.251087000
8	0.931928000	2.306431000	1.492976000	6	-3.133562000	-3.150535000	0.039039000
1	0.948669000	1.813165000	3.452059000	6	-4.257446000	-2.868948000	0.829973000
5	-0.433777000	2.229369000	-0.132358000	1	-4.179578000	-2.138430000	1.625226000
8	0.121197000	3.032779000	-1.093094000	6	-5.469787000	-3.507605000	0.600937000
8	-1.497086000	2.793431000	0.521069000	1	-6.323626000	-3.271498000	1.228498000
6	-0.718269000	4.210502000	-1.172158000	6	-5.592635000	-4.445674000	-0.422841000
6	-1.454235000	4.205035000	0.210779000	1	-6.541750000	-4.942152000	-0.599219000
6	0.170316000	5.416914000	-1.425078000	6	-4.492089000	-4.727044000	-1.226752000
6	-1.682428000	3.993844000	-2.336036000	1	-4.579618000	-5.435223000	-2.045195000
6	-2.883743000	4.722738000	0.178577000	6	-3.281855000	-4.076561000	-1.007503000
6	-0.665933000	4.918415000	1.308580000	1	-2.448259000	-4.252537000	-1.680391000
1	-0.419169000	6.340079000	-1.410797000	6	4.121672000	-1.963286000	-0.432074000
1	0.637823000	5.323013000	-2.409903000	6	4.925088000	-1.194645000	-1.288029000
1	0.962070000	5.487113000	-0.677038000	1	4.492091000	-0.373953000	-1.844212000
1	-2.349524000	3.150663000	-2.129572000	6	6.280027000	-1.472924000	-1.427716000
1	-2.289683000	4.885685000	-2.520272000	1	6.879652000	-0.870382000	-2.102794000
1	-1.109994000	3.767718000	-3.240868000	6	6.868940000	-2.508985000	-0.705713000
1	-2.905761000	5.773872000	-0.129795000	1	7.928595000	-2.717791000	-0.813817000
1	-3.313531000	4.646602000	1.182179000	6	6.090811000	-3.260038000	0.170916000
1	-3.505861000	4.133149000	-0.496790000	1	6.541848000	-4.051298000	0.761686000
1	0.370765000	4.579126000	1.342271000	6	4.735016000	-2.986425000	0.311965000
1	-1.130231000	4.693217000	2.273825000	1	4.145177000	-3.543640000	1.032673000
1	-0.688760000	6.002687000	1.159285000	6	-2.799214000	-0.271888000	0.362954000
				6	-3.283107000	0.347644000	1.530789000
				6	-4.398503000	1.179726000	1.428672000
2-IM2 (in gas phase)				1	-4.789776000	1.655730000	2.324962000
1	-0.313819000	1.096524000	-0.264483000	6	-5.005142000	1.421824000	0.204824000
13	0.174938000	-0.559355000	0.424236000	1	-5.865882000	2.081784000	0.142849000
7	-1.662417000	-1.138015000	0.443512000	6	-4.502489000	0.821667000	-0.943964000
7	0.489096000	-2.356249000	0.230608000	1	-4.979770000	1.014622000	-1.901744000
7	2.101191000	-0.508999000	-0.132335000	6	-3.408816000	-0.042788000	-0.888025000
6	-1.827957000	-2.489152000	0.248701000	6	-2.636308000	0.146321000	2.894030000
6	-0.619771000	-3.194857000	0.151718000	1	-1.748267000	-0.476619000	2.757647000
6	-0.398696000	-4.568571000	-0.023123000	6	-3.565588000	-0.572973000	3.881592000
1	-1.237194000	-5.255358000	0.022646000	1	-3.795708000	-1.593826000	3.564492000
6	0.879032000	-5.040004000	-0.287653000	1	-4.511015000	-0.030778000	3.994839000
1	1.043741000	-6.097781000	-0.456032000	1	-3.093253000	-0.631736000	4.868142000
6	1.955682000	-4.134790000	-0.403530000				

1	0.827030000	-6.000232000	-1.065447000	1	-3.353573000	-1.780164000	3.581506000
6	1.795696000	-4.091942000	-0.923993000	1	-4.072159000	-0.287397000	4.212211000
1	2.767071000	-4.471042000	-1.222150000	6	-1.873255000	1.357533000	3.568404000
6	1.660078000	-2.730013000	-0.602419000	1	-1.490822000	2.067002000	2.829966000
6	2.654462000	-1.748008000	-0.527723000	1	-1.096021000	1.140972000	4.311030000
6	-3.233625000	-3.083205000	-0.048243000	1	-2.694529000	1.855822000	4.096661000
6	-4.238937000	-2.882664000	0.907730000	6	-3.490411000	-0.610761000	-2.072805000
1	-4.065531000	-2.199786000	1.729918000	1	-2.771269000	-1.425069000	-1.971034000
6	-5.457467000	-3.543128000	0.808819000	6	-4.780240000	-1.210832000	-2.646720000
1	-6.218077000	-3.375282000	1.564856000	1	-5.291245000	-1.834593000	-1.906481000
6	-5.704345000	-4.413619000	-0.251553000	1	-4.549490000	-1.830534000	-3.519623000
1	-6.658429000	-4.925826000	-0.327506000	1	-5.474163000	-0.429218000	-2.975168000
6	-4.724167000	-4.607789000	-1.220247000	6	-2.867204000	0.390883000	-3.049254000
1	-4.912357000	-5.263258000	-2.064987000	1	-1.856885000	0.656284000	-2.725431000
6	-3.506076000	-3.942533000	-1.125742000	1	-3.465207000	1.308170000	-3.115242000
1	-2.766515000	-4.059399000	-1.911373000	1	-2.798864000	-0.044040000	-4.052331000
6	4.092407000	-2.078157000	-0.614704000	6	2.974519000	0.611461000	0.015425000
6	5.019190000	-1.254105000	-1.273256000	6	3.651306000	0.634480000	1.261294000
1	4.685388000	-0.335328000	-1.736877000	6	4.299185000	1.813040000	1.650200000
6	6.365717000	-1.595992000	-1.333925000	1	4.817072000	1.839902000	2.606450000
1	7.057399000	-0.941312000	-1.855634000	6	4.297157000	2.937011000	0.842553000
6	6.829531000	-2.763725000	-0.731736000	1	4.795039000	3.846377000	1.165047000
1	7.881894000	-3.025754000	-0.779458000	6	3.666259000	2.889627000	-0.396788000
6	5.930578000	-3.577304000	-0.047392000	1	3.688825000	3.774255000	-1.021506000
1	6.280056000	-4.472857000	0.457883000	6	3.005002000	1.744910000	-0.842850000
6	4.585871000	-3.231309000	0.022871000	6	3.776604000	-0.576043000	2.186839000
1	3.908779000	-3.836459000	0.617513000	1	3.237058000	-1.415782000	1.744341000
6	-2.897131000	-0.235768000	0.413025000	6	3.192006000	-0.364147000	3.592444000
6	-3.183804000	0.340122000	1.666300000	1	2.099216000	-0.381042000	3.587378000
6	-4.304704000	1.164436000	1.783900000	1	3.537396000	0.576456000	4.038341000
1	-4.539308000	1.601642000	2.751516000	1	3.520851000	-1.174707000	4.251133000
6	-5.127047000	1.421909000	0.697175000	6	5.258836000	-0.965355000	2.323000000
1	-5.997474000	2.062518000	0.806245000	1	5.755364000	-1.024348000	1.351556000
6	-4.829573000	0.850917000	-0.534047000	1	5.352322000	-1.937666000	2.818342000
1	-5.475731000	1.052227000	-1.384503000	1	5.792429000	-0.226655000	2.932936000
6	-3.726147000	0.013454000	-0.703261000	6	2.322134000	1.738352000	-2.215229000
6	-2.354697000	0.056971000	2.910164000	1	1.256642000	1.544303000	-2.040814000
1	-1.479947000	-0.521704000	2.608330000	6	2.838971000	0.648857000	-3.167263000
6	-3.127592000	-0.774158000	3.944878000	1	2.275585000	0.693012000	-4.105662000
1	-2.533908000	-0.881093000	4.859159000	1	2.727724000	-0.356990000	-2.759661000

6	2.476212000	-0.539923000	2.907891000	1	3.100899000	0.341101000	2.736668000
6	2.743887000	0.029957000	0.202018000	1	4.554474000	2.745517000	-0.740647000
6	3.038770000	1.385901000	-0.048806000	1	6.223270000	0.985934000	-1.186580000
6	4.303588000	1.708904000	-0.539368000	1	5.658867000	-1.384559000	-0.800241000
6	5.245320000	0.717375000	-0.798363000	1	2.422728000	-2.546136000	0.683515000
6	4.926245000	-0.613964000	-0.575720000	1	4.131761000	-4.195922000	1.184911000
6	3.676122000	-0.986449000	-0.070284000	1	5.382972000	-3.271507000	0.353386000
6	3.364163000	-2.462449000	0.130422000	1	4.700036000	-2.659081000	1.863144000
6	4.456995000	-3.181539000	0.932059000	1	2.945704000	-4.223546000	-1.071729000
6	3.165895000	-3.160750000	-1.220339000	1	2.333642000	-2.722684000	-1.778394000
6	1.980813000	2.455202000	0.179260000	1	4.070888000	-3.082324000	-1.834081000
6	2.188386000	3.699262000	-0.685532000	1	1.022634000	2.009036000	-0.111810000
6	1.863414000	2.855893000	1.655934000	1	1.310270000	4.349754000	-0.615667000
6	-0.021120000	0.171339000	-2.346951000	1	2.336294000	3.442687000	-1.739772000
1	1.341037000	0.504076000	-4.014694000	1	3.051711000	4.286189000	-0.351756000
1	-0.887497000	-0.370168000	-4.276136000	1	1.161838000	3.690998000	1.764679000
1	-1.931284000	-0.765869000	-2.903077000	1	1.496236000	2.034244000	2.278290000
1	-0.514417000	-1.772476000	-3.259978000	1	2.834103000	3.181746000	2.047972000
1	0.030018000	-1.031578000	3.640959000	6	-0.885032000	-0.739837000	-3.237291000
1	-1.064656000	2.077758000	0.314318000	1	1.894569000	-0.768693000	-2.920427000
1	-1.560618000	3.516018000	2.338398000	1	2.045029000	0.925734000	-2.446391000
1	-3.214181000	2.879754000	2.331979000	6	1.391022000	0.206770000	-2.953580000
1	-1.837627000	1.796011000	2.614911000	6	-0.615219000	1.579811000	-2.446667000
1	-1.445942000	4.439527000	0.037663000	1	-0.590636000	1.927906000	-3.493329000
1	-3.196923000	4.267363000	0.119340000	1	-0.067076000	2.323300000	-1.854702000
1	-2.313367000	3.644852000	-1.287316000	1	-1.663488000	1.600382000	-2.128344000
1	-4.564825000	2.710522000	-0.599650000	1	-2.818198000	-1.804315000	2.795879000
1	-6.119986000	0.946156000	-1.340261000	13	0.021935000	-0.734122000	-0.551919000
1	-5.509996000	-1.432508000	-1.085451000				
1	-2.337188000	-2.604239000	0.529515000				
1	-4.605222000	-2.682253000	1.719360000	8	0.014260000	-2.682037000	0.821097000
1	-4.073075000	-4.234331000	1.042460000	7	-1.404356000	-0.101136000	0.726269000
1	-5.309855000	-3.284324000	0.215042000	6	-2.715879000	0.192431000	0.204279000
1	-2.904964000	-4.293109000	-1.207754000	6	-3.063176000	1.547438000	0.012808000
1	-3.989797000	-3.128000000	-1.988393000	6	-4.307128000	1.830415000	-0.551148000
1	-2.245089000	-2.815333000	-1.921386000	6	-5.177037000	0.808883000	-0.920700000
1	-3.248790000	-0.100279000	2.622809000	6	-4.821745000	-0.514566000	-0.708748000
1	-2.164032000	-0.617717000	3.935223000	6	-3.593468000	-0.851726000	-0.130482000
1	2.167926000	-0.561029000	3.953801000	6	-3.262170000	-2.312950000	0.130386000
1	3.099059000	-1.419406000	2.711284000	6	-4.371961000	-3.000632000	0.937072000

3-TS1 (in gas phase)

6	-3.014858000	-3.076639000	-1.176687000	1	-1.625650000	3.850247000	2.184456000
6	-2.120925000	2.671331000	0.428837000	1	-1.850811000	2.138544000	2.544501000
6	-2.340626000	3.971358000	-0.349735000	1	-3.261135000	3.166838000	2.214765000
6	-2.221050000	2.965671000	1.934165000	1	0.033858000	-0.462677000	3.724965000
6	-1.233633000	-0.260217000	2.044444000	1	5.703282000	-1.064423000	-0.701125000
6	0.024260000	-0.316816000	2.652978000	1	6.203546000	1.300566000	-1.196587000
6	1.269957000	-0.144827000	2.037677000	1	4.479465000	3.029469000	-0.852525000
7	1.435057000	-0.026639000	0.714378000	1	0.963007000	2.233225000	-0.212722000
6	2.741290000	0.309401000	0.200911000	1	1.184521000	4.531038000	-0.863675000
6	3.703478000	-0.691100000	-0.011412000	1	2.927339000	4.540376000	-0.590936000
6	4.947131000	-0.304945000	-0.522146000	1	2.245483000	3.586787000	-1.924864000
6	5.229853000	1.022282000	-0.805366000	1	1.039087000	4.008827000	1.558569000
6	4.257273000	1.996826000	-0.604114000	1	2.738978000	3.600461000	1.857674000
6	2.997166000	1.660740000	-0.111856000	1	1.459420000	2.408795000	2.177428000
6	1.911777000	2.714808000	0.051269000	1	2.473392000	-2.253665000	0.773369000
6	2.084534000	3.908030000	-0.890801000	1	4.224897000	-3.818359000	1.408557000
6	1.781619000	3.204813000	1.499880000	1	5.474974000	-2.851549000	0.621319000
6	3.434159000	-2.163108000	0.256424000	1	4.674266000	-2.234550000	2.069244000
6	4.514004000	-2.796951000	1.143982000	1	3.071203000	-3.984843000	-0.876675000
6	3.336372000	-2.940337000	-1.064830000	1	4.295080000	-2.911447000	-1.595566000
6	2.480494000	-0.086564000	2.934452000	1	2.571123000	-2.524515000	-1.726335000
6	-2.441536000	-0.405323000	2.934820000	1	3.122610000	0.761609000	2.682484000
6	-0.082301000	0.345707000	-2.339512000	1	3.076680000	-0.995284000	2.801454000
6	-0.959107000	-0.613799000	-3.165751000	1	2.181779000	-0.015943000	3.980433000
6	-0.674937000	1.748906000	-2.516559000	1	-2.180195000	-0.217219000	3.976894000
6	1.330723000	0.331970000	-2.947616000	1	-2.807353000	-1.435872000	2.851884000
1	-4.599089000	2.862314000	-0.716893000	1	-3.255888000	0.258657000	2.638139000
1	-6.135225000	1.050090000	-1.370512000	1	-0.584969000	-1.644896000	-3.148336000
1	-5.509460000	-1.307526000	-0.989936000	1	-0.973357000	-0.290350000	-4.218078000
1	-2.339762000	-2.362889000	0.715991000	1	-1.999614000	-0.620254000	-2.814823000
1	-4.054251000	-4.007482000	1.224280000	1	-0.132388000	2.525013000	-1.963372000
1	-4.620321000	-2.443225000	1.846137000	1	-0.640421000	2.032313000	-3.580513000
1	-5.290265000	-3.099589000	0.348230000	1	-1.725384000	1.779973000	-2.207959000
1	-2.744800000	-4.115680000	-0.965410000	1	1.988830000	1.081414000	-2.493127000
1	-2.195864000	-2.640452000	-1.754903000	1	1.823773000	-0.643389000	-2.844130000
1	-3.912427000	-3.068079000	-1.806503000	1	1.274351000	0.551892000	-4.025117000
1	-1.096615000	2.332459000	0.229491000	1	0.324377000	-2.011378000	-1.117585000
1	-1.520797000	4.665739000	-0.138049000	6	0.164177000	-3.053010000	-0.339640000
1	-2.378332000	3.805881000	-1.429893000	8	0.216705000	-4.042144000	-1.018417000
1	-3.269160000	4.466775000	-0.044839000	13	0.018862000	-0.387761000	-0.480688000

3-TS1 (in benzene solvent)				1	-2.344512000	-2.358794000	0.705985000
8	0.028476000	-2.740970000	0.800802000	1	-4.052667000	-4.000247000	1.238912000
7	-1.408035000	-0.095315000	0.725331000	1	-4.619212000	-2.438081000	1.860132000
6	-2.723245000	0.199901000	0.209490000	1	-5.298483000	-3.100572000	0.368686000
6	-3.071374000	1.555653000	0.020175000	1	-2.784888000	-4.104891000	-0.981623000
6	-4.320698000	1.839883000	-0.532502000	1	-2.230127000	-2.627217000	-1.765315000
6	-5.195718000	0.819632000	-0.893750000	1	-3.950673000	-3.042761000	-1.802915000
6	-4.839465000	-0.504341000	-0.685597000	1	-1.103806000	2.348881000	0.218563000
6	-3.605332000	-0.842862000	-0.119781000	1	-1.539191000	4.677914000	-0.146420000
6	-3.274456000	-2.305774000	0.132609000	1	-2.415856000	3.821347000	-1.425663000
6	-4.375222000	-2.995039000	0.949356000	1	-3.285279000	4.477974000	-0.026505000
6	-3.046818000	-3.061244000	-1.181859000	1	-1.617839000	3.856741000	2.184445000
6	-2.128225000	2.682087000	0.428714000	1	-1.837392000	2.143968000	2.541357000
6	-2.361347000	3.982325000	-0.345021000	1	-3.250602000	3.171703000	2.229624000
6	-2.213905000	2.971867000	1.935265000	1	0.037615000	-0.476515000	3.718931000
6	-1.232823000	-0.264872000	2.043401000	1	5.711740000	-1.108685000	-0.664331000
6	0.027320000	-0.328370000	2.647191000	1	6.239893000	1.250148000	-1.162686000
6	1.273575000	-0.155618000	2.033736000	1	4.530537000	2.996624000	-0.841863000
7	1.439102000	-0.026279000	0.709297000	1	0.999309000	2.254537000	-0.226752000
6	2.751741000	0.297665000	0.200649000	1	1.270539000	4.555484000	-0.856891000
6	3.706803000	-0.713085000	0.000412000	1	3.008765000	4.529117000	-0.569801000
6	4.960389000	-0.341748000	-0.497416000	1	2.321976000	3.601975000	-1.918290000
6	5.259003000	0.982109000	-0.781779000	1	1.105976000	4.026415000	1.556939000
6	4.294029000	1.967009000	-0.593615000	1	2.784663000	3.561271000	1.876165000
6	3.025425000	1.646117000	-0.110912000	1	1.464764000	2.408283000	2.168246000
6	1.954905000	2.716778000	0.048957000	1	2.457998000	-2.256577000	0.789385000
6	2.157480000	3.913712000	-0.881532000	1	4.180189000	-3.853329000	1.412391000
6	1.821288000	3.198023000	1.500015000	1	5.444104000	-2.921980000	0.606470000
6	3.416119000	-2.181335000	0.266166000	1	4.676674000	-2.281078000	2.063246000
6	4.490852000	-2.839703000	1.140162000	1	3.005315000	-3.988861000	-0.872252000
6	3.291202000	-2.948826000	-1.057114000	1	4.246159000	-2.941552000	-1.595983000
6	2.481383000	-0.108372000	2.932301000	1	2.532573000	-2.512244000	-1.713772000
6	-2.434024000	-0.411611000	2.939967000	1	3.128416000	0.739606000	2.691893000
6	-0.074629000	0.367037000	-2.350147000	1	3.074552000	-1.019540000	2.798235000
6	-0.956621000	-0.591266000	-3.170477000	1	2.179820000	-0.044074000	3.978168000
6	-0.662009000	1.772871000	-2.523151000	1	-2.167822000	-0.212522000	3.979117000
6	1.336276000	0.347621000	-2.960140000	1	-2.790321000	-1.447180000	2.872364000
1	-4.613454000	2.872281000	-0.694248000	1	-3.257792000	0.242522000	2.647049000
1	-6.158325000	1.062169000	-1.333842000	1	-0.585243000	-1.623464000	-3.155429000
1	-5.530552000	-1.296657000	-0.960572000	1	-0.975093000	-0.269609000	-4.223597000

1	-1.996366000	-0.597547000	-2.817657000	6	2.118912000	3.913812000	-0.678707000
1	-0.109389000	2.546852000	-1.976585000	6	1.828416000	3.069174000	1.666473000
1	-0.637036000	2.055600000	-3.587892000	6	3.406761000	-2.229252000	0.118346000
1	-1.709354000	1.811695000	-2.205236000	6	4.500585000	-2.906236000	0.955844000
1	2.000732000	1.090446000	-2.503661000	6	3.270826000	-2.950388000	-1.229917000
1	1.823753000	-0.631601000	-2.865902000	6	2.489175000	-0.287697000	2.893539000
1	1.280870000	0.575249000	-4.036592000	6	-2.430942000	-0.620196000	2.889654000
1	0.260406000	-1.999416000	-1.110014000	6	-0.070502000	0.493987000	-2.331399000
6	0.133655000	-3.039257000	-0.387331000	6	-0.981169000	-0.378591000	-3.219114000
8	0.157614000	-4.015934000	-1.097389000	6	-0.630336000	1.918344000	-2.410395000
13	0.014965000	-0.336863000	-0.482490000	6	1.334054000	0.488865000	-2.961362000
				1	-4.565305000	2.894870000	-0.557615000
				1	-6.105503000	1.140343000	-1.346860000
				1	-5.493413000	-1.241391000	-1.123738000
				1	-2.326833000	-2.419958000	0.505387000
				1	-4.054617000	-4.068348000	0.981007000
				1	-4.570127000	-2.527889000	1.697499000
				1	-5.297589000	-3.092437000	0.189515000
				1	-2.848886000	-4.089229000	-1.252793000
				1	-2.259531000	-2.581659000	-1.976493000
				1	-3.992198000	-2.964284000	-2.004730000
				1	-1.075486000	2.279422000	0.379945000
				1	-1.484233000	4.637487000	0.175039000
				1	-2.336938000	3.877325000	-1.180432000
				1	-3.234438000	4.442486000	0.242510000
				1	-1.605335000	3.658710000	2.432029000
				1	-1.857833000	1.930001000	2.671307000
				1	-3.250600000	2.998345000	2.399904000
				1	0.044597000	-0.700665000	3.674905000
				1	5.670388000	-1.109108000	-0.826533000
				1	6.193752000	1.273164000	-1.199957000
				1	4.498477000	3.001100000	-0.729700000
				1	0.981821000	2.212377000	-0.092614000
				1	1.227812000	4.545759000	-0.604279000
				1	2.973240000	4.515152000	-0.348582000
				1	2.265440000	3.655305000	-1.732315000
				1	1.099741000	3.880120000	1.779922000
				1	2.794743000	3.426765000	2.040238000
				1	1.496629000	2.238822000	2.296235000
				1	2.458293000	-2.332510000	0.655510000
3-IM1 (in gas phase)							
8	0.108357000	-2.160634000	-1.043516000				
6	0.115112000	-3.179720000	-0.223680000				
8	0.041291000	-3.123909000	0.987336000				
7	-1.395628000	-0.172990000	0.703016000				
6	-2.702222000	0.157886000	0.197697000				
6	-3.043473000	1.524686000	0.094624000				
6	-4.280516000	1.852227000	-0.459965000				
6	-5.152465000	0.863707000	-0.906563000				
6	-4.804407000	-0.472743000	-0.783378000				
6	-3.582072000	-0.853795000	-0.220167000				
6	-3.264530000	-2.331010000	-0.052160000				
6	-4.360385000	-3.042118000	0.754444000				
6	-3.076759000	-3.028101000	-1.405260000				
6	-2.098859000	2.611514000	0.594759000				
6	-2.306333000	3.964792000	-0.091112000				
6	-2.210405000	2.802041000	2.115992000				
6	-1.225709000	-0.406397000	2.008134000				
6	0.031482000	-0.487375000	2.614296000				
6	1.272994000	-0.287906000	2.000171000				
7	1.427868000	-0.101769000	0.685074000				
6	2.733419000	0.247186000	0.185605000				
6	3.683570000	-0.749305000	-0.091333000				
6	4.925328000	-0.351840000	-0.597633000				
6	5.221765000	0.985366000	-0.811302000				
6	4.265347000	1.958541000	-0.539219000				
6	3.006825000	1.610790000	-0.050946000				
6	1.938131000	2.666795000	0.189274000				

1	4.204809000	-3.931455000	1.198735000	6	-2.234967000	2.811009000	2.109054000
1	5.446564000	-2.957671000	0.406169000	6	-1.228498000	-0.400490000	2.004507000
1	4.692626000	-2.373615000	1.892404000	6	0.030189000	-0.486010000	2.608625000
1	3.050730000	-4.012314000	-1.070670000	6	1.273774000	-0.284523000	1.997781000
1	4.206211000	-2.882336000	-1.797027000	7	1.431122000	-0.095385000	0.682671000
1	2.467897000	-2.522542000	-1.835356000	6	2.741304000	0.241847000	0.185836000
1	3.144451000	0.560127000	2.677312000	6	3.684559000	-0.764127000	-0.084853000
1	3.070246000	-1.199661000	2.720643000	6	4.933972000	-0.379191000	-0.582843000
1	2.194952000	-0.257950000	3.942920000	6	5.243682000	0.955280000	-0.797389000
1	-2.179756000	-0.453122000	3.938056000	6	4.294079000	1.937759000	-0.533687000
1	-2.754026000	-1.662243000	2.777055000	6	3.029744000	1.603005000	-0.049429000
1	-3.269272000	0.020894000	2.610029000	6	1.975778000	2.673155000	0.196332000
1	-0.620893000	-1.409748000	-3.290942000	6	2.168448000	3.917543000	-0.672103000
1	-1.016281000	0.036707000	-4.239024000	6	1.885869000	3.077600000	1.674071000
1	-2.013824000	-0.402791000	-2.844246000	6	3.391752000	-2.241792000	0.121690000
1	-0.076718000	2.643684000	-1.802492000	6	4.471501000	-2.933183000	0.964518000
1	-0.588692000	2.277644000	-3.451423000	6	3.257494000	-2.958750000	-1.228114000
1	-1.681266000	1.948980000	-2.102156000	6	2.485640000	-0.289921000	2.895311000
1	2.016762000	1.187475000	-2.463870000	6	-2.430000000	-0.611789000	2.890392000
1	1.803333000	-0.503486000	-2.931672000	6	-0.067549000	0.519340000	-2.332085000
1	1.272811000	0.786679000	-4.020565000	6	-0.977023000	-0.345328000	-3.227023000
1	0.196426000	-4.145698000	-0.753518000	6	-0.625161000	1.944728000	-2.396989000
13	0.010327000	-0.417712000	-0.558715000	6	1.335340000	0.519858000	-2.963458000
				1	-4.600339000	2.880457000	-0.550199000
				1	-6.133120000	1.113856000	-1.327000000
				1	-5.502751000	-1.263734000	-1.102684000
				1	-2.322294000	-2.414351000	0.517003000
				1	-4.030337000	-4.074767000	1.001899000
				1	-4.574895000	-2.537531000	1.699850000
				1	-5.282594000	-3.128208000	0.191376000
				1	-2.821032000	-4.091904000	-1.239522000
				1	-2.250177000	-2.580080000	-1.967932000
				1	-3.977261000	-2.983442000	-1.995058000
				1	-1.100407000	2.299158000	0.369443000
				1	-1.533135000	4.650509000	0.154252000
				1	-2.398881000	3.884095000	-1.187486000
				1	-3.280328000	4.443449000	0.246186000
				1	-1.648789000	3.681987000	2.422524000
				1	-1.860051000	1.949041000	2.666283000
				1	-3.277141000	2.984892000	2.401122000
3-IMI (in benzene solvent)							
8	0.100478000	-2.137312000	-1.060817000				
6	0.097835000	-3.178647000	-0.272279000				
8	0.038681000	-3.162310000	0.941588000				
7	-1.399895000	-0.164065000	0.699171000				
6	-2.710383000	0.158449000	0.196579000				
6	-3.062709000	1.522916000	0.092936000				
6	-4.306331000	1.840087000	-0.454668000				
6	-5.174595000	0.844612000	-0.893511000				
6	-4.816161000	-0.489515000	-0.769857000				
6	-3.586964000	-0.860340000	-0.214059000				
6	-3.259100000	-2.335314000	-0.043015000				
6	-4.349737000	-3.055201000	0.761853000				
6	-3.061987000	-3.033439000	-1.393548000				
6	-2.126821000	2.620250000	0.587992000				
6	-2.353587000	3.970262000	-0.098080000				

1	0.042393000	-0.694953000	3.670263000	6	2.118196000	3.337132000	0.537476000
1	5.674505000	-1.143230000	-0.803883000	6	2.419916000	4.629041000	0.107396000
1	6.221240000	1.233956000	-1.179355000	6	1.533950000	5.347546000	-0.689959000
1	4.539308000	2.977846000	-0.723475000	6	0.322747000	4.783302000	-1.058885000
1	1.010091000	2.232190000	-0.076188000	6	-0.031516000	3.493055000	-0.649784000
1	1.288371000	4.564155000	-0.590646000	6	-1.390846000	2.937217000	-1.039772000
1	3.033169000	4.507887000	-0.348595000	6	-2.522150000	3.787938000	-0.448724000
1	2.303960000	3.661916000	-1.728211000	6	-1.547091000	2.849779000	-2.562218000
1	1.181926000	3.909264000	1.793294000	6	3.087523000	2.574064000	1.434659000
1	2.862783000	3.409432000	2.044925000	6	4.548241000	3.005454000	1.262744000
1	1.535701000	2.257467000	2.307789000	6	2.712987000	2.713341000	2.919180000
1	2.438530000	-2.334369000	0.651944000	6	0.023381000	1.187678000	1.721815000
1	4.158310000	-3.952821000	1.211577000	6	-0.024432000	-0.077428000	2.313552000
1	5.418670000	-3.005089000	0.418390000	6	0.438545000	-1.280326000	1.766559000
1	4.670048000	-2.402218000	1.900974000	7	0.981031000	-1.381617000	0.549495000
1	3.015997000	-4.017195000	-1.075086000	6	1.505888000	-2.659042000	0.131069000
1	4.200060000	-2.908955000	-1.785677000	6	0.673472000	-3.603707000	-0.491661000
1	2.471412000	-2.515416000	-1.845077000	6	1.240459000	-4.823896000	-0.874855000
1	3.154151000	0.547281000	2.678351000	6	2.580583000	-5.098913000	-0.649811000
1	3.055905000	-1.211954000	2.736229000	6	3.392235000	-4.144199000	-0.044365000
1	2.187537000	-0.247386000	3.943567000	6	2.876829000	-2.910058000	0.348501000
1	-2.174071000	-0.444989000	3.937987000	6	3.768601000	-1.859111000	0.993815000
1	-2.756758000	-1.653791000	2.783783000	6	5.221515000	-1.927681000	0.516904000
1	-3.270477000	0.030026000	2.619109000	6	3.719975000	-1.932087000	2.526655000
1	-0.613733000	-1.374424000	-3.313995000	6	-0.799991000	-3.353791000	-0.765648000
1	-1.018245000	0.079933000	-4.243227000	6	-1.702479000	-4.377918000	-0.064659000
1	-2.009370000	-0.381014000	-2.852474000	6	-1.085137000	-3.370588000	-2.273090000
1	-0.071053000	2.662521000	-1.780374000	6	0.207095000	-2.519623000	2.596264000
1	-0.582826000	2.318009000	-3.433780000	6	-0.700466000	2.299256000	2.437142000
1	-1.676390000	1.975291000	-2.089888000	1	3.364540000	5.081312000	0.391989000
1	2.019854000	1.213144000	-2.460702000	1	1.791371000	6.349764000	-1.018702000
1	1.806055000	-0.472338000	-2.946606000	1	-0.371472000	5.352045000	-1.671993000
1	1.275847000	0.829410000	-4.020183000	1	-1.494924000	1.928123000	-0.628625000
1	0.154408000	-4.130360000	-0.831046000	1	-3.484155000	3.306302000	-0.643852000
13	0.010618000	-0.398490000	-0.559365000	1	-2.417097000	3.903464000	0.633761000
				1	-2.535165000	4.788908000	-0.895413000
				1	-2.508309000	2.388438000	-2.810916000
				1	-0.745369000	2.254862000	-3.011481000
				1	-1.518341000	3.845462000	-3.019015000
				1	3.014883000	1.510777000	1.171417000
3-TS2 (in gas phase)							
1	-1.593221000	-0.385212000	0.351115000				
7	0.602369000	1.420075000	0.538412000				
6	0.881979000	2.777549000	0.140542000				

6	2.749164000	3.619080000	0.510883000	1	0.554371000	-0.192395000	-3.248379000
6	1.694556000	2.714846000	2.599797000	1	-1.102373000	-5.532308000	1.381115000
6	-2.916424000	2.731479000	-1.421912000	1	-3.507644000	-5.821104000	0.901372000
6	-4.350093000	3.241107000	-1.241101000	1	-4.772918000	-4.020695000	-0.214016000
6	-2.545103000	2.847388000	-2.908442000	1	-3.396802000	-0.640961000	-0.782892000
6	0.066474000	1.170506000	-1.705481000	1	-5.794040000	-0.602878000	-0.981736000
6	0.049154000	-0.097104000	-2.295302000	1	-5.915021000	-2.360397000	-1.027218000
6	-0.498215000	-1.269812000	-1.759693000	1	-5.422124000	-1.547448000	0.471083000
7	-1.062743000	-1.337612000	-0.548950000	1	-4.433277000	-0.894741000	-3.054031000
6	-1.702872000	-2.567662000	-0.149225000	1	-4.174797000	-2.646818000	-2.950735000
6	-0.972448000	-3.574813000	0.504062000	1	-2.790531000	-1.538044000	-2.984532000
6	-1.650618000	-4.741310000	0.875616000	1	0.865800000	-2.486396000	0.439673000
6	-3.001433000	-4.906068000	0.608750000	1	2.404297000	-4.344034000	0.285990000
6	-3.711562000	-3.891099000	-0.026083000	1	1.126474000	-5.530445000	0.613018000
6	-3.083752000	-2.705515000	-0.406658000	1	1.131474000	-4.636621000	-0.910776000
6	-3.870967000	-1.585920000	-1.073709000	1	1.796722000	-3.264802000	2.560302000
6	-5.331406000	-1.527373000	-0.619875000	1	0.494304000	-4.448925000	2.759504000
6	-3.807052000	-1.673839000	-2.604569000	1	0.127729000	-2.721149000	2.849499000
6	0.508398000	-3.446874000	0.823045000	1	-1.168942000	-3.218892000	-2.470151000
6	1.337722000	-4.554411000	0.160652000	1	0.577939000	-3.024795000	-2.265464000
6	0.743030000	-3.467907000	2.338616000	1	-0.228957000	-2.266971000	-3.644850000
6	-0.340637000	-2.519100000	-2.588871000	1	0.881497000	2.039086000	-3.499260000
6	0.840488000	2.242294000	-2.427379000	1	1.866941000	2.205634000	-2.036677000
1	-3.045479000	5.254390000	-0.387691000	1	0.443298000	3.245096000	-2.263389000
1	-1.409249000	6.426117000	1.035817000	6	-2.476467000	0.429761000	2.013396000
1	0.684090000	5.299672000	1.706598000	6	-1.896241000	1.296420000	3.147447000
1	1.615771000	1.820386000	0.653419000	6	-3.718732000	1.163846000	1.502081000
1	3.681251000	3.086553000	0.720496000	6	-2.916570000	-0.905433000	2.637151000
1	2.672052000	3.746530000	-0.573170000	1	-1.055732000	0.807047000	3.651886000
1	2.812302000	4.615984000	0.963141000	1	-2.669451000	1.486414000	3.909851000
1	2.622275000	2.193530000	2.859572000	1	-1.553117000	2.276256000	2.787245000
1	0.854011000	2.165167000	3.035435000	1	-4.199065000	0.676808000	0.645000000
1	1.722053000	3.705131000	3.069164000	1	-4.478099000	1.227877000	2.299140000
1	-2.899551000	1.665871000	-1.158793000	1	-3.472001000	2.190914000	1.213591000
1	-5.045581000	2.557683000	-1.739767000	1	-3.466929000	-1.536437000	1.930154000
1	-4.643148000	3.314290000	-0.190402000	1	-2.067430000	-1.495248000	3.008177000
1	-4.482909000	4.227309000	-1.700219000	1	-3.581607000	-0.721946000	3.497250000
1	-3.337747000	2.410141000	-3.525963000	5	2.795558000	-0.546707000	-0.230119000
1	-1.617150000	2.326569000	-3.153270000	8	3.505347000	0.614060000	-0.511244000
1	-2.434907000	3.899656000	-3.194901000	8	3.589937000	-1.679716000	-0.346222000

6	4.901079000	0.258468000	-0.505284000	6	-0.147516000	-0.084082000	2.255070000
6	4.852826000	-1.257078000	-0.888947000	6	0.328126000	-1.286757000	1.719420000
6	4.782341000	-1.477362000	-2.400501000	7	0.913403000	-1.386852000	0.520477000
6	5.963509000	-2.103025000	-0.286739000	6	1.442854000	-2.664757000	0.106308000
6	5.628249000	1.148827000	-1.500940000	6	0.618789000	-3.602657000	-0.538135000
6	5.451219000	0.486132000	0.902215000	6	1.191031000	-4.816146000	-0.933471000
1	5.275876000	1.527777000	1.189157000	6	2.528655000	-5.093349000	-0.695559000
1	4.948427000	-0.153796000	1.630779000	6	3.329695000	-4.150137000	-0.058855000
1	6.529410000	0.299164000	0.941452000	6	2.808344000	-2.922326000	0.346664000
1	5.602599000	2.185830000	-1.150544000	6	3.686460000	-1.889674000	1.037407000
1	5.158724000	1.113594000	-2.486739000	6	5.150061000	-1.948421000	0.593449000
1	6.677831000	0.850365000	-1.599590000	6	3.598369000	-2.005274000	2.565755000
1	3.991941000	-0.862698000	-2.844669000	6	-0.854164000	-3.351882000	-0.808774000
1	4.543330000	-2.527710000	-2.592776000	6	-1.756111000	-4.390371000	-0.128617000
1	5.730255000	-1.242187000	-2.895302000	6	-1.146246000	-3.335437000	-2.314938000
1	6.946556000	-1.754213000	-0.622542000	6	0.052195000	-2.527322000	2.531700000
1	5.846372000	-3.143471000	-0.605793000	6	-0.843069000	2.287060000	2.359060000
1	5.934672000	-2.078245000	0.804616000	1	3.360982000	5.048878000	0.486148000
8	0.341986000	-0.280666000	1.866457000	1	1.855160000	6.349606000	-0.967805000
6	1.499637000	-0.414569000	2.410866000	1	-0.303619000	5.390315000	-1.693857000
8	2.589231000	-0.449944000	1.852949000	1	-1.500787000	1.980600000	-0.688127000
1	1.464907000	-0.508025000	3.509576000	1	-3.475110000	3.353835000	-0.757529000
13	-0.990707000	0.085710000	0.724677000	1	-2.437019000	3.960872000	0.538362000
3-IM2 (in gas phase)				1	-2.520971000	4.838131000	-0.998710000
1	-1.512537000	-0.358168000	0.176148000	1	-2.452773000	2.441783000	-2.902472000
7	0.545454000	1.425678000	0.513811000	1	-0.682333000	2.300890000	-3.063616000
6	0.854360000	2.784223000	0.138986000	1	-1.452317000	3.890740000	-3.086840000
6	2.084106000	3.323389000	0.580302000	1	2.925730000	1.480734000	1.242882000
6	2.419505000	4.612900000	0.167653000	1	5.102899000	2.221070000	1.923339000
6	1.571489000	5.349761000	-0.653812000	1	4.822350000	2.986950000	0.350767000
6	0.363429000	4.807242000	-1.064067000	1	4.662777000	3.925795000	1.845916000
6	-0.022239000	3.520426000	-0.674258000	1	3.301502000	2.187259000	3.630686000
6	-1.375788000	2.983941000	-1.104273000	1	1.598552000	2.255861000	3.173211000
6	-2.518815000	3.839969000	-0.545389000	1	2.549831000	3.749918000	3.256512000
6	-1.493138000	2.895451000	-2.630313000	1	-0.682059000	-0.156113000	3.194072000
6	3.008344000	2.542710000	1.508609000	1	0.567611000	-5.553833000	-1.432329000
6	4.481790000	2.946735000	1.388519000	1	2.952884000	-6.042624000	-1.008099000
6	2.580558000	2.690652000	2.977598000	1	4.378276000	-4.371121000	0.113806000
6	-0.081498000	1.184329000	1.673161000	1	3.298634000	-0.901167000	0.765338000
				1	5.687782000	-1.076711000	0.980610000

1	5.653677000	-2.839741000	0.983065000	1	-5.388349000	1.682330000	-1.077457000
1	5.243556000	-1.949309000	-0.497184000	1	-5.122065000	-0.010008000	-1.534027000
1	4.277112000	-1.287448000	3.039173000	1	-6.573314000	0.445986000	-0.607519000
1	3.885595000	-3.012052000	2.889433000	1	-5.377758000	2.355449000	1.304215000
1	2.589229000	-1.800962000	2.933965000	1	-4.669904000	1.306609000	2.543371000
1	-1.121581000	-2.373929000	-0.400531000	1	-6.309421000	0.981833000	1.931605000
1	-2.796370000	-4.059537000	-0.197215000	1	-3.275410000	-0.609897000	2.605867000
1	-1.663056000	-5.370495000	-0.610695000	1	-3.830272000	-2.294831000	2.515209000
1	-1.504914000	-4.518508000	0.928370000	1	-4.942715000	-1.028533000	3.080664000
1	-2.182071000	-3.020978000	-2.485401000	1	-6.655605000	-1.572638000	1.159729000
1	-1.019962000	-4.333824000	-2.748885000	1	-5.575435000	-2.956598000	0.903809000
1	-0.472396000	-2.656785000	-2.847114000	1	-5.999018000	-1.910973000	-0.460298000
1	0.789522000	-3.315224000	2.373156000	8	-0.324728000	-0.201529000	-1.987974000
1	-0.929120000	-2.909950000	2.225095000	6	-1.510344000	-0.219212000	-2.430529000
1	0.000353000	-2.282424000	3.593987000	8	-2.579737000	-0.207551000	-1.791722000
1	-0.927640000	2.097257000	3.430746000	1	-1.604173000	-0.250034000	-3.524164000
1	-1.852883000	2.265484000	1.923664000	13	0.979937000	0.057254000	-0.722034000
1	-0.408953000	3.274434000	2.194324000				
6	2.502021000	0.323915000	-1.980911000		3-IM2 (in benzene solvent)		
6	2.024742000	1.276241000	-3.096162000	1	-1.606604000	-0.237408000	0.278019000
6	3.790672000	0.936087000	-1.421524000	7	0.643765000	1.418086000	0.533946000
6	2.839399000	-1.025148000	-2.640856000	6	0.986043000	2.765727000	0.148199000
1	1.166351000	0.871741000	-3.642771000	6	2.244923000	3.266856000	0.552067000
1	2.835186000	1.429218000	-3.826230000	6	2.607168000	4.546397000	0.129782000
1	1.748866000	2.265886000	-2.706568000	6	1.757706000	5.309990000	-0.665812000
1	4.211379000	0.385685000	-0.572092000	6	0.521628000	4.805135000	-1.040088000
1	4.566002000	0.960264000	-2.204103000	6	0.107912000	3.530037000	-0.638107000
1	3.621847000	1.970616000	-1.105224000	6	-1.276184000	3.039823000	-1.028055000
1	3.311203000	-1.725617000	-1.942802000	6	-2.369092000	3.948030000	-0.452871000
1	1.949357000	-1.521627000	-3.050365000	6	-1.433674000	2.942784000	-2.549563000
1	3.539799000	-0.871517000	-3.477391000	6	3.176554000	2.456593000	1.447533000
5	-2.663850000	-0.307696000	-0.141318000	6	4.657087000	2.809585000	1.269862000
8	-3.363194000	0.845447000	0.334299000	6	2.811708000	2.619245000	2.931359000
8	-3.472167000	-1.466445000	0.092903000	6	0.045493000	1.199180000	1.713674000
6	-4.718516000	0.450468000	0.551437000	6	-0.060031000	-0.066869000	2.294164000
6	-4.559452000	-1.059591000	0.918733000	6	0.358103000	-1.287709000	1.749804000
6	-4.133536000	-1.252114000	2.377545000	7	0.905073000	-1.409737000	0.534750000
6	-5.775028000	-1.921659000	0.608410000	6	1.381473000	-2.706215000	0.113660000
6	-5.304843000	1.320557000	1.654173000	6	0.511748000	-3.615630000	-0.511743000
6	-5.505595000	0.645288000	-0.747327000	6	1.030985000	-4.852284000	-0.910341000

6	2.360970000	-5.179230000	-0.692071000	1	-2.914458000	-3.965761000	-0.138715000
6	3.208755000	-4.262820000	-0.076313000	1	-1.814095000	-5.306844000	-0.534663000
6	2.741704000	-3.012642000	0.328772000	1	-1.633542000	-4.436126000	0.991961000
6	3.674134000	-2.005066000	0.985925000	1	-2.289447000	-2.950638000	-2.434767000
6	5.121175000	-2.116973000	0.500887000	1	-1.171618000	-4.299301000	-2.696083000
6	3.628705000	-2.103130000	2.516713000	1	-0.574434000	-2.641688000	-2.812262000
6	-0.955404000	-3.312002000	-0.763628000	1	0.791524000	-3.318603000	2.417408000
6	-1.880979000	-4.317214000	-0.067352000	1	-0.921296000	-2.883866000	2.294777000
6	-1.262661000	-3.294935000	-2.266383000	1	0.043624000	-2.259913000	3.638676000
6	0.072252000	-2.514424000	2.577564000	1	-0.706943000	2.132403000	3.502697000
6	-0.636473000	2.332897000	2.431905000	1	-1.657928000	2.383054000	2.028503000
1	3.570553000	4.953373000	0.420218000	1	-0.152730000	3.297913000	2.273644000
1	2.062504000	6.301320000	-0.987769000	6	2.486573000	0.238858000	-2.015413000
1	-0.144809000	5.409399000	-1.650498000	6	2.000858000	1.180470000	-3.134547000
1	-1.428893000	2.044495000	-0.599669000	6	3.801089000	0.829257000	-1.495860000
1	-3.349872000	3.497940000	-0.629946000	6	2.780215000	-1.125920000	-2.660763000
1	-2.252931000	4.087053000	0.626150000	1	1.115144000	0.789906000	-3.647454000
1	-2.347071000	4.938162000	-0.923269000	1	2.790655000	1.298900000	-3.894097000
1	-2.418163000	2.531036000	-2.799564000	1	1.763390000	2.185428000	-2.759321000
1	-0.661152000	2.309265000	-2.997924000	1	4.230168000	0.278688000	-0.650252000
1	-1.358065000	3.931267000	-3.017253000	1	4.559785000	0.827397000	-2.295788000
1	3.047377000	1.397838000	1.187702000	1	3.664868000	1.870972000	-1.187666000
1	5.273697000	2.057044000	1.772729000	1	3.250683000	-1.826988000	-1.962364000
1	4.959131000	2.847260000	0.219651000	1	1.873495000	-1.610299000	-3.048098000
1	4.894461000	3.777206000	1.726376000	1	3.468802000	-1.002281000	-3.512698000
1	3.547024000	2.100904000	3.556819000	5	-2.749475000	-0.202235000	-0.085472000
1	1.829301000	2.206400000	3.170464000	8	-3.474888000	0.959634000	0.325523000
1	2.815494000	3.678861000	3.211641000	8	-3.563963000	-1.358399000	0.152528000
1	-0.568599000	-0.117710000	3.248771000	6	-4.838474000	0.567750000	0.486698000
1	0.372570000	-5.568245000	-1.396009000	6	-4.699004000	-0.932185000	0.901719000
1	2.742903000	-6.146323000	-1.005405000	6	-4.364646000	-1.088773000	2.387795000
1	4.251232000	-4.523251000	0.078756000	6	-5.894809000	-1.803650000	0.543734000
1	3.311489000	-1.006405000	0.715198000	6	-5.481340000	1.463623000	1.535951000
1	5.699196000	-1.259475000	0.861776000	6	-5.563461000	0.728521000	-0.852145000
1	5.608644000	-3.019109000	0.886595000	1	-5.419788000	1.753470000	-1.210031000
1	5.186539000	-2.134137000	-0.592047000	1	-5.153353000	0.047128000	-1.602359000
1	4.347764000	-1.406130000	2.961753000	1	-6.639464000	0.545246000	-0.758500000
1	3.888231000	-3.116042000	2.845632000	1	-5.549936000	2.488280000	1.155178000
1	2.640877000	-1.856448000	2.916467000	1	-4.888052000	1.484914000	2.453566000
1	-1.182812000	-2.322512000	-0.356314000	1	-6.495176000	1.125633000	1.779346000

6	-1.833861000	-3.931512000	-0.223514000	1	5.362466000	-2.482336000	-0.301705000
6	-1.511724000	-3.902961000	2.257352000	1	4.346214000	-1.987782000	-3.227762000
6	3.452037000	-2.006626000	-1.243868000	1	2.930011000	-3.049224000	-3.104697000
6	4.741562000	-1.606484000	-0.518511000	1	4.468919000	-3.546544000	-2.397769000
6	3.813179000	-2.685843000	-2.572948000	1	-0.133467000	0.012057000	-3.473637000
6	0.358143000	-1.246830000	-1.842025000	1	0.311626000	5.660486000	1.126492000
6	0.156137000	0.016362000	-2.428610000	1	2.738514000	5.904975000	1.529238000
6	0.524324000	1.264295000	-1.896289000	1	4.288013000	4.127230000	0.832836000
7	0.860777000	1.429914000	-0.617012000	1	3.289850000	0.775509000	-0.155958000
6	1.364217000	2.685845000	-0.123299000	1	5.711563000	0.982066000	0.011983000
6	0.472377000	3.714459000	0.231444000	1	5.639904000	2.739347000	-0.036224000
6	0.992044000	4.866226000	0.830896000	1	5.010053000	1.868579000	1.374071000
6	2.352088000	5.007487000	1.055648000	1	4.671640000	1.065218000	-2.236944000
6	3.224845000	3.998087000	0.662796000	1	4.263871000	2.789617000	-2.239725000
6	2.756763000	2.825484000	0.067491000	1	2.995108000	1.571515000	-2.464259000
6	3.730020000	1.750506000	-0.400913000	1	-1.225573000	2.706145000	-0.566027000
6	5.095518000	1.843451000	0.282778000	1	-2.548835000	4.697926000	-1.150683000
6	3.918706000	1.798119000	-1.924094000	1	-1.396909000	5.758200000	-0.342506000
6	-1.022444000	3.632945000	-0.024180000	1	-0.912834000	4.903438000	-1.811704000
6	-1.491736000	4.811982000	-0.886647000	1	-2.893325000	3.467042000	1.059426000
6	-1.825686000	3.574667000	1.276720000	1	-1.680829000	4.487225000	1.867870000
6	0.499525000	2.440273000	-2.840589000	1	-1.540424000	2.717380000	1.889215000
6	0.254185000	-2.422997000	-2.784591000	1	-0.511776000	2.867444000	-2.841620000
6	1.040041000	0.053697000	2.445209000	1	0.729879000	2.124618000	-3.859931000
6	0.480777000	-1.151114000	3.217091000	1	1.195419000	3.225555000	-2.540242000
6	2.568423000	-0.052919000	2.456346000	1	0.902494000	-2.275539000	-3.652174000
6	0.637061000	1.329489000	3.200678000	1	-0.775708000	-2.470131000	-3.157152000
1	4.186730000	-4.324805000	-0.131998000	1	0.495292000	-3.374285000	-2.310901000
1	2.870070000	-5.904465000	1.234234000	1	-0.615095000	-1.202379000	3.184482000
1	0.500525000	-5.420281000	1.733128000	1	0.773483000	-1.094363000	4.278614000
1	-1.210505000	-2.254386000	0.936003000	1	0.868431000	-2.098991000	2.825478000
1	-2.903158000	-3.818058000	-0.023879000	1	3.041049000	0.842212000	2.036208000
1	-1.621431000	-3.427964000	-1.169630000	1	2.938395000	-0.154691000	3.490213000
1	-1.605126000	-4.998945000	-0.332350000	1	2.924367000	-0.929754000	1.899104000
1	-2.507101000	-3.500047000	2.468600000	1	0.995149000	2.243152000	2.708075000
1	-0.854269000	-3.645456000	3.093255000	1	-0.449962000	1.412000000	3.316438000
1	-1.600811000	-4.995005000	2.220283000	1	1.068717000	1.317468000	4.215368000
1	2.892504000	-1.090537000	-1.466637000	1	-3.040164000	-0.709664000	3.920466000
1	5.335012000	-0.937034000	-1.150990000	13	0.268891000	0.081154000	0.613143000
1	4.538791000	-1.097437000	0.428235000				

4 (in gas phase)				6	2.719264000	2.606591000	3.705523000
7	1.499142000	0.005921000	0.803995000	1	2.038698000	1.919727000	4.215671000
7	-1.499092000	-0.006501000	0.803927000	1	2.278319000	3.608835000	3.735508000
6	2.882318000	-0.536547000	-1.616442000	1	3.662097000	2.638733000	4.262917000
6	4.210109000	-0.154919000	-1.383735000	6	2.517585000	-2.777037000	0.853479000
1	4.433224000	0.658974000	-0.697335000	1	1.759396000	-2.369227000	0.178194000
6	5.250396000	-0.817686000	-2.028221000	6	3.487125000	-3.628022000	0.022279000
1	6.276544000	-0.518626000	-1.840404000	1	4.160342000	-3.007860000	-0.573985000
6	4.971874000	-1.857154000	-2.914230000	1	2.928349000	-4.284188000	-0.654191000
1	5.783525000	-2.361967000	-3.429295000	1	4.098290000	-4.269024000	0.667702000
6	3.656424000	-2.263027000	-3.120723000	6	1.812598000	-3.671161000	1.883495000
1	3.438565000	-3.090880000	-3.787927000	1	1.058488000	-3.119735000	2.449375000
6	2.613908000	-1.616882000	-2.461705000	1	2.542595000	-4.078357000	2.592653000
1	1.590877000	-1.950751000	-2.602320000	1	1.331764000	-4.518615000	1.379389000
6	-2.881974000	0.537196000	-1.616273000	6	-2.742784000	0.281742000	1.488323000
6	-4.209895000	0.155869000	-1.383830000	6	-3.225812000	1.611393000	1.525263000
1	-4.433292000	-0.658494000	-0.698082000	6	-4.411447000	1.875978000	2.211395000
6	-5.249973000	0.819564000	-2.027697000	1	-4.786266000	2.895381000	2.241461000
1	-6.276216000	0.520712000	-1.840073000	6	-5.121636000	0.868685000	2.850395000
6	-4.971127000	1.859679000	-2.912837000	1	-6.046717000	1.095901000	3.371624000
1	-5.782622000	2.365240000	-3.427416000	6	-4.628679000	-0.426104000	2.828380000
6	-3.655541000	2.265255000	-3.119041000	1	-5.169472000	-1.216069000	3.343260000
1	-3.437416000	3.093621000	-3.785521000	6	-3.436196000	-0.742322000	2.170059000
6	-2.613232000	1.618190000	-2.460603000	6	-2.516287000	2.776563000	0.853987000
1	-1.590111000	1.951892000	-2.600919000	1	-1.758994000	2.368531000	0.177855000
6	2.742666000	-0.282183000	1.488750000	6	-1.809593000	3.668431000	1.884784000
6	3.435380000	0.741937000	2.171155000	1	-1.055927000	3.115273000	2.449600000
6	4.627563000	0.425928000	2.830095000	1	-2.538706000	4.075589000	2.594875000
1	5.167844000	1.215939000	3.345439000	1	-1.327909000	4.515951000	1.381602000
6	5.120868000	-0.868733000	2.852134000	6	-3.485013000	3.629770000	0.024150000
1	6.045694000	-1.095801000	3.373879000	1	-4.159389000	3.011144000	-0.572411000
6	4.411374000	-1.876074000	2.212464000	1	-2.925583000	4.285751000	-0.651968000
1	4.786472000	-2.895376000	2.242535000	1	-4.094940000	4.271065000	0.670452000
6	3.226071000	-1.611712000	1.525643000	6	-2.940473000	-2.176373000	2.249440000
6	2.939304000	2.175875000	2.250358000	1	-1.970237000	-2.221791000	1.756182000
1	1.969135000	2.220995000	1.756929000	6	-3.890321000	-3.146496000	1.537438000
6	3.889103000	3.146074000	1.538372000	1	-3.492274000	-4.166167000	1.578614000
1	4.020818000	2.882806000	0.483279000	1	-4.021754000	-2.883364000	0.482276000
1	4.876238000	3.149983000	2.014915000	1	-4.877559000	-3.150182000	2.013764000
1	3.490876000	4.165687000	1.579306000	6	-2.720733000	-2.606867000	3.704717000

1	-2.040044000	-1.920093000	4.214836000	1	6.337903000	1.758239000	1.375131000
1	-2.280065000	-3.609221000	3.734975000	6	4.985458000	3.424983000	1.576437000
1	-3.663653000	-2.638591000	4.261994000	1	5.774653000	4.143093000	1.777107000
15	-1.524306000	-0.362314000	-0.799020000	6	3.660532000	3.847159000	1.507500000
6	-1.873270000	-2.130835000	-1.119496000	1	3.413753000	4.894920000	1.645600000
6	-1.101858000	-3.053500000	-0.398937000	6	2.644799000	2.926373000	1.262543000
6	-2.746839000	-2.591969000	-2.105354000	1	1.611466000	3.254065000	1.203985000
6	-1.241333000	-4.415636000	-0.625521000	6	-2.550402000	-0.124157000	1.977068000
1	-0.396052000	-2.699161000	0.352058000	6	-3.941454000	-0.194030000	1.821571000
6	-2.881876000	-3.961971000	-2.335180000	1	-4.419794000	0.252950000	0.952757000
1	-3.323315000	-1.889267000	-2.698590000	6	-4.717248000	-0.841682000	2.778396000
6	-2.140482000	-4.872216000	-1.591249000	1	-5.793785000	-0.893693000	2.651101000
1	-0.652629000	-5.122510000	-0.048862000	6	-4.112308000	-1.423094000	3.892064000
1	-3.568114000	-4.312811000	-3.099604000	1	-4.721076000	-1.921469000	4.640371000
1	-2.252601000	-5.937636000	-1.767328000	6	-2.728664000	-1.376543000	4.037866000
15	1.524407000	0.362189000	-0.798797000	1	-2.252588000	-1.839878000	4.896232000
6	1.872940000	2.130885000	-1.118922000	6	-1.947535000	-0.730752000	3.082558000
6	2.746256000	2.592430000	-2.104815000	1	-0.868092000	-0.691956000	3.198463000
6	1.101282000	3.053216000	-0.398218000	6	2.810892000	-0.440816000	-1.352409000
6	2.880796000	3.962501000	-2.334515000	6	3.343537000	-1.749507000	-1.350790000
1	3.322930000	1.890004000	-2.698183000	6	4.602179000	-1.971432000	-1.916678000
6	1.240219000	4.415423000	-0.624703000	1	5.013757000	-2.977114000	-1.903219000
1	0.395674000	2.698511000	0.352765000	6	5.319856000	-0.945804000	-2.510843000
6	2.139128000	4.872416000	-1.590457000	1	6.298324000	-1.135783000	-2.941619000
1	3.566849000	4.313652000	-3.098963000	6	4.753827000	0.318189000	-2.583479000
1	0.651301000	5.122047000	-0.047956000	1	5.289686000	1.114549000	-3.092211000
1	2.250840000	5.937892000	-1.766460000	6	3.503208000	0.596107000	-2.027069000
6	0.000139000	-0.000198000	-1.532286000	6	2.587313000	-2.956632000	-0.828498000
17	0.000276000	-0.000195000	-3.307038000	1	1.649154000	-2.598674000	-0.402602000
13	-0.000023000	-0.001878000	1.994999000	6	3.372263000	-3.706894000	0.254512000
1	0.035534000	-1.345687000	2.850980000	1	3.684364000	-3.043698000	1.067995000
1	-0.035580000	1.339449000	2.854851000	1	4.269409000	-4.173746000	-0.167337000
				1	2.756665000	-4.505031000	0.684107000
				6	2.237116000	-3.907206000	-1.982238000
4-TS1 (in gas phase)				1	1.635450000	-3.409771000	-2.748921000
7	1.547024000	-0.167250000	-0.687561000	1	1.667023000	-4.764470000	-1.606699000
7	-1.501230000	-0.059659000	-0.672916000	1	3.145440000	-4.292764000	-2.458913000
6	2.951631000	1.571985000	1.105222000	6	2.932574000	1.986436000	-2.263454000
6	4.291341000	1.160177000	1.118832000	1	2.042839000	2.111240000	-1.639020000
1	4.544309000	0.115978000	0.947302000	6	3.920212000	3.108163000	-1.920964000
6	5.303111000	2.084945000	1.360087000				

1	4.379042000	2.963880000	-0.942451000	6	-2.195848000	4.575112000	-0.456601000
1	3.403193000	4.073625000	-1.922245000	1	-0.974557000	2.898819000	-1.026117000
1	4.722310000	3.170216000	-2.664719000	6	-3.637771000	4.237418000	1.448725000
6	2.516234000	2.121945000	-3.736830000	1	-3.551237000	2.296778000	2.368741000
1	1.841026000	1.322195000	-4.047590000	6	-3.156916000	5.056553000	0.433360000
1	3.403185000	2.089408000	-4.380125000	1	-1.807897000	5.216900000	-1.241373000
1	2.007959000	3.078096000	-3.902782000	1	-4.368881000	4.616536000	2.155737000
6	-2.726973000	-0.736086000	-1.067768000	1	-3.519964000	6.075513000	0.339981000
6	-2.927215000	-2.072835000	-0.657709000	15	1.625360000	0.345145000	0.872164000
6	-4.092366000	-2.734584000	-1.047127000	6	2.029435000	-0.990167000	2.068377000
1	-4.246216000	-3.763631000	-0.735468000	6	2.961610000	-0.866816000	3.101991000
6	-5.057717000	-2.098160000	-1.813846000	6	1.207563000	-2.124141000	2.036323000
1	-5.962869000	-2.623418000	-2.103224000	6	3.102071000	-1.882677000	4.048507000
6	-4.848659000	-0.787976000	-2.216908000	1	3.575217000	0.022887000	3.186956000
1	-5.595466000	-0.292447000	-2.831362000	6	1.342522000	-3.133066000	2.979913000
6	-3.687944000	-0.088887000	-1.874103000	1	0.458631000	-2.217283000	1.256241000
6	-1.916860000	-2.813707000	0.198199000	6	2.302234000	-3.017712000	3.985779000
1	-1.302658000	-2.054973000	0.682802000	1	3.835854000	-1.776030000	4.841227000
6	-0.995984000	-3.697994000	-0.650177000	1	0.705078000	-4.010774000	2.926242000
1	-0.436343000	-3.120734000	-1.390984000	1	2.416020000	-3.806143000	4.723314000
1	-1.577491000	-4.453183000	-1.190993000	6	0.101850000	1.030412000	1.330562000
1	-0.270652000	-4.219970000	-0.010961000	17	0.119933000	1.841293000	2.915040000
6	-2.570903000	-3.643177000	1.307249000	13	0.003401000	0.011222000	-1.834848000
1	-3.340322000	-3.072376000	1.833908000	1	0.066238000	1.365833000	-2.640873000
1	-1.813916000	-3.951498000	2.037692000	1	0.396632000	-1.426282000	-2.618476000
1	-3.028885000	-4.555441000	0.909353000	6	-0.693365000	-1.722637000	-3.658120000
6	-3.533071000	1.325701000	-2.409141000	8	-0.434459000	-2.804173000	-4.057263000
1	-2.531612000	1.675714000	-2.148038000	8	-1.392301000	-0.739035000	-3.655030000
6	-4.572951000	2.266804000	-1.784643000				
1	-4.409780000	3.294795000	-2.125286000		4-IM1 (in gas phase)		
1	-4.533795000	2.265109000	-0.691691000	7	1.500009000	-0.095950000	-0.631701000
1	-5.583820000	1.969226000	-2.087225000	7	-1.469068000	-0.054205000	-0.723242000
6	-3.657875000	1.385848000	-3.938249000	6	2.785209000	1.757009000	1.130898000
1	-2.960395000	0.702926000	-4.423180000	6	4.114646000	1.332784000	1.258336000
1	-3.449736000	2.404925000	-4.281436000	1	4.359449000	0.273886000	1.207043000
1	-4.674016000	1.133654000	-4.261721000	6	5.128784000	2.265800000	1.456147000
15	-1.510872000	0.759311000	0.763843000	1	6.155200000	1.929435000	1.561017000
6	-2.243731000	2.429469000	0.657336000	6	4.824114000	3.624265000	1.513470000
6	-1.732475000	3.271592000	-0.338473000	1	5.614225000	4.350221000	1.679135000
6	-3.179735000	2.925385000	1.566044000	6	3.511947000	4.052877000	1.329011000

1	3.276996000	5.112278000	1.342084000	1	1.756210000	1.145070000	-3.897316000
6	2.494404000	3.124567000	1.127517000	1	3.317035000	1.824168000	-4.371930000
1	1.472126000	3.457446000	0.977157000	1	1.977632000	2.903062000	-3.921038000
6	-2.549143000	-0.333484000	1.892647000	6	-2.584351000	-0.795836000	-1.263413000
6	-3.826512000	-0.840958000	1.605612000	6	-2.682501000	-2.184858000	-1.036749000
1	-4.330687000	-0.580146000	0.678270000	6	-3.863311000	-2.837654000	-1.399211000
6	-4.454947000	-1.691813000	2.508614000	1	-3.959862000	-3.902132000	-1.201762000
1	-5.435698000	-2.091996000	2.271966000	6	-4.904974000	-2.158003000	-2.014568000
6	-3.824853000	-2.035671000	3.704076000	1	-5.820119000	-2.679980000	-2.277289000
1	-4.317942000	-2.704023000	4.403431000	6	-4.742140000	-0.818845000	-2.347321000
6	-2.567604000	-1.519063000	4.002167000	1	-5.521808000	-0.305749000	-2.903452000
1	-2.073523000	-1.778386000	4.933391000	6	-3.582225000	-0.121998000	-2.001979000
6	-1.931692000	-0.666940000	3.101351000	6	-1.535349000	-3.016300000	-0.486351000
1	-0.950237000	-0.269852000	3.338235000	1	-0.667077000	-2.351813000	-0.400819000
6	2.811037000	-0.417924000	-1.182468000	6	-1.177396000	-4.147559000	-1.464356000
6	3.374310000	-1.706928000	-1.024890000	1	-1.033945000	-3.791662000	-2.486899000
6	4.666278000	-1.941123000	-1.509509000	1	-1.965883000	-4.908171000	-1.479270000
1	5.104235000	-2.925930000	-1.374507000	1	-0.253396000	-4.639480000	-1.142687000
6	5.389314000	-0.963047000	-2.169673000	6	-1.826933000	-3.630327000	0.888734000
1	6.388371000	-1.171766000	-2.539835000	1	-1.966924000	-2.878071000	1.668281000
6	4.806518000	0.277887000	-2.375669000	1	-0.996265000	-4.284691000	1.181928000
1	5.352221000	1.040420000	-2.923141000	1	-2.733664000	-4.244903000	0.849560000
6	3.530817000	0.575107000	-1.895951000	6	-3.375892000	1.282591000	-2.543493000
6	2.672233000	-2.897061000	-0.385561000	1	-2.522997000	1.726824000	-2.029199000
1	1.659153000	-2.589260000	-0.109681000	6	-4.578983000	2.203547000	-2.331191000
6	3.409154000	-3.372414000	0.875722000	1	-4.333493000	3.217908000	-2.661968000
1	3.562963000	-2.565275000	1.597446000	1	-4.865888000	2.251285000	-1.275588000
1	4.391187000	-3.779648000	0.610358000	1	-5.448445000	1.872191000	-2.909688000
1	2.842131000	-4.167983000	1.370521000	6	-3.003169000	1.193427000	-4.031113000
6	2.565044000	-4.078874000	-1.365995000	1	-2.114183000	0.571631000	-4.180352000
1	2.053850000	-3.821483000	-2.298194000	1	-2.795821000	2.192678000	-4.428707000
1	2.023524000	-4.903928000	-0.890278000	1	-3.824342000	0.756351000	-4.610933000
1	3.559470000	-4.455169000	-1.627949000	15	-1.665588000	0.737452000	0.710148000
6	2.962308000	1.943400000	-2.236875000	6	-2.675873000	2.260476000	0.648430000
1	2.110855000	2.146399000	-1.583215000	6	-2.180473000	3.325208000	-0.117191000
6	3.969221000	3.080359000	-2.029304000	6	-3.869314000	2.419679000	1.355834000
1	4.471860000	3.001822000	-1.062740000	6	-2.890826000	4.515326000	-0.201060000
1	3.452219000	4.044581000	-2.073033000	1	-1.238006000	3.208627000	-0.647758000
1	4.734187000	3.088177000	-2.813296000	6	-4.575544000	3.619793000	1.274976000
6	2.466879000	1.950630000	-3.691477000	1	-4.247593000	1.620557000	1.983805000

6	-4.092528000	4.662516000	0.492716000	1	-7.774440000	-3.034126000	0.113183000
1	-2.505644000	5.331552000	-0.804125000	1	-7.019684000	-3.585670000	1.621854000
1	-5.501616000	3.735960000	1.829066000	1	-6.403013000	-4.168799000	0.068575000
1	-4.645387000	5.594758000	0.428515000	1	-5.678464000	-0.145524000	1.408916000
15	1.466949000	0.522573000	0.905275000	1	-7.366064000	-0.669753000	1.176036000
6	1.752717000	-0.731490000	2.206372000	1	-6.386335000	-1.365829000	2.487976000
6	2.606401000	-0.547626000	3.297310000	1	-7.414568000	-0.763493000	-1.392543000
6	0.898549000	-1.841513000	2.191681000	1	-6.065685000	-0.210373000	-2.401833000
6	2.647380000	-1.493429000	4.321934000	1	-6.235438000	0.412403000	-0.752461000
1	3.235535000	0.333135000	3.361609000	1	-4.869979000	-3.592309000	-1.552587000
6	0.934232000	-2.778860000	3.214707000	1	-4.981846000	-2.362558000	-2.824088000
1	0.182789000	-1.957260000	1.381326000	1	-6.465719000	-3.087654000	-2.165542000
6	1.822801000	-2.612307000	4.277329000	13	-0.011953000	-0.569586000	-1.202738000
1	3.320898000	-1.345242000	5.160071000	7	-0.521809000	0.985701000	-0.232729000
1	0.261112000	-3.630597000	3.187002000	7	1.434164000	-1.235703000	-0.171640000
1	1.857941000	-3.345847000	5.076908000	1	0.309587000	-0.235348000	-2.716987000
6	-0.085721000	1.268713000	1.201734000	6	-1.901211000	1.365920000	0.029442000
17	-0.134066000	2.217933000	2.710891000	15	0.631206000	2.180138000	-0.268518000
13	0.037306000	0.437004000	-1.764925000	6	1.640352000	-2.666849000	-0.144132000
1	0.770791000	-2.212343000	-2.134748000	15	2.660859000	-0.189470000	0.166737000
6	0.514342000	-1.868775000	-3.155703000	6	-2.690124000	1.862880000	-1.033166000
8	0.116065000	-0.611780000	-3.198886000	6	-2.450577000	1.252764000	1.331444000
8	0.603852000	-2.607593000	-4.103080000	6	2.182505000	1.394797000	-0.389440000
1	-0.054237000	1.960454000	-2.186387000	6	0.606478000	3.332978000	-1.696600000
				6	0.424295000	3.286067000	1.162828000
				6	2.038239000	-3.344632000	-1.323492000
				6	1.346376000	-3.401150000	1.025293000
				6	4.190650000	-0.722344000	-0.660462000
				6	3.079299000	-0.089397000	1.946387000
				6	-3.956797000	2.378798000	-0.750877000
				6	-2.268591000	1.763807000	-2.491076000
				6	-3.713041000	1.806201000	1.559534000
				6	-1.790886000	0.525092000	2.502205000
				17	3.524358000	2.565803000	-0.467340000
				6	0.363441000	4.702993000	-1.570225000
				6	0.923051000	2.808551000	-2.957816000
				6	-0.771195000	3.993523000	1.364367000
				6	1.470291000	3.419843000	2.080191000
				6	2.185415000	-4.733139000	-1.281497000
				6	2.242286000	-2.658580000	-2.667231000
4-TS2 (in gas phase)							
1	-2.586863000	-1.518703000	0.866859000				
5	-3.595347000	-1.884861000	0.345715000				
8	-4.588232000	-2.545688000	1.075422000				
8	-4.150998000	-1.138988000	-0.696033000				
8	-2.674375000	-3.396834000	-0.512844000				
6	-5.853970000	-2.127555000	0.554106000				
6	-5.488613000	-1.618215000	-0.878414000				
6	-1.580279000	-3.078515000	-0.964243000				
6	-6.821541000	-3.302062000	0.583904000				
6	-6.360631000	-1.000994000	1.456674000				
6	-6.357550000	-0.473274000	-1.380321000				
6	-5.456569000	-2.744080000	-1.914456000				
8	-1.212985000	-1.861365000	-1.163239000				
1	-0.846968000	-3.857128000	-1.232883000				

6	1.526366000	-4.787493000	1.017305000	1	-5.433329000	2.814360000	0.752638000
6	0.789617000	-2.766885000	2.286269000	1	-1.994417000	3.912539000	-2.791779000
6	4.904026000	-1.812155000	-0.143977000	1	-3.545989000	3.292950000	-3.390319000
6	4.628519000	-0.107396000	-1.837429000	1	-2.061284000	2.956911000	-4.282429000
6	2.024199000	0.263597000	2.798790000	1	-2.875822000	-0.334986000	-2.606006000
6	4.377665000	-0.141210000	2.461106000	1	-2.639213000	0.465081000	-4.187871000
1	-4.565241000	2.762536000	-1.565119000	1	-4.082634000	0.800381000	-3.204974000
6	-4.454324000	2.392407000	0.542873000	1	-0.275609000	2.006271000	3.150558000
1	-1.204921000	1.531829000	-2.531393000	1	-0.838290000	0.891172000	4.407882000
6	-2.481498000	3.060632000	-3.276689000	1	-1.877451000	2.212913000	3.861465000
6	-3.005914000	0.596843000	-3.163683000	1	-3.443200000	-0.947081000	2.664517000
1	-4.134176000	1.757959000	2.559481000	1	-3.431828000	0.301573000	3.924317000
1	-1.028448000	-0.143628000	2.080636000	1	-2.248874000	-0.995719000	3.969197000
6	-1.144452000	1.469384000	3.527565000	6	0.683892000	4.996639000	-3.944497000
6	-2.798599000	-0.332634000	3.293333000	1	0.210200000	6.592658000	-2.581523000
6	0.400043000	5.529786000	-2.692892000	1	1.185898000	3.213989000	-5.047368000
1	0.162500000	5.141153000	-0.599645000	1	-1.847775000	5.338293000	2.641727000
6	0.950535000	3.633659000	-4.074307000	6	0.125095000	4.922003000	3.404773000
1	1.142627000	1.748705000	-3.055073000	1	2.131148000	4.322880000	3.913200000
1	-1.591269000	3.907894000	0.655685000	1	2.075729000	-6.534484000	-0.109844000
6	-0.915462000	4.805228000	2.484275000	1	0.112087000	-2.674474000	-3.198098000
6	1.317372000	4.233901000	3.200353000	1	1.036972000	-4.057370000	-3.814439000
1	2.397342000	2.875720000	1.932075000	1	1.206970000	-2.458336000	-4.566780000
1	2.485077000	-5.257150000	-2.184858000	1	4.404311000	-2.968503000	-2.641369000
6	1.949859000	-5.456153000	-0.120260000	1	3.756481000	-2.413908000	-4.196767000
1	2.262163000	-1.576593000	-2.512466000	1	3.530651000	-4.090834000	-3.696609000
6	1.075697000	-2.980356000	-3.613142000	1	1.359907000	-2.413621000	4.352143000
6	3.563975000	-3.058052000	-3.332434000	1	2.742958000	-2.528821000	3.250630000
1	1.306851000	-5.350439000	1.920483000	1	1.863587000	-3.992785000	3.729994000
1	0.658761000	-1.702365000	2.087214000	1	-1.312090000	-3.190460000	1.824134000
6	1.749454000	-2.933962000	3.470748000	1	-0.984350000	-2.853498000	3.529340000
6	-0.590207000	-3.341899000	2.632349000	1	-0.533792000	-4.416174000	2.839424000
1	4.540321000	-2.336980000	0.736495000	1	6.642390000	-3.059456000	-0.337267000
6	6.088872000	-2.222264000	-0.750134000	6	6.554084000	-1.562892000	-1.885581000
6	5.812148000	-0.522769000	-2.440470000	1	6.155510000	-0.029831000	-3.344282000
1	4.047439000	0.699655000	-2.272134000	6	3.544765000	0.403180000	4.661849000
6	2.251886000	0.502845000	4.146881000	1	1.423473000	0.778645000	4.791444000
1	1.019160000	0.369724000	2.394311000	1	5.616312000	0.042217000	4.207063000
6	4.604485000	0.093102000	3.817532000	1	0.709003000	5.641302000	-4.817801000
1	5.220849000	-0.348678000	1.812114000	1	0.004835000	5.552232000	4.280703000

1	7.483136000	-1.876151000	-2.351806000	6	2.171163000	1.366347000	-0.420966000
1	3.724930000	0.585796000	5.716747000	6	0.630379000	3.341055000	-1.713490000
4-IM2 (in gas phase)				6	0.456518000	3.287821000	1.146236000
1	-2.499873000	-1.426873000	0.809784000	6	1.912255000	-3.365532000	-1.334575000
5	-3.440937000	-1.972259000	0.287835000	6	1.226590000	-3.409684000	1.017039000
8	-4.452487000	-2.536807000	1.109696000	6	4.145734000	-0.794220000	-0.643107000
8	-4.047414000	-1.283777000	-0.795734000	6	3.038556000	-0.097527000	1.940991000
8	-2.615613000	-3.341704000	-0.355435000	6	-3.929190000	2.532657000	-0.731264000
6	-5.714392000	-2.100369000	0.609036000	6	-2.293440000	1.849883000	-2.497304000
6	-5.394443000	-1.746076000	-0.879431000	6	-3.670794000	1.957557000	1.577392000
6	-1.559247000	-3.088023000	-0.947744000	6	-1.789922000	0.596675000	2.490231000
6	-6.737873000	-3.213720000	0.790759000	17	3.534269000	2.512105000	-0.510671000
6	-6.134082000	-0.866737000	1.411741000	6	0.430766000	4.717294000	-1.577866000
6	-6.255360000	-0.635223000	-1.466755000	6	0.919826000	2.813756000	-2.979929000
6	-5.436882000	-2.976176000	-1.791570000	6	-0.718548000	4.027406000	1.354036000
8	-1.179767000	-1.914063000	-1.262668000	6	1.512330000	3.398243000	2.055371000
1	-0.906229000	-3.922669000	-1.242669000	6	1.993514000	-4.759978000	-1.304561000
1	-7.696890000	-2.942783000	0.333944000	6	2.165453000	-2.683546000	-2.672556000
1	-6.903749000	-3.385955000	1.858581000	6	1.340363000	-4.803248000	0.995649000
1	-6.385815000	-4.147605000	0.347779000	6	0.739883000	-2.761199000	2.300160000
1	-5.421146000	-0.052106000	1.248910000	6	4.822638000	-1.893626000	-0.098467000
1	-7.137272000	-0.520218000	1.140120000	6	4.620527000	-0.205344000	-1.818873000
1	-6.128698000	-1.124196000	2.475692000	6	1.989524000	0.264684000	2.796671000
1	-7.320797000	-0.883167000	-1.394381000	6	4.341238000	-0.139293000	2.446827000
1	-6.009021000	-0.499283000	-2.524692000	1	-4.532849000	2.942535000	-1.536142000
1	-6.069753000	0.309824000	-0.949402000	6	-4.403684000	2.571681000	0.570979000
1	-4.869578000	-3.804216000	-1.357478000	1	-1.240940000	1.572026000	-2.552681000
1	-4.981176000	-2.711679000	-2.751167000	6	-2.462580000	3.157042000	-3.276748000
1	-6.464194000	-3.309523000	-1.974047000	6	-3.094007000	0.720263000	-3.161408000
13	-0.045129000	-0.547082000	-1.226495000	1	-4.076516000	1.929163000	2.584582000
7	-0.543080000	1.011026000	-0.259630000	1	-1.023024000	-0.062182000	2.062934000
7	1.375284000	-1.243193000	-0.174731000	6	-1.157682000	1.522048000	3.541153000
1	0.271141000	-0.215045000	-2.740537000	6	-2.807972000	-0.282969000	3.241239000
6	-1.907116000	1.434839000	0.018375000	6	0.482722000	5.548379000	-2.696624000
15	0.635482000	2.183013000	-0.290322000	1	0.251732000	5.156148000	-0.603355000
6	1.543806000	-2.679559000	-0.149862000	6	0.962835000	3.643619000	-4.092407000
15	2.620689000	-0.217157000	0.162169000	1	1.107090000	1.748581000	-3.084755000
6	-2.689769000	1.963085000	-1.033325000	1	-1.545117000	3.963551000	0.650623000
6	-2.438574000	1.347901000	1.329203000	6	-0.833630000	4.845166000	2.472859000
				6	1.388859000	4.218948000	3.174406000

6	3.949466000	0.642280000	2.474772000	6	6.591507000	-1.139370000	-1.237437000
6	1.601663000	0.271599000	2.873378000	1	6.295710000	0.324810000	-2.788138000
15	0.332130000	2.252214000	-0.453883000	6	3.012385000	1.040714000	4.667303000
17	3.183464000	2.757623000	-0.475350000	1	5.080896000	1.347453000	4.159299000
6	-2.157277000	1.538464000	0.029103000	1	0.897017000	0.657705000	4.863814000
1	1.589867000	-5.400415000	1.709871000	6	-0.975673000	4.411874000	0.802981000
6	2.216007000	-5.288891000	-0.337602000	6	1.041478000	3.620474000	1.877269000
1	0.541379000	-1.884449000	2.148822000	6	0.395871000	2.392471000	-3.202931000
6	2.057144000	-2.875379000	3.320149000	6	0.192247000	4.555328000	-2.148084000
6	-0.257860000	-3.714103000	2.874875000	6	-3.816400000	2.256506000	1.637579000
1	2.758454000	-4.875251000	-2.366651000	6	-1.644316000	1.356639000	2.531917000
1	2.242323000	-1.218561000	-2.414272000	6	-4.322482000	2.328082000	-0.703651000
6	3.797605000	-2.523744000	-3.143562000	6	-2.742898000	1.549728000	-2.483472000
6	1.400054000	-2.620887000	-3.794974000	1	7.604667000	-1.378323000	-1.545913000
1	4.289613000	-1.999901000	1.105161000	1	3.138926000	1.342930000	5.702325000
6	6.016458000	-1.809655000	-0.159106000	1	-1.722952000	4.331996000	0.016278000
6	5.860199000	-0.179533000	-1.931490000	6	-1.110816000	5.391090000	1.783261000
1	3.984024000	0.862948000	-2.092164000	6	0.894367000	4.593294000	2.862711000
6	4.103024000	1.039016000	3.802969000	1	1.880411000	2.931657000	1.920840000
1	4.807327000	0.655449000	1.809963000	6	0.397749000	2.998880000	-4.451640000
6	1.755637000	0.658783000	4.198430000	1	0.493804000	1.311515000	-3.122635000
1	0.624269000	-0.008237000	2.500553000	6	0.202940000	5.161992000	-3.404275000
6	0.116247000	3.533184000	0.832112000	1	0.147015000	5.175201000	-1.259791000
6	0.262957000	3.164965000	-2.040321000	1	-4.119298000	2.419934000	2.667419000
6	-2.552543000	1.730626000	1.375291000	6	-4.698983000	2.564541000	0.609098000
6	-3.057544000	1.818613000	-1.021731000	1	-0.620654000	1.460164000	2.173946000
1	2.452095000	-6.346649000	-0.408489000	6	-1.863704000	-0.105819000	2.942632000
1	2.912295000	-2.288042000	2.971508000	6	-1.787147000	2.277715000	3.745646000
1	2.404027000	-3.896555000	3.517445000	1	-5.020215000	2.539803000	-1.509626000
1	1.720973000	-2.441832000	4.268475000	1	-1.697106000	1.255016000	-2.555339000
1	-1.116272000	-3.734611000	2.202309000	6	-2.946337000	2.789242000	-3.360891000
1	-0.576088000	-3.265681000	3.822623000	6	-3.572822000	0.370455000	-3.004797000
1	0.039360000	-4.746968000	3.088746000	1	-1.956942000	6.070141000	1.750198000
1	4.526803000	-2.518675000	-2.331168000	6	-0.170743000	5.488288000	2.807733000
1	4.079246000	-1.755604000	-3.871365000	1	1.619140000	4.651689000	3.668615000
1	3.866937000	-3.491980000	-3.652045000	6	0.292953000	4.386426000	-4.554132000
1	0.377205000	-2.321368000	-3.580280000	1	0.485809000	2.389791000	-5.345793000
1	1.403498000	-3.699442000	-3.990071000	1	0.146837000	6.243492000	-3.477716000
1	1.741085000	-2.112964000	-4.704740000	1	-5.681128000	2.970008000	0.833602000
1	6.572320000	-2.578629000	0.367508000	1	-1.766427000	-0.797046000	2.098611000

1	-2.869929000	-0.241739000	3.353096000	5 (in gas phase)			
1	-1.150558000	-0.401217000	3.724198000	13	0.000046000	-0.462193000	-0.000711000
1	-1.762376000	3.331250000	3.453917000	7	-1.746002000	-0.243820000	1.044626000
1	-0.961471000	2.101032000	4.443213000	7	1.746175000	-0.241064000	-1.045341000
1	-2.718834000	2.089311000	4.290856000	8	-0.837890000	0.383284000	-1.372970000
1	-2.631495000	2.574429000	-4.387298000	8	0.838638000	0.377710000	1.374536000
1	-2.360455000	3.641180000	-2.999303000	6	-4.746008000	-0.912056000	-1.055083000
1	-3.999960000	3.088053000	-3.394475000	6	-3.067150000	-2.564874000	-0.158698000
1	-3.418952000	-0.532844000	-2.403815000	6	-2.778708000	2.460519000	0.791437000
1	-3.290507000	0.142549000	-4.038357000	6	-3.747559000	3.329308000	1.602641000
1	-4.643089000	0.612213000	-2.993019000	6	-2.089103000	3.296701000	-0.295022000
1	-0.277660000	6.253773000	3.570410000	6	-2.546279000	-3.065008000	-1.511142000
1	0.296314000	4.860567000	-5.530893000	6	-4.123403000	-3.524649000	0.402056000
5	-2.673870000	-2.730779000	0.035236000	6	-2.973133000	-0.053524000	0.326851000
8	-1.784263000	-3.879365000	0.018914000	6	-1.772808000	-0.343423000	2.348862000
8	-3.363587000	-2.627667000	1.245922000	6	-0.574809000	-0.319522000	3.132576000
8	-3.528117000	-2.522001000	-1.061961000	6	0.629361000	0.116319000	2.631331000
6	-1.011539000	-4.085021000	-1.025362000	6	-3.471586000	1.254259000	0.175857000
6	-4.726667000	-2.299292000	0.932114000	6	-3.085493000	-0.402895000	3.091026000
6	-4.850494000	-2.761625000	-0.556705000	6	1.822974000	0.370478000	3.505744000
1	-0.546679000	-5.081231000	-1.009328000	6	-5.249322000	0.371318000	-1.221305000
8	-0.801791000	-3.274052000	-1.898721000	6	5.249589000	0.368071000	1.221957000
6	-5.633516000	-3.041269000	1.903546000	6	4.612008000	1.440700000	0.609088000
6	-4.908547000	-0.795248000	1.077915000	6	3.472133000	1.254571000	-0.173291000
6	-5.124977000	-4.262538000	-0.682228000	6	2.973420000	-0.052749000	-0.327283000
6	-5.852121000	-1.974245000	-1.386464000	6	3.602965000	-1.149601000	0.282995000
1	-5.479892000	-2.652250000	2.914469000	6	4.746055000	-0.914830000	1.052730000
1	-5.412998000	-4.110513000	1.913413000	6	3.066837000	-2.565209000	0.152477000
1	-6.686462000	-2.897038000	1.636481000	6	2.779322000	2.462305000	-0.786034000
1	-4.643216000	-0.497632000	2.094995000	6	3.748466000	3.334013000	-1.593726000
1	-4.255835000	-0.258312000	0.382080000	6	2.088143000	3.294788000	0.302265000
1	-5.944036000	-0.491671000	0.891519000	6	2.545290000	-3.068077000	1.503640000
1	-6.144906000	-4.515733000	-0.375988000	6	4.122998000	-3.524106000	-0.409946000
1	-4.421255000	-4.837377000	-0.071833000	6	-3.602908000	-1.148827000	-0.285961000
1	-4.989888000	-4.554794000	-1.727350000	6	1.772667000	-0.337168000	-2.349842000
1	-6.867192000	-2.115083000	-0.998177000	6	0.574449000	-0.310759000	-3.133156000
1	-5.825817000	-2.329063000	-2.421295000	6	-0.629289000	0.124628000	-2.630468000
1	-5.618340000	-0.907929000	-1.384604000	6	-4.611480000	1.442402000	-0.606011000
				6	3.085158000	-0.394946000	-3.092480000
				6	-1.823039000	0.381611000	-3.503868000

6	3.404551000	1.473398000	-0.003414000	1	3.582009000	1.141690000	-2.908306000
6	3.097948000	0.177421000	-3.099951000	1	2.963069000	0.061545000	-4.175723000
6	-1.833434000	0.846102000	-3.496382000	1	3.774169000	-0.597234000	-2.729227000
6	5.267275000	0.478234000	1.191277000	1	-2.642942000	0.151787000	-3.244534000
6	-5.175725000	1.087723000	-1.074911000	1	-1.618530000	0.797960000	-4.564847000
6	-4.349807000	2.019118000	-0.456911000	1	-2.187273000	1.849043000	-3.233307000
6	-3.211612000	1.622221000	0.245478000	1	6.163941000	0.593497000	1.792635000
6	-2.921296000	0.248038000	0.326411000	1	-6.055494000	1.414453000	-1.620901000
6	-3.741940000	-0.708617000	-0.290804000	1	-4.587849000	3.077692000	-0.527931000
6	-4.867400000	-0.263221000	-0.989872000	1	-5.508917000	-0.992370000	-1.477610000
6	-3.411535000	-2.189309000	-0.268390000	1	-2.629953000	-2.347107000	0.479914000
6	-2.315286000	2.683472000	0.866913000	1	-1.478880000	2.183433000	1.366922000
6	-3.066959000	3.506152000	1.921142000	1	-2.394446000	4.231734000	2.390061000
6	-1.724160000	3.603833000	-0.208382000	1	-3.483776000	2.870255000	2.708461000
6	-2.862727000	-2.630907000	-1.631116000	1	-3.895348000	4.062018000	1.468666000
6	-4.605685000	-3.059304000	0.137910000	1	-1.083398000	4.363192000	0.252111000
6	3.667869000	-0.961733000	0.065783000	1	-2.516417000	4.124024000	-0.758482000
6	-1.774110000	-0.377727000	2.294034000	1	-1.128942000	3.028606000	-0.923511000
6	-0.606490000	-0.518526000	3.105659000	1	-2.516237000	-3.667539000	-1.587614000
6	0.647786000	-0.164298000	2.666494000	1	-2.012551000	-2.011592000	-1.931671000
6	4.558982000	1.597524000	0.770481000	1	-3.645096000	-2.547097000	-2.395504000
6	-3.111481000	-0.449547000	2.989939000	1	-4.285321000	-4.100689000	0.238790000
6	1.831973000	-0.065729000	3.582440000	1	-5.400109000	-3.029778000	-0.615327000
1	-0.481719000	-2.814943000	1.450730000	1	-5.037665000	-2.737287000	1.091506000
1	5.375808000	-1.664067000	1.162116000	1	-0.739368000	-0.761537000	4.151681000
1	2.318475000	-2.296487000	-0.913975000	1	4.905715000	2.588244000	1.053201000
1	1.861494000	2.441372000	-1.125356000	1	-3.631327000	0.510516000	2.914481000
1	2.942900000	4.605313000	-1.443608000	1	-2.991590000	-0.708611000	4.042098000
1	4.083017000	3.336543000	-1.930498000	1	-3.751129000	-1.193132000	2.503931000
1	4.281788000	4.163778000	-0.380652000	1	2.641552000	-0.689602000	3.187984000
1	1.385156000	4.238902000	0.527044000	1	1.594781000	-0.360165000	4.605708000
1	2.668138000	3.613344000	1.579060000	1	2.198008000	0.966753000	3.570535000
1	1.234536000	2.620846000	1.256610000	6	-0.328254000	-3.072369000	0.381626000
1	2.286035000	-4.045741000	0.787518000	8	-0.000099000	-2.047921000	-0.372443000
1	2.020575000	-2.478121000	1.571594000	8	-0.453347000	-4.207273000	-0.010461000
1	3.605966000	-3.259880000	1.684422000				
1	3.869872000	-4.173336000	-1.247169000		5-TS2 (in gas phase)		
1	5.149159000	-3.337676000	-0.356876000	1	2.089966000	-0.407867000	-3.339981000
1	4.593388000	-2.697110000	-1.908983000	6	1.856061000	-0.620846000	-2.284048000
1	0.708481000	0.212633000	-4.261091000	8	0.739395000	-0.129337000	-1.903755000

8	2.657978000	-1.294517000	-1.637715000	6	1.677358000	1.836452000	2.403700000
5	3.088495000	-1.137403000	0.275570000	6	-3.205302000	-4.750853000	-0.231627000
8	3.490598000	0.204346000	0.355158000	6	-0.161358000	5.201812000	1.069550000
8	4.190746000	-1.989207000	0.353537000	6	-1.049712000	4.358897000	1.729953000
6	4.910530000	0.231775000	0.149583000	6	-1.482090000	3.167213000	1.145413000
6	5.339501000	-1.187479000	0.645662000	6	-1.034950000	2.864112000	-0.153893000
6	6.553162000	-1.769558000	-0.064652000	6	-0.083144000	3.662337000	-0.804691000
6	5.545656000	-1.235106000	2.161503000	6	0.335445000	4.837183000	-0.173814000
6	5.189732000	0.446996000	-1.339628000	6	0.563471000	3.242364000	-2.113748000
6	5.489213000	1.392236000	0.948200000	6	-2.385822000	2.208133000	1.908903000
1	5.115948000	2.336026000	0.537153000	6	-3.866213000	2.406938000	1.551227000
1	5.198775000	1.338075000	2.000009000	6	-2.196517000	2.300062000	3.425377000
1	6.583177000	1.401257000	0.886818000	6	2.020952000	2.826659000	-1.856623000
1	4.657881000	1.346641000	-1.666893000	6	0.496560000	4.338866000	-3.182777000
1	4.833919000	-0.398653000	-1.931360000	6	-1.067131000	-3.602928000	-0.245797000
1	6.259565000	0.590477000	-1.524436000	6	-2.617226000	1.838724000	-1.570011000
1	6.366222000	-1.881824000	-1.134241000	6	-3.271412000	0.781750000	-2.241656000
1	6.777067000	-2.757871000	0.347465000	6	-2.779129000	-0.513778000	-2.286725000
1	7.432221000	-1.130809000	0.078231000	6	-3.817837000	-3.610120000	0.280284000
1	6.451405000	-0.702875000	2.469949000	6	-3.182681000	3.222908000	-1.792375000
1	5.631502000	-2.281033000	2.468513000	6	-3.488205000	-1.610279000	-3.028464000
1	4.684848000	-0.797513000	2.677795000	1	-1.378222000	-5.598921000	-0.972823000
13	-0.515675000	0.008816000	-0.596653000	1	0.803362000	-2.595790000	-0.422070000
7	-0.894111000	-1.354105000	0.751534000	1	-3.195593000	-0.341880000	0.633151000
7	-1.542934000	1.675669000	-0.802781000	1	-4.409202000	-0.242206000	2.892230000
8	-1.689902000	-0.865924000	-1.719025000	1	-2.768397000	-0.893377000	2.972551000
8	0.602610000	0.880102000	0.549588000	1	-4.164594000	-1.990493000	3.019859000
6	-1.847762000	-4.730329000	-0.517576000	1	-5.571781000	-0.047635000	0.711104000
6	0.380411000	-3.562603000	-0.699802000	1	-5.877982000	-1.764151000	0.981516000
6	-3.766637000	-1.188295000	1.038925000	1	-5.233190000	-1.214870000	-0.579620000
6	-3.770464000	-1.071482000	2.570376000	1	1.489651000	-3.562111000	-2.559200000
6	-5.194930000	-1.054015000	0.502731000	1	-0.145558000	-2.869387000	-2.691782000
6	0.451228000	-3.662802000	-2.229072000	1	0.070171000	-4.628340000	-2.581350000
6	1.252828000	-4.636698000	-0.044159000	1	2.297870000	-4.490168000	-0.334755000
6	-1.684658000	-2.501752000	0.363935000	1	0.945002000	-5.643130000	-0.351701000
6	-0.430161000	-1.348516000	2.001868000	1	1.201514000	-4.587919000	1.048014000
6	0.309791000	-0.284664000	2.558780000	1	0.586835000	-0.350704000	3.602612000
6	0.814178000	0.767865000	1.807503000	1	-0.398889000	-2.310155000	3.925616000
6	-3.077655000	-2.461191000	0.564043000	1	0.027829000	-3.350536000	2.553582000
6	-0.642757000	-2.551721000	2.890457000	1	-1.660062000	-2.942322000	2.834274000

1	2.664145000	1.751554000	1.937551000	6	5.156202000	-0.911835000	0.530032000
1	1.762304000	1.742670000	3.488041000	6	6.548979000	-1.339563000	0.088615000
1	1.260533000	2.815437000	2.141802000	6	4.865579000	-1.429424000	1.943276000
1	-3.795267000	-5.638839000	-0.437538000	6	5.499093000	1.218242000	-0.857394000
1	0.164709000	6.124566000	1.539657000	6	5.272451000	1.438344000	1.623905000
1	-1.393050000	4.623510000	2.725014000	1	5.061868000	2.497982000	1.442969000
1	1.071059000	5.468972000	-0.664625000	1	4.713111000	1.124384000	2.508835000
1	0.033436000	2.364734000	-2.496822000	1	6.344033000	1.336727000	1.830409000
1	-2.097169000	1.189862000	1.614743000	1	5.061383000	2.207647000	-1.024781000
1	-4.505708000	1.824991000	2.223097000	1	5.282447000	0.594626000	-1.728829000
1	-4.089310000	2.091646000	0.527059000	1	6.584498000	1.328789000	-0.759421000
1	-4.144187000	3.462248000	1.656904000	1	6.712644000	-1.106142000	-0.965573000
1	-2.714706000	1.467196000	3.910895000	1	6.658419000	-2.420701000	0.217979000
1	-2.615579000	3.227203000	3.831783000	1	7.321289000	-0.842839000	0.687289000
1	-1.137459000	2.248581000	3.697779000	1	5.620076000	-1.106432000	2.668771000
1	2.468212000	2.434579000	-2.778059000	1	4.852472000	-2.523199000	1.915497000
1	2.091495000	2.060797000	-1.077396000	1	3.880188000	-1.082592000	2.275168000
1	2.613813000	3.693737000	-1.539685000	13	-0.502639000	0.008353000	-0.632768000
1	0.918377000	3.973088000	-4.124270000	7	-0.612879000	-1.454358000	0.659698000
1	1.073023000	5.221528000	-2.885906000	7	-1.769043000	1.514382000	-0.742720000
1	-0.532106000	4.661876000	-3.373540000	8	-1.561075000	-0.999791000	-1.750365000
1	-4.174235000	1.010868000	-2.791869000	8	0.513516000	1.011625000	0.490861000
1	-4.891071000	-3.611096000	0.444433000	6	-1.252746000	-4.895618000	-0.615593000
1	-3.281518000	3.782547000	-0.860292000	6	0.807917000	-3.448472000	-0.922078000
1	-4.151486000	3.166271000	-2.289743000	6	-3.483848000	-1.624161000	1.104365000
1	-2.494567000	3.788893000	-2.430568000	6	-3.438447000	-1.517232000	2.636047000
1	-2.846569000	-1.965889000	-3.841010000	6	-4.939859000	-1.663007000	0.629041000
1	-4.445863000	-1.283928000	-3.437395000	6	1.055212000	-4.175827000	-2.247221000
1	-3.639633000	-2.451662000	-2.342330000	6	1.910272000	-3.800430000	0.084368000
1	2.022395000	-1.467726000	0.696097000	6	-1.300069000	-2.672537000	0.291669000
				6	-0.063272000	-1.438992000	1.877435000
				6	0.624855000	-0.330119000	2.410353000
				6	0.884836000	0.838877000	1.704744000
				6	-2.669279000	-2.801413000	0.582353000
				6	-0.167492000	-2.657727000	2.769481000
				6	1.597177000	2.002914000	2.319420000
				6	-2.573479000	-5.085759000	-0.227941000
				6	-0.823357000	5.173278000	1.155586000
				6	-1.528807000	4.188796000	1.839802000
				6	-1.812121000	2.958766000	1.244008000
5-IM2 (in gas phase)							
1	1.912158000	0.376201000	-3.591645000	6	0.884836000	0.838877000	1.704744000
6	1.826635000	0.107877000	-2.530404000	6	-2.669279000	-2.801413000	0.582353000
8	0.660725000	0.175572000	-2.052215000	6	-0.167492000	-2.657727000	2.769481000
8	2.887626000	-0.232304000	-1.973734000	6	1.597177000	2.002914000	2.319420000
5	3.070707000	-0.581259000	-0.375431000	6	-2.573479000	-5.085759000	-0.227941000
8	3.453496000	0.641911000	0.273471000	6	-0.823357000	5.173278000	1.155586000
8	4.190741000	-1.473728000	-0.347987000	6	-1.528807000	4.188796000	1.839802000
6	4.873641000	0.617047000	0.404663000	6	-1.812121000	2.958766000	1.244008000

6	-1.407581000	2.754074000	-0.088144000	1	-1.845874000	4.375301000	2.860902000
6	-0.633159000	3.705688000	-0.767427000	1	0.237016000	5.665738000	-0.640530000
6	-0.360249000	4.917313000	-0.126510000	1	-0.400940000	2.477021000	-2.498813000
6	-0.003713000	3.424420000	-2.120999000	1	-2.124175000	0.903338000	1.678547000
6	-2.524405000	1.865190000	2.026967000	1	-4.560903000	1.215991000	2.455195000
6	-4.037603000	1.882732000	1.762710000	1	-4.280676000	1.561335000	0.744808000
6	-2.251107000	1.938976000	3.531573000	1	-4.435090000	2.893895000	1.909579000
6	1.515402000	3.263692000	-1.947430000	1	-2.637249000	1.038591000	4.019184000
6	-0.313313000	4.512622000	-3.155329000	1	-2.748620000	2.798093000	3.994507000
6	-0.597538000	-3.683388000	-0.387853000	1	-1.178010000	2.005870000	3.738189000
6	-2.893306000	1.526615000	-1.451915000	1	1.981334000	2.976997000	-2.897961000
6	-3.410596000	0.393966000	-2.122188000	1	1.760897000	2.512215000	-1.189509000
6	-2.727123000	-0.806499000	-2.239775000	1	1.964671000	4.213640000	-1.634940000
6	-3.283165000	-4.032637000	0.336394000	1	0.112701000	4.242296000	-4.126782000
6	-3.676073000	2.810238000	-1.607262000	1	0.119837000	5.475181000	-2.863604000
6	-3.306678000	-1.982980000	-2.970837000	1	-1.390580000	4.658123000	-3.285239000
1	-0.724358000	-5.698356000	-1.120559000	1	-4.369719000	0.490211000	-2.613355000
1	0.895636000	-2.378023000	-1.132002000	1	-4.334385000	-4.164804000	0.573274000
1	-3.039123000	-0.711687000	0.684280000	1	-3.790773000	3.341404000	-0.660643000
1	-4.188629000	-0.806044000	2.996167000	1	-4.658200000	2.611135000	-2.037475000
1	-2.461683000	-1.179028000	2.995089000	1	-3.129112000	3.478504000	-2.282117000
1	-3.658169000	-2.490009000	3.091682000	1	-2.653620000	-2.240914000	-3.810356000
1	-5.425056000	-0.708391000	0.855987000	1	-4.315336000	-1.788244000	-3.338789000
1	-5.511859000	-2.448245000	1.135187000	1	-3.316441000	-2.842824000	-2.290431000
1	-5.004701000	-1.830728000	-0.450910000	1	2.001021000	-1.020697000	-0.036796000
1	1.990067000	-3.814563000	-2.686402000				
1	0.242548000	-3.996762000	-2.958804000				
1	1.159077000	-5.257670000	-2.107996000	13	-0.084197000	0.036826000	-0.095225000
1	2.895096000	-3.665944000	-0.372085000	7	-1.029673000	-1.364847000	0.959250000
1	1.803973000	-4.839955000	0.419298000	7	-1.138656000	1.526601000	-0.871431000
1	1.891191000	-3.138888000	0.954472000	8	-0.380655000	-0.986679000	-1.615379000
1	0.998760000	-0.406762000	3.422670000	8	0.133364000	1.046485000	1.453278000
1	0.285987000	-2.456401000	3.740389000	6	-1.146462000	-4.764802000	-0.543135000
1	0.343259000	-3.507737000	2.309672000	6	0.875147000	-3.409710000	0.194789000
1	-1.206080000	-2.962710000	2.913187000	6	-3.769930000	-1.371199000	-0.025933000
1	2.478789000	2.204642000	1.705815000	6	-4.472154000	-1.272809000	1.337516000
1	1.893322000	1.807818000	3.351975000	6	-4.809273000	-1.328731000	-1.150579000
1	0.937626000	2.878062000	2.278722000	6	1.699570000	-4.212885000	-0.812660000
1	-3.061663000	-6.039705000	-0.402947000	6	1.346731000	-3.721172000	1.619883000
1	-0.611574000	6.124227000	1.634595000	6	-1.516384000	-2.537339000	0.270080000

5-TS3 (in gas phase)

6	-1.166053000	-1.386098000	2.282892000	1	1.047115000	-4.732445000	1.922202000
6	-0.765628000	-0.327779000	3.130825000	1	0.950240000	-3.007304000	2.348794000
6	-0.138686000	0.825657000	2.681813000	1	-0.939198000	-0.437022000	4.193005000
6	-2.862092000	-2.591087000	-0.127584000	1	-1.858041000	-2.418435000	4.041382000
6	-1.755644000	-2.600689000	2.971076000	1	-1.105817000	-3.467706000	2.819523000
6	0.288780000	1.911385000	3.628528000	1	-2.729035000	-2.869293000	2.557476000
6	-2.501813000	-4.884596000	-0.832370000	1	1.382153000	1.978661000	3.617120000
6	-0.945494000	5.282411000	1.054601000	1	-0.052224000	1.732840000	4.649718000
6	-1.895357000	4.342995000	1.445914000	1	-0.099543000	2.867926000	3.261872000
6	-1.967388000	3.093382000	0.830116000	1	-2.892831000	-5.813787000	-1.235852000
6	-1.067614000	2.813426000	-0.215744000	1	-0.903051000	6.249613000	1.546383000
6	-0.086766000	3.735932000	-0.607321000	1	-2.583324000	4.585442000	2.249938000
6	-0.047091000	4.972192000	0.045036000	1	0.709817000	5.696799000	-0.242384000
6	0.971131000	3.394657000	-1.641146000	1	0.670441000	2.490577000	-2.177741000
6	-3.006391000	2.070982000	1.266174000	1	-2.551246000	1.076235000	1.171391000
6	-4.239280000	2.126163000	0.351007000	1	-5.047687000	1.505913000	0.750776000
6	-3.439650000	2.230021000	2.725767000	1	-4.015754000	1.770884000	-0.659736000
6	2.288380000	3.068874000	-0.926427000	1	-4.610060000	3.155300000	0.279513000
6	1.178308000	4.503900000	-2.677017000	1	-4.044022000	1.367535000	3.024391000
6	-0.622259000	-3.586381000	-0.008202000	1	-4.054413000	3.125366000	2.870380000
6	-1.801511000	1.477602000	-2.018969000	1	-2.578855000	2.291126000	3.399293000
6	-1.955025000	0.298424000	-2.789385000	1	3.037636000	2.715802000	-1.639240000
6	-1.242471000	-0.864263000	-2.558564000	1	2.142031000	2.270157000	-0.192681000
6	-3.343014000	-3.793021000	-0.657042000	1	2.668773000	3.957279000	-0.405374000
6	-2.407925000	2.732246000	-2.603403000	1	1.863766000	4.153681000	-3.454587000
6	-1.412686000	-2.080229000	-3.423431000	1	1.620600000	5.399981000	-2.227810000
1	1.751112000	-1.256535000	-3.751125000	1	0.238363000	4.800633000	-3.155330000
1	-0.480470000	-5.595709000	-0.753694000	1	-2.601057000	0.343155000	-3.656341000
1	1.104080000	-2.357587000	0.003790000	1	-4.385241000	-3.870162000	-0.951200000
1	-3.132144000	-0.485965000	-0.146948000	1	-2.858016000	3.373753000	-1.844400000
1	-5.280691000	-0.535927000	1.302254000	1	-3.150599000	2.479881000	-3.361672000
1	-3.783902000	-0.971733000	2.133644000	1	-1.609058000	3.309894000	-3.084257000
1	-4.916722000	-2.237748000	1.609210000	1	-0.443844000	-2.367639000	-3.844131000
1	-5.294918000	-0.347602000	-1.164831000	1	-2.128214000	-1.919252000	-4.231584000
1	-5.594760000	-2.078830000	-1.006880000	1	-1.748566000	-2.910850000	-2.791039000
1	-4.344374000	-1.495902000	-2.127285000	6	2.085768000	-0.601952000	-2.931871000
1	2.739789000	-3.881529000	-0.759007000	8	1.962385000	0.592744000	-2.946473000
1	1.340955000	-4.047720000	-1.833688000	8	2.630570000	-1.335699000	-1.961912000
1	1.671983000	-5.288359000	-0.600407000	1	1.513767000	-0.042762000	-0.280420000
1	2.438527000	-3.654866000	1.656761000	5	3.171305000	-0.756715000	-0.797895000

8	3.935474000	0.388254000	-0.777824000	6	-2.691782000	-1.159452000	-0.645490000
8	3.438657000	-1.601774000	0.263571000	6	-3.503363000	-1.637606000	0.398987000
6	4.872162000	0.241766000	0.304911000	6	-4.751187000	-2.163523000	0.065891000
6	4.174498000	-0.819606000	1.221102000	6	-5.180182000	-2.197341000	-1.257546000
6	5.127115000	-1.738666000	1.970016000	6	-4.376540000	-1.686180000	-2.268631000
6	3.173255000	-0.190824000	2.190669000	6	-3.121214000	-1.143809000	-1.982188000
6	6.175119000	-0.276274000	-0.303464000	6	-2.254754000	-0.569036000	-3.091640000
6	5.093748000	1.598916000	0.954041000	6	-3.037477000	0.387597000	-3.996895000
1	5.562832000	2.274219000	0.232467000	6	-1.612922000	-1.693932000	-3.914955000
1	4.149938000	2.046151000	1.272112000	6	-3.009929000	-1.604252000	1.836882000
1	5.756286000	1.507506000	1.822003000	6	-2.280693000	-2.910274000	2.182445000
1	6.497538000	0.418229000	-1.083721000	6	-4.126745000	-1.338581000	2.849128000
1	6.023868000	-1.259197000	-0.760445000	1	0.931690000	-2.665150000	1.684170000
1	6.968597000	-0.354796000	0.446194000	1	1.338474000	-1.833923000	3.986695000
1	5.736261000	-2.326402000	1.280336000	1	3.054248000	-1.599488000	3.603180000
1	4.553246000	-2.429018000	2.595724000	1	1.821978000	-0.624800000	2.787043000
1	5.788932000	-1.158119000	2.621988000	1	1.288326000	-4.286561000	3.398666000
1	3.688533000	0.314950000	3.014508000	1	3.042694000	-4.172057000	3.282342000
1	2.540319000	-0.982801000	2.606699000	1	2.113381000	-4.876869000	1.943939000
1	2.524141000	0.524498000	1.678492000	1	4.403874000	-3.867232000	1.588576000
				1	5.979383000	-3.364895000	-0.233202000
6 (in gas phase)				1	5.431406000	-1.678018000	-1.935816000
7	-1.366897000	-0.683416000	-0.325588000	1	2.673588000	0.705697000	-1.673022000
6	-1.242458000	0.675496000	-0.038299000	1	5.118436000	0.752599000	-2.286777000
6	1.239617000	0.475258000	0.412436000	1	4.015143000	1.188146000	-3.602974000
7	1.371920000	-0.792272000	0.035395000	1	4.773521000	-0.402716000	-3.588707000
6	2.656959000	-1.451900000	-0.013883000	1	1.837968000	-0.025457000	-3.902547000
6	2.934385000	-2.426919000	0.958114000	1	2.495380000	-1.651017000	-3.615053000
6	1.957058000	-2.703952000	2.092586000	1	1.166844000	-1.031423000	-2.622915000
6	2.045487000	-1.622763000	3.178326000	1	3.295189000	0.562731000	1.018275000
6	2.114116000	-4.094516000	2.708159000	1	2.209397000	1.669307000	1.899830000
6	4.150010000	-3.107479000	0.857642000	1	-2.168761000	2.588942000	0.137614000
6	5.038404000	-2.828050000	-0.172873000	1	-3.242447000	1.176463000	-0.395669000
6	4.726474000	-1.873013000	-1.135318000	1	-5.399385000	-2.549452000	0.846218000
6	3.523064000	-1.169339000	-1.085681000	1	-6.152125000	-2.615415000	-1.499006000
6	3.138714000	-0.160405000	-2.161506000	1	-4.730893000	-1.704953000	-3.295157000
6	4.336653000	0.371744000	-2.950408000	1	-1.453633000	0.018180000	-2.625860000
6	2.102553000	-0.753087000	-3.128200000	1	-2.362433000	0.859761000	-4.717364000
6	2.439295000	1.228545000	0.926999000	1	-3.810727000	-0.136348000	-4.567084000
6	-2.267927000	1.542109000	-0.101766000	1	-3.521000000	1.174928000	-3.410997000

6	3.509833000	-0.127037000	-1.291748000	1	-5.246416000	-4.100224000	-1.097754000
6	2.805973000	0.719930000	-2.350509000	1	-4.359072000	-2.698974000	-2.924189000
6	3.782035000	1.388183000	-3.322350000	1	-1.696101000	-0.096368000	-2.409494000
6	1.752810000	-0.067758000	-3.145552000	1	-3.110432000	0.596029000	-4.277263000
6	2.004140000	2.151375000	0.692030000	1	-4.201370000	-0.769616000	-4.031660000
6	-2.680205000	1.086733000	0.161902000	1	-4.088632000	0.498681000	-2.800060000
6	-2.347988000	-1.651225000	-0.401248000	1	-1.183870000	-1.045254000	-4.646740000
6	-2.853655000	-2.428957000	0.658294000	1	-0.746307000	-2.209321000	-3.380806000
6	-3.904484000	-3.306374000	0.378893000	1	-2.228136000	-2.437471000	-4.315252000
6	-4.433958000	-3.408068000	-0.901136000	1	-1.412134000	-1.712191000	2.061271000
6	-3.931865000	-2.617663000	-1.928726000	1	-1.582206000	-3.499610000	3.715723000
6	-2.889841000	-1.718412000	-1.699655000	1	-1.341564000	-4.239150000	2.121623000
6	-2.373633000	-0.846926000	-2.834433000	1	-2.942764000	-4.239229000	2.874473000
6	-3.513044000	-0.087387000	-3.523188000	1	-2.970602000	-1.362704000	3.947075000
6	-1.585023000	-1.682207000	-3.851321000	1	-3.549131000	-0.524053000	2.491382000
6	-2.341650000	-2.294006000	2.083454000	1	-4.301182000	-2.047534000	2.998442000
6	-2.032973000	-3.648509000	2.729789000	1	1.932777000	2.963612000	-0.035607000
6	-3.351325000	-1.506342000	2.930533000	13	0.367917000	-1.572324000	-0.326258000
1	1.756481000	-1.445572000	2.143376000	1	0.864529000	-2.635154000	-1.500968000
1	2.718250000	-0.513552000	4.229851000	7	-0.287675000	1.378167000	0.379505000
1	4.275776000	-0.283799000	3.412608000	6	-0.600019000	2.786730000	0.576033000
1	2.857236000	0.636538000	2.888629000	6	-0.630432000	3.608852000	-0.559852000
1	2.576859000	-3.027262000	3.749649000	6	-0.878155000	3.243833000	1.869169000
1	4.245391000	-2.858296000	3.212791000	6	-0.938600000	4.955335000	-0.362509000
1	3.056964000	-3.640993000	2.158219000	6	-1.177484000	4.601070000	2.011928000
1	5.347159000	-2.198105000	1.458113000	6	-1.205653000	5.448311000	0.910628000
1	6.481978000	-1.664213000	-0.661442000	1	-0.976559000	5.625567000	-1.216504000
1	5.348814000	-0.330730000	-2.385740000	1	-1.399380000	4.996337000	2.999073000
1	2.278610000	1.531329000	-1.831889000	1	-1.443833000	6.498650000	1.043418000
1	4.578243000	1.920812000	-2.794701000	6	-0.896500000	2.325482000	3.080855000
1	3.243277000	2.108950000	-3.943554000	1	-0.615571000	1.315539000	2.756679000
1	4.242071000	0.657489000	-3.995398000	6	-0.374613000	3.078396000	-1.962957000
1	1.369143000	0.544295000	-3.969073000	1	-0.053470000	2.031093000	-1.889699000
1	2.180295000	-0.982175000	-3.569853000	6	-2.310196000	2.245764000	3.672853000
1	0.881504000	-0.346354000	-2.539449000	1	-2.333495000	1.534733000	4.504292000
1	3.018762000	1.756761000	0.699626000	1	-2.626947000	3.221216000	4.056454000
1	1.766690000	2.580480000	1.668375000	1	-3.035493000	1.921735000	2.921486000
1	-2.860027000	2.127308000	0.380465000	6	0.103329000	2.777526000	4.153392000
1	-3.533411000	0.450141000	-0.032840000	1	-0.161390000	3.764175000	4.546385000
1	-4.316914000	-3.915700000	1.177817000	1	0.098279000	2.074929000	4.992014000

1	1.127301000	2.837963000	3.770318000	6	-1.527487000	-1.643146000	-3.878433000
6	0.735528000	3.856071000	-2.681037000	6	-2.116731000	-2.592897000	2.009984000
1	0.940299000	3.400492000	-3.655713000	6	-1.739776000	-3.969468000	2.566251000
1	0.440633000	4.894565000	-2.860816000	6	-3.125750000	-1.894210000	2.930813000
1	1.670552000	3.871945000	-2.109767000	1	1.916101000	-1.285061000	2.135228000
6	-1.665690000	3.097084000	-2.792423000	1	2.925764000	-0.423080000	4.221116000
1	-1.483389000	2.669555000	-3.784175000	1	4.467492000	-0.166147000	3.383813000
1	-2.453808000	2.516671000	-2.303946000	1	3.046708000	0.784504000	2.927207000
1	-2.025839000	4.122337000	-2.928059000	1	2.819840000	-2.936836000	3.620866000
6	1.075289000	-3.792256000	-0.340304000	1	4.470211000	-2.685956000	3.057633000
8	0.704664000	-3.143881000	0.651399000	1	3.286013000	-3.455447000	1.992706000
8	1.474835000	-4.745437000	-0.853095000	1	5.534199000	-1.807053000	1.349430000

6-TSI (in benzene solvent)

7	-1.159074000	-0.879019000	-0.167678000	1	5.307957000	0.094486000	-2.470680000
6	-1.486851000	0.437637000	0.146481000	1	2.154301000	1.742532000	-1.829041000
6	0.944768000	1.118996000	0.397782000	1	4.385979000	2.254927000	-2.879176000
7	1.481682000	-0.051836000	0.073456000	1	3.007868000	2.349890000	-3.986792000
6	2.903683000	-0.254008000	-0.112745000	1	4.088198000	0.958870000	-4.055291000
6	3.615824000	-0.955486000	0.874913000	1	1.239554000	0.707423000	-3.954253000
6	3.008028000	-1.291682000	2.228704000	1	2.108754000	-0.783841000	-3.554759000
6	3.381247000	-0.207384000	3.249250000	1	0.807393000	-0.177096000	-2.505740000
6	3.421037000	-2.672524000	2.745841000	1	2.887303000	1.943597000	0.761106000
6	4.951906000	-1.271801000	0.605919000	1	1.579014000	2.651917000	1.743965000
6	5.542759000	-0.906960000	-0.594372000	1	-3.000342000	1.916837000	0.428431000
6	4.818512000	-0.197101000	-1.548440000	1	-3.562290000	0.208604000	-0.011350000
6	3.483947000	0.147982000	-1.335010000	1	-4.021522000	-4.268338000	1.066189000
6	2.700262000	0.956855000	-2.367937000	1	-4.998760000	-4.390289000	-1.194711000
6	3.606402000	1.668895000	-3.374854000	1	-4.231467000	-2.853144000	-2.967161000
6	1.659850000	0.120317000	-3.130109000	1	-1.720930000	-0.123690000	-2.376871000
6	1.847661000	2.265958000	0.757291000	1	-3.199688000	0.552900000	-4.202517000
6	-2.750540000	0.894645000	0.192856000	1	-4.195055000	-0.890992000	-4.006727000
6	-2.236548000	-1.801096000	-0.430123000	1	-4.156040000	0.330882000	-2.724841000
6	-2.665807000	-2.667851000	0.594171000	1	-1.165515000	-0.953111000	-4.648540000
6	-3.668873000	-3.593325000	0.291601000	1	-0.658840000	-2.142765000	-3.432192000
6	-4.223893000	-3.660995000	-0.979544000	1	-2.130196000	-2.413060000	-4.372942000
6	-3.791294000	-2.792771000	-1.975776000	1	-1.209683000	-1.978070000	1.995460000
6	-2.800798000	-1.843435000	-1.720977000	1	-1.223783000	-3.858849000	3.525446000
6	-2.355647000	-0.896834000	-2.825273000	1	-1.080474000	-4.517471000	1.885530000
6	-3.547881000	-0.186507000	-3.474136000	1	-2.626186000	-4.587201000	2.742836000
				1	-2.721247000	-1.798703000	3.944287000

1	-3.370905000	-0.893996000	2.559409000	7	-1.398283000	-0.428619000	-0.347602000
1	-4.055830000	-2.470587000	2.991704000	6	-1.253933000	0.911940000	-0.003842000
1	1.727425000	3.089748000	0.049121000	6	1.250281000	0.685742000	0.303757000
13	0.477402000	-1.530947000	-0.353140000	7	1.344265000	-0.601915000	-0.013797000
1	1.047593000	-2.563924000	-1.512314000	6	2.578450000	-1.349609000	0.096556000
7	-0.384567000	1.344097000	0.424180000	6	2.698222000	-2.230825000	1.190634000
6	-0.794233000	2.724892000	0.646200000	6	1.643714000	-2.273344000	2.290924000
6	-0.864028000	3.569022000	-0.472407000	6	1.825416000	-1.101037000	3.265490000
6	-1.123981000	3.137223000	1.942656000	6	1.611564000	-3.601567000	3.047194000
6	-1.273380000	4.885444000	-0.254884000	6	3.845350000	-3.021979000	1.253776000
6	-1.524671000	4.465876000	2.106683000	6	4.824737000	-2.943649000	0.267959000
6	-1.598133000	5.331328000	1.022045000	6	4.674681000	-2.072257000	-0.801713000
1	-1.343633000	5.568615000	-1.096758000	6	3.546179000	-1.255424000	-0.915945000
1	-1.789407000	4.821402000	3.098464000	6	3.411769000	-0.320876000	-2.108549000
1	-1.914869000	6.358904000	1.170501000	6	4.617939000	0.620074000	-2.225255000
6	-1.091782000	2.200525000	3.139218000	6	3.223361000	-1.116154000	-3.407463000
1	-0.726229000	1.222257000	2.805226000	6	2.499502000	1.438046000	0.676066000
6	-0.542776000	3.091771000	-1.881011000	6	-2.286576000	1.766056000	0.096545000
1	-0.130209000	2.076294000	-1.821978000	6	-2.734565000	-0.967957000	-0.375309000
6	-2.503555000	2.003026000	3.705854000	6	-3.258162000	-1.511010000	0.814033000
1	-2.488028000	1.269542000	4.518435000	6	-4.521091000	-2.101645000	0.761307000
1	-2.894571000	2.942727000	4.111182000	6	-5.243494000	-2.141161000	-0.426254000
1	-3.196018000	1.650014000	2.936055000	6	-4.719572000	-1.573234000	-1.580991000
6	-0.150720000	2.713394000	4.235686000	6	-3.460871000	-0.966847000	-1.578637000
1	-0.504841000	3.665477000	4.644388000	6	-2.928922000	-0.313021000	-2.843356000
1	-0.106822000	1.995093000	5.060402000	6	-3.873384000	0.790825000	-3.335144000
1	0.869301000	2.868733000	3.868834000	6	-2.688523000	-1.351181000	-3.946237000
6	0.501110000	3.980305000	-2.567710000	6	-2.510530000	-1.434882000	2.136286000
1	0.753579000	3.569940000	-3.551436000	6	-2.212839000	-2.826951000	2.705632000
1	0.115816000	4.992659000	-2.727558000	6	-3.284449000	-0.578744000	3.146385000
1	1.426027000	4.066344000	-1.985986000	1	0.651294000	-2.154381000	1.833388000
6	-1.818002000	3.014465000	-2.730572000	1	1.054837000	-1.130111000	4.043253000
1	-1.586977000	2.611118000	-3.722867000	1	2.805594000	-1.154401000	3.750544000
1	-2.568489000	2.371758000	-2.260063000	1	1.753062000	-0.131248000	2.760449000
1	-2.256334000	4.009528000	-2.865794000	1	0.748393000	-3.622494000	3.717864000
6	1.351110000	-3.694883000	-0.317843000	1	2.505465000	-3.735866000	3.664362000
8	0.919824000	-3.066294000	0.656616000	1	1.531248000	-4.449775000	2.361006000
8	1.832902000	-4.615277000	-0.820968000	1	3.977726000	-3.711616000	2.080058000
				1	5.708981000	-3.568947000	0.336188000
				1	5.444563000	-2.024647000	-1.566486000

6-IMI (in gas phase)

6	4.653391000	0.544035000	-2.127600000	1	-1.922182000	0.095070000	-2.643163000
6	3.299781000	-1.197151000	-3.343332000	1	-3.353320000	1.288004000	-4.241831000
6	2.508055000	1.402295000	0.719378000	1	-4.787018000	0.424064000	-3.670957000
6	-2.260557000	1.798803000	0.037056000	1	-3.953034000	1.557887000	-2.594790000
6	-2.743106000	-0.936898000	-0.386449000	1	-2.285508000	-0.939238000	-4.867882000
6	-3.290595000	-1.449648000	0.806350000	1	-2.047631000	-2.197913000	-3.643663000
6	-4.565668000	-2.014505000	0.752511000	1	-3.673209000	-1.843602000	-4.247249000
6	-5.276911000	-2.063666000	-0.441603000	1	-1.572610000	-0.910736000	1.956786000
6	-4.727570000	-1.533547000	-1.602472000	1	-1.768886000	-2.662186000	3.689241000
6	-3.456367000	-0.952742000	-1.598251000	1	-1.741268000	-3.399377000	2.071882000
6	-2.902580000	-0.337130000	-2.873099000	1	-3.263374000	-3.259562000	2.962478000
6	-3.802865000	0.800289000	-3.370357000	1	-2.736666000	-0.346151000	4.043584000
6	-2.714733000	-1.392418000	-3.968245000	1	-3.459605000	0.537217000	2.681128000
6	-2.553859000	-1.367848000	2.134726000	1	-4.284555000	-0.874579000	3.367748000
6	-2.316554000	-2.753510000	2.744471000	1	2.848420000	2.005175000	-0.130964000
6	-3.304295000	-0.456912000	3.112904000	13	-0.094305000	-1.579654000	-0.608135000
1	0.586828000	-2.156675000	1.872729000	1	0.104256000	-4.652032000	-1.802755000
1	0.977549000	-1.092790000	4.065651000	7	0.110426000	1.376505000	0.261773000
1	2.731693000	-1.155976000	3.802642000	6	0.238095000	2.819332000	0.415541000
1	1.717626000	-0.130604000	2.777890000	6	0.532794000	3.565831000	-0.733011000
1	0.655739000	-3.588099000	3.795995000	6	0.045929000	3.392390000	1.679689000
1	2.411069000	-3.724698000	3.747961000	6	0.670366000	4.947047000	-0.581134000
1	1.428690000	-4.453564000	2.458825000	6	0.197943000	4.777365000	1.778717000
1	3.863088000	-3.791734000	2.155179000	6	0.511877000	5.546350000	0.663293000
1	5.624663000	-3.691089000	0.438602000	1	0.897075000	5.559408000	-1.449393000
1	5.428710000	-2.137188000	-1.466697000	1	0.063378000	5.259365000	2.743230000
1	2.544983000	0.227364000	-1.939874000	1	0.624612000	6.621337000	0.763449000
1	4.781632000	1.128056000	-1.210461000	6	-0.329808000	2.577331000	2.908009000
1	4.538684000	1.238941000	-2.965452000	1	-0.419090000	1.524680000	2.612967000
1	5.576861000	-0.020278000	-2.293572000	6	0.660858000	2.929711000	-2.108428000
1	3.178304000	-0.521035000	-4.195883000	1	0.600869000	1.839802000	-1.998244000
1	4.192194000	-1.806154000	-3.523352000	6	-1.691004000	3.021906000	3.458249000
1	2.434978000	-1.866982000	-3.310183000	1	-1.980929000	2.393929000	4.306729000
1	3.293732000	0.696993000	0.984887000	1	-1.650734000	4.058186000	3.810924000
1	2.327751000	2.082883000	1.550514000	1	-2.472709000	2.952531000	2.696202000
1	-2.133360000	2.839442000	0.290044000	6	0.738035000	2.678916000	4.004750000
1	-3.262063000	1.445312000	-0.170644000	1	0.822772000	3.706888000	4.373205000
1	-5.009124000	-2.416524000	1.659803000	1	0.468437000	2.042419000	4.853847000
1	-6.266649000	-2.509252000	-0.464236000	1	1.728527000	2.369582000	3.654617000
1	-5.295238000	-1.562308000	-2.528942000	6	2.004649000	3.255157000	-2.769428000

1	2.102823000	2.707820000	-3.713169000	1	0.705932000	-3.913982000	3.313439000
1	2.086532000	4.323041000	-2.997254000	6	1.860655000	-1.405171000	3.112608000
1	2.852990000	2.988060000	-2.129083000	1	2.405903000	-0.599013000	2.609703000
6	-0.507956000	3.360623000	-3.003755000	1	2.593985000	-2.148338000	3.444280000
1	-0.450335000	2.858888000	-3.975475000	1	1.386806000	-0.985047000	4.006272000
1	-1.468689000	3.111406000	-2.541693000	6	-0.625579000	2.784404000	0.472966000
1	-0.484562000	4.441581000	-3.180499000	6	-1.017316000	3.779882000	-0.443391000
6	0.035195000	-3.635273000	-1.411399000	6	-0.661677000	5.101964000	-0.166938000
8	-0.243309000	-3.402534000	-0.190297000	1	-0.946484000	5.886009000	-0.863278000
8	0.230593000	-2.613914000	-2.146431000	6	0.045640000	5.431031000	0.981024000
6-TS2 (in gas phase)				1	0.314717000	6.464189000	1.176007000
13	0.514164000	0.558132000	-0.585856000	6	0.402656000	4.438961000	1.885662000
7	-0.064340000	-1.182478000	-0.432967000	1	0.945481000	4.711560000	2.784450000
7	-2.280625000	-0.558750000	0.092406000	6	0.077228000	3.101016000	1.656227000
7	-0.862969000	1.394759000	0.166604000	6	-1.832172000	3.478973000	-1.692948000
6	0.948701000	-2.213827000	-0.355532000	1	-2.068461000	2.408892000	-1.703516000
6	1.504961000	-2.726872000	-1.536174000	6	-1.052674000	3.805616000	-2.972342000
6	2.502063000	-3.695616000	-1.410206000	1	-0.138480000	3.210358000	-3.045335000
1	2.943757000	-4.123814000	-2.305901000	1	-0.776221000	4.864544000	-3.006546000
6	2.936643000	-4.121430000	-0.160452000	1	-1.664493000	3.591653000	-3.854745000
1	3.707297000	-4.882462000	-0.085004000	6	-3.158301000	4.251198000	-1.673170000
6	2.389317000	-3.572004000	0.993735000	1	-3.746357000	4.010586000	-0.782359000
1	2.738965000	-3.908279000	1.966429000	1	-3.755884000	4.004143000	-2.556062000
6	1.387434000	-2.601282000	0.924145000	1	-2.985698000	5.332128000	-1.682665000
6	1.055550000	-2.274915000	-2.915182000	6	0.416222000	2.046672000	2.701798000
1	0.313492000	-1.476552000	-2.795058000	1	0.491480000	1.073426000	2.201517000
6	0.379534000	-3.421141000	-3.678607000	6	-0.729221000	1.924343000	3.717336000
1	-0.479610000	-3.820251000	-3.129566000	1	-0.509729000	1.138536000	4.449101000
1	1.080655000	-4.245213000	-3.846418000	1	-1.673625000	1.683187000	3.220059000
1	0.030122000	-3.073683000	-4.655483000	1	-0.859129000	2.867090000	4.259826000
6	2.230960000	-1.698499000	-3.713825000	6	1.748415000	2.304209000	3.410535000
1	2.726760000	-0.901619000	-3.152158000	1	2.569690000	2.437898000	2.699589000
1	1.877921000	-1.293836000	-4.667087000	1	1.993025000	1.456898000	4.058467000
1	2.971562000	-2.474780000	-3.935299000	1	1.697194000	3.189972000	4.051307000
6	0.794788000	-2.038041000	2.209802000	1	2.342528000	2.636085000	-2.926705000
1	0.079763000	-1.245042000	1.956165000	6	2.131890000	2.104211000	-1.991942000
6	0.027376000	-3.123370000	2.976568000	8	1.195683000	1.191547000	-2.086128000
1	-0.744134000	-3.590937000	2.356268000	8	2.732269000	2.349741000	-0.955517000
1	-0.455423000	-2.693953000	3.860754000	6	-2.117123000	0.853646000	0.404539000
				6	-3.169277000	1.557810000	0.856771000

1	-2.688800000	-1.097406000	3.151437000	1	-2.025086000	1.546301000	-4.045663000
1	-1.802230000	-1.524088000	4.633337000	1	-1.638439000	3.262336000	-4.060689000
1	-2.888994000	-2.700691000	3.884483000	1	-2.411695000	2.310598000	3.119826000
6	-0.791511000	-1.946442000	-2.272610000	6	-2.148568000	1.882557000	2.145896000
1	-0.105614000	-1.139463000	-1.986243000	8	-1.188535000	0.995119000	2.175443000
6	0.014813000	-2.972899000	-3.077834000	8	-2.721990000	2.215234000	1.114331000
1	0.803784000	-3.434385000	-2.475219000	6	2.106865000	0.890052000	-0.354367000
1	0.479898000	-2.494536000	-3.946557000	6	3.152587000	1.632787000	-0.757459000
1	-0.634923000	-3.775465000	-3.444068000	6	1.379063000	-1.483966000	0.152505000
6	-1.877838000	-1.315644000	-3.149710000	1	4.139875000	1.227826000	-0.912617000
1	-2.446089000	-0.547765000	-2.612622000	1	2.996799000	2.685535000	-0.954360000
1	-2.587686000	-2.066942000	-3.513601000	6	1.856889000	-2.909237000	0.200760000
1	-1.419312000	-0.845187000	-4.026536000	1	2.364927000	-3.185693000	-0.725636000
6	0.580381000	2.791871000	-0.410268000	1	1.023453000	-3.586126000	0.376065000
6	0.961667000	3.775509000	0.523583000	1	2.585239000	-3.016316000	1.011195000
6	0.614435000	5.103234000	0.260623000	1	-1.858541000	0.526539000	-0.508569000
1	0.893333000	5.876717000	0.971402000	5	-3.050885000	0.571969000	-0.132553000
6	-0.082745000	5.448586000	-0.888471000	8	-3.947442000	1.030278000	-1.032630000
1	-0.347499000	6.485173000	-1.072942000	8	-3.502080000	-0.328012000	0.781855000
6	-0.441442000	4.467702000	-1.805258000	6	-5.180174000	0.284829000	-0.763580000
1	-0.984212000	4.752270000	-2.700478000	6	-4.962955000	-0.235020000	0.702480000
6	-0.119385000	3.126081000	-1.591596000	6	-5.425748000	0.753643000	1.768017000
6	1.745232000	3.453908000	1.788063000	6	-5.534096000	-1.613397000	0.978157000
1	1.976455000	2.382774000	1.788892000	6	-6.354536000	1.229956000	-0.934312000
6	0.931655000	3.766313000	3.049073000	6	-5.239831000	-0.843177000	-1.786003000
1	-0.005956000	3.203359000	3.073770000	1	-5.165585000	-0.418965000	-2.791519000
1	0.685969000	4.832137000	3.107184000	1	-4.415073000	-1.549654000	-1.644639000
1	1.503937000	3.505536000	3.945892000	1	-6.184609000	-1.389734000	-1.710631000
6	3.074056000	4.219102000	1.819836000	1	-6.425500000	1.537703000	-1.981230000
1	3.688687000	3.990641000	0.943639000	1	-6.243006000	2.126223000	-0.321444000
1	3.644567000	3.955387000	2.716284000	1	-7.289106000	0.728351000	-0.662693000
1	2.906549000	5.301202000	1.842196000	1	-5.062877000	1.765747000	1.575408000
6	-0.471716000	2.079449000	-2.641236000	1	-5.048491000	0.426916000	2.742895000
1	-0.621279000	1.118959000	-2.134569000	1	-6.518159000	0.777522000	1.819309000
6	0.701720000	1.882549000	-3.610735000	1	-6.620687000	-1.607009000	0.842959000
1	0.476165000	1.087996000	-4.332043000	1	-5.321885000	-1.895971000	2.013883000
1	1.619478000	1.615290000	-3.077152000	1	-5.097422000	-2.367620000	0.321353000
1	0.893240000	2.804507000	-4.171515000	6	3.691319000	-0.953876000	-0.102005000
6	-1.759278000	2.393656000	-3.405410000	6	4.275543000	-1.416737000	-1.289090000
1	-2.598595000	2.581663000	-2.728630000	6	4.392479000	-0.840824000	1.106076000

6	5.622228000	-1.784631000	-1.232237000	6	-0.246949000	3.364268000	1.189373000
6	5.732218000	-1.232779000	1.111743000	6	0.557752000	2.790394000	2.357834000
6	6.342347000	-1.700136000	-0.046205000	6	0.845765000	3.826983000	3.447062000
1	6.115370000	-2.137428000	-2.133268000	6	-0.033440000	1.530675000	2.996950000
1	6.304125000	-1.160283000	2.032631000	6	2.518928000	2.334735000	-0.380383000
1	7.387229000	-1.993575000	-0.026753000	6	2.264585000	-2.386871000	0.523481000
6	3.756400000	-0.287427000	2.371478000	6	-0.522986000	-2.653797000	0.456150000
1	2.716182000	-0.017219000	2.151834000	6	-0.534353000	-3.604738000	-0.584201000
6	3.524108000	-1.504929000	-2.609567000	6	-1.197801000	-4.815728000	-0.370465000
1	2.461712000	-1.299088000	-2.421671000	6	-1.829877000	-5.089541000	0.832029000
6	4.471944000	0.991528000	2.819458000	6	-1.798405000	-4.150164000	1.854998000
1	4.488881000	1.731962000	2.013654000	6	-1.147346000	-2.925907000	1.693989000
1	3.961354000	1.428725000	3.684513000	6	-1.099587000	-1.928216000	2.842033000
1	5.505894000	0.781244000	3.113761000	6	0.299952000	-1.880442000	3.471544000
6	3.741582000	-1.328252000	3.496115000	6	-2.130646000	-2.185504000	3.943813000
1	4.759434000	-1.614279000	3.781738000	6	0.131914000	-3.387914000	-1.935198000
1	3.247663000	-0.920492000	4.383970000	6	-0.892471000	-3.447776000	-3.078695000
1	3.208647000	-2.238892000	3.200226000	6	1.224491000	-4.437941000	-2.182187000
6	3.637092000	-2.901781000	-3.234084000	1	-0.029397000	1.919060000	-2.579459000
1	3.029123000	-2.960283000	-4.142298000	1	0.679864000	3.441599000	-4.380239000
1	4.670755000	-3.123902000	-3.518612000	1	0.040667000	4.835158000	-3.495558000
1	3.307234000	-3.694441000	-2.553940000	1	1.415559000	3.934578000	-2.843812000
6	4.039174000	-0.450786000	-3.599156000	1	-1.614938000	2.330767000	-4.414251000
1	5.088860000	-0.640484000	-3.849787000	1	-2.278203000	3.739826000	-3.592373000
1	3.460222000	-0.485878000	-4.528002000	1	-2.544269000	2.141619000	-2.905145000
1	3.964521000	0.559325000	-3.187454000	1	-1.762465000	5.177282000	-1.911161000
				1	-2.010172000	6.157058000	0.341908000
				1	-0.947140000	5.078075000	2.277449000
				1	1.536007000	2.500942000	1.950247000
				1	1.279034000	4.743318000	3.036374000
				1	1.554401000	3.408658000	4.167099000
				1	-0.061735000	4.090441000	4.000240000
				1	0.645712000	1.166738000	3.776023000
				1	-0.999904000	1.739842000	3.467218000
				1	-0.161489000	0.721064000	2.271964000
				1	1.976709000	3.277610000	-0.391594000
				1	3.009756000	2.194914000	-1.349445000
				1	3.341641000	-2.344135000	0.529448000
				1	1.792516000	-3.333299000	0.748535000
				1	-1.223681000	-5.553655000	-1.167511000
6-IM2 (in gas phase)							
7	0.090737000	-1.356060000	0.250254000				
6	1.483284000	-1.320661000	0.269917000				
6	1.571846000	1.179939000	-0.160150000				
7	0.259046000	1.400355000	-0.207790000				
6	-0.248991000	2.753354000	-0.088644000				
6	-0.734216000	3.415443000	-1.225855000				
6	-0.503574000	2.902989000	-2.638252000				
6	0.467410000	3.833657000	-3.380810000				
6	-1.809873000	2.764136000	-3.427261000				
6	-1.371215000	4.649571000	-1.045874000				
6	-1.498468000	5.208742000	0.214407000				
6	-0.909875000	4.584908000	1.312915000				

6	-0.254095000	2.759861000	-0.114023000	1	0.619510000	1.191389000	3.756315000
6	-0.748453000	3.409018000	-1.254840000	1	-1.018293000	1.784945000	3.449930000
6	-0.530186000	2.881600000	-2.663599000	1	-0.197416000	0.753306000	2.253327000
6	0.434140000	3.802258000	-3.424742000	1	1.975450000	3.289237000	-0.413355000
6	-1.842512000	2.734098000	-3.439048000	1	3.018062000	2.204250000	-1.354401000
6	-1.388300000	4.643168000	-1.083702000	1	3.346416000	-2.330973000	0.530952000
6	-1.506563000	5.215963000	0.171433000	1	1.801436000	-3.320932000	0.751528000
6	-0.911462000	4.604112000	1.273479000	1	-1.218394000	-5.546549000	-1.168757000
6	-0.249628000	3.381719000	1.159144000	1	-2.331440000	-6.032658000	0.980143000
6	0.551291000	2.810527000	2.331596000	1	-2.267783000	-4.380880000	2.802611000
6	0.849431000	3.849178000	3.414885000	1	-1.328739000	-0.942739000	2.426575000
6	-0.055921000	1.562055000	2.977154000	1	0.313203000	-1.167832000	4.326512000
6	2.516586000	2.346106000	-0.391130000	1	0.638043000	-2.829989000	3.806468000
6	2.269331000	-2.373454000	0.522100000	1	1.055167000	-1.479992000	2.743258000
6	-0.512392000	-2.648668000	0.460141000	1	-2.123887000	-1.361942000	4.656612000
6	-0.526332000	-3.599642000	-0.580969000	1	-3.113257000	-2.369044000	3.585008000
6	-1.188991000	-4.811591000	-0.368624000	1	-1.812469000	-3.092752000	4.543344000
6	-1.815713000	-5.088226000	0.836299000	1	0.601700000	-2.388595000	-1.941729000
6	-1.777517000	-4.152441000	1.862534000	1	-0.453878000	-3.060440000	-4.005458000
6	-1.130045000	-2.925457000	1.700964000	1	-1.800820000	-2.882012000	-2.849002000
6	-1.088848000	-1.926140000	2.849045000	1	-1.200584000	-4.478133000	-3.263315000
6	0.315834000	-1.840476000	3.461443000	1	1.708143000	-4.263959000	-3.152323000
6	-2.099165000	-2.209007000	3.962671000	1	2.003221000	-4.392509000	-1.407095000
6	0.135279000	-3.379997000	-1.933834000	1	0.804858000	-5.435818000	-2.187738000
6	-0.890055000	-3.444376000	-3.076049000	1	3.296820000	2.386706000	0.369376000
6	1.230297000	-4.426696000	-2.180589000	13	-0.903474000	-0.042434000	-0.500007000
1	-0.055090000	1.899035000	-2.598783000	1	-1.893487000	-0.318151000	-4.137101000
1	0.642593000	3.394355000	-4.419234000	7	2.123605000	-0.025888000	-0.003956000
1	0.005822000	4.801712000	-3.554513000	6	3.580195000	-0.074889000	-0.020076000
1	1.385737000	3.912920000	-2.894886000	6	4.262226000	0.068651000	1.197417000
1	-1.657871000	2.285404000	-4.421382000	6	4.228979000	-0.279489000	-1.243490000
1	-2.310562000	3.709119000	-3.612927000	6	5.656127000	0.007205000	1.159648000
1	-2.575560000	2.121051000	-2.903673000	6	5.624939000	-0.336538000	-1.226528000
1	-1.787374000	5.158353000	-1.953075000	6	6.332282000	-0.194355000	-0.038961000
1	-2.019287000	6.164905000	0.292651000	1	6.217189000	0.111107000	2.084344000
1	-0.946601000	5.107529000	2.233077000	1	6.161653000	-0.501847000	-2.156380000
1	1.526256000	2.506060000	1.927398000	1	7.416649000	-0.244046000	-0.046058000
1	1.300477000	4.756496000	3.002153000	6	3.475260000	-0.475277000	-2.548592000
1	1.548800000	3.424412000	4.141020000	1	2.407999000	-0.300371000	-2.363182000
1	-0.054603000	4.132029000	3.964700000	6	3.545780000	0.263136000	2.525150000

1	2.963387000	-0.738359000	-3.015871000	6	-5.704490000	-1.450042000	-0.841132000
1	2.807142000	-3.975193000	-2.750601000	6	-6.180274000	-1.928342000	0.374490000
1	3.359892000	-5.291071000	-0.736366000	1	-5.746272000	-2.295434000	2.443192000
1	2.343552000	-4.723434000	1.432502000	1	-6.360785000	-1.435696000	-1.706377000
1	-0.436774000	-2.383890000	1.845976000	1	-7.200619000	-2.289805000	0.451080000
1	0.055406000	-4.748624000	2.541798000	6	-3.902881000	-0.424102000	-2.291017000
1	-0.032441000	-3.595466000	3.885342000	1	-2.823418000	-0.241576000	-2.212922000
1	1.535595000	-4.174185000	3.333524000	6	-3.182948000	-1.442143000	2.682353000
1	0.786080000	-1.169806000	3.572671000	1	-2.204842000	-1.013681000	2.428731000
1	2.332443000	-1.820491000	2.990713000	6	-4.576706000	0.924501000	-2.575945000
1	1.432212000	-0.665798000	2.000026000	1	-4.169553000	1.368697000	-3.490693000
1	-0.963395000	-3.480935000	-0.850049000	1	-5.655807000	0.795944000	-2.712908000
1	-2.546079000	-2.801251000	-1.293957000	1	-4.416349000	1.621104000	-1.748011000
1	-4.088966000	1.128411000	1.056557000	6	-4.128697000	-1.400208000	-3.451650000
1	-2.989381000	2.619817000	1.104181000	1	-5.195608000	-1.563979000	-3.631501000
1	-1.017330000	5.914955000	-0.980736000	1	-3.699441000	-0.993042000	-4.371899000
1	0.093731000	6.556316000	1.126395000	1	-3.668992000	-2.376582000	-3.265623000
1	0.664428000	4.835095000	2.801870000	6	-2.963126000	-2.850253000	3.250555000
1	0.082138000	1.167582000	2.284486000	1	-2.338374000	-2.799281000	4.148044000
1	-0.528277000	1.551922000	4.638689000	1	-3.914762000	-3.309802000	3.536216000
1	-0.614788000	3.298159000	4.354375000	1	-2.472475000	-3.520413000	2.536102000
1	-1.762056000	2.214034000	3.544484000	6	-3.808066000	-0.537529000	3.753337000
1	1.923059000	1.416017000	3.861899000	1	-3.150767000	-0.480376000	4.626491000
1	2.409942000	2.206408000	2.345904000	1	-3.962784000	0.475999000	3.374642000
1	1.887673000	3.175572000	3.729651000	1	-4.773402000	-0.932013000	4.086783000
1	-1.940957000	2.381724000	-1.848649000	6	2.085474000	1.849507000	-2.369226000
1	-1.565826000	3.592675000	-3.979486000	8	1.088577000	1.124768000	-2.117829000
1	-0.034330000	3.374590000	-3.118718000	8	3.072439000	2.021688000	-1.597835000
1	-0.837863000	4.950464000	-3.110448000	5	3.342522000	1.161381000	-0.393584000
1	-3.732022000	3.859596000	-2.715429000	1	1.992686000	1.181498000	0.304387000
1	-3.747168000	3.859909000	-0.941178000	8	3.531257000	-0.193769000	-0.643196000
1	-3.065569000	5.234479000	-1.825510000	8	4.266896000	1.719177000	0.442054000
1	-2.238776000	-3.262962000	0.370636000	6	5.099325000	0.633027000	0.921677000
13	0.646256000	0.585195000	-0.409674000	6	4.882020000	-0.474993000	-0.170345000
1	2.113016000	2.388386000	-3.318071000	6	4.922748000	-1.895845000	0.357127000
7	-2.221186000	-0.528348000	0.074998000	6	5.808566000	-0.315680000	-1.372799000
6	-3.590035000	-1.016859000	0.180064000	6	4.585113000	0.233168000	2.298687000
6	-4.042019000	-1.471445000	1.426262000	6	6.529298000	1.140412000	1.019595000
6	-4.396020000	-0.980179000	-0.964997000	1	5.894219000	-2.103496000	0.818150000
6	-5.357877000	-1.934637000	1.494999000	1	4.133389000	-2.066692000	1.093492000

1	4.773230000	-2.597904000	-0.467039000	6	-0.872902000	3.851072000	-3.120786000
1	5.777716000	0.706450000	-1.764279000	6	-3.102292000	4.083307000	-1.991610000
1	6.843398000	-0.557318000	-1.115081000	1	0.460170000	-1.173011000	-2.755615000
1	5.190474000	-0.566768000	2.734827000	1	0.117733000	-2.460122000	-4.824242000
1	4.629025000	1.103112000	2.959455000	1	1.032843000	-3.823129000	-4.161556000
1	7.205114000	0.323590000	1.293773000	1	-0.509368000	-3.355489000	-3.428944000
1	6.865232000	1.577320000	0.077895000	1	2.089772000	-0.798097000	-4.509644000
1	6.590090000	1.909167000	1.793941000	1	3.021067000	-2.225736000	-4.050613000
1	5.480704000	-0.998824000	-2.161600000	1	2.991665000	-0.833366000	-2.966487000
1	3.546080000	-0.100492000	2.244103000	1	2.826927000	-4.067388000	-2.624838000

6-TS3 (in benzene solvent)

7	-0.837770000	1.439656000	0.073918000	1	2.354959000	-4.661121000	1.582817000
6	-2.075815000	0.886323000	0.346355000	1	-0.424620000	-2.304963000	1.910541000
6	-1.278398000	-1.450107000	-0.225924000	1	0.059645000	-4.639152000	2.707114000
7	0.028233000	-1.189052000	-0.343425000	1	-0.008650000	-3.426913000	3.998425000
6	0.953573000	-2.310251000	-0.420453000	1	1.550270000	-4.041001000	3.459466000
6	1.505952000	-2.677140000	-1.655170000	1	0.817183000	-1.026183000	3.576237000
6	1.143220000	-1.999850000	-2.965849000	1	2.356077000	-1.710486000	3.016411000
6	0.402013000	-2.968029000	-3.896797000	1	1.462897000	-0.590726000	1.980715000
6	2.383760000	-1.424491000	-3.659858000	1	-0.958660000	-3.517745000	-0.742813000
6	2.390338000	-3.761738000	-1.677999000	1	-2.528944000	-2.853058000	-1.239773000
6	2.696092000	-4.463383000	-0.522852000	1	-4.097321000	1.143873000	0.992434000
6	2.120583000	-4.092197000	0.689695000	1	-3.006085000	2.637933000	1.020550000
6	1.240777000	-3.014451000	0.769199000	1	-1.052045000	5.905210000	-1.052905000
6	0.611832000	-2.613282000	2.096931000	1	-0.042901000	6.590339000	1.094415000
6	0.551778000	-3.751176000	3.116611000	1	0.512215000	4.891609000	2.799625000
6	1.349863000	-1.412550000	2.699798000	1	0.013096000	1.211364000	2.297965000
6	-1.770834000	-2.858049000	-0.452465000	1	-0.570764000	1.633922000	4.653747000
6	-3.128798000	1.582876000	0.815460000	1	-0.640327000	3.376854000	4.350737000
6	-0.669792000	2.841615000	0.361510000	1	-1.810921000	2.297323000	3.569866000
6	-1.030237000	3.804293000	-0.602630000	1	1.879710000	1.489177000	3.850581000
6	-0.786561000	5.149976000	-0.317612000	1	2.338269000	2.236235000	2.303762000
6	-0.224162000	5.539278000	0.891619000	1	1.847196000	3.245544000	3.669446000
6	0.091940000	4.581647000	1.846592000	1	-1.840942000	2.347752000	-1.934213000
6	-0.127339000	3.223604000	1.605671000	1	-1.336100000	3.503764000	-4.050214000
6	0.185900000	2.216112000	2.699307000	1	0.138159000	3.436699000	-3.065859000
6	-0.767506000	2.392165000	3.887342000	1	-0.778661000	4.940647000	-3.181056000
6	1.647319000	2.301022000	3.151352000	1	-3.619196000	3.774009000	-2.905958000
6	-1.713844000	3.436195000	-1.909421000	1	-3.723592000	3.804069000	-1.134829000
				1	-3.023394000	5.175800000	-2.008963000

6	-0.460909000	5.153981000	-0.435919000	1	0.549109000	3.481928000	4.264574000
6	-0.348880000	5.585979000	0.879074000	1	-0.847429000	2.280169000	-2.214351000
6	-0.387344000	4.661778000	1.915693000	1	0.483376000	3.347714000	-3.993754000
6	-0.543673000	3.297836000	1.662872000	1	1.429748000	3.443829000	-2.478294000
6	-0.622001000	2.324493000	2.827817000	1	0.580754000	4.854492000	-3.084543000
6	-1.966853000	2.469717000	3.551581000	1	-2.081249000	3.620257000	-3.888425000
6	0.552237000	2.492426000	3.796947000	1	-2.899082000	3.689945000	-2.316910000
6	-0.745417000	3.371279000	-2.190683000	1	-1.933635000	5.065756000	-2.878140000
6	0.509784000	3.766895000	-2.981051000	1	-2.657907000	-2.952580000	0.689643000
6	-1.990470000	3.972391000	-2.855343000	13	0.723157000	0.530182000	-0.003472000
1	0.604697000	-1.670238000	-2.235569000	1	1.804008000	1.118915000	-3.698471000
1	0.192090000	-3.441834000	-3.912834000	7	-2.282936000	-0.425094000	-0.158514000
1	1.025036000	-4.626557000	-2.892788000	6	-3.658026000	-0.862095000	-0.344786000
1	-0.494571000	-3.908042000	-2.346535000	6	-4.479063000	-0.989999000	0.783722000
1	2.251738000	-1.914417000	-4.016303000	6	-4.095139000	-1.130326000	-1.648887000
1	3.104697000	-3.186016000	-3.149813000	6	-5.783708000	-1.441932000	0.573743000
1	3.140422000	-1.545366000	-2.508407000	6	-5.413118000	-1.563280000	-1.805601000
1	2.948389000	-4.432879000	-1.268705000	6	-6.247039000	-1.726529000	-0.705392000
1	3.306386000	-5.169324000	1.060707000	1	-6.448992000	-1.563041000	1.423784000
1	2.035018000	-4.127015000	2.899995000	1	-5.792060000	-1.775704000	-2.800664000
1	-0.653103000	-1.578496000	2.377975000	1	-7.266478000	-2.070795000	-0.846660000
1	-0.926371000	-3.962825000	3.172577000	6	-3.198375000	-0.934650000	-2.862218000
1	-1.042256000	-2.739250000	4.452382000	1	-2.159607000	-0.851465000	-2.517038000
1	0.422005000	-3.706272000	4.291598000	6	-4.014884000	-0.633034000	2.189139000
1	0.488808000	-0.706729000	4.405514000	1	-3.010714000	-0.195493000	2.126117000
1	1.949660000	-1.619401000	3.978052000	6	-3.551418000	0.379262000	-3.574059000
1	1.391893000	-0.298154000	2.934407000	1	-2.889585000	0.539855000	-4.431670000
1	-1.078337000	-3.533453000	0.108892000	1	-4.582189000	0.348224000	-3.943229000
1	-2.342111000	-3.026629000	-1.033510000	1	-3.456172000	1.230209000	-2.893125000
1	-4.209298000	1.422196000	-0.226515000	6	-3.266482000	-2.115864000	-3.836660000
1	-3.077924000	2.876052000	-0.042567000	1	-4.248044000	-2.185214000	-4.315177000
1	-0.429563000	5.881207000	-1.243215000	1	-2.526436000	-1.986836000	-4.632339000
1	-0.231766000	6.642794000	1.096706000	1	-3.069330000	-3.071354000	-3.338740000
1	-0.301597000	5.007973000	2.941878000	6	-3.943062000	-1.868298000	3.096708000
1	-0.579131000	1.304568000	2.425161000	1	-3.620248000	-1.576855000	4.101511000
1	-2.062670000	1.716370000	4.342168000	1	-4.923640000	-2.347241000	3.186583000
1	-2.055033000	3.458740000	4.014568000	1	-3.236948000	-2.618489000	2.724855000
1	-2.797900000	2.347849000	2.849488000	6	-4.935369000	0.425536000	2.810160000
1	0.491275000	1.752293000	4.601018000	1	-4.554333000	0.727810000	3.790268000
1	1.510373000	2.365135000	3.281544000	1	-4.996172000	1.314743000	2.176010000

1	-5.948232000	0.035470000	2.952970000	6	1.093778000	-2.120854000	2.378660000
6	2.099409000	0.981009000	-2.656665000	6	0.409283000	-1.156201000	3.335566000
8	1.262077000	0.620730000	-1.829157000	6	-0.429850000	-1.919110000	4.368004000
8	3.342521000	1.248842000	-2.427667000	6	1.421084000	-0.233184000	4.022014000
5	4.079815000	0.812508000	-1.292410000	6	-1.896200000	-2.783478000	0.467699000
1	1.876340000	1.002565000	0.940368000	6	-3.145874000	1.735385000	-0.627522000
8	3.696018000	-0.260018000	-0.567165000	6	-0.750804000	2.922767000	0.285737000
8	5.231490000	1.409627000	-0.962125000	6	-0.609042000	3.730779000	-0.857640000
6	5.622639000	0.800760000	0.310853000	6	-0.491943000	5.113747000	-0.691797000
6	4.851080000	-0.567891000	0.285796000	6	-0.500047000	5.682543000	0.573379000
6	4.339902000	-1.033353000	1.634421000	6	-0.603807000	4.870203000	1.697985000
6	5.609772000	-1.681356000	-0.425923000	6	-0.727254000	3.484940000	1.581358000
6	5.135938000	1.746106000	1.402896000	6	-0.826210000	2.598117000	2.814859000
6	7.134606000	0.671916000	0.337127000	6	-2.266130000	2.117728000	3.036029000
1	5.180528000	-1.213305000	2.312920000	6	-0.296200000	3.254935000	4.089249000
1	3.672198000	-0.296898000	2.085591000	6	-0.520331000	3.138987000	-2.255910000
1	3.790671000	-1.970558000	1.508295000	6	0.911106000	3.295987000	-2.787709000
1	5.965788000	-1.357586000	-1.409618000	6	-1.523847000	3.765687000	-3.228440000
1	6.469815000	-2.010263000	0.163484000	1	0.304830000	-2.412374000	-1.576520000
1	5.442705000	1.393633000	2.391339000	1	0.146508000	-4.606282000	-2.724429000
1	5.572532000	2.733503000	1.234637000	1	1.136976000	-5.360561000	-1.471627000
1	7.451889000	0.146943000	1.243779000	1	-0.472044000	-4.754056000	-1.067552000
1	7.508227000	0.130838000	-0.533805000	1	1.966921000	-2.882335000	-3.288237000
1	7.584986000	1.667410000	0.343416000	1	2.969661000	-3.799328000	-2.160389000
1	4.933785000	-2.530738000	-0.561679000	1	2.811883000	-2.059954000	-1.945787000
1	4.045098000	1.843544000	1.388977000	1	2.794064000	-4.714250000	0.027646000
				1	3.353769000	-4.670883000	2.434149000
				1	2.247281000	-3.047673000	3.936282000
				1	-0.279452000	-0.524632000	2.762279000
				1	-1.170932000	-2.564461000	3.883784000
				1	-0.962000000	-1.217227000	5.018321000
				1	0.200924000	-2.550376000	5.003326000
				1	0.908359000	0.449489000	4.708022000
				1	2.149845000	-0.806700000	4.605602000
				1	1.969031000	0.369330000	3.289874000
				1	-1.150325000	-3.420137000	0.938023000
				1	-2.167099000	-3.209398000	-0.504114000
				1	-4.109087000	1.319265000	-0.875821000
				1	-3.036932000	2.810511000	-0.666965000
				1	-0.383299000	5.749210000	-1.566911000
6-IM3 (in benzene solvent)							
7	-0.865252000	1.493328000	0.153693000				
6	-2.097738000	0.989583000	-0.223207000				
6	-1.366172000	-1.386551000	0.282896000				
7	-0.083594000	-1.138356000	0.479684000				
6	0.806922000	-2.149730000	1.002365000				
6	1.400537000	-3.084337000	0.133503000				
6	1.043527000	-3.189136000	-1.342250000				
6	0.421741000	-4.554095000	-1.665797000				
6	2.267662000	-2.961102000	-2.236840000				
6	2.324021000	-3.980365000	0.677508000				
6	2.637263000	-3.961045000	2.032518000				
6	2.017020000	-3.045396000	2.874107000				

6	0.890061000	-1.997158000	-0.041058000	1	2.290547000	0.236149000	3.749305000
6	1.180443000	-2.776959000	-1.170772000	1	3.292215000	-1.168672000	3.393011000
6	0.267352000	-2.846491000	-2.383815000	1	3.171288000	0.157699000	2.211855000
6	-0.253451000	-4.273628000	-2.602342000	1	-0.850007000	-3.490633000	0.534740000
6	0.981132000	-2.336360000	-3.642446000	1	-2.402243000	-3.306988000	-0.319097000
6	2.371006000	-3.508795000	-1.160563000	1	-4.584840000	1.066070000	0.583818000
6	3.234588000	-3.460069000	-0.075860000	1	-3.632584000	2.609491000	0.201507000
6	2.919594000	-2.681572000	1.034480000	1	-1.551120000	5.461164000	-2.450987000
6	1.749543000	-1.923044000	1.072711000	1	-0.849894000	6.714782000	-0.443895000
6	1.394578000	-1.103118000	2.305702000	1	-0.490185000	5.537136000	1.696066000
6	0.637271000	-1.973073000	3.318342000	1	-1.007387000	1.833852000	2.113469000
6	2.612576000	-0.434434000	2.947242000	1	-1.676288000	2.903207000	4.211116000
6	-1.775100000	-2.918295000	0.490093000	1	-1.508913000	4.513414000	3.500229000
6	-3.649810000	1.534264000	0.320573000	1	-2.764629000	3.414499000	2.904751000
6	-1.265539000	2.881688000	-0.269149000	1	0.780191000	2.473447000	3.722367000
6	-1.528770000	3.542461000	-1.482678000	1	1.393302000	2.517272000	2.056571000
6	-1.365085000	4.929177000	-1.521847000	1	0.990152000	4.023196000	2.894961000
6	-0.975583000	5.637931000	-0.392007000	1	-2.139070000	1.745222000	-2.452757000
6	-0.767948000	4.971764000	0.810390000	1	-1.356034000	2.341487000	-4.736721000
6	-0.920377000	3.587299000	0.900221000	1	-0.027323000	2.477120000	-3.569452000
6	-0.755793000	2.893066000	2.243433000	1	-0.842672000	3.933853000	-4.163946000
6	-1.736159000	3.466507000	3.274285000	1	-3.760481000	2.739662000	-4.006304000
6	0.686912000	2.980048000	2.755636000	1	-4.112403000	3.271398000	-2.350275000
6	-2.013509000	2.801617000	-2.717943000	1	-3.319965000	4.372243000	-3.490103000
6	-0.996596000	2.892335000	-3.861824000	1	-2.334696000	-3.044003000	1.418187000
6	-3.383174000	3.328763000	-3.164318000	13	0.247262000	0.626472000	-0.513021000
1	-0.598756000	-2.196617000	-2.207338000	1	2.789296000	1.873685000	-1.285760000
1	-0.954233000	-4.295562000	-3.442637000	7	-2.508245000	-0.598788000	0.287220000
1	0.569010000	-4.956850000	-2.837720000	6	-3.826330000	-1.173698000	0.498201000
1	-0.764979000	-4.663527000	-1.716616000	6	-4.291553000	-1.336420000	1.810013000
1	0.293329000	-2.342539000	-4.493553000	6	-4.579925000	-1.504115000	-0.635126000
1	1.830021000	-2.979843000	-3.895600000	6	-5.576116000	-1.860143000	1.967851000
1	1.353650000	-1.318776000	-3.501300000	6	-5.857007000	-2.026891000	-0.422698000
1	2.625595000	-4.119787000	-2.021801000	6	-6.351364000	-2.201527000	0.864847000
1	4.156922000	-4.031904000	-0.091378000	1	-5.976637000	-1.997968000	2.968070000
1	3.590228000	-2.675193000	1.887620000	1	-6.474378000	-2.291837000	-1.276408000
1	0.713990000	-0.295329000	2.007136000	1	-7.348547000	-2.604221000	1.010464000
1	-0.273990000	-2.395148000	2.878673000	6	-4.065227000	-1.283951000	-2.049112000
1	0.350861000	-1.383826000	4.195462000	1	-3.031164000	-0.922176000	-1.991739000
1	1.262849000	-2.807152000	3.653265000	6	-3.463990000	-0.953025000	3.027682000

1	-1.825843000	-1.016065000	4.322310000	6	5.964767000	-1.242397000	-0.347875000
1	-2.424655000	-3.746529000	3.349355000	6	6.113711000	-1.597401000	-1.682970000
1	-3.610012000	-4.698021000	1.408451000	1	5.153333000	-1.830646000	-3.589115000
1	-2.839468000	-4.222973000	-0.876473000	1	6.827967000	-1.258121000	0.311424000
1	0.348614000	-2.692736000	-1.641005000	1	7.088039000	-1.894041000	-2.057640000
1	-0.959781000	-4.722998000	-2.312132000	6	4.594075000	-0.414935000	1.609679000
1	-0.653938000	-3.579473000	-3.630263000	1	3.542636000	-0.173767000	1.809090000
1	-2.253663000	-3.656814000	-2.896007000	6	2.580597000	-1.125328000	-3.046232000
1	-0.601976000	-1.119117000	-3.232722000	1	1.676329000	-0.895118000	-2.470349000
1	-2.175658000	-1.155644000	-2.410152000	6	5.413782000	0.858533000	1.856659000
1	-0.776886000	-0.430050000	-1.617873000	1	5.266278000	1.212251000	2.881662000
1	1.323007000	-3.550175000	0.494401000	1	6.482893000	0.666324000	1.717711000
1	2.941224000	-2.889867000	0.843315000	1	5.116197000	1.655344000	1.169626000
1	3.962751000	1.432526000	-1.211629000	6	5.020879000	-1.522573000	2.581320000
1	2.791483000	2.843847000	-0.949210000	1	6.078032000	-1.774594000	2.450810000
1	0.568834000	5.669692000	1.841949000	1	4.885140000	-1.189088000	3.614407000
1	-0.400833000	6.568576000	-0.239559000	1	4.441494000	-2.441536000	2.444311000
1	-0.696548000	5.102920000	-2.205078000	6	2.351819000	-2.460574000	-3.765452000
1	0.368737000	1.505138000	-2.265564000	1	1.459303000	-2.395995000	-4.397223000
1	0.538401000	2.401995000	-4.531987000	1	3.195425000	-2.710751000	-4.416546000
1	0.124396000	4.027675000	-3.980909000	1	2.213874000	-3.293715000	-3.067117000
1	1.646906000	3.284531000	-3.463855000	6	2.765105000	0.005555000	-4.066835000
1	-1.708809000	1.549716000	-3.622145000	1	1.891520000	0.064539000	-4.724995000
1	-2.098829000	1.750499000	-1.908529000	1	2.884888000	0.969995000	-3.565303000
1	-2.107977000	3.156305000	-2.986427000	1	3.646515000	-0.172502000	-4.692150000
1	1.531464000	2.083571000	2.327340000	6	-2.303217000	0.915109000	2.295173000
1	1.141975000	3.101781000	4.515696000	8	-0.976608000	0.861518000	2.593122000
1	-0.364395000	3.141271000	3.585344000	8	-2.285616000	0.576624000	0.818979000
1	0.607981000	4.615127000	3.782778000	5	-3.524350000	0.363580000	0.196381000
1	3.392078000	3.353526000	3.331169000	1	-2.748028000	1.910130000	2.380649000
1	3.449373000	3.476831000	1.559622000	8	-3.667080000	0.044301000	-1.105940000
1	2.849167000	4.835264000	2.527105000	8	-4.664834000	0.504375000	0.912522000
1	2.444249000	-3.117688000	-0.824625000	6	-5.740461000	0.498660000	-0.077852000
13	-0.385255000	0.457532000	0.985534000	6	-5.083232000	-0.279621000	-1.269718000
1	-2.911853000	0.144610000	2.777652000	6	-5.520810000	0.176073000	-2.649558000
7	2.333271000	-0.448312000	-0.238117000	6	-5.198534000	-1.793445000	-1.129746000
6	3.642719000	-0.848308000	-0.730423000	6	-6.029826000	1.958576000	-0.409265000
6	3.758911000	-1.186628000	-2.086776000	6	-6.957705000	-0.174895000	0.527695000
6	4.722723000	-0.852147000	0.159416000	1	-6.598974000	0.032384000	-2.772621000
6	5.021575000	-1.564722000	-2.544103000	1	-5.282524000	1.227839000	-2.818072000

1	-5.008921000	-0.418573000	-3.411148000	6	1.078120000	3.792036000	3.386420000
1	-4.877314000	-2.127892000	-0.137758000	6	3.299799000	3.592177000	2.234801000
1	-6.225723000	-2.127695000	-1.299258000	1	-0.201236000	-0.864161000	3.000562000
1	-6.867063000	2.045254000	-1.106901000	1	0.280291000	-2.258928000	4.988990000
1	-6.289683000	2.487146000	0.511136000	1	-0.873158000	-3.480510000	4.426016000
1	-7.747417000	-0.273242000	-0.223970000	1	0.595321000	-3.157539000	3.492602000
1	-6.716055000	-1.165303000	0.917289000	1	-1.470636000	-0.307715000	4.962131000
1	-7.343576000	0.434226000	1.348922000	1	-2.616819000	-1.626418000	4.707758000
1	-4.552397000	-2.267881000	-1.874617000	1	-2.617999000	-0.248335000	3.602807000
1	-5.155609000	2.446309000	-0.853455000	1	-3.109717000	-3.213990000	3.198501000
				1	-4.120487000	-4.315364000	1.234538000
				1	-3.164172000	-3.986473000	-1.002773000
				1	0.083010000	-2.648649000	-1.648704000
				1	-1.409041000	-4.526016000	-2.388276000
				1	-0.939537000	-3.419491000	-3.687151000
				1	-2.563195000	-3.324927000	-3.006719000
				1	-0.783649000	-1.039148000	-3.361010000
				1	-2.225821000	-0.765452000	-2.370477000
				1	-0.622104000	-0.296812000	-1.781813000
				1	0.728160000	-3.516651000	0.826366000
				1	2.403966000	-3.060100000	1.221095000
				1	4.265732000	0.844525000	-0.998611000
				1	3.303819000	2.429536000	-0.957125000
				1	1.184559000	5.760266000	1.463703000
				1	0.401486000	6.618649000	-0.711484000
				1	0.077821000	5.074855000	-2.611779000
				1	0.756516000	1.387584000	-2.407659000
				1	1.318889000	2.126794000	-4.675242000
				1	1.101697000	3.822057000	-4.227127000
				1	2.418754000	2.882165000	-3.505087000
				1	-1.097653000	1.650773000	-4.037743000
				1	-1.685083000	1.992259000	-2.397879000
				1	-1.347570000	3.321834000	-3.516766000
				1	1.733731000	2.130515000	2.199977000
				1	1.469782000	3.341633000	4.303433000
				1	0.002866000	3.596634000	3.347158000
				1	1.220994000	4.873982000	3.469565000
				1	3.750163000	3.205381000	3.154949000
				1	3.846893000	3.180721000	1.382310000
				1	3.425635000	4.680385000	2.227290000
6-TS5 (in gas phase)							
7	1.057561000	1.403645000	-0.028489000				
6	2.242801000	0.750802000	-0.309392000				
6	1.260889000	-1.499458000	0.324222000				
7	0.028487000	-1.084770000	0.598182000				
6	-1.063805000	-2.017227000	0.780794000				
6	-1.579189000	-2.210683000	2.070334000				
6	-0.939059000	-1.610154000	3.310168000				
6	-0.187947000	-2.691336000	4.099458000				
6	-1.972616000	-0.904700000	4.195330000				
6	-2.694722000	-3.042541000	2.209624000				
6	-3.262148000	-3.662511000	1.109179000				
6	-2.719817000	-3.469611000	-0.159602000				
6	-1.616076000	-2.640280000	-0.361256000				
6	-0.996967000	-2.472474000	-1.749300000				
6	-1.510636000	-3.502023000	-2.758623000				
6	-1.172641000	-1.063261000	-2.336286000				
6	1.599452000	-2.959906000	0.487385000				
6	3.344447000	1.361904000	-0.783833000				
6	0.986679000	2.827749000	-0.235487000				
6	1.227461000	3.701439000	0.845704000				
6	1.003696000	5.066799000	0.647291000				
6	0.573614000	5.554964000	-0.580541000				
6	0.389075000	4.683809000	-1.646912000				
6	0.601306000	3.311695000	-1.501293000				
6	0.447415000	2.396052000	-2.705351000				
6	1.378690000	2.835063000	-3.842659000				
6	-1.007313000	2.334215000	-3.186291000				
6	1.809993000	3.222959000	2.166505000				

6	1.245296000	5.064039000	0.704334000	1	-1.047039000	3.450231000	-3.508123000
6	1.085185000	5.639563000	-0.552588000	1	1.880296000	2.049175000	2.072565000
6	0.948141000	4.839207000	-1.679571000	1	0.097304000	2.218244000	3.781457000
6	0.958477000	3.446102000	-1.575140000	1	-0.668223000	2.249112000	2.178925000
6	0.810774000	2.568185000	-2.807423000	1	-0.468033000	3.744459000	3.072710000
6	1.667057000	3.056599000	-3.979667000	1	2.450496000	3.242638000	4.100599000
6	-0.664750000	2.464913000	-3.220919000	1	3.255718000	4.042583000	2.737597000
6	1.398886000	3.023680000	2.222987000	1	1.815680000	4.763772000	3.480195000
6	0.016273000	2.788051000	2.849421000	1	1.893907000	-3.400296000	-0.295081000
6	2.283142000	3.819023000	3.185632000	13	-0.543896000	0.699178000	0.040400000
1	-1.267671000	-0.121022000	2.400796000	7	2.214238000	-0.661450000	0.057914000
1	-0.013787000	-0.995177000	4.371314000	6	3.523437000	-1.294779000	0.009849000
1	-0.477826000	-2.649239000	3.935510000	6	3.961384000	-1.805173000	-1.219138000
1	0.593359000	-1.719041000	2.875384000	6	4.291563000	-1.322849000	1.180515000
1	-2.363967000	-0.118078000	4.526025000	6	5.231942000	-2.383382000	-1.248806000
1	-2.890123000	-1.792304000	4.364934000	6	5.554683000	-1.911424000	1.096148000
1	-3.560359000	-0.539150000	3.284253000	6	6.020019000	-2.437200000	-0.104346000
1	-3.550564000	-2.972620000	2.650348000	1	5.612736000	-2.787915000	-2.182280000
1	-4.130334000	-4.430473000	0.752587000	1	6.184354000	-1.952455000	1.980286000
1	-2.932337000	-4.240933000	-1.383752000	1	7.006292000	-2.887576000	-0.149413000
1	0.218043000	-2.645582000	-1.881444000	6	3.804055000	-0.726869000	2.492062000
1	-1.141715000	-4.563815000	-2.748744000	1	2.763388000	-0.403248000	2.360990000
1	-0.675706000	-3.399436000	-3.996137000	6	3.130040000	-1.714223000	-2.490358000
1	-2.330775000	-3.405185000	-3.380176000	1	2.148397000	-1.292974000	-2.236874000
1	-0.955685000	-1.056809000	-3.661773000	6	4.626238000	0.514079000	2.866074000
1	-2.101250000	-0.718808000	-2.355848000	1	4.247820000	0.951619000	3.795437000
1	-0.356078000	-0.368244000	-2.179354000	1	5.677747000	0.250966000	3.022288000
1	0.563596000	-3.444263000	0.889641000	1	4.574444000	1.273166000	2.080065000
1	2.216731000	-2.994952000	1.382833000	6	3.832390000	-1.755178000	3.630022000
1	4.353024000	0.832206000	-0.550341000	1	4.856639000	-2.068088000	3.855513000
1	3.419492000	2.424972000	-0.708070000	1	3.412306000	-1.318039000	4.540838000
1	1.366383000	5.704239000	1.572200000	1	3.255439000	-2.654428000	3.389176000
1	1.075743000	6.720135000	-0.653426000	6	2.898804000	-3.091792000	-3.124727000
1	0.835270000	5.303397000	-2.654635000	1	2.243121000	-2.997543000	-3.996316000
1	1.172231000	1.564929000	-2.548084000	1	3.840130000	-3.532956000	-3.467051000
1	1.621227000	2.336005000	-4.801968000	1	2.436857000	-3.799574000	-2.427577000
1	1.313229000	4.016430000	-4.368306000	6	3.783893000	-0.762092000	-3.501417000
1	2.713558000	3.173516000	-3.682444000	1	3.163388000	-0.680493000	-4.399452000
1	-0.781164000	1.793587000	-4.078567000	1	3.909310000	0.237650000	-3.076286000
1	-1.308268000	2.099527000	-2.410003000	1	4.767997000	-1.133833000	-3.805304000

8	-2.110822000	1.253872000	0.029158000	6	3.457602000	-1.975903000	1.574667000
5	-3.421373000	0.883462000	-0.045510000	6	3.137053000	0.969212000	-2.233438000
8	-4.142588000	0.953873000	-1.204354000	6	0.566912000	1.924224000	-1.751335000
8	-4.123352000	0.400325000	1.025534000	6	0.799907000	3.300631000	-1.586346000
6	-5.512282000	0.356106000	0.611434000	6	0.087853000	4.183815000	-2.397254000
6	-5.390132000	0.263015000	-0.948885000	6	-0.813423000	3.720312000	-3.349953000
6	-6.504406000	0.950716000	-1.718108000	6	-0.984245000	2.354363000	-3.536050000
6	-5.196700000	-1.169955000	-1.435021000	6	-0.285680000	1.431326000	-2.753689000
6	-6.155644000	1.658376000	1.078751000	6	-0.431272000	-0.054715000	-3.038317000
6	-6.179102000	-0.840102000	1.269123000	6	0.042530000	-0.382634000	-4.460068000
1	-7.471684000	0.499084000	-1.474671000	6	-1.865050000	-0.545125000	-2.811276000
1	-6.546363000	2.017540000	-1.491867000	6	1.807059000	3.845432000	-0.586816000
1	-6.334033000	0.834970000	-2.791730000	6	1.141139000	4.734325000	0.470839000
1	-4.396059000	-1.661441000	-0.871730000	6	2.914901000	4.621290000	-1.312178000
1	-6.111531000	-1.760141000	-1.327935000	1	1.412057000	0.685933000	3.052548000
1	-7.226001000	1.676336000	0.855537000	1	2.769689000	0.879519000	5.107844000
1	-6.024238000	1.750444000	2.159997000	1	2.074696000	-0.628657000	5.726302000
1	-7.202086000	-0.961927000	0.898297000	1	3.096897000	-0.656248000	4.281954000
1	-5.620011000	-1.758784000	1.076576000	1	0.492037000	2.004867000	4.874626000
1	-6.227652000	-0.684635000	2.350984000	1	-0.204614000	0.585079000	5.650657000
1	-4.918456000	-1.149970000	-2.493089000	1	-0.858842000	1.152969000	4.105854000
1	-5.685374000	2.523494000	0.600672000	1	-0.359356000	-1.606220000	5.441754000
				1	-1.210485000	-3.834216000	4.817086000
				1	-0.779597000	-4.750530000	2.572935000
6-TS5' (in gas phase)				1	1.495324000	-3.181885000	0.121377000
7	1.171836000	0.984000000	-0.836762000	1	1.367034000	-5.456512000	1.198278000
6	2.456191000	0.549718000	-1.151280000	1	0.988944000	-5.433780000	-0.534082000
6	2.552538000	-1.041729000	0.813728000	1	-0.312600000	-5.583212000	0.641740000
7	1.295627000	-0.883857000	1.213753000	1	-0.270547000	-3.462487000	-1.549707000
6	0.708356000	-1.727500000	2.232583000	1	-1.518992000	-3.530701000	-0.289218000
6	0.509980000	-1.198580000	3.516967000	1	-0.650826000	-2.031515000	-0.584587000
6	1.085052000	0.142244000	3.947323000	1	3.849390000	-2.757334000	0.919733000
6	2.333150000	-0.080001000	4.814617000	1	2.923431000	-2.429278000	2.406958000
6	0.062763000	1.017042000	4.681135000	1	4.143115000	0.651658000	-2.456090000
6	-0.190217000	-1.985085000	4.438377000	1	2.661924000	1.668420000	-2.907791000
6	-0.664589000	-3.241294000	4.090486000	1	0.237923000	5.253921000	-2.279512000
6	-0.424405000	-3.755387000	2.818190000	1	-1.363524000	4.425801000	-3.965349000
6	0.268324000	-3.015299000	1.861119000	1	-1.660634000	1.996428000	-4.308131000
6	0.530636000	-3.574732000	0.467197000	1	0.227518000	-0.601993000	-2.352648000
6	0.651012000	-5.100675000	0.451257000	1	0.000160000	-1.462784000	-4.635519000
6	-0.534596000	-3.121529000	-0.542138000				

1	-0.590659000	0.102636000	-5.210073000	6	3.490435000	-2.356792000	-3.660640000
1	1.072178000	-0.046808000	-4.616148000	1	2.628484000	-2.865495000	-4.103693000
1	-2.553843000	-0.064923000	-3.517199000	1	3.432202000	-1.295627000	-3.916782000
1	-1.925566000	-1.628003000	-2.965801000	1	4.395477000	-2.772933000	-4.115266000
1	-2.212915000	-0.331577000	-1.794640000	8	-1.570266000	0.064911000	0.607820000
1	2.275277000	2.996466000	-0.074005000	6	-2.339827000	-0.782905000	1.454040000
1	1.885657000	5.095118000	1.187862000	1	-2.113238000	-1.822245000	1.202360000
1	0.359185000	4.194334000	1.010674000	1	-2.096279000	-0.571021000	2.498745000
1	0.675908000	5.610202000	0.005045000	8	-3.683850000	-0.501009000	1.272539000
1	3.675677000	4.957137000	-0.600175000	5	-4.385634000	-1.138884000	0.287485000
1	3.403000000	4.001498000	-2.070784000	8	-3.870006000	-2.120998000	-0.521767000
1	2.510209000	5.508517000	-1.810284000	8	-5.687713000	-0.822135000	0.039483000
1	4.318305000	-1.417584000	1.953816000	6	-5.011950000	-2.680102000	-1.226483000
13	0.131273000	0.332513000	0.454212000	6	-6.033280000	-1.492704000	-1.195266000
7	3.080887000	-0.394607000	-0.240487000	6	-5.803372000	-0.485419000	-2.319343000
6	4.449793000	-0.744899000	-0.589394000	6	-7.492123000	-1.912083000	-1.138839000
6	4.647676000	-1.794505000	-1.497309000	6	-4.577171000	-3.107913000	-2.616651000
6	5.494635000	-0.005256000	-0.022869000	6	-5.481773000	-3.885034000	-0.415865000
6	5.967187000	-2.110234000	-1.825866000	1	-4.650468000	-4.587591000	-0.309618000
6	6.795255000	-0.357844000	-0.389407000	1	-5.808854000	-3.582512000	0.583962000
6	7.030305000	-1.400291000	-1.278520000	1	-6.309350000	-4.400342000	-0.910917000
1	6.164022000	-2.916472000	-2.526901000	1	-3.830665000	-3.904254000	-2.538921000
1	7.634212000	0.194349000	0.023567000	1	-4.140598000	-2.277806000	-3.174613000
1	8.048670000	-1.658217000	-1.550714000	1	-5.432758000	-3.496968000	-3.178295000
6	5.249452000	1.156446000	0.926626000	1	-4.748399000	-0.193590000	-2.372364000
1	4.190279000	1.151956000	1.214237000	1	-6.396349000	0.409679000	-2.113795000
6	3.497497000	-2.557128000	-2.139290000	1	-6.105690000	-0.889299000	-3.289860000
1	2.550931000	-2.154589000	-1.755988000	1	-7.755377000	-2.502609000	-2.022559000
6	5.527478000	2.489382000	0.218510000	1	-8.127352000	-1.022736000	-1.120581000
1	5.305468000	3.328307000	0.886239000	1	-7.703409000	-2.500357000	-0.244102000
1	6.581092000	2.558026000	-0.072974000	1	-0.200764000	1.659231000	1.679040000
1	4.914279000	2.590107000	-0.681716000	5	-1.401845000	1.927563000	1.375536000
6	6.081188000	1.041064000	2.209548000	8	-2.367432000	1.983412000	2.326336000
1	7.151192000	1.134017000	2.000113000	8	-1.538585000	2.769475000	0.315684000
1	5.812555000	1.843635000	2.902654000	6	-3.273576000	3.051940000	1.893856000
1	5.924247000	0.084242000	2.718766000	6	-2.916220000	3.240213000	0.370896000
6	3.549027000	-4.052846000	-1.801175000	6	-3.729440000	2.360248000	-0.573043000
1	2.693086000	-4.567625000	-2.250110000	6	-2.930519000	4.681430000	-0.111517000
1	4.458434000	-4.514876000	-2.198466000	6	-4.702615000	2.606624000	2.149157000
1	3.526925000	-4.238969000	-0.721524000	6	-2.917653000	4.265621000	2.745573000

1	-3.026951000	3.999972000	3.800102000	6	0.125249000	-2.387028000	1.183072000
1	-1.881943000	4.578087000	2.575990000	6	-0.462454000	-2.331989000	2.454038000
1	-3.577323000	5.110529000	2.529599000	6	-0.232327000	-1.180951000	3.420900000
1	-4.860715000	2.490310000	3.224674000	6	0.747377000	-1.606634000	4.524076000
1	-4.918338000	1.653680000	1.663381000	6	-1.539733000	-0.654310000	4.023536000
1	-5.401215000	3.366215000	1.782407000	6	-1.226320000	-3.431237000	2.860203000
1	-3.731592000	1.322180000	-0.237189000	6	-1.379681000	-4.536935000	2.038156000
1	-3.270150000	2.407707000	-1.566151000	6	-0.762126000	-4.574538000	0.790169000
1	-4.764536000	2.707424000	-0.643291000	6	-0.001966000	-3.502401000	0.332240000
1	-3.935165000	5.105971000	-0.015310000	6	0.646306000	-3.527432000	-1.044908000
1	-2.642170000	4.706384000	-1.166238000	6	1.006435000	-4.938150000	-1.516230000
1	-2.228601000	5.301229000	0.450191000	6	-0.247882000	-2.837271000	-2.084095000
6-TS6 (in gas phase)				6	2.947040000	-2.308296000	1.295582000
				6	3.300945000	1.766736000	-1.264872000
1	-1.043100000	0.939706000	1.513031000	6	0.572278000	2.458543000	-1.179416000
5	-2.132565000	1.311449000	0.945007000	6	0.661838000	3.700976000	-0.527907000
8	-3.338377000	0.910201000	1.458105000	6	0.064187000	4.804378000	-1.136975000
8	-2.078135000	2.600966000	0.511678000	6	-0.588644000	4.685471000	-2.358527000
6	-4.170570000	2.112641000	1.474722000	6	-0.636597000	3.455443000	-3.002962000
6	-3.457500000	3.053325000	0.434942000	6	-0.058103000	2.320242000	-2.430836000
6	-3.923559000	2.850306000	-1.002836000	6	-0.072369000	1.007100000	-3.198212000
6	-3.476207000	4.530100000	0.793159000	6	0.965863000	1.045226000	-4.328654000
6	-5.583510000	1.714315000	1.087932000	6	-1.458837000	0.644206000	-3.740159000
6	-4.117199000	2.646997000	2.901608000	6	1.383950000	3.875898000	0.798235000
1	-4.461857000	1.866556000	3.585302000	6	0.412081000	4.263276000	1.920044000
1	-3.093962000	2.920684000	3.180282000	6	2.505335000	4.915432000	0.676026000
1	-4.758239000	3.524554000	3.023094000	1	0.244842000	-0.354962000	2.879348000
1	-6.004532000	1.058406000	1.856182000	1	0.936899000	-0.774577000	5.209076000
1	-5.587671000	1.186061000	0.131980000	1	0.335695000	-2.438286000	5.105268000
1	-6.221734000	2.600633000	1.010604000	1	1.705723000	-1.932412000	4.105973000
1	-3.936931000	1.793327000	-1.280259000	1	-1.343242000	0.248442000	4.610809000
1	-3.226479000	3.374357000	-1.663599000	1	-1.985747000	-1.390557000	4.699971000
1	-4.926093000	3.263308000	-1.151031000	1	-2.279281000	-0.412231000	3.253560000
1	-4.503722000	4.907517000	0.815219000	1	-1.689900000	-3.422888000	3.842458000
1	-2.920123000	5.084624000	0.031561000	1	-1.968145000	-5.385170000	2.375091000
1	-3.008692000	4.716441000	1.762098000	1	-0.878848000	-5.455349000	0.167360000
7	1.062216000	1.274774000	-0.514547000	1	1.586672000	-2.963666000	-0.995786000
6	2.416040000	0.990254000	-0.613623000	1	1.597172000	-5.474072000	-0.766893000
6	2.166970000	-1.193442000	0.646236000	1	1.590941000	-4.882787000	-2.438927000
7	0.835459000	-1.223801000	0.689032000	1	0.112642000	-5.530521000	-1.735480000

1	0.256426000	-2.789679000	-3.055501000	6	4.751355000	2.411613000	2.133662000
1	-1.185190000	-3.391656000	-2.198603000	1	4.240955000	2.974135000	2.922622000
1	-0.516587000	-1.815875000	-1.790668000	1	5.828106000	2.584007000	2.236838000
1	2.274647000	-3.025273000	1.760639000	1	4.431238000	2.804568000	1.164151000
1	3.615675000	-1.889032000	2.052237000	6	4.859370000	0.378043000	3.623672000
1	4.356568000	1.551816000	-1.308473000	1	5.928387000	0.536537000	3.795717000
1	2.938077000	2.656772000	-1.761516000	1	4.318346000	0.901918000	4.417185000
1	0.109607000	5.773171000	-0.646343000	1	4.661474000	-0.694048000	3.727663000
1	-1.047290000	5.556478000	-2.816818000	6	4.192490000	-3.080254000	-2.375580000
1	-1.128314000	3.375015000	-3.968469000	1	3.573883000	-3.420551000	-3.212588000
1	0.239780000	0.204198000	-2.519150000	1	5.225742000	-3.374627000	-2.585906000
1	0.991043000	0.087176000	-4.859435000	1	3.870320000	-3.619067000	-1.477553000
1	0.717264000	1.827915000	-5.053450000	6	4.495831000	-0.860666000	-3.521464000
1	1.965596000	1.250556000	-3.933522000	1	3.858468000	-1.189223000	-4.348212000
1	-1.765003000	1.327943000	-4.538607000	1	4.409313000	0.225482000	-3.431829000
1	-1.439533000	-0.364058000	-4.169599000	1	5.531709000	-1.103330000	-3.780038000
1	-2.222106000	0.675249000	-2.956700000	8	-1.819343000	0.107624000	-0.478655000
1	1.846664000	2.919056000	1.066197000	5	-2.850050000	-0.808257000	-0.623062000
1	-0.375965000	3.514933000	2.041564000	8	-4.033212000	-0.489428000	-1.217875000
1	-0.075160000	5.219360000	1.697706000	8	-2.755002000	-2.099509000	-0.195205000
1	0.950099000	4.373467000	2.867439000	6	-4.744086000	-1.744297000	-1.390211000
1	3.059168000	4.991481000	1.617219000	6	-4.102090000	-2.639720000	-0.278025000
1	3.210870000	4.647355000	-0.116846000	6	-4.731615000	-2.429459000	1.095713000
1	2.102546000	5.907684000	0.448155000	6	-4.032754000	-4.116560000	-0.622395000
1	3.577108000	-2.818162000	0.563161000	6	-6.232992000	-1.498513000	-1.224278000
13	-0.195557000	0.193386000	0.124440000	6	-4.427923000	-2.229306000	-2.802182000
7	2.877780000	-0.208962000	0.065690000	1	-4.722883000	-1.455925000	-3.516172000
6	4.323325000	-0.381325000	0.048548000	1	-3.354247000	-2.412253000	-2.922143000
6	4.894858000	-1.046675000	-1.044507000	1	-4.968902000	-3.149126000	-3.040728000
6	5.070232000	0.147808000	1.108209000	1	-6.588143000	-0.842054000	-2.023354000
6	6.282495000	-1.201936000	-1.038768000	1	-6.456892000	-1.028515000	-0.264665000
6	6.454456000	-0.028715000	1.061870000	1	-6.783258000	-2.442875000	-1.289007000
6	7.054739000	-0.700986000	0.003343000	1	-4.788739000	-1.362927000	1.338558000
1	6.765171000	-1.712624000	-1.867239000	1	-4.097261000	-2.916012000	1.842761000
1	7.070252000	0.369837000	1.862774000	1	-5.733654000	-2.864765000	1.147380000
1	8.132300000	-0.828488000	-0.013649000	1	-5.037850000	-4.508670000	-0.809831000
6	4.429868000	0.915679000	2.253355000	1	-3.600414000	-4.669011000	0.215627000
1	3.340279000	0.806858000	2.178490000	1	-3.417608000	-4.294435000	-1.507809000
6	4.075399000	-1.558187000	-2.220753000				
1	3.019710000	-1.311485000	-2.048232000				

6-TS7 (in gas phase)

7	1.372783000	-0.653538000	-0.255709000	1	-0.659952000	-1.784482000	2.193822000
6	1.295560000	0.737787000	-0.243601000	1	-1.825648000	0.231113000	3.038260000
6	-1.172680000	0.725631000	0.337121000	1	-1.026813000	-0.648589000	4.352484000
7	-1.366236000	-0.574341000	0.191937000	1	-2.784029000	-0.774833000	4.135444000
6	-2.625293000	-1.231900000	0.451048000	1	-0.614123000	-3.156418000	4.153675000
6	-3.644520000	-1.217836000	-0.517121000	1	-2.365721000	-3.338314000	4.190695000
6	-3.580595000	-0.385911000	-1.789664000	1	-1.427024000	-4.090248000	2.885509000
6	-4.690377000	0.676231000	-1.800735000	1	-3.175504000	0.995102000	1.046036000
6	-3.690623000	-1.257692000	-3.046920000	1	-2.608654000	2.254323000	-0.079194000
6	-4.783774000	-1.988136000	-0.260719000	1	2.293095000	2.616067000	-0.433434000
6	-4.900545000	-2.740558000	0.899912000	1	3.300485000	1.089762000	-0.728017000
6	-3.877846000	-2.734827000	1.843582000	1	4.854836000	-2.446451000	-2.689569000
6	-2.720154000	-1.984147000	1.641046000	1	6.147851000	-2.924815000	-0.643743000
6	-1.625679000	-1.925089000	2.697517000	1	5.264319000	-2.278660000	1.564905000
6	-1.827273000	-0.704937000	3.607602000	1	2.126294000	-0.297448000	2.010309000
6	-1.507475000	-3.205369000	3.524634000	1	3.496009000	-0.128124000	4.009012000
6	-2.321846000	1.604324000	0.753339000	1	4.700617000	-1.242292000	3.370909000
6	2.346994000	1.540371000	-0.487952000	1	4.480850000	0.343921000	2.610545000
6	2.688530000	-1.230164000	-0.379753000	1	1.741671000	-1.996283000	3.770040000
6	3.193857000	-1.559137000	-1.649535000	1	1.440358000	-2.724591000	2.176079000
6	4.446428000	-2.177895000	-1.718980000	1	2.947241000	-3.066303000	3.029466000
6	5.178125000	-2.442921000	-0.570851000	1	1.499758000	-0.757095000	-2.674661000
6	4.675844000	-2.078336000	0.674926000	1	1.504157000	-2.294068000	-4.590089000
6	3.433161000	-1.458900000	0.795178000	1	1.605647000	-3.252781000	-3.099446000
6	2.885841000	-1.074101000	2.160246000	1	3.048015000	-2.995838000	-4.083116000
6	3.957526000	-0.491221000	3.085473000	1	2.668625000	-0.000386000	-4.703610000
6	2.209785000	-2.283478000	2.821436000	1	3.450024000	0.666358000	-3.257408000
6	2.447101000	-1.242364000	-2.934941000	1	4.191947000	-0.689287000	-4.124079000
6	2.130788000	-2.519714000	-3.721843000	1	-2.029513000	2.253402000	1.580662000
6	3.238222000	-0.256747000	-3.804637000	13	-0.031085000	-1.746160000	-0.338760000
1	-2.611872000	0.128117000	-1.826351000	1	-0.137524000	-4.334903000	-1.816378000
1	-4.599404000	1.308942000	-2.688888000	7	0.012009000	1.325934000	0.101378000
1	-5.677515000	0.203737000	-1.829581000	6	0.019691000	2.779092000	0.153967000
1	-4.658305000	1.317417000	-0.915017000	6	0.333690000	3.404873000	1.367485000
1	-3.611690000	-0.635208000	-3.943251000	6	-0.256846000	3.478995000	-1.027330000
1	-4.656160000	-1.772179000	-3.085105000	6	0.358385000	4.800592000	1.375351000
1	-2.897993000	-2.008404000	-3.086514000	6	-0.222010000	4.873588000	-0.965315000
1	-5.594003000	-1.992339000	-0.984439000	6	0.083141000	5.528188000	0.222493000
1	-5.794059000	-3.331035000	1.074853000	1	0.601124000	5.324716000	2.295216000
1	-3.984558000	-3.323018000	2.748788000	1	-0.427511000	5.453146000	-1.860872000

6	-1.911023000	-0.431047000	3.789277000	1	0.436363000	-4.836532000	-1.305970000
6	-0.880301000	-3.134855000	-1.666040000	1	-1.137015000	-5.279229000	-1.987085000
6	-1.959377000	-2.710493000	-2.668947000	1	4.010760000	1.646367000	-0.261773000
6	-0.341125000	-4.528050000	-2.012109000	13	-0.692762000	0.498083000	0.155136000
1	-0.280676000	1.484642000	-2.434717000	7	2.251812000	-0.463072000	-0.226576000
1	0.396582000	2.166010000	-4.708677000	6	3.627007000	-0.917097000	-0.377228000
1	0.621460000	3.834930000	-4.155140000	6	4.464490000	-0.862396000	0.745650000
1	1.664427000	2.549569000	-3.527716000	6	4.037902000	-1.405408000	-1.623447000
1	-2.056587000	2.080965000	-3.972099000	6	5.777413000	-1.308089000	0.582062000
1	-1.911057000	3.796909000	-3.600314000	6	5.359577000	-1.842544000	-1.732390000
1	-2.526426000	2.678825000	-2.370900000	6	6.221887000	-1.792233000	-0.643243000
1	-0.772377000	5.206024000	-2.343885000	1	6.457844000	-1.284064000	1.428585000
1	-0.066547000	6.631730000	-0.460203000	1	5.716090000	-2.232182000	-2.681350000
1	1.153408000	5.664655000	1.447113000	1	7.245252000	-2.137698000	-0.748231000
1	2.425398000	2.197685000	1.551204000	6	3.097252000	-1.498695000	-2.813756000
1	3.476937000	4.465809000	1.875061000	1	2.168557000	-0.968861000	-2.565339000
1	3.358114000	3.486999000	3.348879000	6	3.990931000	-0.373280000	2.106724000
1	2.240199000	4.822526000	3.095512000	1	2.936025000	-0.080078000	2.028141000
1	1.320884000	1.985152000	3.732862000	6	2.732166000	-2.964029000	-3.085327000
1	0.209203000	3.310176000	3.334560000	1	2.009112000	-3.029985000	-3.905145000
1	0.103776000	1.778272000	2.463576000	1	3.621331000	-3.536238000	-3.371092000
1	2.874814000	2.685460000	-1.159388000	1	2.294813000	-3.429436000	-2.197228000
1	3.559499000	1.219206000	-1.904137000	6	3.685855000	-0.847371000	-4.071066000
1	2.848712000	-2.969897000	0.482003000	1	4.569451000	-1.388886000	-4.422443000
1	1.113100000	-3.454474000	0.915968000	1	2.949299000	-0.862392000	-4.879773000
1	-2.789632000	-4.705353000	-0.573404000	1	3.981248000	0.193078000	-3.899324000
1	-3.667628000	-4.704130000	1.734482000	6	4.792187000	0.847471000	2.577906000
1	-2.759061000	-3.133018000	3.407099000	1	4.407881000	1.199284000	3.541140000
1	-0.106356000	-0.590637000	2.644460000	1	5.848252000	0.594541000	2.715972000
1	0.416610000	-1.424539000	4.896441000	1	4.741322000	1.680847000	1.868177000
1	-0.688229000	-2.790837000	4.676911000	6	4.071680000	-1.495004000	3.150835000
1	0.764481000	-2.661702000	3.669414000	1	3.677246000	-1.145688000	4.110149000
1	-2.601197000	-1.061956000	4.359062000	1	3.491311000	-2.366735000	2.837555000
1	-1.460646000	0.280320000	4.490268000	1	5.108437000	-1.809400000	3.309173000
1	-2.489783000	0.126493000	3.046340000	8	-1.980080000	1.308248000	0.939049000
1	-0.047612000	-2.426576000	-1.745608000	1	-1.937171000	0.339712000	-1.214206000
1	-1.555231000	-2.695812000	-3.686464000	5	-3.039441000	0.381971000	-0.609421000
1	-2.352317000	-1.716299000	-2.434131000	8	-3.984200000	1.281049000	-0.992551000
1	-2.802874000	-3.409534000	-2.653233000	8	-3.499972000	-0.770523000	-0.056102000
1	0.086658000	-4.533807000	-3.019551000	6	-5.230090000	0.798740000	-0.389610000

6	-4.946859000	-0.732320000	-0.199703000	6	4.924864000	-1.531066000	-2.151586000
6	-5.567689000	-1.352139000	1.040238000	1	5.989734000	-1.438940000	-1.965229000
6	-5.276896000	-1.564666000	-1.434354000	6	4.447704000	-2.499423000	-3.034916000
6	-5.410898000	1.526564000	0.937810000	1	5.145971000	-3.158984000	-3.540473000
6	-6.370198000	1.123421000	-1.338032000	6	3.080452000	-2.624507000	-3.269536000
1	-6.491704000	2.207478000	-1.408935000	1	2.712037000	-3.379076000	-3.956574000
1	-6.182148000	0.732095000	-2.339183000	6	2.183058000	-1.773269000	-2.630024000
1	-7.306804000	0.698607000	-0.962703000	1	1.114350000	-1.852292000	-2.810166000
1	-5.413715000	2.605727000	0.761536000	6	-2.761628000	0.242829000	1.391744000
1	-4.602469000	1.283836000	1.634250000	6	-3.492974000	-0.804235000	1.978615000
1	-6.361785000	1.252685000	1.403231000	6	-4.725453000	-0.494415000	2.564500000
1	-5.195649000	-0.880912000	1.952245000	1	-5.310807000	-1.289967000	3.017382000
1	-5.305433000	-2.412716000	1.077377000	6	-5.203197000	0.807111000	2.591028000
1	-6.658639000	-1.263949000	1.009425000	1	-6.163433000	1.024719000	3.047624000
1	-6.357487000	-1.655269000	-1.576945000	6	-4.437981000	1.839043000	2.055488000
1	-4.854051000	-2.564141000	-1.297031000	1	-4.807432000	2.858241000	2.106627000
1	-4.838953000	-1.127638000	-2.337634000	6	-3.207652000	1.581837000	1.454917000
6	-2.307616000	2.653796000	1.267059000	6	-2.976510000	-2.230424000	2.062534000
1	-2.776976000	2.667752000	2.254591000	1	-2.012600000	-2.273998000	1.547780000
1	-1.418217000	3.288488000	1.281058000	6	-3.912005000	-3.226566000	1.369901000
1	-3.010835000	3.035404000	0.521356000	1	-4.068675000	-2.963928000	0.318547000
7 (in gas phase)				1	-4.889326000	-3.257356000	1.863147000
13	0.000065000	-0.000002000	1.735970000	1	-3.487219000	-4.234651000	1.408868000
7	-1.503315000	-0.026509000	0.723473000	6	-2.736466000	-2.628835000	3.525294000
7	-0.000043000	0.000342000	-1.492475000	1	-2.052389000	-1.932544000	4.021974000
7	1.503372000	0.026570000	0.723376000	1	-2.305699000	-3.633895000	3.578326000
6	-2.660126000	0.798486000	-1.748640000	1	-3.673167000	-2.635778000	4.092051000
6	-4.035557000	0.680619000	-1.502654000	6	-2.347390000	2.725232000	0.938558000
1	-4.412601000	-0.069359000	-0.810706000	1	-1.728095000	2.339102000	0.125161000
6	-4.925127000	1.530919000	-2.151461000	6	-3.152809000	3.886965000	0.354311000
1	-5.989982000	1.438711000	-1.965055000	1	-3.879251000	3.528637000	-0.381138000
6	-4.448078000	2.499275000	-3.034854000	1	-2.478304000	4.589205000	-0.146189000
1	-5.146418000	3.158752000	-3.540417000	1	-3.687959000	4.445292000	1.129120000
6	-3.080843000	2.624461000	-3.269508000	6	-1.413285000	3.225940000	2.050342000
1	-2.712496000	3.379030000	-3.956584000	1	-0.759573000	2.433457000	2.445700000
6	-2.183358000	1.773344000	-2.629961000	1	-1.992916000	3.599532000	2.900581000
1	-1.114661000	1.852485000	-2.810110000	1	-0.771235000	4.038395000	1.690796000
6	2.659930000	-0.798429000	-1.748749000	6	2.761620000	-0.242872000	1.391730000
6	4.035380000	-0.680681000	-1.502770000	6	3.207551000	-1.581921000	1.454825000
1	4.412512000	0.069284000	-0.810856000	6	4.437772000	-1.839277000	2.055545000

6	3.467038000	0.509303000	1.965305000	1	-1.075272000	2.721589000	2.452950000
6	4.686501000	0.116271000	2.526218000	1	-2.493875000	3.745941000	2.683437000
1	5.235517000	0.8222006000	3.143363000	1	-1.205057000	4.269516000	1.588771000
6	5.202763000	-1.152947000	2.313804000	6	-3.346783000	3.731445000	0.009814000
1	6.151516000	-1.437368000	2.757417000	1	-3.965503000	3.244081000	-0.748442000
6	4.492146000	-2.064057000	1.541866000	1	-2.697729000	4.457664000	-0.490351000
1	4.890939000	-3.063245000	1.393417000	1	-4.004122000	4.290913000	0.683323000
6	3.274957000	-1.723297000	0.952322000	6	-3.023509000	-2.306847000	1.793127000
6	2.952240000	1.906744000	2.271141000	1	-2.012894000	-2.321724000	1.378421000
1	1.964366000	2.016779000	1.816912000	6	-3.894685000	-3.230745000	0.933249000
6	3.859543000	2.983776000	1.663868000	1	-3.493010000	-4.249081000	0.941828000
1	3.951583000	2.866980000	0.578921000	1	-3.936957000	-2.892795000	-0.107249000
1	4.863814000	2.936240000	2.098358000	1	-4.918444000	-3.269131000	1.320754000
1	3.452850000	3.980353000	1.863210000	6	-2.945759000	-2.838110000	3.231238000
6	2.790549000	2.127226000	3.780913000	1	-2.396351000	-2.157362000	3.889910000
1	2.156166000	1.360728000	4.238353000	1	-2.446775000	-3.811889000	3.248955000
1	2.335886000	3.104222000	3.972367000	1	-3.943957000	-2.968947000	3.660917000
1	3.757119000	2.105160000	4.293913000	1	-0.018254000	0.726673000	2.984615000
6	2.530276000	-2.780795000	0.151024000	15	-1.441318000	-0.217204000	-1.116889000
1	1.749535000	-2.284483000	-0.432331000	6	-1.762903000	-1.943513000	-1.565397000
6	3.432098000	-3.521412000	-0.842336000	6	-1.039925000	-2.943051000	-0.902164000
1	4.016625000	-2.828260000	-1.451262000	6	-2.642588000	-2.295575000	-2.592137000
1	2.818507000	-4.134493000	-1.510515000	6	-1.215857000	-4.278146000	-1.239631000
1	4.126176000	-4.194094000	-0.327782000	1	-0.342766000	-2.680902000	-0.108013000
6	1.859499000	-3.793709000	1.089930000	6	-2.818735000	-3.637500000	-2.927708000
1	1.135558000	-3.324901000	1.762863000	1	-3.192869000	-1.530626000	-3.130346000
1	2.610981000	-4.292261000	1.711406000	6	-2.113838000	-4.626311000	-2.249748000
1	1.344798000	-4.566510000	0.508191000	1	-0.663396000	-5.048859000	-0.711582000
6	-2.800700000	0.196933000	1.208732000	1	-3.509190000	-3.906366000	-3.720260000
6	-3.287974000	1.522189000	1.277090000	1	-2.258461000	-5.670219000	-2.508717000
6	-4.530026000	1.741662000	1.870792000	15	1.443625000	0.500076000	-1.048269000
1	-4.919911000	2.753322000	1.928499000	6	1.780636000	2.282322000	-1.119507000
6	-5.279156000	0.690387000	2.386129000	6	2.679867000	2.840690000	-2.031666000
1	-6.248559000	0.880857000	2.835388000	6	1.043091000	3.124936000	-0.278646000
6	-4.774302000	-0.599764000	2.338512000	6	2.861016000	4.222737000	-2.074893000
1	-5.352488000	-1.417297000	2.760079000	1	3.240189000	2.206190000	-2.710160000
6	-3.528351000	-0.874173000	1.764216000	6	1.222873000	4.500615000	-0.324580000
6	-2.491413000	2.713755000	0.770054000	1	0.327126000	2.706196000	0.426238000
1	-1.737154000	2.348634000	0.067589000	6	2.141316000	5.050338000	-1.220185000
6	-1.769232000	3.398175000	1.939769000	1	3.566302000	4.649173000	-2.780511000

1	-3.981855000	-4.319400000	-0.227292000	7-TS2 (in gas phase)			
6	-3.043452000	2.113104000	-2.058089000	13	-0.277188000	-0.616311000	-0.617403000
1	-2.028819000	2.182564000	-1.657903000	7	-0.913530000	1.020421000	-0.145897000
6	-3.928715000	3.090126000	-1.273883000	7	1.589494000	1.698560000	0.556495000
1	-3.547973000	4.111829000	-1.371713000	7	1.455887000	-0.893837000	-0.119388000
1	-3.961076000	2.842474000	-0.207968000	6	-0.429368000	3.514877000	1.184292000
1	-4.954378000	3.074269000	-1.658259000	6	-1.578779000	4.261451000	0.888756000
6	-2.984205000	2.522263000	-3.535614000	1	-2.155656000	4.056009000	-0.010286000
1	-2.391126000	1.816947000	-4.124727000	6	-1.978093000	5.276415000	1.751255000
1	-2.530112000	3.513037000	-3.633135000	1	-2.866071000	5.857285000	1.525032000
1	-3.984469000	2.570119000	-3.977378000	6	-1.236971000	5.547005000	2.902678000
1	-0.001607000	-0.001188000	-4.890202000	1	-1.549506000	6.344450000	3.569412000
15	-1.445267000	0.353094000	1.051989000	6	-0.101704000	4.798202000	3.200606000
6	-1.784902000	2.112288000	1.327989000	1	0.470445000	5.008887000	4.098057000
6	-1.074695000	3.047810000	0.565632000	6	0.306809000	3.780769000	2.341230000
6	-2.659537000	2.556376000	2.322844000	1	1.197146000	3.195015000	2.552108000
6	-1.256757000	4.408188000	0.774135000	6	3.999933000	0.349054000	0.322892000
1	-0.382771000	2.715296000	-0.206040000	6	4.846981000	-0.749252000	0.525042000
6	-2.843174000	3.923301000	2.528135000	1	4.451552000	-1.691859000	0.896663000
1	-3.199963000	1.843746000	2.937366000	6	6.204883000	-0.628202000	0.251909000
6	-2.149842000	4.846597000	1.752870000	1	6.863526000	-1.476222000	0.407194000
1	-0.712429000	5.127817000	0.170732000	6	6.717509000	0.581959000	-0.218169000
1	-3.529888000	4.262994000	3.296381000	1	7.779313000	0.673710000	-0.423721000
1	-2.299606000	5.909689000	1.911485000	6	5.873757000	1.669711000	-0.426269000
15	1.445330000	-0.352485000	1.051976000	1	6.274934000	2.608134000	-0.794626000
6	1.784902000	-2.111591000	1.328580000	6	4.511817000	1.557140000	-0.155332000
6	2.659635000	-2.555223000	2.323571000	1	3.840248000	2.398277000	-0.301771000
6	1.074739000	-3.047486000	0.566648000	6	-2.341260000	1.249862000	0.002235000
6	2.843386000	-3.922042000	2.529429000	6	-3.143593000	1.464812000	-1.136381000
1	3.200002000	-1.842295000	2.937794000	6	-4.510421000	1.685182000	-0.951093000
6	1.256912000	-4.407764000	0.775712000	1	-5.138318000	1.866334000	-1.819399000
1	0.382776000	-2.715366000	-0.205148000	6	-5.081633000	1.664663000	0.313815000
6	2.150079000	-4.845707000	1.754578000	1	-6.146687000	1.837018000	0.435659000
1	3.530156000	-4.261377000	3.297783000	6	-4.282653000	1.416164000	1.422502000
1	0.712629000	-5.127677000	0.172610000	1	-4.731730000	1.394757000	2.411837000
1	2.299946000	-5.908724000	1.913606000	6	-2.906472000	1.212012000	1.296187000
6	-0.001025000	-0.000857000	-3.798371000	6	-2.599905000	1.458056000	-2.555211000
8	-0.031683000	-1.081226000	-3.130605000	1	-1.546338000	1.176928000	-2.516866000
8	0.030373000	1.079840000	-3.131272000	6	-2.687087000	2.850120000	-3.192757000
				1	-2.136477000	3.596671000	-2.609959000

1	-3.729226000	3.179010000	-3.270121000	1	2.993805000	-4.552523000	2.250152000
1	-2.262871000	2.833364000	-4.201907000	6	0.397409000	-4.710161000	1.260750000
6	-3.309147000	0.413628000	-3.425767000	1	-0.283221000	-4.670386000	0.407326000
1	-3.244074000	-0.576574000	-2.966467000	1	-0.202808000	-4.723604000	2.175745000
1	-2.843107000	0.374833000	-4.415676000	1	0.949583000	-5.654722000	1.217392000
1	-4.366854000	0.661506000	-3.567947000	1	-0.501076000	-2.960847000	-3.379077000
6	-2.097274000	0.967155000	2.561814000	15	2.260382000	0.268738000	0.779773000
1	-1.033785000	1.017012000	2.308583000	6	2.246469000	-0.163957000	2.542432000
6	-2.362177000	2.028901000	3.637371000	6	1.069641000	-0.650671000	3.121999000
1	-2.307992000	3.040782000	3.231655000	6	3.374670000	0.038808000	3.343735000
1	-1.622172000	1.936230000	4.439166000	6	1.030546000	-0.962630000	4.475689000
1	-3.352040000	1.896128000	4.086914000	1	0.183376000	-0.807316000	2.511742000
6	-2.389535000	-0.417948000	3.154398000	6	3.330919000	-0.269947000	4.701627000
1	-2.166245000	-1.242092000	2.467424000	1	4.290930000	0.428497000	2.911816000
1	-3.447387000	-0.499499000	3.426615000	6	2.165031000	-0.778124000	5.265342000
1	-1.804712000	-0.564035000	4.068384000	1	0.123558000	-1.366806000	4.913522000
6	2.132176000	-2.047867000	-0.694211000	1	4.212545000	-0.118167000	5.315565000
6	2.793331000	-1.913756000	-1.937471000	1	2.137314000	-1.031383000	6.320267000
6	3.381499000	-3.049889000	-2.497707000	15	0.195181000	2.270107000	0.043104000
1	3.892675000	-2.962164000	-3.452354000	6	0.440554000	3.118609000	-1.542852000
6	3.336483000	-4.281337000	-1.858933000	6	0.469103000	4.512493000	-1.639249000
1	3.807485000	-5.148565000	-2.310721000	6	0.673088000	2.345240000	-2.687102000
6	2.681105000	-4.396581000	-0.642204000	6	0.697083000	5.122167000	-2.872096000
1	2.639090000	-5.361408000	-0.145634000	1	0.311121000	5.126666000	-0.758637000
6	2.058603000	-3.298068000	-0.043693000	6	0.897711000	2.954778000	-3.914447000
6	2.917134000	-0.603845000	-2.704756000	1	0.665122000	1.257500000	-2.633369000
1	2.533040000	0.208346000	-2.078197000	6	0.902449000	4.346900000	-4.008243000
6	2.110066000	-0.630174000	-4.011626000	1	0.710822000	6.204897000	-2.940900000
1	1.037050000	-0.744483000	-3.838573000	1	1.057030000	2.346378000	-4.798903000
1	2.442610000	-1.457385000	-4.648154000	1	1.069964000	4.824158000	-4.968415000
1	2.277424000	0.298294000	-4.568684000	6	-0.681394000	-2.586970000	-2.364003000
6	4.380641000	-0.277876000	-3.036206000	8	-0.553261000	-1.292387000	-2.231912000
1	5.031365000	-0.390073000	-2.167255000	8	-0.984402000	-3.335681000	-1.445117000
1	4.459649000	0.751998000	-3.399314000	1	-1.223960000	-1.708001000	0.439889000
1	4.756784000	-0.935181000	-3.827398000	5	-2.205431000	-2.345229000	0.016065000
6	1.351273000	-3.508344000	1.285016000	8	-2.669956000	-3.346838000	0.793773000
1	0.753884000	-2.617081000	1.493279000	8	-3.099917000	-1.758490000	-0.822122000
6	2.369790000	-3.668486000	2.422424000	6	-4.110585000	-3.396741000	0.536155000
1	1.855255000	-3.797817000	3.380240000	6	-4.243216000	-2.672712000	-0.849051000
1	3.028475000	-2.798250000	2.512132000	6	-4.059868000	-3.612746000	-2.036904000

6	-1.791852000	5.460063000	1.412129000	6	-2.114506000	2.392246000	3.685522000
1	-2.678704000	6.034626000	1.166145000	1	-2.107639000	3.378727000	3.215442000
6	-0.998160000	5.825364000	2.500199000	1	-1.315333000	2.359645000	4.433271000
1	-1.267992000	6.689913000	3.098481000	1	-3.064916000	2.272972000	4.216403000
6	0.136251000	5.085017000	2.821573000	6	-2.123940000	-0.086437000	3.326814000
1	0.750811000	5.369210000	3.669412000	1	-1.852473000	-0.923357000	2.672116000
6	0.488249000	3.979144000	2.050986000	1	-3.175744000	-0.214707000	3.605371000
1	1.374460000	3.395372000	2.283050000	1	-1.525850000	-0.154246000	4.241616000
6	4.017547000	0.290469000	0.110762000	6	2.009569000	-2.136687000	-0.570774000
6	4.867826000	-0.797998000	0.349375000	6	2.581939000	-2.142964000	-1.868661000
1	4.490731000	-1.697762000	0.830577000	6	3.050197000	-3.356066000	-2.379632000
6	6.205624000	-0.720195000	-0.021834000	1	3.496711000	-3.372328000	-3.370170000
1	6.867418000	-1.559401000	0.165152000	6	2.967419000	-4.535485000	-1.650860000
6	6.693645000	0.436196000	-0.632451000	1	3.341601000	-5.464370000	-2.069368000
1	7.739848000	0.495642000	-0.915357000	6	2.404627000	-4.515503000	-0.383996000
6	5.845208000	1.511749000	-0.881440000	1	2.339600000	-5.436409000	0.187687000
1	6.227617000	2.407967000	-1.358786000	6	1.912548000	-3.332622000	0.176517000
6	4.504745000	1.443766000	-0.507116000	6	2.736123000	-0.907593000	-2.748240000
1	3.832631000	2.280365000	-0.677453000	1	2.406359000	-0.031118000	-2.181406000
6	-2.314710000	1.332510000	0.106747000	6	1.899997000	-0.996180000	-4.034927000
6	-3.172566000	1.522165000	-0.996667000	1	0.824108000	-0.994897000	-3.844408000
6	-4.505767000	1.858439000	-0.746638000	1	2.152147000	-1.902349000	-4.597056000
1	-5.173908000	2.026919000	-1.586967000	1	2.131059000	-0.142342000	-4.680539000
6	-4.993854000	1.969755000	0.547778000	6	4.202645000	-0.687337000	-3.150134000
1	-6.034989000	2.225222000	0.719137000	1	4.878314000	-0.760990000	-2.297467000
6	-4.143372000	1.747685000	1.623661000	1	4.319381000	0.302653000	-3.602549000
1	-4.527791000	1.835382000	2.635771000	1	4.515862000	-1.428486000	-3.893564000
6	-2.793739000	1.443914000	1.431316000	6	1.326614000	-3.393157000	1.577968000
6	-2.712214000	1.417020000	-2.441716000	1	0.806348000	-2.452073000	1.768359000
1	-1.686253000	1.043496000	-2.442350000	6	2.443142000	-3.531492000	2.622319000
6	-2.717589000	2.793117000	-3.120882000	1	2.019661000	-3.548994000	3.631835000
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1	-3.735199000	3.196858000	-3.165789000	1	2.995901000	-4.464992000	2.468588000
1	-2.340984000	2.712703000	-4.145796000	6	0.307384000	-4.526798000	1.744027000
6	-3.556253000	0.424186000	-3.250020000	1	-0.461991000	-4.511978000	0.967931000
1	-3.535807000	-0.567506000	-2.791978000	1	-0.193209000	-4.433473000	2.712879000
1	-3.164074000	0.351504000	-4.269922000	1	0.792372000	-5.508161000	1.722583000
1	-4.598853000	0.752653000	-3.325163000	1	-0.079793000	-3.149853000	-2.988653000
6	-1.904700000	1.275032000	2.656126000	15	2.317530000	0.276331000	0.705196000
1	-0.859911000	1.325996000	2.335500000	6	2.448171000	-0.034780000	2.491103000

1	-5.575540000	3.344392000	0.465201000	1	4.756979000	-1.454107000	-2.269674000
6	-3.839009000	2.559170000	1.462803000	1	4.367302000	-0.334067000	-3.588731000
1	-4.232558000	2.762853000	2.454466000	1	4.285527000	-2.078629000	-3.856404000
6	-2.569223000	1.993116000	1.338382000	6	0.817984000	-3.458357000	1.619360000
6	-2.390318000	1.731179000	-2.519152000	1	0.499777000	-2.435263000	1.816057000
1	-1.423812000	1.227078000	-2.463878000	6	1.884488000	-3.818950000	2.661623000
6	-2.210098000	3.022912000	-3.326181000	1	1.465028000	-3.755196000	3.671083000
1	-1.499140000	3.704886000	-2.848168000	1	2.739869000	-3.136449000	2.614997000
1	-3.164763000	3.548857000	-3.436724000	1	2.251821000	-4.839709000	2.508374000
1	-1.834362000	2.795520000	-4.329021000	6	-0.414638000	-4.355192000	1.777447000
6	-3.360515000	0.783085000	-3.235289000	1	-1.178532000	-4.136270000	1.024237000
1	-3.481999000	-0.149042000	-2.676770000	1	-0.860409000	-4.198776000	2.765581000
1	-2.982987000	0.547310000	-4.236156000	1	-0.159994000	-5.417047000	1.698009000
1	-4.348158000	1.241603000	-3.358194000	1	-0.310040000	-2.951204000	-3.032635000
6	-1.797053000	1.666016000	2.607445000	15	2.344274000	-0.000255000	0.719954000
1	-0.748337000	1.504639000	2.341098000	6	2.375655000	-0.305067000	2.514454000
6	-1.833296000	2.802634000	3.635303000	6	1.158324000	-0.456303000	3.190420000
1	-1.603763000	3.767524000	3.176998000	6	3.567615000	-0.315754000	3.244064000
1	-1.097534000	2.610610000	4.423102000	6	1.134240000	-0.644623000	4.566578000
1	-2.814524000	2.876641000	4.116113000	1	0.217778000	-0.441936000	2.641917000
6	-2.332149000	0.375441000	3.243490000	6	3.541631000	-0.504625000	4.625114000
1	-2.211082000	-0.484782000	2.577386000	1	4.519418000	-0.179882000	2.740686000
1	-3.398970000	0.477142000	3.475027000	6	2.329583000	-0.675776000	5.285128000
1	-1.806639000	0.165466000	4.181846000	1	0.186526000	-0.777531000	5.078806000
6	1.690732000	-2.346585000	-0.537683000	1	4.472547000	-0.518612000	5.182419000
6	2.267423000	-2.457262000	-1.828054000	1	2.312536000	-0.830118000	6.359248000
6	2.533604000	-3.732963000	-2.332049000	15	0.586077000	2.229214000	-0.086422000
1	2.981305000	-3.827327000	-3.317897000	6	0.907644000	2.871521000	-1.753942000
6	2.246674000	-4.879453000	-1.601718000	6	1.192540000	4.219070000	-1.989878000
1	2.463134000	-5.859752000	-2.014178000	6	0.939797000	1.963125000	-2.817993000
6	1.687507000	-4.758915000	-0.338568000	6	1.472809000	4.655799000	-3.283825000
1	1.470108000	-5.653230000	0.238332000	1	1.191987000	4.931487000	-1.171202000
6	1.398225000	-3.507430000	0.215230000	6	1.215463000	2.401591000	-4.106900000
6	2.619623000	-1.263905000	-2.706566000	1	0.727910000	0.911440000	-2.636820000
1	2.446484000	-0.347461000	-2.134905000	6	1.475212000	3.752234000	-4.341264000
6	1.755790000	-1.209456000	-3.975859000	1	1.685238000	5.704756000	-3.462598000
1	0.701347000	-1.010515000	-3.760438000	1	1.213290000	1.696704000	-4.932188000
1	1.826734000	-2.150052000	-4.534443000	1	1.681838000	4.097019000	-5.349411000
1	2.117608000	-0.414466000	-4.635805000	6	-0.930859000	-2.535125000	-2.234635000
6	4.097317000	-1.287170000	-3.122711000	8	-0.796254000	-1.351662000	-1.895151000

8	-1.763276000	-3.378369000	-1.722215000	6	3.542957000	-2.180715000	0.143088000
1	-1.452230000	-1.539789000	0.758298000	6	3.505458000	-3.577020000	0.260674000
5	-2.916030000	-3.039657000	-0.956376000	1	2.625966000	-4.074306000	0.664441000
8	-3.523976000	-3.981301000	-0.218480000	6	4.605927000	-4.330108000	-0.134495000
8	-3.500580000	-1.826945000	-1.024977000	1	4.581765000	-5.410733000	-0.040414000
6	-4.584345000	-3.283054000	0.507485000	6	5.736224000	-3.695692000	-0.651291000
6	-4.790130000	-1.975479000	-0.348808000	1	6.594706000	-4.286726000	-0.954289000
6	-5.829815000	-2.131411000	-1.452371000	6	5.765983000	-2.309812000	-0.784015000
6	-5.036139000	-0.715299000	0.458716000	1	6.644609000	-1.820217000	-1.190904000
6	-5.798962000	-4.192436000	0.571161000	6	4.670579000	-1.547568000	-0.384597000
6	-4.039548000	-3.017222000	1.905756000	1	4.682380000	-0.464165000	-0.467441000
1	-3.783381000	-3.972872000	2.371002000	6	-0.713959000	2.606799000	-0.031599000
1	-3.135257000	-2.403084000	1.864862000	6	-1.113947000	3.310695000	-1.185534000
1	-4.782667000	-2.511862000	2.528984000	6	-2.001593000	4.380702000	-1.032442000
1	-5.558797000	-5.077978000	1.164551000	1	-2.308678000	4.939359000	-1.912090000
1	-6.112967000	-4.519146000	-0.421403000	6	-2.499349000	4.736541000	0.211618000
1	-6.633760000	-3.673072000	1.053152000	1	-3.187205000	5.570809000	0.306358000
1	-5.634805000	-3.018907000	-2.062498000	6	-2.121119000	4.011997000	1.335196000
1	-5.790959000	-1.252258000	-2.101193000	1	-2.522478000	4.284152000	2.307076000
1	-6.837483000	-2.210430000	-1.035750000	6	-1.229347000	2.944122000	1.241069000
1	-5.959939000	-0.806506000	1.039666000	6	-0.628284000	2.972305000	-2.584836000
1	-5.135313000	0.137650000	-0.218578000	1	-0.042253000	2.053194000	-2.526146000
1	-4.205611000	-0.508704000	1.138437000	6	0.274470000	4.081160000	-3.140685000
				1	1.138014000	4.267463000	-2.493782000
				1	-0.283218000	5.018857000	-3.241594000
				1	0.650399000	3.804503000	-4.131097000
				6	-1.796700000	2.708436000	-3.542439000
				1	-2.467222000	1.940800000	-3.149379000
				1	-1.413353000	2.370696000	-4.510616000
				1	-2.382296000	3.616740000	-3.718505000
				6	-0.875160000	2.173228000	2.503030000
				1	0.018544000	1.577350000	2.299317000
				6	-0.540233000	3.086309000	3.686676000
				1	0.184564000	3.854277000	3.404866000
				1	-0.113931000	2.492983000	4.502541000
				1	-1.433967000	3.584774000	4.076475000
				6	-2.015154000	1.216953000	2.883283000
				1	-2.223803000	0.489962000	2.090093000
				1	-2.936181000	1.780710000	3.069259000
				1	-1.769452000	0.667779000	3.799622000
7-TS4 (in gas phase)							
13	-0.434628000	-0.163801000	-0.488066000				
7	0.223375000	1.501471000	-0.131184000				
7	2.544473000	0.379424000	0.633481000				
7	0.796046000	-1.480207000	-0.164189000				
6	2.133475000	3.041133000	1.327050000				
6	1.744628000	4.360951000	1.058660000				
1	1.233583000	4.609508000	0.130909000				
6	2.020707000	5.360756000	1.985195000				
1	1.722726000	6.383324000	1.778586000				
6	2.679732000	5.048219000	3.174781000				
1	2.898636000	5.833008000	3.892010000				
6	3.054826000	3.735012000	3.446424000				
1	3.564258000	3.494216000	4.373678000				
6	2.783914000	2.727777000	2.523188000				
1	3.079942000	1.699932000	2.713845000				

6	0.500633000	-2.785488000	-0.721761000	1	3.396466000	-3.140034000	5.123622000
6	1.036055000	-3.122711000	-1.986210000	1	1.364584000	-2.276266000	6.249889000
6	0.718832000	-4.368246000	-2.528791000	15	1.863531000	1.726088000	0.123803000
1	1.123609000	-4.640801000	-3.499254000	6	2.679601000	2.251464000	-1.408156000
6	-0.103449000	-5.263042000	-1.855826000	6	3.601689000	3.300387000	-1.439170000
1	-0.332411000	-6.229287000	-2.294030000	6	2.432616000	1.514000000	-2.572611000
6	-0.635155000	-4.911798000	-0.623941000	6	4.245251000	3.626018000	-2.632444000
1	-1.280093000	-5.611795000	-0.099851000	1	3.818651000	3.867139000	-0.539378000
6	-0.355063000	-3.674069000	-0.035874000	6	3.076697000	1.838847000	-3.758996000
6	1.915640000	-2.180285000	-2.793717000	1	1.721462000	0.689831000	-2.559306000
1	2.228373000	-1.360686000	-2.140826000	6	3.979436000	2.902671000	-3.790210000
6	1.134507000	-1.583981000	-3.973683000	1	4.954128000	4.447214000	-2.653467000
1	0.255850000	-1.020045000	-3.648236000	1	2.869674000	1.272011000	-4.661234000
1	0.789504000	-2.380520000	-4.642084000	1	4.477090000	3.163040000	-4.718881000
1	1.782350000	-0.921029000	-4.558522000	6	-2.426532000	-0.681573000	-1.530490000
6	3.190228000	-2.859049000	-3.307148000	8	-1.310524000	-0.330449000	-2.075695000
1	3.717375000	-3.385360000	-2.508173000	8	-3.444481000	0.145087000	-1.614935000
1	3.865083000	-2.106447000	-3.728178000	1	-1.946549000	-0.542143000	0.129434000
1	2.966427000	-3.578950000	-4.101514000	5	-4.665106000	-0.224630000	-1.023493000
6	-0.958167000	-3.366470000	1.325830000	8	-4.812852000	-1.422872000	-0.403029000
1	-0.733061000	-2.326243000	1.568406000	8	-5.733867000	0.591757000	-1.023364000
6	-0.328777000	-4.249020000	2.411705000	6	-6.077827000	-1.317144000	0.321005000
1	-0.721957000	-3.980960000	3.397803000	6	-6.832908000	-0.217794000	-0.504666000
1	0.759452000	-4.134208000	2.442999000	6	-7.566841000	-0.782562000	-1.716072000
1	-0.554295000	-5.305759000	2.230672000	6	-7.746870000	0.674464000	0.315226000
6	-2.484569000	-3.516300000	1.340729000	6	-6.744049000	-2.679950000	0.337204000
1	-2.972909000	-2.859106000	0.613702000	6	-5.723922000	-0.863688000	1.733619000
1	-2.868272000	-3.258907000	2.334259000	1	-5.022800000	-1.580423000	2.169887000
1	-2.792360000	-4.545203000	1.127414000	1	-5.248885000	0.122951000	1.725109000
1	-2.664904000	-1.740240000	-1.384575000	1	-6.613647000	-0.816017000	2.367279000
15	2.173940000	-1.165271000	0.725784000	1	-6.137112000	-3.376332000	0.922539000
6	1.932300000	-1.595249000	2.474270000	1	-6.857226000	-3.083580000	-0.670372000
6	0.798267000	-1.090583000	3.122652000	1	-7.732084000	-2.612066000	0.803449000
6	2.874036000	-2.322645000	3.206008000	1	-6.917315000	-1.437806000	-2.305289000
6	0.593383000	-1.332649000	4.474354000	1	-7.887469000	0.045489000	-2.352664000
1	0.062544000	-0.513122000	2.565780000	1	-8.450188000	-1.350684000	-1.412074000
6	2.664638000	-2.568060000	4.562728000	1	-8.530184000	0.076916000	0.792575000
1	3.770754000	-2.699892000	2.725249000	1	-8.226377000	1.406059000	-0.339782000
6	1.525950000	-2.080452000	5.194675000	1	-7.194165000	1.214331000	1.085997000
1	-0.292976000	-0.945387000	4.967314000				

7-IM4 (in gas phase)			1	-1.512196000	3.698528000	-3.163427000	
1	-0.853460000	-3.258017000	-1.937453000	1	-3.182564000	3.391827000	-3.677335000
13	-0.243563000	-0.604894000	-0.800479000	1	-1.835007000	2.685581000	-4.580060000
7	-0.546131000	1.123546000	-0.309911000	6	-3.129337000	0.611058000	-3.295269000
7	2.106156000	1.342257000	0.049201000	1	-3.169366000	-0.265717000	-2.637330000
7	1.324948000	-1.216362000	-0.057329000	1	-2.753277000	0.290629000	-4.271761000
6	0.476463000	3.485531000	0.926659000	1	-4.155736000	0.973975000	-3.420730000
6	-0.545666000	4.428476000	0.744288000	6	-1.628080000	1.349153000	2.393433000
1	-1.212359000	4.361946000	-0.112742000	1	-0.571477000	1.256475000	2.129323000
6	-0.702690000	5.459937000	1.664228000	6	-1.711690000	2.328055000	3.567386000
1	-1.488828000	6.193789000	1.520286000	1	-1.488879000	3.350662000	3.251438000
6	0.145213000	5.547274000	2.768809000	1	-0.985226000	2.039033000	4.334522000
1	0.019892000	6.355652000	3.482285000	1	-2.702722000	2.319631000	4.033920000
6	1.146958000	4.599645000	2.961262000	6	-2.130398000	-0.035569000	2.825275000
1	1.801769000	4.664383000	3.824010000	1	-1.908004000	-0.802647000	2.073637000
6	1.318246000	3.570310000	2.039062000	1	-3.217443000	-0.025812000	2.956201000
1	2.107899000	2.835963000	2.171502000	1	-1.671072000	-0.330472000	3.774384000
6	4.098303000	-0.544074000	0.337195000	6	1.678582000	-2.545543000	-0.525480000
6	4.613821000	-1.752920000	0.819119000	6	2.423606000	-2.713962000	-1.716874000
1	3.959875000	-2.482085000	1.292268000	6	2.664455000	-4.016747000	-2.160193000
6	5.972721000	-2.018733000	0.692578000	1	3.239439000	-4.162658000	-3.070169000
1	6.376358000	-2.956484000	1.059687000	6	2.182660000	-5.124196000	-1.476465000
6	6.814719000	-1.076265000	0.100746000	1	2.388710000	-6.124753000	-1.843035000
1	7.876527000	-1.283064000	0.012059000	6	1.422829000	-4.942009000	-0.330046000
6	6.300033000	0.126980000	-0.375283000	1	1.032898000	-5.807478000	0.197415000
1	6.958299000	0.856702000	-0.835363000	6	1.145035000	-3.662062000	0.155725000
6	4.938112000	0.397262000	-0.260415000	6	2.974553000	-1.573544000	-2.565368000
1	4.517381000	1.331419000	-0.621457000	1	2.786156000	-0.623292000	-2.052514000
6	-1.885243000	1.652357000	-0.144613000	6	2.297566000	-1.504155000	-3.943657000
6	-2.660667000	1.990816000	-1.269913000	1	1.218680000	-1.364175000	-3.864940000
6	-3.920632000	2.560228000	-1.060282000	1	2.482713000	-2.425384000	-4.506934000
1	-4.525751000	2.836563000	-1.920045000	1	2.728124000	-0.676909000	-4.519816000
6	-4.413730000	2.765814000	0.220981000	6	4.490607000	-1.712718000	-2.772424000
1	-5.390390000	3.218723000	0.364070000	1	5.020273000	-1.919154000	-1.840839000
6	-3.657657000	2.373194000	1.319765000	1	4.895810000	-0.793353000	-3.206931000
1	-4.056093000	2.513581000	2.320511000	1	4.708181000	-2.527789000	-3.470983000
6	-2.390164000	1.813193000	1.163416000	6	0.297783000	-3.523424000	1.409594000
6	-2.223899000	1.692654000	-2.693555000	1	-0.053802000	-2.489648000	1.458850000
1	-1.213522000	1.283122000	-2.669345000	6	1.143514000	-3.797983000	2.659378000
6	-2.188671000	2.942938000	-3.576669000	1	0.554626000	-3.648464000	3.571123000

6	6.223016000	0.757830000	-0.275648000	1	1.592821000	-5.668109000	-0.204995000
1	6.794258000	1.597575000	-0.657653000	6	1.517965000	-3.526032000	-0.063058000
6	4.846024000	0.878739000	-0.100013000	6	3.073180000	-1.061331000	-2.637994000
1	4.329171000	1.805285000	-0.333427000	1	2.816201000	-0.186226000	-2.031495000
6	-2.035238000	1.535847000	-0.108055000	6	2.410960000	-0.898301000	-4.014866000
6	-2.763630000	1.837759000	-1.273558000	1	1.327659000	-0.780821000	-3.951812000
6	-4.082946000	2.280250000	-1.138103000	1	2.621729000	-1.765250000	-4.650425000
1	-4.653680000	2.523834000	-2.030797000	1	2.828215000	-0.017905000	-4.516223000
6	-4.676271000	2.401718000	0.110301000	6	4.596795000	-1.069718000	-2.837234000
1	-5.700145000	2.753305000	0.196997000	1	5.131124000	-1.311785000	-1.917480000
6	-3.955942000	2.059566000	1.248734000	1	4.934043000	-0.089134000	-3.187845000
1	-4.430917000	2.133085000	2.222787000	1	4.881285000	-1.806743000	-3.596096000
6	-2.635388000	1.620904000	1.165955000	6	0.754808000	-3.573154000	1.250970000
6	-2.208830000	1.630138000	-2.671335000	1	0.344616000	-2.578948000	1.434849000
1	-1.171498000	1.306386000	-2.585537000	6	1.702928000	-3.911510000	2.409361000
6	-2.214230000	2.914164000	-3.505505000	1	1.158914000	-3.921770000	3.359667000
1	-1.621771000	3.698803000	-3.022485000	1	2.511125000	-3.177472000	2.498644000
1	-3.231001000	3.293963000	-3.651157000	1	2.152390000	-4.899802000	2.261699000
1	-1.782393000	2.725532000	-4.493675000	6	-0.427400000	-4.548930000	1.219480000
6	-2.977668000	0.503050000	-3.371921000	1	-1.094534000	-4.351922000	0.374501000
1	-3.003862000	-0.393354000	-2.739918000	1	-1.010343000	-4.447489000	2.141306000
1	-2.505704000	0.247410000	-4.326383000	1	-0.095387000	-5.590579000	1.162202000
1	-4.016786000	0.789648000	-3.568578000	1	-1.859943000	-2.445683000	-2.847380000
6	-1.921872000	1.188975000	2.435407000	15	2.365230000	0.007214000	0.752798000
1	-0.845873000	1.182941000	2.241856000	6	2.236278000	-0.310398000	2.538835000
6	-2.155315000	2.134482000	3.616801000	6	1.003166000	-0.651960000	3.101848000
1	-1.974805000	3.175695000	3.336322000	6	3.344759000	-0.128853000	3.374245000
1	-1.473256000	1.875042000	4.433351000	6	0.882502000	-0.833802000	4.475332000
1	-3.176054000	2.054451000	4.005407000	1	0.134255000	-0.789342000	2.465768000
6	-2.348338000	-0.238345000	2.807393000	6	3.220635000	-0.308779000	4.749531000
1	-2.044457000	-0.966473000	2.046605000	1	4.307506000	0.146588000	2.955264000
1	-3.438607000	-0.300645000	2.889407000	6	1.993615000	-0.667166000	5.299908000
1	-1.913047000	-0.528948000	3.769362000	1	-0.073331000	-1.118563000	4.903433000
6	1.901223000	-2.313833000	-0.681260000	1	4.086658000	-0.173343000	5.389080000
6	2.611806000	-2.316863000	-1.906311000	1	1.901598000	-0.817486000	6.370773000
6	2.928731000	-3.551160000	-2.479165000	15	0.585189000	2.225350000	-0.027070000
1	3.473429000	-3.570472000	-3.419062000	6	0.875044000	3.060240000	-1.612219000
6	2.568487000	-4.749723000	-1.877553000	6	0.905258000	4.448888000	-1.753052000
1	2.830004000	-5.694579000	-2.343305000	6	1.132120000	2.248272000	-2.725054000
6	1.872665000	-4.730866000	-0.676838000	6	1.158626000	5.016884000	-3.002023000

6	-2.580104000	1.447737000	3.755315000	6	3.932203000	-0.605334000	2.917083000
1	-2.600347000	2.538254000	3.669313000	6	1.627491000	-0.808846000	4.483657000
1	-1.906837000	1.182596000	4.576848000	1	0.549801000	-0.279187000	2.705091000
1	-3.581654000	1.101705000	4.030373000	6	4.029069000	-0.944092000	4.267111000
6	-2.173154000	-0.725631000	2.553814000	1	4.834086000	-0.506681000	2.322246000
1	-1.752686000	-1.235027000	1.674339000	6	2.882218000	-1.053003000	5.045789000
1	-3.218505000	-1.045844000	2.613868000	1	0.731853000	-0.880576000	5.093044000
1	-1.642972000	-1.092757000	3.440450000	1	5.005123000	-1.119040000	4.707389000
6	1.946220000	-2.261847000	-0.630009000	1	2.962351000	-1.319802000	6.094667000
6	2.519298000	-2.308982000	-1.919381000	15	0.410936000	2.253930000	0.188179000
6	3.065612000	-3.514800000	-2.351972000	6	0.657787000	3.249186000	-1.304228000
1	3.525625000	-3.575100000	-3.332950000	6	0.518370000	4.637774000	-1.334047000
6	3.025567000	-4.648341000	-1.544478000	6	1.073698000	2.569826000	-2.457098000
1	3.462315000	-5.578305000	-1.894273000	6	0.761008000	5.334276000	-2.518445000
6	2.396792000	-4.597885000	-0.309624000	1	0.230524000	5.181625000	-0.440443000
1	2.326315000	-5.498690000	0.293822000	6	1.312965000	3.264369000	-3.634082000
6	1.830855000	-3.410961000	0.169008000	1	1.208677000	1.488913000	-2.432345000
6	2.466793000	-1.100589000	-2.841580000	6	1.148216000	4.650802000	-3.665720000
1	2.520216000	-0.201246000	-2.222599000	1	0.648578000	6.413199000	-2.538864000
6	1.127561000	-1.081808000	-3.595238000	1	1.629231000	2.730661000	-4.524995000
1	0.256685000	-1.112005000	-2.923432000	1	1.332145000	5.196285000	-4.585691000
1	1.040109000	-1.962731000	-4.239355000	8	-1.354774000	-1.848884000	-0.925370000
1	1.039894000	-0.187985000	-4.223985000	5	-2.650859000	-2.240954000	-0.783622000
6	3.633822000	-1.019894000	-3.826279000	8	-3.085964000	-3.503754000	-1.076203000
1	4.592360000	-1.107007000	-3.305850000	8	-3.636449000	-1.412930000	-0.302193000
1	3.614039000	-0.056406000	-4.345581000	6	-4.414500000	-3.612040000	-0.513970000
1	3.579508000	-1.802415000	-4.589950000	6	-4.885866000	-2.119091000	-0.483388000
6	1.054304000	-3.437757000	1.474601000	6	-5.469401000	-1.653091000	-1.814324000
1	0.704581000	-2.422286000	1.684733000	6	-5.823560000	-1.766318000	0.658449000
6	1.924364000	-3.873500000	2.657838000	6	-5.252429000	-4.527685000	-1.389129000
1	1.346287000	-3.836687000	3.586770000	6	-4.249337000	-4.203908000	0.884268000
1	2.797924000	-3.223487000	2.773669000	1	-3.719345000	-5.156684000	0.803436000
1	2.279017000	-4.901424000	2.527253000	1	-3.658276000	-3.536947000	1.522824000
6	-0.185586000	-4.334710000	1.342301000	1	-5.216333000	-4.380231000	1.363906000
1	-0.815581000	-4.031372000	0.499663000	1	-4.849188000	-5.542977000	-1.349583000
1	-0.781636000	-4.288398000	2.260651000	1	-5.246515000	-4.198401000	-2.429740000
1	0.101934000	-5.379656000	1.184839000	1	-6.287311000	-4.555828000	-1.032387000
15	2.441198000	0.109288000	0.619176000	1	-4.816725000	-1.930891000	-2.648485000
6	2.678162000	-0.384363000	2.345045000	1	-5.554377000	-0.562239000	-1.791422000
6	1.528786000	-0.472623000	3.141306000	1	-6.460497000	-2.081378000	-1.989598000

1	-6.746336000	-2.352100000	0.591785000	6	0.543387000	-3.519135000	0.850913000
1	-6.082409000	-0.705290000	0.599913000	6	1.910620000	-1.241855000	3.671727000
1	-5.360303000	-1.953264000	1.629876000	1	1.930863000	-0.368484000	3.015497000
7-TSS' (in gas phase)				6	3.355624000	-1.533572000	4.098690000
1	-3.133867000	-0.876507000	2.256576000	1	4.001273000	-1.743837000	3.239300000
13	0.258632000	0.305879000	0.897560000	1	3.388307000	-2.398546000	4.770382000
7	1.351101000	-1.176039000	0.746060000	1	3.776290000	-0.674705000	4.631689000
7	2.500753000	-0.104854000	-1.420265000	6	1.055487000	-0.877719000	4.891373000
7	0.339421000	1.333188000	-0.631908000	1	0.008119000	-0.723649000	4.620959000
6	3.399697000	-2.635536000	-0.666368000	1	1.424951000	0.048989000	5.341948000
6	3.835038000	-3.576254000	0.277550000	1	1.104089000	-1.657590000	5.658452000
1	3.703994000	-3.392611000	1.341724000	6	0.239983000	-3.596872000	-0.640890000
6	4.446716000	-4.748243000	-0.152386000	1	0.614033000	-2.690661000	-1.129920000
1	4.785130000	-5.478055000	0.575645000	6	0.904618000	-4.811928000	-1.305089000
6	4.626046000	-4.982724000	-1.516916000	1	1.950704000	-4.922526000	-1.018341000
1	5.110452000	-5.896088000	-1.847526000	1	0.850337000	-4.713130000	-2.393989000
6	4.185281000	-4.052334000	-2.453823000	1	0.382308000	-5.735906000	-1.033921000
1	4.323165000	-4.238788000	-3.513781000	6	-1.271322000	-3.684884000	-0.893443000
6	3.572799000	-2.874165000	-2.030999000	1	-1.791188000	-2.785017000	-0.561102000
1	3.235816000	-2.130438000	-2.747694000	1	-1.697817000	-4.546799000	-0.367332000
6	2.034294000	2.218909000	-2.799520000	1	-1.466828000	-3.813310000	-1.963329000
6	1.246904000	3.200507000	-3.416305000	6	-0.193483000	2.691614000	-0.642596000
1	0.164785000	3.187313000	-3.316097000	6	0.642595000	3.760006000	-0.245707000
6	1.856099000	4.207394000	-4.156261000	6	0.139124000	5.061710000	-0.301729000
1	1.246628000	4.971985000	-4.626455000	1	0.777986000	5.888010000	-0.003806000
6	3.244246000	4.230942000	-4.297829000	6	-1.151487000	5.320279000	-0.739716000
1	3.713992000	5.014893000	-4.883529000	1	-1.519995000	6.340257000	-0.789148000
6	4.026454000	3.253002000	-3.690729000	6	-1.966086000	4.261158000	-1.113863000
1	5.105872000	3.271663000	-3.800063000	1	-2.974267000	4.462789000	-1.464260000
6	3.424430000	2.246954000	-2.938002000	6	-1.516565000	2.937859000	-1.070512000
1	4.020569000	1.477373000	-2.457538000	6	2.076891000	3.587641000	0.232185000
6	1.077840000	-2.384219000	1.508184000	1	2.409563000	2.570374000	-0.000280000
6	1.328862000	-2.413091000	2.897380000	6	2.173898000	3.795656000	1.750240000
6	1.048929000	-3.584435000	3.606100000	1	1.608920000	3.042694000	2.309070000
1	1.247739000	-3.614483000	4.673484000	1	1.776253000	4.779345000	2.023896000
6	0.525393000	-4.703175000	2.976451000	1	3.220845000	3.757394000	2.069141000
1	0.314710000	-5.604031000	3.543963000	6	3.042564000	4.555155000	-0.467785000
6	0.274806000	-4.659730000	1.612642000	1	2.866729000	4.597374000	-1.545098000
1	-0.132392000	-5.537162000	1.118118000	1	4.075632000	4.235768000	-0.295943000
				1	2.943673000	5.569804000	-0.067626000

6	-2.463517000	1.850808000	-1.551623000	8	-4.130243000	-1.326489000	-1.570605000
1	-2.030894000	0.884285000	-1.292351000	6	-5.982782000	-2.035359000	-0.289838000
6	-2.636662000	1.906096000	-3.076622000	6	-5.341433000	-2.115966000	-1.720349000
1	-3.273665000	1.077956000	-3.406163000	6	-4.900784000	-3.530732000	-2.086468000
1	-1.682584000	1.821635000	-3.607221000	6	-6.180375000	-1.506630000	-2.829660000
1	-3.111699000	2.847398000	-3.376775000	6	-6.729334000	-3.285295000	0.143459000
6	-3.840242000	1.926573000	-0.880668000	6	-6.851498000	-0.797274000	-0.090090000
1	-3.756244000	1.805401000	0.201908000	1	-7.103398000	-0.711311000	0.970054000
1	-4.472226000	1.130899000	-1.287738000	1	-6.323871000	0.113285000	-0.391233000
1	-4.344088000	2.877071000	-1.086437000	1	-7.780480000	-0.868315000	-0.662532000
1	-1.982918000	-2.161482000	1.718877000	1	-7.137010000	-3.138087000	1.146891000
15	1.298139000	0.824662000	-1.916179000	1	-6.073764000	-4.157596000	0.164506000
6	0.277779000	-0.034938000	-3.143307000	1	-7.563154000	-3.485568000	-0.537168000
6	-0.791031000	-0.836177000	-2.730529000	1	-4.279245000	-3.966523000	-1.296930000
6	0.578281000	0.071399000	-4.506208000	1	-4.312053000	-3.496591000	-3.007651000
6	-1.571936000	-1.497749000	-3.672462000	1	-5.760487000	-4.185050000	-2.255148000
1	-1.043895000	-0.923163000	-1.676230000	1	-7.136330000	-2.032283000	-2.921298000
6	-0.197741000	-0.603111000	-5.444494000	1	-5.648164000	-1.596474000	-3.780844000
1	1.407075000	0.690352000	-4.836999000	1	-6.375669000	-0.448083000	-2.645960000
6	-1.277275000	-1.378677000	-5.029050000	1	0.168953000	1.358790000	2.168853000
1	-2.427701000	-2.073279000	-3.335852000	5	-1.389269000	0.998893000	2.574317000
1	0.034114000	-0.511321000	-6.500579000	8	-1.442133000	1.065121000	3.941641000
1	-1.893055000	-1.886524000	-5.764786000	8	-2.213813000	1.898884000	1.940467000
15	2.758208000	-1.032359000	-0.152770000	6	-2.442715000	2.071982000	4.260302000
6	4.089645000	-0.317262000	0.862993000	6	-2.513773000	2.908026000	2.937109000
6	5.400344000	-0.800752000	0.795578000	6	-3.872530000	3.508153000	2.620932000
6	3.809411000	0.777973000	1.687688000	6	-1.428813000	3.976094000	2.852094000
6	6.403334000	-0.217230000	1.567154000	6	-3.741772000	1.328002000	4.555205000
1	5.643954000	-1.636094000	0.147454000	6	-1.981638000	2.849105000	5.480773000
6	4.809033000	1.355582000	2.460845000	1	-1.965457000	2.189010000	6.352150000
1	2.801414000	1.182875000	1.747729000	1	-0.978111000	3.253899000	5.338358000
6	6.107982000	0.851716000	2.406638000	1	-2.669894000	3.674742000	5.689479000
1	7.415371000	-0.604783000	1.513133000	1	-3.560163000	0.592292000	5.342814000
1	4.572666000	2.187817000	3.116059000	1	-4.107054000	0.803899000	3.665505000
1	6.887743000	1.295708000	3.017042000	1	-4.523997000	2.013935000	4.892994000
6	-2.316449000	-1.128406000	1.576556000	1	-4.641369000	2.738291000	2.525266000
8	-1.203006000	-0.297434000	1.873227000	1	-3.810585000	4.053223000	1.673923000
8	-2.642572000	-0.885193000	0.246169000	1	-4.171992000	4.211417000	3.404853000
5	-3.845232000	-1.339211000	-0.237332000	1	-1.644874000	4.811456000	3.524791000
8	-4.814879000	-1.869784000	0.561232000	1	-1.384677000	4.350666000	1.825518000

1	-0.447716000	3.567016000	3.111922000	6	2.467559000	-4.212880000	0.716965000
				1	1.621445000	-4.358887000	1.384893000
7-TS6 (in gas phase)							
5	-3.057462000	-0.538691000	-0.999997000	6	3.158583000	-5.315946000	0.227016000
8	-3.079537000	-1.875835000	-0.823905000	1	2.849503000	-6.315201000	0.515517000
8	-4.112225000	-0.002242000	-1.657956000	6	4.242633000	-5.137449000	-0.633211000
6	-4.268942000	-2.361399000	-1.513157000	1	4.780250000	-6.001748000	-1.010306000
6	-5.123723000	-1.051743000	-1.696308000	6	4.633779000	-3.856044000	-1.011463000
6	-5.868769000	-0.956121000	-3.016449000	1	5.473172000	-3.716741000	-1.684851000
6	-6.069072000	-0.785500000	-0.530155000	6	3.952461000	-2.745980000	-0.518103000
6	-3.810177000	-2.966422000	-2.832625000	1	4.261394000	-1.742351000	-0.795454000
6	-4.913973000	-3.423705000	-0.639525000	6	0.422715000	2.834592000	-0.542692000
1	-4.241828000	-4.282404000	-0.564992000	6	-0.281251000	3.223563000	-1.698856000
1	-5.103114000	-3.049446000	0.368746000	6	-0.731713000	4.541673000	-1.799084000
1	-5.859139000	-3.757658000	-1.079697000	1	-1.259683000	4.853937000	-2.695956000
1	-3.081666000	-3.754136000	-2.619574000	6	-0.528651000	5.449914000	-0.771591000
1	-3.336514000	-2.214804000	-3.471345000	1	-0.882592000	6.472239000	-0.865334000
1	-4.652603000	-3.404731000	-3.374932000	6	0.116939000	5.037577000	0.386931000
1	-6.412709000	-0.008968000	-3.058213000	1	0.247973000	5.743003000	1.202809000
1	-6.594868000	-1.770803000	-3.102611000	6	0.598446000	3.736113000	0.532106000
1	-5.188891000	-0.997740000	-3.869013000	6	-0.605390000	2.265332000	-2.830607000
1	-6.868576000	-1.530476000	-0.493213000	1	-0.365197000	1.255521000	-2.487545000
1	-6.524465000	0.198894000	-0.669776000	6	0.243772000	2.569288000	-4.070485000
1	-5.533811000	-0.783032000	0.424387000	1	1.314067000	2.554716000	-3.841166000
13	-0.326613000	0.254462000	0.303951000	1	-0.003123000	3.560783000	-4.465660000
7	0.878682000	1.458227000	-0.419512000	1	0.055043000	1.834807000	-4.861782000
7	2.809616000	-0.098096000	0.601294000	6	-2.099554000	2.274850000	-3.176675000
7	0.459822000	-1.392082000	0.497802000	1	-2.714504000	2.154586000	-2.280662000
6	3.585117000	2.438919000	-0.130173000	1	-2.333031000	1.456900000	-3.867342000
6	3.583478000	3.557351000	-0.972379000	1	-2.391794000	3.209779000	-3.666322000
1	2.858943000	3.639239000	-1.779573000	6	1.226854000	3.361750000	1.868303000
6	4.517481000	4.567931000	-0.773440000	1	1.697921000	2.376598000	1.781809000
1	4.515468000	5.439282000	-1.419848000	6	2.300762000	4.362687000	2.314645000
6	5.459952000	4.455607000	0.249649000	1	3.003003000	4.595537000	1.511933000
1	6.194336000	5.241626000	0.394619000	1	2.863758000	3.957135000	3.161367000
6	5.463081000	3.340224000	1.083293000	1	1.844283000	5.301161000	2.646595000
1	6.197311000	3.255775000	1.877840000	6	0.147537000	3.262885000	2.954842000
6	4.523195000	2.328413000	0.898012000	1	-0.643201000	2.570375000	2.659108000
1	4.512117000	1.448235000	1.534482000	1	-0.309468000	4.243550000	3.129294000
6	2.870629000	-2.920794000	0.349029000	1	0.585038000	2.923547000	3.900839000
				6	-0.273124000	-2.633494000	0.341403000

7	-1.534553000	-0.060329000	-0.583679000	1	2.340669000	-3.993449000	-3.100029000
6	2.710738000	0.885577000	1.747632000	1	3.800498000	-3.140580000	-3.626602000
6	4.075972000	0.629556000	1.555857000	6	2.473485000	2.626793000	-1.079024000
1	4.401257000	-0.201171000	0.933258000	1	1.714907000	2.321230000	-0.353595000
6	5.021423000	1.442073000	2.172294000	6	3.314683000	3.715331000	-0.407034000
1	6.078073000	1.243603000	2.026561000	1	3.929932000	3.303501000	0.397515000
6	4.611215000	2.507222000	2.974837000	1	2.655125000	4.477853000	0.020316000
1	5.353002000	3.135036000	3.458362000	1	3.974021000	4.217933000	-1.122323000
6	3.255646000	2.769576000	3.154852000	6	1.760409000	3.193613000	-2.315316000
1	2.938748000	3.600563000	3.776319000	1	1.080015000	2.463927000	-2.769902000
6	2.302015000	1.959237000	2.543366000	1	2.493253000	3.477976000	-3.077931000
1	1.240658000	2.143505000	2.684228000	1	1.185459000	4.089174000	-2.054358000
6	-2.728141000	-0.048341000	2.010330000	6	-2.763526000	-0.514175000	-1.199686000
6	-4.072419000	0.235339000	1.733843000	6	-3.228067000	-1.825396000	-0.939215000
1	-4.347049000	0.794259000	0.841779000	6	-4.363500000	-2.270638000	-1.619520000
6	-5.060120000	-0.192328000	2.614440000	1	-4.731734000	-3.274867000	-1.428819000
1	-6.101738000	0.028422000	2.406018000	6	-5.032318000	-1.461050000	-2.528086000
6	-4.709480000	-0.903111000	3.763212000	1	-5.915559000	-1.828919000	-3.040453000
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6	-3.374442000	-1.196160000	4.029619000	1	-5.090929000	0.456976000	-3.482156000
1	-3.106424000	-1.751737000	4.922235000	6	-3.427599000	0.317449000	-2.129955000
6	-2.378403000	-0.767372000	3.155027000	6	-2.567935000	-2.778743000	0.047564000
1	-1.330418000	-0.974170000	3.353512000	1	-1.768186000	-2.241191000	0.566735000
6	2.782603000	0.085120000	-1.308369000	6	-1.952425000	-3.997252000	-0.655508000
6	3.516628000	-1.026035000	-1.767927000	1	-1.159871000	-3.721477000	-1.355141000
6	4.772659000	-0.801334000	-2.341505000	1	-2.718016000	-4.547811000	-1.212916000
1	5.351963000	-1.651011000	-2.692526000	1	-1.536103000	-4.682384000	0.091087000
6	5.285094000	0.479557000	-2.477716000	6	-3.563376000	-3.270870000	1.107639000
1	6.263187000	0.632461000	-2.922656000	1	-4.113953000	-2.446797000	1.564519000
6	4.530968000	1.568854000	-2.057635000	1	-3.030058000	-3.810880000	1.896601000
1	4.925593000	2.572292000	-2.185059000	1	-4.290790000	-3.962382000	0.668874000
6	3.277659000	1.398862000	-1.471254000	6	-2.974074000	1.734052000	-2.444812000
6	2.993503000	-2.450783000	-1.715469000	1	-1.985446000	1.878404000	-2.005799000
1	2.004072000	-2.433735000	-1.258111000	6	-3.917354000	2.763730000	-1.809307000
6	3.885353000	-3.363392000	-0.866929000	1	-3.565486000	3.780251000	-2.013161000
1	3.971620000	-2.994493000	0.160580000	1	-3.971421000	2.642187000	-0.722289000
1	4.893292000	-3.435372000	-1.289214000	1	-4.929910000	2.664209000	-2.215518000
1	3.465744000	-4.373814000	-0.828132000	6	-2.842445000	1.985123000	-3.951275000
6	2.831449000	-3.015559000	-3.132587000	1	-2.182219000	1.250887000	-4.425784000
1	2.230005000	-2.345876000	-3.757422000	1	-2.420195000	2.978982000	-4.128502000

1	3.991397000	-3.413610000	-0.720600000	6	-3.035036000	-2.146876000	-2.449500000
1	2.617756000	-4.526217000	-0.589150000	6	-1.414398000	-4.219433000	-1.508756000
1	3.783245000	-4.418442000	0.729767000	1	-0.298463000	-2.690306000	-0.497412000
6	1.439485000	-3.324645000	1.638595000	6	-3.300757000	-3.466835000	-2.815802000
1	0.747570000	-2.581337000	2.061429000	1	-3.656307000	-1.346484000	-2.837344000
1	2.004270000	-3.738870000	2.480827000	6	-2.499654000	-4.499692000	-2.341883000
1	0.835553000	-4.130129000	1.205031000	1	-0.779809000	-5.023232000	-1.148438000
6	-2.747011000	0.119654000	1.295182000	1	-4.134678000	-3.682842000	-3.475368000
6	-3.221711000	1.435344000	1.486129000	1	-2.712237000	-5.525134000	-2.626469000
6	-4.445861000	1.605509000	2.128176000	15	1.429081000	0.380697000	-1.145135000
1	-4.841212000	2.605318000	2.275498000	6	1.874473000	2.112847000	-1.429921000
6	-5.171008000	0.508809000	2.586558000	6	2.916502000	2.511783000	-2.268766000
1	-6.127014000	0.658846000	3.078017000	6	1.073297000	3.082611000	-0.811963000
6	-4.657252000	-0.771542000	2.443815000	6	3.174421000	3.869945000	-2.458005000
1	-5.207465000	-1.618359000	2.844828000	1	3.522500000	1.773848000	-2.783752000
6	-3.430487000	-0.994191000	1.808529000	6	1.332939000	4.432496000	-1.000107000
6	-2.384660000	2.633517000	1.066127000	1	0.243005000	2.776380000	-0.176424000
1	-1.814101000	2.347082000	0.178948000	6	2.392493000	4.826417000	-1.820280000
6	-1.386438000	2.989949000	2.178928000	1	3.986800000	4.176020000	-3.108728000
1	-0.762265000	2.136957000	2.485045000	1	0.711833000	5.177915000	-0.513183000
1	-1.918748000	3.311011000	3.080251000	1	2.599000000	5.881605000	-1.967479000
1	-0.720165000	3.803103000	1.867368000	6	0.921683000	-0.817273000	4.182312000
6	-3.209672000	3.859683000	0.674382000	1	0.839430000	-0.169472000	5.059034000
1	-3.968189000	3.599233000	-0.070062000	1	1.966351000	-0.832941000	3.847678000
1	-2.555618000	4.623698000	0.242007000	8	0.053327000	-0.340671000	3.176786000
1	-3.709037000	4.310157000	1.538183000				
6	-2.851627000	-2.398212000	1.782299000		7-TS8 (in gas phase)		
1	-1.922917000	-2.371522000	1.205839000	1	-1.651454000	-3.543506000	-2.443451000
6	-3.782789000	-3.404576000	1.100805000	13	-0.475151000	-0.710948000	-0.169376000
1	-3.308193000	-4.390150000	1.059151000	7	1.336722000	-0.976206000	-0.063200000
1	-4.020821000	-3.097603000	0.076923000	7	1.725616000	1.644689000	0.390555000
1	-4.722842000	-3.512138000	1.652172000	7	-0.850862000	1.086243000	-0.123893000
6	-2.491579000	-2.843989000	3.206431000	6	3.999566000	0.076663000	0.095173000
1	-1.802403000	-2.131887000	3.672147000	6	4.770315000	-1.070574000	0.327651000
1	-2.017762000	-3.831362000	3.185974000	1	4.333010000	-1.943145000	0.807730000
1	-3.385025000	-2.912926000	3.835784000	6	6.107946000	-1.088927000	-0.052555000
1	0.624808000	-1.831851000	4.469714000	1	6.707348000	-1.975055000	0.128069000
15	-1.500839000	-0.185011000	-1.104208000	6	6.676297000	0.030772000	-0.661511000
6	-1.965802000	-1.864245000	-1.597890000	1	7.722471000	0.014462000	-0.950296000
6	-1.147977000	-2.907714000	-1.144052000	6	5.907386000	1.166618000	-0.901109000

1	6.351300000	2.034976000	-1.376735000	1	0.633084000	-0.894909000	-3.548848000
6	4.567084000	1.193815000	-0.522144000	1	1.741457000	-1.944119000	-4.446699000
1	3.955154000	2.075605000	-0.690521000	1	1.897394000	-0.185036000	-4.564302000
6	-0.134727000	3.640008000	0.963250000	6	-2.255593000	1.427720000	0.031005000
6	-1.230004000	4.456403000	0.647225000	6	-2.790749000	1.569928000	1.331815000
1	-1.859789000	4.228179000	-0.210013000	6	-4.153077000	1.845423000	1.458437000
6	-1.503620000	5.573307000	1.429608000	1	-4.579372000	1.960247000	2.451463000
1	-2.347390000	6.209634000	1.183912000	6	-4.972322000	1.978217000	0.343950000
6	-0.695560000	5.872070000	2.527580000	1	-6.027856000	2.201327000	0.466146000
1	-0.910112000	6.747462000	3.132404000	6	-4.433309000	1.823182000	-0.924509000
6	0.380716000	5.050620000	2.851935000	1	-5.076449000	1.918257000	-1.795021000
1	1.004489000	5.282537000	3.708916000	6	-3.078823000	1.534590000	-1.108021000
6	0.666704000	3.934815000	2.068318000	6	-1.967292000	1.424206000	2.604886000
1	1.514537000	3.294716000	2.296294000	1	-0.907452000	1.400411000	2.333281000
6	1.884149000	-2.224786000	-0.558905000	6	-2.300440000	0.117946000	3.338004000
6	1.758694000	-3.406265000	0.202194000	1	-2.070331000	-0.765619000	2.735352000
6	2.251333000	-4.598577000	-0.337468000	1	-3.366163000	0.078768000	3.589341000
1	2.166017000	-5.513818000	0.240978000	1	-1.736041000	0.060386000	4.275247000
6	2.844290000	-4.635204000	-1.590449000	6	-2.164562000	2.600386000	3.569374000
1	3.217795000	-5.572040000	-1.991420000	1	-2.059336000	3.562340000	3.064759000
6	2.961485000	-3.463533000	-2.327723000	1	-1.422584000	2.548030000	4.372884000
1	3.430415000	-3.494082000	-3.307172000	1	-3.155135000	2.567119000	4.035443000
6	2.494614000	-2.243569000	-1.834669000	6	-2.567479000	1.345108000	-2.527000000
6	1.150607000	-3.441782000	1.595669000	1	-1.536213000	0.985668000	-2.468991000
1	0.657914000	-2.483795000	1.778145000	6	-2.562626000	2.675859000	-3.290946000
6	2.244903000	-3.610970000	2.658402000	1	-2.161477000	2.537539000	-4.300351000
1	2.984031000	-2.804132000	2.616911000	1	-1.952143000	3.432415000	-2.787060000
1	2.769320000	-4.563020000	2.519795000	1	-3.581952000	3.067033000	-3.382567000
1	1.804817000	-3.608167000	3.660971000	6	-3.378017000	0.294985000	-3.298789000
6	0.088253000	-4.537356000	1.746038000	1	-3.440869000	-0.644526000	-2.743027000
1	-0.682363000	-4.465228000	0.974042000	1	-2.914003000	0.111785000	-4.274492000
1	-0.396715000	-4.445278000	2.723570000	1	-4.400365000	0.639126000	-3.487235000
1	0.534061000	-5.536419000	1.699566000	15	0.339075000	2.262642000	-0.100347000
6	2.661077000	-1.005538000	-2.706736000	6	0.569954000	2.991962000	-1.747522000
1	2.457672000	-0.118964000	-2.099582000	6	0.735148000	2.122630000	-2.830475000
6	4.089229000	-0.868745000	-3.249151000	6	0.656426000	4.371157000	-1.956037000
1	4.833172000	-1.000350000	-2.460175000	6	0.942013000	2.620091000	-4.110300000
1	4.223974000	0.124420000	-3.689545000	1	0.687284000	1.049403000	-2.669057000
1	4.290082000	-1.605747000	-4.033898000	6	0.867146000	4.869485000	-3.240975000
6	1.671241000	-1.009021000	-3.879640000	1	0.558751000	5.061196000	-1.124838000

1	3.946390000	-4.958364000	4.937198000	1	5.714584000	3.791554000	2.771463000
13	-0.263664000	0.110865000	-0.661629000	1	4.607698000	6.154896000	-0.640935000
1	-0.458376000	0.682783000	-4.262085000	1	6.039794000	5.797256000	1.351051000
6	-0.024243000	0.568868000	-3.262204000	1	1.445190000	-0.150638000	-0.710825000
8	-0.868915000	0.156116000	-2.347699000	5	2.210970000	-0.534098000	-1.597256000
8	1.151016000	0.813275000	-3.032546000	8	3.440938000	0.007030000	-1.597775000
6	-0.257598000	1.957151000	0.083137000	8	2.039121000	-1.747624000	-2.154007000
6	-1.642571000	3.514293000	1.301823000	6	4.307954000	-1.058922000	-2.130419000
1	-2.654407000	3.868358000	1.466986000	6	3.291851000	-1.974316000	-2.903695000
6	-0.544968000	4.046948000	1.958991000	6	3.039036000	-1.519659000	-4.335456000
1	-0.651589000	4.834731000	2.690498000	6	3.609197000	-3.456778000	-2.850372000
6	0.704243000	3.611377000	1.540813000	6	5.374487000	-0.423135000	-3.001655000
1	1.625160000	4.057290000	1.901410000	6	4.926964000	-1.738546000	-0.914494000
6	-2.658325000	1.947838000	-0.297886000	1	5.464576000	-0.990861000	-0.326119000
1	-2.636967000	0.883663000	-0.000959000	1	4.162152000	-2.196245000	-0.275919000
6	2.191613000	2.249640000	0.135969000	1	5.634759000	-2.515845000	-1.213917000
1	2.090025000	2.123315000	-0.945700000	1	6.030513000	0.196370000	-2.385292000
7	-1.491545000	2.547013000	0.400482000	1	4.936108000	0.204172000	-3.779102000
7	0.832377000	2.648932000	0.629451000	1	5.984679000	-1.198853000	-3.475011000
1	-2.446804000	2.010028000	-1.369255000	1	2.818718000	-0.450240000	-4.385044000
1	2.413089000	1.272495000	0.581510000	1	2.184071000	-2.071563000	-4.735392000
6	-3.988423000	2.550053000	0.044833000	1	3.906973000	-1.731299000	-4.965584000
6	-4.507356000	3.591230000	-0.728738000	1	4.581753000	-3.649623000	-3.313875000
6	-4.706924000	2.079338000	1.149054000	1	2.852475000	-4.014672000	-3.407437000
6	-5.735244000	4.158224000	-0.399494000	1	3.631267000	-3.829390000	-1.824102000
1	-3.954949000	3.952949000	-1.592380000				
6	-5.934273000	2.647120000	1.477008000		8-IM2 (in gas phase)		
1	-4.305090000	1.262793000	1.746994000	6	-0.894464000	0.532195000	1.535259000
6	-6.446711000	3.687243000	0.702333000	7	-2.315249000	0.573393000	1.756203000
1	-6.138972000	4.962288000	-1.005419000	6	-2.948307000	-0.475918000	2.290518000
1	-6.491805000	2.278468000	2.331549000	1	-4.035233000	-0.431363000	2.307059000
1	-7.405104000	4.128247000	0.955601000	6	-2.243703000	-1.509409000	2.877369000
6	3.274929000	3.232721000	0.469841000	1	-2.750782000	-2.341912000	3.342752000
6	4.087078000	3.032060000	1.588308000	6	-0.881593000	-1.257019000	3.129165000
6	3.464386000	4.362556000	-0.331220000	1	-0.306447000	-1.827524000	3.852080000
6	5.080241000	3.954644000	1.906670000	7	-0.255734000	-0.281837000	2.501448000
1	3.949905000	2.146422000	2.205023000	6	-3.038248000	1.863136000	1.582879000
6	4.456396000	5.283730000	-0.012446000	1	-2.497763000	2.419817000	0.817967000
1	2.843267000	4.512652000	-1.211053000	6	1.183287000	-0.059460000	2.722284000
6	5.262857000	5.080392000	1.106935000	1	1.504155000	0.586831000	1.899072000

13	-0.190610000	0.936049000	-0.228892000	1	7.843828000	-1.890678000	-1.160062000
1	-2.524672000	2.957543000	-2.389617000	6	2.003054000	-1.326759000	2.742107000
6	0.422293000	-0.755512000	-1.130933000	6	1.716954000	-2.380240000	1.866993000
7	1.748613000	-1.190700000	-1.151959000	6	3.105078000	-1.420868000	3.591584000
6	2.118673000	-2.449886000	-1.383661000	6	2.530754000	-3.509000000	1.839130000
1	3.183724000	-2.652578000	-1.348647000	1	0.835780000	-2.327300000	1.225515000
6	1.178750000	-3.424841000	-1.678225000	6	3.924433000	-2.549431000	3.558030000
1	1.467662000	-4.443937000	-1.892554000	1	3.326526000	-0.613487000	4.284692000
6	-0.143373000	-3.016105000	-1.750460000	6	3.640197000	-3.592745000	2.681024000
1	-0.950193000	-3.688274000	-2.021335000	1	2.291773000	-4.332783000	1.172734000
7	-0.486931000	-1.753995000	-1.495934000	1	4.774605000	-2.616621000	4.228779000
6	2.777843000	-0.139557000	-0.867628000	1	4.269489000	-4.476427000	2.664572000
1	2.577461000	0.662079000	-1.581663000	6	-2.897303000	-2.450382000	-1.749061000
6	-1.920348000	-1.334666000	-1.532086000	6	-3.320842000	-3.219758000	-0.660904000
1	-1.999686000	-0.566428000	-2.303649000	6	-3.376495000	-2.734018000	-3.030089000
1	-2.959632000	2.421945000	2.522715000	6	-4.215764000	-4.266851000	-0.854082000
1	1.314418000	0.525286000	3.638741000	1	-2.950962000	-2.988714000	0.337201000
1	2.552509000	0.227844000	0.141722000	6	-4.274566000	-3.780894000	-3.221493000
1	-2.090401000	-0.863840000	-0.551808000	1	-3.053058000	-2.133045000	-3.876632000
6	-4.478004000	1.673384000	1.181295000	6	-4.692147000	-4.546353000	-2.134729000
6	-5.509260000	2.075764000	2.028350000	1	-4.548838000	-4.860610000	-0.009357000
6	-4.786342000	1.077491000	-0.046880000	1	-4.650968000	-3.995464000	-4.215986000
6	-6.839230000	1.896318000	1.648845000	1	-5.394353000	-5.359751000	-2.284567000
1	-5.275912000	2.538479000	2.983934000	6	-1.563180000	2.602693000	-2.009646000
6	-6.111282000	0.890124000	-0.420998000	8	-1.590498000	1.599799000	-1.219628000
1	-3.980793000	0.764644000	-0.708822000	8	-0.539100000	3.209907000	-2.379891000
6	-7.139980000	1.302806000	0.427331000	1	1.150717000	1.809934000	-2.732294000
1	-7.636745000	2.219399000	2.309441000	5	0.949827000	2.768003000	-2.026322000
1	-6.346512000	0.428241000	-1.374473000	8	1.752833000	3.898956000	-2.061091000
1	-8.174601000	1.161889000	0.132784000	8	0.935157000	2.337332000	-0.540943000
6	4.197129000	-0.612971000	-0.945308000	6	2.336775000	4.189190000	-0.793145000
6	4.903136000	-0.512765000	-2.147419000	6	1.345948000	3.552410000	0.226571000
6	4.809298000	-1.172207000	0.180237000	6	1.971102000	3.137540000	1.542503000
6	6.214502000	-0.973235000	-2.222649000	6	0.099430000	4.394335000	0.467252000
1	4.430972000	-0.065222000	-3.018892000	6	3.723041000	3.545891000	-0.743141000
6	6.118662000	-1.635140000	0.100652000	6	2.455496000	5.699730000	-0.641763000
1	4.262573000	-1.237808000	1.118645000	1	3.178644000	6.072724000	-1.370572000
6	6.820051000	-1.536276000	-1.100347000	1	1.501779000	6.194609000	-0.832521000
1	6.765626000	-0.886014000	-3.152886000	1	2.810128000	5.970645000	0.358086000
1	6.593911000	-2.063518000	0.977198000	1	4.288199000	3.887169000	-1.613105000

1	3.666140000	2.452276000	-0.788161000	1	-2.410285000	1.203544000	0.343111000
1	4.273422000	3.829253000	0.158470000	1	2.131664000	1.905803000	-1.639288000
1	2.754966000	2.387005000	1.405714000	6	4.625896000	-1.428147000	-0.960311000
1	1.204922000	2.759235000	2.226735000	6	4.927071000	-2.790998000	-1.049505000
1	2.429014000	4.014856000	2.010351000	6	5.657098000	-0.496977000	-0.832923000
1	0.345593000	5.252884000	1.097596000	6	6.250447000	-3.215719000	-1.007862000
1	-0.649137000	3.798416000	1.002301000	1	4.125116000	-3.517805000	-1.158240000
1	-0.323800000	4.771220000	-0.466330000	6	6.982108000	-0.923571000	-0.791474000

8-TS3 (in gas phase)

6	1.096820000	-0.947025000	0.298750000	1	6.482630000	-4.272545000	-1.085917000
7	2.493711000	-1.120767000	0.330408000	1	7.780960000	-0.194702000	-0.699860000
6	3.166302000	-1.384512000	1.445859000	1	8.310618000	-2.614472000	-0.849766000
1	4.245800000	-1.451163000	1.356792000	6	-3.616010000	2.979095000	0.304966000
6	2.498119000	-1.623579000	2.640389000	6	-4.045847000	4.081072000	-0.440981000
1	3.034698000	-1.848248000	3.550447000	6	-4.311037000	2.612558000	1.459757000
6	1.121556000	-1.793792000	2.552629000	6	-5.156601000	4.810136000	-0.030488000
1	0.530550000	-2.191880000	3.371242000	1	-3.514807000	4.361192000	-1.347762000
7	0.471247000	-1.523437000	1.427313000	6	-5.425191000	3.341305000	1.869045000
6	3.196268000	-0.970860000	-0.975994000	1	-3.985144000	1.747026000	2.033475000
1	3.134437000	0.089837000	-1.246171000	6	-5.845438000	4.440762000	1.124859000
6	-0.999296000	-1.702350000	1.319446000	1	-5.491771000	5.660388000	-0.614961000
1	-1.430673000	-0.688554000	1.349858000	1	-5.966607000	3.048722000	2.762447000
13	0.087311000	0.312563000	-0.837269000	1	-6.715111000	5.007585000	1.440256000
1	0.660417000	-0.149719000	-4.558063000	6	-1.602689000	-2.564992000	2.389849000
6	0.043799000	2.262676000	-0.390903000	6	-2.220658000	-1.988651000	3.501507000
7	-1.108306000	2.829884000	0.215942000	6	-1.538673000	-3.958032000	2.278491000
6	-1.049961000	3.813293000	1.112477000	6	-2.769185000	-2.795484000	4.495659000
1	-1.992754000	4.116541000	1.556454000	1	-2.276555000	-0.905449000	3.587594000
6	0.142929000	4.450670000	1.411303000	6	-2.085705000	-4.763270000	3.271514000
1	0.189619000	5.262736000	2.121682000	1	-1.066623000	-4.407682000	1.407658000
6	1.236012000	4.098244000	0.629227000	6	-2.700218000	-4.181621000	4.380438000
1	2.179322000	4.635455000	0.662893000	1	-3.252478000	-2.343732000	5.355491000
7	1.165946000	3.083886000	-0.226599000	1	-2.039251000	-5.843238000	3.179588000
6	-2.411031000	2.194883000	-0.127961000	1	-3.129955000	-4.810933000	5.152723000
1	-2.399178000	2.036736000	-1.210667000	6	3.597012000	2.620340000	-0.189633000
6	2.365129000	2.794575000	-1.046941000	6	3.527861000	1.885582000	1.000236000
1	2.488619000	3.615999000	-1.759207000	6	4.806518000	3.197162000	-0.575460000
1	2.598627000	-1.543171000	-1.690010000	6	4.662695000	1.726687000	1.788874000
1	-1.180605000	-2.111913000	0.319418000	1	2.575020000	1.459164000	1.318772000

6	5.944885000	3.031372000	0.214710000	1	-3.892786000	3.378166000	-0.854892000
1	4.863719000	3.782119000	-1.489828000	7	-2.492891000	1.896535000	-1.108741000
6	5.874321000	2.297209000	1.395452000	6	-2.885511000	-1.772501000	-1.101543000
1	4.600194000	1.171535000	2.720430000	1	-2.220097000	-2.087390000	-0.289817000
1	6.880483000	3.490026000	-0.087803000	6	-1.442624000	2.863596000	-1.529037000
1	6.756830000	2.179758000	2.015627000	1	-0.669686000	2.816741000	-0.745668000
6	0.172350000	-0.216182000	-3.583992000	13	-0.149841000	0.144303000	-0.787094000
8	0.797469000	0.187642000	-2.577556000	1	1.440977000	-3.120658000	-1.945720000
8	-0.999557000	-0.700043000	-3.615260000	6	0.475656000	0.216875000	1.108162000
1	-1.383212000	-0.184895000	-1.136091000	7	1.368220000	1.253992000	1.505685000
5	-2.017231000	-1.112342000	-2.658224000	6	1.251956000	1.894407000	2.665005000
8	-3.225713000	-0.514337000	-2.748163000	1	1.944092000	2.713711000	2.837146000
8	-1.986716000	-2.362796000	-2.125666000	6	0.349199000	1.478665000	3.633490000
6	-4.140281000	-1.385476000	-2.014552000	1	0.266623000	1.984320000	4.583929000
6	-3.398443000	-2.767258000	-2.071073000	6	-0.251075000	0.242425000	3.409362000
6	-3.609166000	-3.654768000	-0.858823000	1	-0.784062000	-0.299776000	4.185195000
6	-3.672529000	-3.536421000	-3.358660000	7	-0.156419000	-0.353427000	2.227912000
6	-4.264017000	-0.830547000	-0.598317000	6	2.422020000	1.650068000	0.524721000
6	-5.487533000	-1.360843000	-2.714219000	1	2.689556000	0.732818000	-0.003638000
1	-5.931248000	-0.366293000	-2.622466000	6	-0.734565000	-1.702711000	2.063583000
1	-5.391106000	-1.596403000	-3.775053000	1	-0.086744000	-2.415496000	2.583695000
1	-6.168233000	-2.082632000	-2.251804000	1	-2.325232000	-1.814473000	-2.039004000
1	-4.584367000	0.214933000	-0.651345000	1	-1.006373000	2.459737000	-2.445624000
1	-3.306789000	-0.882030000	-0.067067000	1	1.958955000	2.331187000	-0.198992000
1	-5.006908000	-1.388714000	-0.022013000	1	-0.660778000	-1.933240000	0.996671000
1	-3.313198000	-3.163489000	0.071426000	6	-4.104447000	-2.647050000	-1.144467000
1	-3.023583000	-4.571519000	-0.970231000	6	-4.824995000	-2.790600000	-2.333536000
1	-4.663891000	-3.936398000	-0.778126000	6	-4.539759000	-3.294941000	0.013285000
1	-4.694572000	-3.923589000	-3.376958000	6	-5.972189000	-3.577043000	-2.362146000
1	-2.981482000	-4.380280000	-3.423168000	1	-4.483935000	-2.291895000	-3.237772000
1	-3.526291000	-2.902817000	-4.239180000	6	-5.689102000	-4.079833000	-0.016132000
				1	-3.974079000	-3.188482000	0.935895000
				6	-6.405095000	-4.220158000	-1.203001000
				1	-6.524873000	-3.694231000	-3.288266000
				1	-6.020243000	-4.586078000	0.884929000
				1	-7.297820000	-4.836359000	-1.228213000
				6	3.632981000	2.271025000	1.163546000
				6	4.608320000	1.450982000	1.739212000
				6	3.792072000	3.657937000	1.191138000
				6	5.725127000	2.016560000	2.344715000
8-IM3 (in gas phase)							
6	-2.078639000	0.545717000	-1.019873000				
7	-3.173223000	-0.329023000	-0.870186000				
6	-4.393210000	0.069941000	-0.521361000				
1	-5.139837000	-0.707380000	-0.399751000				
6	-4.690529000	1.415998000	-0.373526000				
1	-5.682423000	1.750152000	-0.107044000				
6	-3.706405000	2.313106000	-0.771385000				

1	4.497586000	0.370282000	1.691120000	6	6.248223000	-0.877839000	-2.320069000
6	4.911821000	4.223693000	1.797236000	6	6.929436000	-1.848626000	-0.111242000
1	3.044954000	4.297701000	0.726287000	1	7.179571000	-0.825091000	0.180388000
6	5.875848000	3.402904000	2.376400000	1	6.597695000	-2.392250000	0.775202000
1	6.482936000	1.378470000	2.787871000	1	7.837311000	-2.323488000	-0.495702000
1	5.034234000	5.301579000	1.810011000	1	6.368658000	0.131342000	-1.918693000
1	6.749723000	3.842338000	2.845988000	1	5.481119000	-0.851042000	-3.100705000
6	-1.925868000	4.271927000	-1.716702000	1	7.193183000	-1.184351000	-2.775699000
6	-1.896160000	5.175550000	-0.651305000	1	5.877722000	-3.023451000	-3.792248000
6	-2.424092000	4.681144000	-2.956358000	1	5.662899000	-4.692823000	-3.236347000
6	-2.362028000	6.475898000	-0.822086000	1	7.132579000	-3.805026000	-2.806765000
1	-1.502590000	4.860407000	0.312910000	1	6.474090000	-4.573946000	-0.376191000
6	-2.887986000	5.981838000	-3.127612000	1	4.920549000	-5.195632000	-0.957226000
1	-2.439858000	3.983254000	-3.789928000	1	4.961943000	-3.961587000	0.320531000
6	-2.858006000	6.878111000	-2.060682000				
1	-2.331980000	7.176261000	0.005922000		8-TS4 (in gas phase)		
1	-3.265941000	6.298255000	-4.093969000	6	0.245132591	-0.653423591	1.898430000
1	-3.215881000	7.893302000	-2.196534000	7	0.792499295	-1.838320295	2.460659295
6	-2.157680000	-1.792735000	2.558463000	6	1.655472295	-1.809025000	3.477979295
6	-3.058986000	-0.753835000	2.302821000	1	2.044328591	-2.769170000	3.807899295
6	-2.587091000	-2.923608000	3.252607000	6	1.970284000	-0.631321000	4.131319000
6	-4.379784000	-0.855022000	2.728557000	1	2.658034000	-0.610094000	4.963456000
1	-2.716514000	0.143985000	1.785839000	6	1.151837000	0.461827000	3.829875000
6	-3.913076000	-3.025567000	3.674005000	1	1.126376705	1.359758000	4.440964000
1	-1.887867000	-3.727104000	3.469376000	7	0.320959295	0.422949705	2.801107000
6	-4.810165000	-1.993747000	3.410629000	6	0.348395295	-3.143085000	1.926724295
1	-5.071563000	-0.038797000	2.541241000	1	-0.658169000	-2.994577000	1.528742591
1	-4.238038000	-3.905346000	4.219547000	6	-0.586181000	1.573199000	2.577637000
1	-5.838457000	-2.068412000	3.748677000	1	-1.144854000	1.350405000	1.662329295
6	1.273520000	-2.149751000	-1.468792000	13	-0.082473886	-0.365445932	-0.014493409
8	0.129059000	-1.695513000	-1.339083000	6	1.121051295	0.761867705	-1.108309295
8	2.297186000	-1.487149000	-1.041496000	7	0.930243000	2.137951000	-1.314498000
1	0.787766000	0.937672000	-1.772625000	6	1.930129000	2.989721000	-1.540149000
5	3.642525000	-1.933634000	-1.213343000	1	1.660522000	4.036674000	-1.630052000
8	4.626710000	-1.265161000	-0.598839000	6	3.229318000	2.538004000	-1.701374000
8	3.954036000	-3.000023000	-1.964788000	1	4.040717000	3.217432000	-1.918150000
6	5.860275000	-1.818559000	-1.186507000	6	3.418973295	1.159671000	-1.702942000
6	5.387597000	-3.232496000	-1.686798000	1	4.372882295	0.702119295	-1.938919000
6	6.053437000	-3.709793000	-2.962478000	7	2.417461295	0.333770000	-1.424906000
6	5.440328000	-4.301854000	-0.603874000	6	-0.480166000	2.618702000	-1.225798000

7	-2.278919000	1.439122000	1.956005000	1	-7.521664000	1.357670000	-1.299943000
6	-2.883350000	0.761835000	2.936278000	6	3.108802000	-1.971171000	-1.333996000
1	-3.931404000	0.987540000	3.105457000	6	3.434504000	-2.440764000	-2.609986000
6	-2.195327000	-0.121094000	3.743451000	6	3.880359000	-2.352616000	-0.234736000
1	-2.678690000	-0.643776000	4.555367000	6	4.522304000	-3.290872000	-2.781832000
6	-0.800445000	-0.108892000	3.607646000	1	2.842295000	-2.134054000	-3.469394000
1	-0.136830000	-0.563435000	4.336945000	6	4.969925000	-3.202256000	-0.408643000
7	-0.231347000	0.484348000	2.572920000	1	3.638160000	-1.964819000	0.751567000
6	-2.983178000	2.611692000	1.341414000	6	5.289273000	-3.672092000	-1.680827000
1	-2.265269000	3.067480000	0.658385000	1	4.778128000	-3.648965000	-3.773385000
6	1.242041000	0.436820000	2.441557000	1	5.571063000	-3.491545000	0.447500000
1	1.491355000	0.847588000	1.457701000	1	6.140778000	-4.330450000	-1.818044000
13	-0.454273000	1.013529000	-0.345840000	6	1.786481000	-0.961887000	2.614911000
6	-0.475160000	-0.833314000	-1.020548000	6	1.086454000	-2.065031000	2.112636000
7	0.616664000	-1.710214000	-1.079907000	6	3.001660000	-1.158993000	3.269864000
6	0.492011000	-3.035035000	-1.024371000	6	1.599887000	-3.349190000	2.265805000
1	1.415501000	-3.605271000	-1.029320000	1	0.121195000	-1.918320000	1.625154000
6	-0.758826000	-3.633470000	-1.006662000	6	3.517923000	-2.447051000	3.417615000
1	-0.869317000	-4.707744000	-0.983578000	1	3.543482000	-0.308665000	3.675905000
6	-1.861258000	-2.795286000	-1.167712000	6	2.818341000	-3.542301000	2.917864000
1	-2.872489000	-3.168107000	-1.295131000	1	1.041411000	-4.202782000	1.892465000
7	-1.708925000	-1.479904000	-1.196481000	1	4.457548000	-2.592693000	3.940395000
6	1.945235000	-1.045537000	-1.139330000	1	3.212681000	-4.544760000	3.047428000
1	1.871555000	-0.320225000	-1.956959000	6	-4.212229000	-1.172115000	-1.285222000
6	-2.852787000	-0.544399000	-1.343957000	6	-4.819256000	-1.380134000	-0.044650000
1	-2.688099000	0.018696000	-2.267952000	6	-4.888606000	-1.516369000	-2.457472000
1	-3.174787000	3.317028000	2.156741000	6	-6.096013000	-1.926689000	0.024842000
1	1.671353000	1.128652000	3.172697000	1	-4.296944000	-1.086234000	0.864881000
1	2.061833000	-0.493315000	-0.198605000	6	-6.166792000	-2.063752000	-2.387509000
1	-2.754490000	0.156912000	-0.499831000	1	-4.422726000	-1.341077000	-3.424272000
6	-4.262024000	2.263389000	0.612235000	6	-6.769642000	-2.267144000	-1.147578000
6	-5.454286000	2.031116000	1.308657000	1	-6.571813000	-2.077117000	0.988373000
6	-4.276715000	2.227852000	-0.785306000	1	-6.694117000	-2.324608000	-3.299001000
6	-6.618344000	1.693751000	0.624758000	1	-7.768237000	-2.688377000	-1.094851000
1	-5.498051000	2.162533000	2.387788000	6	0.107743000	2.936612000	-1.623954000
6	-5.445745000	1.900996000	-1.469823000	8	-1.084423000	2.312866000	-1.379597000
1	-3.372670000	2.477679000	-1.336073000	8	1.064992000	2.044256000	-0.861895000
6	-6.612130000	1.613858000	-0.766494000	1	0.425665000	2.913513000	-2.668785000
1	-7.536599000	1.520631000	1.176444000	5	2.431419000	2.335079000	-0.750916000
1	-5.447576000	1.883260000	-2.555388000	8	3.245937000	1.557516000	0.003727000

8	2.986616000	3.381289000	-1.385079000	6	0.711436000	3.678526000	-0.715813000
6	4.606191000	2.007007000	-0.346201000	1	0.817407000	4.746098000	-0.589091000
6	4.349933000	3.473882000	-0.843350000	6	1.818046000	2.860383000	-0.927846000
6	4.293297000	4.489147000	0.291340000	1	2.830400000	3.244349000	-1.000345000
6	5.278313000	3.941317000	-1.948012000	7	1.671750000	1.550343000	-1.073622000
6	5.478707000	1.891228000	0.888622000	6	-1.986462000	1.110367000	-1.127675000
6	5.096831000	1.080043000	-1.451708000	1	-1.901781000	0.447782000	-1.994963000
1	5.091209000	0.047823000	-1.091057000	6	2.831548000	0.641486000	-1.292333000
1	4.456818000	1.142381000	-2.339241000	1	2.674709000	0.167124000	-2.265997000
1	6.117349000	1.334983000	-1.748869000	1	3.181696000	-3.326703000	1.896379000
1	5.580280000	0.837762000	1.164884000	1	-1.607933000	-1.477373000	3.106050000
1	5.056638000	2.436963000	1.734682000	1	-2.121534000	0.489127000	-0.234479000
1	6.478724000	2.285044000	0.682977000	1	2.738720000	-0.129455000	-0.516818000
1	3.629634000	4.154782000	1.095980000	6	4.409924000	-2.223423000	0.504776000
1	3.914366000	5.437214000	-0.097327000	6	5.548141000	-2.119299000	1.312991000
1	5.287197000	4.662655000	0.711905000	6	4.540162000	-2.023114000	-0.871701000
1	6.315342000	3.930634000	-1.598154000	6	6.773693000	-1.751981000	0.764952000
1	5.026078000	4.966618000	-2.228795000	1	5.488192000	-2.361943000	2.372214000
1	5.199010000	3.311851000	-2.835790000	6	5.768320000	-1.668578000	-1.424117000
1	0.197853000	3.934678000	-1.187959000	1	3.676996000	-2.164010000	-1.518440000
8-TS5 (in gas phase)				6	6.882339000	-1.513578000	-0.603764000
6	0.968193000	-1.190534000	1.361783000	1	7.648712000	-1.677462000	1.402252000
7	2.335106000	-1.419083000	1.689335000	1	5.857422000	-1.520648000	-2.495711000
6	2.926591000	-0.706767000	2.677396000	1	7.839477000	-1.236014000	-1.032804000
1	4.010582000	-0.763588000	2.731830000	6	-3.141621000	2.055529000	-1.263844000
6	2.186132000	-0.017238000	3.596101000	6	-3.423070000	2.669923000	-2.487914000
1	2.644283000	0.530002000	4.407213000	6	-3.953897000	2.305940000	-0.156661000
6	0.784834000	-0.196350000	3.532559000	6	-4.505908000	3.536216000	-2.597992000
1	0.115275000	0.107715000	4.330043000	1	-2.801052000	2.463013000	-3.356123000
7	0.233671000	-0.727729000	2.457255000	6	-5.038985000	3.171494000	-0.268902000
6	3.068170000	-2.579283000	1.102354000	1	-3.746512000	1.799898000	0.782889000
1	2.407070000	-2.997989000	0.342796000	6	-5.312715000	3.787857000	-1.487938000
6	-1.248056000	-0.749825000	2.372349000	1	-4.728134000	4.007078000	-3.549722000
1	-1.521168000	-1.146491000	1.390968000	1	-5.672850000	3.358095000	0.592217000
13	0.288795000	-1.004275000	-0.462269000	1	-6.160583000	4.458920000	-1.578128000
6	0.439264000	0.890450000	-0.990890000	6	-1.850402000	0.616414000	2.616019000
7	-0.653400000	1.766165000	-0.995986000	6	-1.178980000	1.781465000	2.228568000
6	-0.535789000	3.080492000	-0.813943000	6	-3.095785000	0.716640000	3.235805000
1	-1.462494000	3.644587000	-0.783072000	6	-1.746377000	3.030077000	2.467548000
				1	-0.193260000	1.712138000	1.765561000

1	-1.241695000	-2.402148000	4.911444000	6	5.508908000	4.260489000	-1.620470000
1	-0.017344000	-3.663612000	5.111670000	1	4.653099000	5.627022000	-0.193652000
1	1.548119000	-1.588214000	5.565669000	1	6.139806000	2.703899000	-2.968071000
1	0.252818000	-0.480057000	5.088329000	1	6.357159000	4.900441000	-1.840065000
1	1.814596000	-0.437993000	4.239917000	6	-2.007139000	0.487452000	0.788865000
13	-0.431020000	-0.184438000	-0.146116000	7	-2.033898000	1.682210000	1.533697000
8	-0.204624000	-1.931986000	0.000581000	6	-3.123865000	2.428716000	1.660515000
6	0.056687000	0.862974000	-1.717582000	1	-3.018474000	3.350536000	2.222989000
7	-0.719782000	0.848681000	-2.880714000	6	-4.340101000	2.005538000	1.137937000
6	-0.794769000	1.868605000	-3.724841000	1	-5.233906000	2.602356000	1.244897000
1	-1.448279000	1.740408000	-4.582884000	6	-4.396607000	0.693896000	0.676554000
6	-0.035337000	3.020251000	-3.516960000	1	-5.331734000	0.198820000	0.435690000
1	-0.098614000	3.866136000	-4.185142000	7	-3.293022000	-0.035428000	0.565730000
6	0.946701000	2.939014000	-2.542884000	6	-0.730150000	2.068448000	2.117821000
1	1.715503000	3.697649000	-2.430872000	1	-0.436122000	1.250353000	2.783433000
7	1.038912000	1.880763000	-1.738523000	6	-3.336834000	-1.467809000	0.149415000
6	-1.513424000	-0.368535000	-3.163287000	1	-2.686830000	-1.997171000	0.851729000
1	-1.087839000	-0.850556000	-4.048528000	1	-0.032842000	2.082385000	1.263034000
6	2.160429000	1.721782000	-0.770822000	1	-2.873322000	-1.513488000	-0.845608000
1	2.454152000	0.669143000	-0.818573000	6	-0.712140000	3.403858000	2.799815000
1	-1.334232000	-1.060644000	-2.330517000	6	-0.894083000	3.495120000	4.180854000
1	1.752913000	1.933544000	0.229000000	6	-0.529579000	4.567281000	2.046191000
6	-2.982065000	-0.066548000	-3.344851000	6	-0.891533000	4.740600000	4.803732000
6	-3.716966000	-0.747427000	-4.315189000	1	-1.029917000	2.591102000	4.769392000
6	-3.614256000	0.884485000	-2.535940000	6	-0.530302000	5.811568000	2.667845000
6	-5.078980000	-0.488430000	-4.470601000	1	-0.387322000	4.493769000	0.968758000
1	-3.228657000	-1.476414000	-4.956745000	6	-0.710895000	5.896791000	4.047948000
6	-4.971632000	1.144291000	-2.696658000	1	-1.025720000	4.808031000	5.878065000
1	-3.035358000	1.435851000	-1.793216000	1	-0.385639000	6.712917000	2.081557000
6	-5.706713000	0.456122000	-3.662879000	1	-0.706269000	6.866308000	4.534894000
1	-5.642466000	-1.015415000	-5.233469000	6	-4.719588000	-2.046024000	0.098569000
1	-5.454296000	1.895679000	-2.078422000	6	-5.418065000	-2.073921000	-1.109584000
1	-6.763259000	0.665944000	-3.793114000	6	-5.324281000	-2.527601000	1.263180000
6	3.336795000	2.611313000	-1.049305000	6	-6.715304000	-2.577267000	-1.154494000
6	3.464671000	3.847048000	-0.411317000	1	-4.939853000	-1.710598000	-2.016183000
6	4.303207000	2.199624000	-1.971451000	6	-6.620138000	-3.031220000	1.216791000
6	4.550498000	4.671230000	-0.696528000	1	-4.776715000	-2.514158000	2.202729000
1	2.720802000	4.159514000	0.319578000	6	-7.316095000	-3.053987000	0.008368000
6	5.386225000	3.025213000	-2.256059000	1	-7.252048000	-2.604385000	-2.097352000
1	4.208300000	1.222856000	-2.438990000	1	-7.085206000	-3.413145000	2.119408000

7	-0.491273000	-2.576988000	-0.625979000	1	4.632279000	-1.826648000	-0.053634000
6	-3.489721000	-1.177076000	0.982790000	6	6.993500000	-0.291394000	1.852654000
1	-3.299626000	-0.094664000	1.024080000	1	6.592631000	1.152098000	3.400554000
6	0.790864000	-3.111074000	-0.139982000	1	7.092984000	-1.758185000	0.279276000
1	0.944953000	-2.667671000	0.850047000	1	8.067768000	-0.266836000	2.002771000
13	-0.554555000	-0.111033000	1.123636000	6	1.935418000	-2.836963000	-1.091120000
6	0.921154000	1.039364000	0.453075000	6	1.994011000	-1.640572000	-1.816053000
7	2.262880000	0.720231000	0.369334000	6	2.953466000	-3.779886000	-1.238024000
6	3.119955000	1.366943000	-0.431908000	6	3.066039000	-1.390001000	-2.668626000
1	4.140207000	0.996986000	-0.444311000	1	1.179080000	-0.918894000	-1.734635000
6	2.711573000	2.475887000	-1.148577000	6	4.025343000	-3.528393000	-2.094179000
1	3.393837000	3.015538000	-1.790568000	1	2.906872000	-4.718975000	-0.692708000
6	1.422782000	2.938949000	-0.913363000	6	4.084734000	-2.333517000	-2.807565000
1	1.043080000	3.867068000	-1.327592000	1	3.094997000	-0.471146000	-3.247105000
7	0.586048000	2.249040000	-0.139419000	1	4.804481000	-4.274083000	-2.213490000
6	2.754245000	-0.390473000	1.257502000	1	4.911416000	-2.145461000	-3.484709000
1	2.205724000	-0.264097000	2.197113000	6	-1.119155000	4.076521000	-0.469941000
6	-0.821496000	2.722994000	0.098798000	6	-1.590756000	4.203230000	-1.780144000
1	-0.966939000	2.687317000	1.181886000	6	-0.906065000	5.218869000	0.307087000
1	-3.127730000	-1.619575000	1.915684000	6	-1.846183000	5.464480000	-2.309742000
1	0.680421000	-4.187713000	0.028791000	1	-1.768032000	3.314439000	-2.382066000
1	2.461758000	-1.323363000	0.772700000	6	-1.163095000	6.479011000	-0.224176000
1	-1.455159000	1.947637000	-0.362427000	1	-0.551978000	5.121093000	1.330452000
6	-4.951273000	-1.447103000	0.775920000	6	-1.631449000	6.600909000	-1.531391000
6	-5.496607000	-2.671078000	1.174760000	1	-2.220649000	5.561023000	-3.323244000
6	-5.767036000	-0.489678000	0.168838000	1	-1.006827000	7.363937000	0.383355000
6	-6.846618000	-2.933175000	0.967525000	1	-1.837226000	7.583795000	-1.942172000
1	-4.865363000	-3.414097000	1.656543000	6	-2.080447000	0.364948000	3.573637000
6	-7.118489000	-0.752628000	-0.037841000	8	-1.245946000	0.637532000	2.469579000
1	-5.347437000	0.467600000	-0.132512000	1	-3.132396000	0.533988000	3.316593000
6	-7.656744000	-1.974088000	0.360821000	1	-1.964462000	-0.668340000	3.919839000
1	-7.269270000	-3.879850000	1.286771000	1	-1.815311000	1.037356000	4.392264000
1	-7.751628000	-0.003273000	-0.500821000				
1	-8.711181000	-2.176948000	0.205617000				
6	4.236428000	-0.366602000	1.482251000	8-TS8 (in gas phase)			
6	4.786941000	0.474096000	2.453951000	13	0.412757000	0.115109000	-0.319144000
6	5.067616000	-1.168929000	0.696317000	8	0.592088000	-0.918470000	-1.700679000
6	6.164891000	0.509241000	2.638715000	5	0.269973000	-2.384490000	-0.101260000
1	4.138477000	1.089167000	3.073647000	8	1.298694000	-3.246560000	-0.261755000
6	6.446888000	-1.129528000	0.882894000	8	-0.983063000	-2.872337000	-0.281757000
				6	0.688806000	-4.445383000	-0.862527000

6	-0.805547000	-4.325886000	-0.400937000	1	1.842755000	7.297381000	-2.328939000
6	-1.823453000	-4.856127000	-1.393682000	1	-0.281873000	7.485054000	1.400502000
6	-1.051529000	-4.900423000	0.989671000	1	0.805730000	8.627372000	-0.511403000
6	0.845379000	-4.326608000	-2.373191000	6	4.689810000	-1.316690000	0.568103000
6	1.420804000	-5.664942000	-0.334644000	6	5.260500000	-1.881648000	1.709606000
1	2.449559000	-5.663968000	-0.703341000	6	5.446742000	-1.193198000	-0.601167000
1	1.445095000	-5.679998000	0.756198000	6	6.582595000	-2.321001000	1.683220000
1	0.934296000	-6.579197000	-0.688977000	1	4.669531000	-1.989827000	2.616045000
1	1.906617000	-4.239476000	-2.620591000	6	6.766074000	-1.629304000	-0.625272000
1	0.316518000	-3.449068000	-2.759446000	1	4.997857000	-0.761228000	-1.493453000
1	0.453973000	-5.216262000	-2.873689000	6	7.333713000	-2.192928000	0.518039000
1	-1.758981000	-4.336820000	-2.352188000	1	7.021980000	-2.766579000	2.569292000
1	-2.830629000	-4.722017000	-0.989482000	1	7.350679000	-1.538542000	-1.534601000
1	-1.667891000	-5.926213000	-1.563185000	1	8.362132000	-2.537838000	0.496662000
1	-1.001364000	-5.992336000	0.980599000	6	-1.388822000	0.797486000	-0.053929000
1	-2.048996000	-4.605397000	1.326599000	7	-2.197963000	0.687826000	1.080713000
1	-0.317629000	-4.526270000	1.710761000	6	-3.050804000	1.633513000	1.428097000
6	1.985910000	1.228667000	0.122314000	1	-3.635498000	1.462271000	2.325400000
7	1.950563000	2.632402000	0.220893000	6	-3.201721000	2.787253000	0.635660000
6	2.894542000	3.353301000	0.837941000	1	-3.850190000	3.593831000	0.946170000
1	2.736132000	4.426289000	0.860843000	6	-2.699160000	2.716524000	-0.643892000
6	4.005529000	2.753684000	1.389086000	1	-2.977625000	3.425459000	-1.419850000
1	4.780543000	3.331201000	1.871661000	7	-1.890723000	1.709836000	-1.008263000
6	4.106012000	1.367316000	1.257969000	6	-1.989288000	-0.534198000	1.919069000
1	4.964544000	0.806916000	1.613264000	1	-2.006076000	-1.375500000	1.220577000
7	3.151127000	0.667144000	0.662954000	6	-1.799721000	1.351473000	-2.460416000
6	0.720054000	3.260353000	-0.286684000	1	-0.837005000	0.863073000	-2.624058000
1	0.537658000	2.824933000	-1.279187000	1	-0.973702000	-0.433147000	2.327992000
6	3.270739000	-0.827470000	0.586195000	1	-1.822214000	2.291052000	-3.019899000
1	2.756457000	-1.124960000	-0.330354000	6	-2.999546000	-0.704647000	3.014536000
1	-0.078744000	2.896881000	0.385315000	6	-4.216988000	-1.334438000	2.738877000
1	2.718224000	-1.232351000	1.441583000	6	-2.743390000	-0.224113000	4.300892000
6	0.736151000	4.758685000	-0.357830000	6	-5.168795000	-1.481406000	3.742541000
6	1.345975000	5.406967000	-1.436588000	1	-4.413677000	-1.713060000	1.738343000
6	0.150131000	5.511139000	0.662813000	6	-3.696291000	-0.372498000	5.305128000
6	1.372158000	6.796383000	-1.489666000	1	-1.793032000	0.257688000	4.519846000
1	1.797497000	4.822789000	-2.235366000	6	-4.908172000	-1.000123000	5.024953000
6	0.175807000	6.902632000	0.607904000	1	-6.110038000	-1.976263000	3.527977000
1	-0.330023000	5.006502000	1.498449000	1	-3.491014000	-0.006112000	6.305382000
6	0.787302000	7.543467000	-0.467090000	1	-5.648935000	-1.120108000	5.808569000

6	-2.936930000	0.439830000	-2.839737000	1	-3.843826000	-0.063795000	1.445274000
6	-4.118967000	0.973707000	-3.355046000	1	-3.823716000	-1.648329000	0.687525000
6	-2.830052000	-0.935675000	-2.614630000	6	-5.131670000	-0.227498000	-0.284798000
6	-5.194405000	0.139218000	-3.645758000	1	-5.170528000	-0.748863000	-1.246601000
1	-4.196279000	2.041413000	-3.550478000	1	-6.019911000	-0.510835000	0.285190000
6	-3.911215000	-1.765072000	-2.899005000	1	-5.191907000	0.847278000	-0.485352000
1	-1.901349000	-1.354726000	-2.232051000	7	1.755259000	-1.442236000	-0.021821000
6	-5.091238000	-1.230238000	-3.413149000	6	1.361786000	-2.659977000	-0.787703000
1	-6.106241000	0.555249000	-4.060964000	6	1.739202000	-1.767691000	1.427397000
1	-3.830193000	-2.834221000	-2.730660000	1	0.731755000	-2.065772000	1.722459000
1	-5.927666000	-1.882085000	-3.643161000	1	2.436436000	-2.587336000	1.632246000
1	0.425064000	-1.411512000	0.669712000	1	2.040552000	-0.893223000	2.006976000
6	1.656373000	-1.065201000	-2.625976000	6	3.125601000	-1.053526000	-0.433006000
1	2.294761000	-1.906467000	-2.332591000	1	3.811437000	-1.897178000	-0.298357000
1	1.244332000	-1.269629000	-3.617432000	1	3.120018000	-0.757152000	-1.484876000
1	2.266018000	-0.153969000	-2.678563000	1	0.347823000	-2.956098000	-0.507970000
				1	2.051556000	-3.478389000	-0.555941000
				1	1.396280000	-2.443981000	-1.857364000
				1	3.472970000	-0.222733000	0.185357000
9 (in gas phase)				9-TS1 (in gas phase)			
6	1.418581000	1.841258000	1.428802000	6	1.431081000	-0.332380000	-2.477887000
7	0.953975000	1.762730000	0.023271000	7	0.878264000	-1.141422000	-1.361375000
6	1.994293000	2.319372000	-0.880473000	6	1.865957000	-2.188110000	-0.984425000
6	-0.277256000	2.591451000	-0.118623000	6	-0.357468000	-1.808877000	-1.874778000
1	-0.037787000	3.641685000	0.079370000	1	-0.095975000	-2.420999000	-2.744015000
1	-0.664194000	2.498623000	-1.137627000	1	-0.789598000	-2.439372000	-1.098977000
1	-1.032671000	2.249639000	0.591293000	1	-1.080829000	-1.046488000	-2.171674000
1	1.555319000	2.887971000	1.722025000	1	1.576325000	-0.968812000	-3.356910000
1	0.678448000	1.378589000	2.086544000	1	0.730536000	0.467278000	-2.730846000
1	2.912323000	1.736035000	-0.794566000	1	2.762362000	-1.720326000	-0.570745000
1	2.204724000	3.358575000	-0.605415000	1	2.137967000	-2.775200000	-1.867944000
1	1.637761000	2.276632000	-1.910631000	1	1.425022000	-2.852924000	-0.240164000
1	2.376470000	1.325479000	1.528716000	1	2.395145000	0.089872000	-2.193782000
13	0.338442000	-0.087796000	-0.548521000	13	0.341509000	0.006807000	0.221558000
1	0.502920000	-0.006783000	-2.119164000	6	-1.286008000	1.017847000	-0.190571000
6	-1.288517000	-0.537620000	0.450333000	1	-1.294579000	1.991076000	0.320725000
1	-1.309514000	-1.617562000	0.664979000	1	-1.261686000	1.282252000	-1.262986000
1	-1.308897000	-0.063805000	1.445140000	6	-2.617155000	0.307958000	0.111032000
6	-2.590142000	-0.188888000	-0.300457000				
1	-2.602342000	-0.693493000	-1.276480000				
1	-2.632818000	0.886670000	-0.526219000				
6	-3.852390000	-0.572539000	0.472542000				

1	-2.690452000	0.101589000	1.186864000	1	-2.399092000	0.828189000	-1.970485000
1	-2.649547000	-0.677902000	-0.373946000	13	-0.303092000	-0.042677000	0.281163000
6	-3.838510000	1.115781000	-0.328032000	6	1.315757000	-0.832715000	-0.487163000
1	-3.771276000	1.310879000	-1.406526000	1	1.319857000	-1.927813000	-0.387956000
1	-3.813712000	2.096748000	0.163457000	1	1.297476000	-0.666566000	-1.579337000
6	-5.152885000	0.408670000	-0.008911000	6	2.647178000	-0.295985000	0.067598000
1	-5.251399000	0.232506000	1.066975000	1	2.710877000	-0.506168000	1.143503000
1	-6.012233000	1.002031000	-0.330748000	1	2.683676000	0.799370000	-0.012595000
1	-5.208992000	-0.562199000	-0.512081000	6	3.870535000	-0.887081000	-0.632368000
7	1.759638000	1.577968000	0.321043000	1	3.810694000	-0.666483000	-1.706452000
6	1.443857000	2.218773000	1.629342000	1	3.841508000	-1.980531000	-0.541856000
6	1.606804000	2.612341000	-0.733190000	6	5.183767000	-0.354429000	-0.065533000
1	0.564459000	2.932142000	-0.781115000	1	5.274632000	-0.590889000	0.999497000
1	2.238281000	3.477324000	-0.501111000	1	6.045121000	-0.788577000	-0.579227000
1	1.909565000	2.212390000	-1.701018000	1	5.244121000	0.733760000	-0.171201000
6	3.171008000	1.129393000	0.378365000	7	-1.729883000	-1.503995000	-0.201717000
1	3.826005000	1.975088000	0.616560000	6	-1.417309000	-2.626003000	0.733916000
1	3.278026000	0.365979000	1.152417000	6	-1.605972000	-2.039370000	-1.581075000
1	0.412615000	2.576720000	1.626581000	1	-0.568689000	-2.321315000	-1.770707000
1	2.115571000	3.068283000	1.793358000	1	-2.244869000	-2.922250000	-1.694283000
1	1.579777000	1.496359000	2.436525000	1	-1.918811000	-1.291501000	-2.309175000
1	3.478658000	0.718913000	-0.585279000	6	-3.136305000	-1.101160000	0.048616000
1	1.212980000	-0.545524000	1.563834000	1	-3.800946000	-1.962713000	-0.082552000
6	0.218397000	-1.741808000	1.971087000	1	-3.227732000	-0.725889000	1.068959000
8	0.623810000	-2.197110000	2.959792000	1	-0.385296000	-2.949571000	0.586370000
8	-0.566112000	-1.674081000	1.034264000	1	-2.086725000	-3.467645000	0.525544000
				1	-1.557782000	-2.295884000	1.762609000
				1	-3.439136000	-0.326327000	-0.658400000
				1	-0.313057000	1.082323000	3.532309000
				6	-0.265070000	0.805873000	2.475127000
				8	0.588560000	1.259262000	1.693120000
				8	-1.120741000	-0.023835000	1.991581000
9-IMI (in gas phase)				9-TS2 (in gas phase)			
6	-1.430751000	1.316246000	-2.080763000	6	-2.821168000	-0.834144000	2.476722000
7	-0.853055000	1.617098000	-0.746607000	7	-1.556817000	-0.835728000	1.698308000
6	-1.817151000	2.448078000	0.023261000	6	-1.061460000	-2.236407000	1.569271000
6	0.389124000	2.417645000	-0.981176000	6	-0.564462000	-0.052752000	2.501707000
1	0.129844000	3.316053000	-1.550816000	1	-0.549727000	-0.453916000	3.520562000
1	0.834043000	2.697135000	-0.027827000	1	0.431021000	-0.148563000	2.069850000
1	1.099585000	1.817573000	-1.553823000				
1	-1.573339000	2.248026000	-2.637976000				
1	-0.746422000	0.671758000	-2.637829000				
1	-2.712828000	1.865115000	0.249506000				
1	-2.095695000	3.329564000	-0.563826000				
1	-1.345620000	2.774331000	0.950920000				

8	-1.419625000	-2.047755000	-0.026998000	7	-2.127002000	-0.567947000	0.045473000
1	-0.163490000	-0.279457000	-1.155280000	6	-2.612664000	-1.558297000	-0.944853000
5	1.359447000	-1.430060000	-0.674499000	7	0.031804000	1.201234000	-0.059787000
8	2.360059000	-1.209961000	-1.551856000	7	2.126371000	-0.595021000	0.042586000
8	1.555398000	-0.924360000	0.591861000	6	2.744015000	-1.858367000	-0.415031000
6	3.315752000	-0.341318000	-0.888757000	6	-2.835755000	-0.799996000	1.324031000
6	2.980042000	-0.572101000	0.628146000	1	-3.914502000	-0.646689000	1.202585000
6	3.699122000	-1.779395000	1.222173000	1	-2.650849000	-1.824607000	1.651352000
6	3.171488000	0.650343000	1.506661000	1	-2.454792000	-0.126288000	2.093971000
6	4.714616000	-0.778684000	-1.292167000	6	2.816168000	-0.152405000	1.270466000
6	3.044588000	1.079835000	-1.362771000	1	2.724761000	-0.935074000	2.025211000
1	3.120055000	1.105964000	-2.452775000	1	3.877157000	0.041351000	1.070831000
1	2.040954000	1.402198000	-1.080473000	1	2.359381000	0.754088000	1.668957000
1	3.771844000	1.783587000	-0.947415000	6	-0.240180000	1.967340000	1.184687000
1	4.859589000	-0.587259000	-2.358155000	1	0.599045000	1.858651000	1.871097000
1	4.873368000	-1.843067000	-1.111765000	1	-0.386715000	3.028776000	0.953826000
1	5.466499000	-0.207706000	-0.737744000	1	-1.125573000	1.579694000	1.686718000
1	3.565718000	-2.667220000	0.595928000	6	-1.081453000	1.389140000	-1.032949000
1	3.285821000	-1.990151000	2.212311000	6	2.188278000	0.418447000	-1.029284000
1	4.770320000	-1.589668000	1.329247000	6	1.343301000	1.631710000	-0.646366000
1	4.220538000	0.962817000	1.488183000	1	-3.148729000	0.805650000	-1.232271000
1	2.913869000	0.410466000	2.542897000	1	-2.741135000	1.432284000	0.355631000
1	2.558024000	1.490670000	1.171733000	1	-1.206777000	2.454872000	-1.261582000
7	-3.332656000	-0.403186000	-1.064365000	1	-0.799490000	0.867772000	-1.954339000
6	-3.016844000	-0.223291000	-2.507781000	1	3.223170000	0.726900000	-1.229099000
6	-4.360542000	0.602136000	-0.682559000	1	1.792644000	-0.049554000	-1.936391000
1	-3.958262000	1.609559000	-0.758135000	1	1.863250000	2.242591000	0.094559000
1	-5.227260000	0.507823000	-1.346616000	1	1.173202000	2.266884000	-1.520791000
1	-4.687406000	0.416059000	0.341936000	1	0.008678000	-1.263201000	1.778910000
6	-3.966864000	-1.736605000	-0.902770000	1	0.033241000	-1.627222000	-1.133324000
1	-4.941918000	-1.737216000	-1.402599000	1	-2.163138000	-1.359089000	-1.918216000
1	-3.341671000	-2.507706000	-1.347203000	1	-3.705212000	-1.507969000	-1.021097000
1	-2.610207000	0.775569000	-2.675440000	1	-2.313904000	-2.560981000	-0.632382000
1	-3.924912000	-0.350006000	-3.108663000	1	2.608597000	-2.619405000	0.357368000
1	-2.274993000	-0.965055000	-2.813757000	1	3.816065000	-1.716805000	-0.595858000
1	-4.104981000	-1.958606000	0.157146000	1	2.254519000	-2.192646000	-1.330206000

10 (in gas phase)

6	-2.370745000	0.808501000	-0.461195000
13	0.027162000	-0.844177000	0.250738000

10-TS1 (in gas phase)

6	2.315413000	-1.231117000	-0.621808000
13	-0.012230000	0.194777000	0.526093000

7	2.109643000	0.012473000	0.183943000	10-IM1 (in gas phase)			
6	2.678788000	1.164036000	-0.556287000	6	-2.344717000	1.075763000	-0.550636000
7	-0.076492000	-1.721718000	-0.307590000	13	0.015100000	-0.374225000	0.565234000
7	-2.106305000	0.120705000	0.202547000	7	-2.118648000	-0.183541000	0.225740000
6	-2.750962000	1.436240000	0.000856000	6	-2.756857000	-1.309951000	-0.503728000
6	2.809350000	-0.085645000	1.488877000	7	0.046044000	1.558956000	-0.238376000
1	3.885632000	-0.226844000	1.337784000	7	2.108907000	-0.231980000	0.240911000
1	2.636960000	0.834224000	2.051651000	6	2.825840000	-1.511263000	0.031918000
1	2.403355000	-0.915985000	2.067920000	6	-2.771046000	-0.102506000	1.558338000
6	-2.781984000	-0.561086000	1.328609000	1	-3.849238000	0.057525000	1.444885000
1	-2.704960000	0.066609000	2.217497000	1	-2.593976000	-1.038064000	2.092990000
1	-3.837741000	-0.738443000	1.091387000	1	-2.335020000	0.706582000	2.144314000
1	-2.294164000	-1.510277000	1.550624000	6	2.729298000	0.439891000	1.406424000
6	0.185944000	-2.783834000	0.695462000	1	2.648224000	-0.213226000	2.276240000
1	-0.632573000	-2.816304000	1.414018000	1	3.784643000	0.655347000	1.201412000
1	0.281191000	-3.758081000	0.201902000	1	2.207777000	1.367718000	1.638673000
1	1.094435000	-2.567257000	1.255217000	6	-0.230713000	2.585864000	0.799702000
6	1.023485000	-1.671050000	-1.304651000	1	0.590722000	2.616710000	1.514120000
6	-2.209263000	-0.662981000	-1.052237000	1	-0.348561000	3.570606000	0.332687000
6	-1.405650000	-1.956938000	-0.950232000	1	-1.130690000	2.336898000	1.358394000
1	3.089691000	-1.067038000	-1.378030000	6	-1.060382000	1.538940000	-1.231596000
1	2.685041000	-2.019159000	0.037681000	6	2.234622000	0.598836000	-0.982392000
1	1.162428000	-2.653894000	-1.773354000	6	1.367970000	1.852252000	-0.875728000
1	0.734587000	-0.953983000	-2.078953000	1	-3.121419000	0.919581000	-1.305488000
1	-3.258997000	-0.893952000	-1.276314000	1	-2.719174000	1.846575000	0.126392000
1	-1.819982000	-0.032843000	-1.856072000	1	-1.203046000	2.538659000	-1.661891000
1	-1.946488000	-2.690349000	-0.348276000	1	-0.777878000	0.850371000	-2.032069000
1	-1.275557000	-2.396057000	-1.944702000	1	3.281718000	0.889468000	-1.140294000
1	-0.006771000	-0.191546000	2.063307000	1	1.918022000	-0.016636000	-1.825703000
1	-0.022812000	0.999116000	-0.967255000	1	1.872350000	2.607644000	-0.269285000
1	2.174117000	1.275815000	-1.517663000	1	1.220414000	2.288581000	-1.868621000
1	3.751295000	1.011424000	-0.720432000	1	0.004641000	0.003050000	2.105131000
1	2.549344000	2.075541000	0.031169000	1	-0.014435000	-3.289888000	-1.236372000
1	-2.624527000	2.043975000	0.899433000	1	-2.371360000	-1.356107000	-1.522064000
1	-3.821587000	1.309336000	-0.196955000	1	-3.841846000	-1.161336000	-0.534699000
1	-2.296734000	1.941526000	-0.854737000	1	-2.545745000	-2.245426000	0.017043000
6	0.062461000	2.620911000	-0.224205000	1	2.642891000	-2.172268000	0.880703000
8	0.039952000	3.360124000	-1.116892000	1	3.902152000	-1.327503000	-0.062843000
8	0.110098000	2.246240000	0.926312000	1	2.474142000	-1.984728000	-0.885687000
				6	-0.007284000	-2.346462000	-0.679977000

8	-0.048875000	-2.331663000	0.581848000	1	-2.971034000	-2.692239000	1.727968000
8	0.040611000	-1.233016000	-1.277833000	1	-4.167673000	-2.244785000	0.498653000
				6	-2.638492000	2.795129000	1.095354000
10-TS2 (in gas phase)				1	-2.902247000	2.559428000	2.127785000
1	0.422569000	-0.188737000	-0.756472000	1	-2.349400000	3.849737000	1.020258000
5	1.597092000	-0.145937000	-0.546580000	1	-3.515429000	2.610722000	0.473608000
8	2.413114000	-1.201117000	-0.775338000	6	-4.158783000	0.458427000	-1.525671000
8	2.220544000	1.015217000	-0.204913000	1	-4.613428000	1.246564000	-0.925731000
6	3.740499000	-0.797383000	-0.325754000	1	-4.393399000	0.615544000	-2.585036000
6	3.649727000	0.770159000	-0.367544000	1	-4.587632000	-0.485605000	-1.191895000
6	4.393859000	1.477118000	0.751790000	6	-2.066794000	-0.608628000	-2.134883000
6	4.030624000	1.358797000	-1.722773000	6	-1.089271000	2.266332000	-0.709909000
6	3.922453000	-1.356497000	1.081520000	6	-2.155124000	1.810753000	-1.698196000
6	4.770252000	-1.394597000	-1.270680000	1	-1.870930000	-2.754921000	-2.032447000
1	4.756226000	-2.483825000	-1.181336000	1	-3.489637000	-2.171391000	-1.679713000
1	4.566757000	-1.133216000	-2.310635000	1	-2.408419000	-0.549472000	-3.176473000
1	5.774196000	-1.044997000	-1.008836000	1	-0.983687000	-0.463893000	-2.123346000
1	3.801806000	-2.442476000	1.042924000	1	-0.936253000	3.349373000	-0.802455000
1	3.174024000	-0.955545000	1.768311000	1	-0.127741000	1.784562000	-0.894192000
1	4.923291000	-1.135042000	1.463171000	1	-2.990260000	2.514484000	-1.700465000
1	4.017155000	1.176106000	1.730958000	1	-1.751204000	1.793755000	-2.716027000
1	4.270749000	2.558670000	0.648901000	1	-0.021000000	-2.177244000	-0.320715000
1	5.463564000	1.250202000	0.700563000	1	-0.941550000	-3.703465000	-0.214995000
1	3.770075000	2.420384000	-1.734585000	1	-0.655184000	-2.721549000	1.238773000
1	3.490313000	0.861663000	-2.534505000	1	-0.652574000	1.982844000	2.607404000
1	5.103451000	1.263857000	-1.910742000	1	-0.111542000	3.288686000	1.521340000
1	-0.044730000	-0.879519000	3.680651000	1	0.509157000	1.630634000	1.295550000
6	-0.138238000	-0.688017000	2.600757000				
8	0.831647000	-0.678530000	1.870671000	10-IM2 (in gas phase)			
8	-1.376615000	-0.491350000	2.230197000	1	0.047635000	-0.652179000	3.858990000
13	-2.272205000	-0.012186000	0.737887000	6	-0.063138000	-0.459492000	2.787525000
1	-3.773717000	0.129262000	1.199994000	8	1.009846000	-0.435258000	2.124755000
6	-2.428996000	-1.957443000	-1.532439000	8	-1.231295000	-0.293481000	2.348960000
7	-2.136045000	-1.963174000	-0.069347000	1	-0.076867000	0.041113000	0.236903000
6	-0.852000000	-2.681893000	0.170127000	5	1.125804000	-0.094120000	0.602755000
7	-2.686440000	0.468569000	-1.324925000	8	1.716359000	-1.135996000	-0.148664000
7	-1.500339000	1.933393000	0.676866000	8	1.896475000	1.085429000	0.481578000
6	-0.359222000	2.223008000	1.584874000	6	3.091365000	-0.748806000	-0.361918000
6	-3.196836000	-2.715572000	0.660010000	6	2.981436000	0.809952000	-0.426399000
1	-3.223164000	-3.753885000	0.311577000	6	4.221300000	1.550227000	0.051196000

1	3.077213000	2.657887000	-1.274082000	13	-0.000842000	0.000481000	-0.000051000
1	2.161387000	1.198280000	-3.036512000	7	-1.450930000	1.559619000	-0.267547000
1	0.734082000	0.832279000	-2.038259000	6	-2.632852000	1.207257000	0.548553000
1	1.312329000	-3.280068000	-1.320485000	7	1.451494000	1.558938000	0.267650000
1	0.225521000	-1.899349000	-1.060701000	7	1.451496000	-1.559298000	-0.267572000
1	3.072260000	-1.909271000	-2.162471000	6	1.866803000	1.839844000	1.656918000
1	1.623297000	-1.241626000	-2.893537000	1	2.274183000	0.946855000	2.125488000
1	-0.394746000	2.230399000	-0.237368000	1	2.622115000	2.636304000	1.662758000
1	0.302115000	3.790702000	0.305336000	1	1.008061000	2.145710000	2.252051000
1	-0.010727000	2.474662000	1.465893000	6	0.724070000	2.740293000	-0.256104000
1	0.940853000	-2.586049000	2.312565000	6	2.633068000	-1.207125000	0.548683000
1	0.667605000	-3.833740000	1.076030000	6	2.633224000	1.206499000	-0.548552000
1	-0.315543000	-2.351932000	1.055113000	1	-1.228119000	3.668106000	-0.044006000
1	0.163951000	-0.010894000	0.077659000	1	-0.742360000	2.692262000	1.348513000
5	-1.807559000	-0.148463000	0.990845000	1	1.229561000	3.667552000	0.044365000
8	-2.295994000	1.043878000	0.560366000	1	0.743414000	2.692110000	-1.348270000
8	-2.251645000	-1.244492000	0.321216000	1	3.316272000	2.065821000	-0.614820000
6	-3.382005000	0.714266000	-0.353131000	1	2.259696000	1.003257000	-1.556548000
6	-3.014534000	-0.742670000	-0.812428000	7	-1.451781000	-1.559554000	0.267535000
6	-4.208314000	-1.656780000	-1.030805000	6	-2.633397000	-1.206736000	-0.548673000
6	-2.096710000	-0.770975000	-2.030117000	6	-3.420936000	0.000396000	0.000000000
6	-4.666971000	0.774418000	0.466929000	6	0.723328000	-2.740128000	0.256214000
6	-3.409309000	1.746873000	-1.466422000	6	-0.723618000	-2.740235000	-0.256552000
1	-3.651950000	2.727201000	-1.048279000	6	-1.867203000	-1.840924000	1.656610000
1	-2.444632000	1.817583000	-1.974626000	6	3.421125000	-0.000351000	0.000066000
1	-4.176173000	1.492769000	-2.205073000	1	4.084732000	-0.330281000	-0.805711000
1	-4.758459000	1.770018000	0.907770000	1	3.316164000	-2.066410000	0.615146000
1	-4.652841000	0.040422000	1.278681000	1	2.259578000	-1.003731000	1.556678000
1	-5.545555000	0.587792000	-0.156404000	1	-2.259470000	1.003859000	1.556585000
1	-4.799541000	-1.768184000	-0.120743000	1	-3.315841000	2.066589000	0.614789000
1	-3.860936000	-2.646938000	-1.336810000	1	-4.084621000	-0.329251000	0.805813000
1	-4.850606000	-1.259955000	-1.823592000	1	-4.084550000	0.330325000	-0.805747000
1	-1.768379000	-1.800100000	-2.202892000	1	-2.259911000	-1.003436000	-1.556682000
1	-1.215761000	-0.142692000	-1.863331000	1	-3.316851000	-2.065725000	-0.615030000
1	-2.617454000	-0.424068000	-2.926649000	1	-0.742817000	-2.691628000	-1.348700000
13	1.710225000	0.049961000	0.634875000	1	-1.228631000	-3.667903000	0.043497000
1	3.150237000	0.069027000	1.330221000	1	1.228492000	-3.667693000	-0.043892000
				1	0.742368000	-2.691679000	1.348386000
11 (in gas phase)				1	-2.622498000	-2.637409000	1.662172000
6	-0.723007000	2.740625000	0.256352000	1	-1.008526000	-2.147005000	2.251764000

1	-2.274633000	-0.948045000	2.125419000	1	3.603604000	-1.647674000	-0.094761000
6	-1.866204000	1.840860000	-1.656834000	1	2.547527000	-0.846060000	1.061456000
6	1.866878000	-1.840564000	-1.656696000	1	-2.494598000	0.734028000	1.303785000
1	-2.620840000	2.637929000	-1.662488000	1	-3.612806000	1.664730000	0.294760000
1	-1.007250000	2.145831000	-2.252110000	1	-4.040031000	-0.866183000	0.481692000
1	-2.274507000	0.948120000	-2.125104000	1	-4.144276000	-0.164005000	-1.110935000
1	2.274496000	-0.947809000	-2.125526000	1	-2.123272000	-1.137128000	-1.887098000
1	2.622007000	-2.637224000	-1.662379000	1	-2.973050000	-2.397807000	-0.989880000
1	1.008140000	-2.146463000	-2.251842000	1	-0.474551000	-2.669106000	-1.741991000
1	4.084832000	0.329540000	0.805780000	1	-0.801349000	-3.699805000	-0.344729000
1	-0.000531000	-0.000992000	-1.630664000	1	1.646621000	-3.446409000	-0.563838000
1	-0.000848000	0.000058000	1.630607000	1	1.137781000	-2.559611000	0.882767000
11-TS1 (in gas phase)				1	-2.327325000	-2.920937000	1.189868000
6	-1.098880000	2.621256000	0.104322000	1	-0.777363000	-2.377142000	1.878144000
7	-1.668265000	1.380813000	-0.493154000	1	-2.133145000	-1.259518000	1.831704000
6	-2.839935000	0.884820000	0.281833000	6	-2.122847000	1.701428000	-1.871315000
7	1.181783000	1.674781000	-0.000389000	6	1.986296000	-1.530706000	-2.171630000
7	1.615411000	-1.321180000	-0.752586000	1	-2.949679000	2.418881000	-1.815779000
6	1.704355000	2.001769000	1.358629000	1	-1.310285000	2.124910000	-2.458348000
1	2.210070000	1.144981000	1.801192000	1	-2.457325000	0.803988000	-2.386938000
1	2.413717000	2.831553000	1.262674000	1	2.303615000	-0.594002000	-2.626411000
1	0.885950000	2.281142000	2.017672000	1	2.802942000	-2.259871000	-2.233590000
6	0.318783000	2.817295000	-0.430598000	1	1.131139000	-1.890450000	-2.741471000
6	2.819058000	-0.885278000	0.002527000	1	4.007517000	0.861298000	0.308902000
6	2.349898000	1.530466000	-0.920688000	1	0.637345000	-0.522663000	1.206883000
1	-1.724638000	3.484951000	-0.150910000	6	0.279949000	-0.257720000	2.299644000
1	-1.089870000	2.494586000	1.188515000	8	0.926160000	-0.862992000	3.131542000
1	0.744923000	3.758572000	-0.066378000	8	-0.654669000	0.563000000	2.282207000
1	0.326524000	2.853691000	-1.523468000	13	-0.039020000	0.040601000	-0.474789000
1	2.861279000	2.499469000	-0.990361000	1	-0.081689000	0.098009000	-2.076393000
1	1.942646000	1.304196000	-1.910554000	11-IMI (in gas phase)			
7	-1.228280000	-1.632149000	-0.068802000	6	0.812214000	-2.610874000	-0.396673000
6	-2.459504000	-1.432719000	-0.888951000	13	-0.063609000	0.087425000	-0.296767000
6	-3.440116000	-0.403132000	-0.307483000	7	1.428125000	-1.324423000	-0.821341000
6	1.060254000	-2.589684000	-0.209615000	6	2.695480000	-1.026004000	-0.106225000
6	-0.395850000	-2.729723000	-0.653033000	7	-1.412996000	-1.561409000	-0.151501000
6	-1.645702000	-2.069513000	1.295811000	7	-1.592163000	1.576833000	-0.289134000
6	3.369453000	0.465452000	-0.486839000	6	-1.826060000	-2.089911000	1.171335000
1	4.031561000	0.311594000	-1.345079000	1	-2.260028000	-1.302307000	1.783937000

1	2.635774000	-4.316497000	-0.728049000	6	0.000221000	3.008231000	1.219314000
6	2.706017000	-1.251699000	0.496001000	6	-1.252362000	2.615237000	0.469786000
1	4.415550000	-2.651234000	0.469493000	6	-2.439850000	3.317870000	0.355386000
13	0.000002000	0.000014000	0.512050000	7	-1.399489000	1.356088000	-0.061004000
6	-4.786191000	0.000914000	1.019273000	6	-3.367406000	2.444121000	-0.269454000
1	-5.210219000	0.885575000	1.507019000	1	-2.627989000	4.327683000	0.698808000
1	-5.084413000	0.000622000	-0.033386000	6	-2.701483000	1.251503000	-0.504227000
1	-5.210455000	-0.883345000	1.507551000	1	-4.399960000	2.664695000	-0.509743000
6	-2.943761000	0.001202000	2.671701000	6	1.252800000	2.615047000	0.469886000
1	-3.376649000	-0.893039000	3.139547000	6	2.440515000	3.317364000	0.355886000
1	-1.866049000	0.000817000	2.841332000	7	1.399655000	1.355978000	-0.061165000
1	-3.375965000	0.896099000	3.138933000	6	3.367933000	2.443493000	-0.268987000
6	-0.001154000	-4.512216000	-1.470761000	1	2.628878000	4.327050000	0.699558000
1	0.885472000	-4.796804000	-2.047922000	6	2.701705000	1.251122000	-0.504151000
1	-0.001226000	-5.070178000	-0.528976000	1	4.400589000	2.663828000	-0.509054000
1	-0.888003000	-4.796459000	-2.047790000	6	3.256248000	-0.000200000	-1.162875000
6	-0.001135000	-2.282045000	-2.575531000	6	2.701464000	-1.251509000	-0.504309000
1	0.895396000	-2.550318000	-3.148763000	6	3.367404000	-2.444112000	-0.269518000
1	-0.898085000	-2.550042000	-3.148217000	7	1.399485000	-1.356086000	-0.061037000
1	-0.000909000	-1.198121000	-2.427734000	6	2.439876000	-3.317846000	0.355386000
6	0.000964000	4.512297000	-1.470649000	1	4.399951000	-2.664686000	-0.509836000
1	0.000660000	5.070224000	-0.528843000	6	1.252387000	-2.615218000	0.469803000
1	0.887935000	4.796661000	-2.047413000	1	2.628033000	-4.327647000	0.698833000
1	-0.885535000	4.796813000	-2.048051000	6	-0.000169000	-3.008202000	1.219383000
6	0.001262000	2.282136000	-2.575555000	6	-1.252772000	-2.615041000	0.469984000
1	-0.895205000	2.550391000	-3.148882000	6	-2.440467000	-3.317390000	0.355970000
1	0.898262000	2.550188000	-3.148137000	7	-1.399665000	-1.355965000	-0.061037000
1	0.001097000	1.198206000	-2.427812000	6	-3.367910000	-2.443533000	-0.268884000
6	4.786273000	-0.000914000	1.018613000	1	-2.628801000	-4.327087000	0.699626000
1	5.210449000	-0.885525000	1.506314000	6	-2.701718000	-1.251136000	-0.504022000
1	5.084257000	-0.000719000	-0.034122000	1	-4.400560000	-2.663893000	-0.508953000
1	5.210618000	0.883406000	1.506692000	13	-0.000012000	-0.000003000	-0.467421000
6	2.944239000	-0.001327000	2.671544000	6	4.786242000	-0.000357000	-1.018292000
1	3.377015000	0.893030000	3.139286000	1	5.215957000	0.880764000	-1.505191000
1	1.866562000	-0.001249000	2.841402000	1	5.090791000	-0.000462000	0.033090000
1	3.376809000	-0.896156000	3.138565000	1	5.215791000	-0.881486000	-1.505320000
				6	2.961506000	-0.000049000	-2.680949000
12 (in THF solvent)				1	3.399848000	-0.890743000	-3.148044000
1	-0.000074000	-0.000044000	-2.089042000	1	1.888757000	0.000120000	-2.879456000
6	-3.256304000	0.000177000	-1.162729000	1	3.400102000	0.890593000	-3.147905000

6	-0.000243000	-4.514394000	1.492133000	6	-2.346240000	3.548644000	-0.282727000
1	-0.883437000	-4.798531000	2.073384000	7	-1.343506000	1.540769000	-0.014227000
1	-0.000405000	-5.089586000	0.560281000	6	-3.310277000	2.631778000	0.205087000
1	0.883062000	-4.798654000	2.073157000	1	-2.506795000	4.590165000	-0.532427000
6	-0.000066000	-2.281720000	2.584583000	6	-2.668300000	1.415401000	0.347067000
1	-0.891953000	-2.549494000	3.163952000	1	-4.350865000	2.839219000	0.420559000
1	0.892353000	-2.548784000	3.163461000	6	-3.249329000	0.119406000	0.868783000
1	-0.000558000	-1.195593000	2.445800000	6	-2.714084000	-1.070040000	0.090711000
6	0.000310000	4.514428000	1.492035000	6	-3.396943000	-2.228210000	-0.236033000
1	0.000445000	5.089603000	0.560172000	7	-1.429716000	-1.137545000	-0.404742000
1	-0.882976000	4.798702000	2.073081000	6	-2.499650000	-3.041738000	-0.971878000
1	0.883522000	4.798574000	2.073254000	1	-4.424894000	-2.461414000	0.012314000
6	0.000163000	2.281779000	2.584532000	6	-1.311462000	-2.341959000	-1.051025000
1	0.892067000	2.549571000	3.163865000	1	-2.703418000	-4.016567000	-1.397442000
1	-0.892239000	2.548852000	3.163432000	6	-0.067986000	-2.685920000	-1.834442000
1	0.000657000	1.195648000	2.445776000	6	1.187763000	-2.420387000	-1.039708000
6	-4.786291000	0.000334000	-1.018042000	6	2.335707000	-3.185314000	-0.963484000
1	-5.216038000	-0.880797000	-1.504893000	7	1.371011000	-1.229219000	-0.383952000
1	-5.090766000	0.000458000	0.033362000	6	3.275468000	-2.427375000	-0.221060000
1	-5.215876000	0.881452000	-1.505056000	1	2.486447000	-4.166798000	-1.395806000
6	-2.961672000	-0.000002000	-2.680825000	6	2.656766000	-1.235309000	0.112375000
1	-3.400048000	0.890684000	-3.147904000	1	4.288779000	-2.718031000	0.026828000
1	-1.888937000	-0.000175000	-2.879410000	13	0.006000000	0.089963000	0.137979000
1	-3.400302000	-0.890653000	-3.147732000	6	-2.966225000	-0.004047000	2.384504000
				1	-1.913396000	0.156412000	2.612921000
				1	-3.541646000	0.758098000	2.926578000
				1	-3.254922000	-0.998332000	2.747096000
				6	-4.777570000	0.153477000	0.708042000
				1	-5.197830000	1.007205000	1.250311000
				1	-5.058341000	0.228581000	-0.346538000
				1	-5.220967000	-0.755980000	1.127638000
				6	0.156718000	4.823729000	-1.147620000
				1	0.168195000	5.251880000	-0.140481000
				1	1.054395000	5.154098000	-1.681064000
				1	-0.716063000	5.210134000	-1.684688000
				6	0.094297000	2.762170000	-2.539831000
				1	-0.789387000	3.134226000	-3.072998000
				1	1.003236000	3.074886000	-3.068664000
				1	0.057831000	1.668301000	-2.543332000
				6	-0.112319000	-4.154662000	-2.262450000
12-TS1 (in gas phase)							
8	-0.233133000	-2.515770000	2.132896000				
6	-0.106103000	-1.531920000	2.784006000				
8	-0.014634000	-0.995403000	3.850981000				
1	-0.020292000	-0.313738000	1.780378000				
6	3.253161000	-0.079192000	0.895300000				
6	0.108241000	3.294214000	-1.085867000				
6	1.345558000	2.767029000	-0.402830000				
6	2.569102000	3.395688000	-0.269713000				
7	1.443122000	1.453399000	-0.006424000				
6	3.471609000	2.422138000	0.225902000				
1	2.794847000	4.425142000	-0.518990000				
6	2.755330000	1.247781000	0.364946000				
1	4.521422000	2.565387000	0.448655000				
6	-1.162728000	2.845889000	-0.408426000				

1	-0.136761000	-4.809339000	-1.386011000	7	-1.410035000	-1.189644000	-0.393088000
1	-1.003531000	-4.345318000	-2.870617000	6	-2.417146000	-3.138786000	-0.922567000
1	0.770093000	-4.401379000	-2.863233000	1	-4.343466000	-2.624217000	0.099346000
6	-0.033893000	-1.816886000	-3.113540000	6	-1.261186000	-2.389972000	-1.044008000
1	0.858099000	-2.049226000	-3.708841000	1	-2.598034000	-4.119607000	-1.344805000
1	-0.933505000	-1.990900000	-3.717212000	6	-0.025971000	-2.679453000	-1.863604000
1	-0.000508000	-0.755072000	-2.851127000	6	1.231988000	-2.385381000	-1.080306000
6	2.943289000	-0.183503000	2.406437000	6	2.402180000	-3.119436000	-1.021026000
1	3.193993000	-1.184490000	2.779027000	7	1.387787000	-1.199766000	-0.404124000
1	3.535932000	0.562121000	2.952812000	6	3.327984000	-2.344758000	-0.273433000
1	1.892690000	0.009903000	2.618349000	1	2.580494000	-4.086775000	-1.474180000
6	4.782325000	-0.135356000	0.753317000	6	2.679275000	-1.173680000	0.081125000
1	5.165438000	-1.070983000	1.174754000	1	4.351346000	-2.610733000	-0.040303000
1	5.080603000	-0.073463000	-0.297372000	13	-0.002488000	0.082484000	0.132949000
1	5.245521000	0.690166000	1.304232000	6	-2.959146000	-0.049758000	2.402056000
12-TS1 (in THF solvent)				1	-1.909965000	0.152479000	2.615099000
8	0.063705000	-2.477140000	2.327217000	1	-3.555790000	0.702356000	2.933057000
6	0.015426000	-1.448633000	2.912987000	1	-3.211984000	-1.040699000	2.799031000
8	-0.022999000	-0.810618000	3.917711000	6	-4.786463000	0.008114000	0.735810000
1	-0.005130000	-0.272237000	1.774286000	1	-5.232312000	0.857993000	1.261860000
6	3.254309000	-0.013222000	0.876721000	1	-5.086715000	0.051048000	-0.315717000
6	0.019275000	3.282019000	-1.111950000	1	-5.202745000	-0.901977000	1.179670000
6	1.263575000	2.790216000	-0.411328000	6	0.023135000	4.812952000	-1.176404000
6	2.465821000	3.455618000	-0.255312000	1	0.010651000	5.254465000	-0.174863000
7	1.399936000	1.475847000	-0.022121000	1	0.913555000	5.171113000	-1.703021000
6	3.394725000	2.505587000	0.242817000	1	-0.850717000	5.175739000	-1.726815000
1	2.664542000	4.492430000	-0.495476000	6	0.041037000	2.745228000	-2.563981000
6	2.715882000	1.306262000	0.362973000	1	-0.841560000	3.090051000	-3.115779000
1	4.436645000	2.681816000	0.478086000	1	0.942845000	3.085476000	-3.086843000
6	-1.245765000	2.794169000	-0.445953000	1	0.038897000	1.649513000	-2.572118000
6	-2.454009000	3.458437000	-0.339674000	6	-0.030921000	-4.138012000	-2.328278000
7	-1.388990000	1.488797000	-0.029297000	1	-0.014285000	-4.827029000	-1.477349000
6	-3.392317000	2.518501000	0.159718000	1	-0.925211000	-4.344591000	-2.925250000
1	-2.648724000	4.488881000	-0.608852000	1	0.842019000	-4.341489000	-2.956971000
6	-2.713480000	1.325285000	0.329735000	6	-0.045782000	-1.779420000	-3.120468000
1	-4.439492000	2.698522000	0.367070000	1	0.839140000	-1.964866000	-3.741138000
6	-3.256804000	0.024906000	0.886153000	1	-0.944846000	-1.970801000	-3.718706000
6	-2.686557000	-1.164357000	0.129995000	1	-0.046383000	-0.720080000	-2.841679000
6	-3.329954000	-2.354117000	-0.169577000	6	2.958382000	-0.138645000	2.389600000
				1	3.194142000	-1.147303000	2.750513000

1	3.569737000	0.582924000	2.945665000	6	-3.382764000	2.507863000	0.207025000
1	1.914836000	0.079014000	2.612901000	1	-2.639390000	4.480417000	-0.554125000
6	4.784064000	-0.030787000	0.727196000	6	-2.709653000	1.307522000	0.350457000
1	5.196916000	-0.953499000	1.147840000	1	-4.424703000	2.693096000	0.435465000
1	5.086396000	0.038656000	-0.322312000	13	0.000061000	0.079502000	0.153621000
1	5.231667000	0.803307000	1.276286000	6	3.066617000	-0.084445000	2.419707000
12-IM1 (in gas phase)				1	2.022563000	0.058117000	2.695499000
8	-0.002107000	-0.276019000	1.945612000	1	3.398159000	-1.062522000	2.790368000
6	-0.006167000	-1.484912000	2.443043000	1	3.661204000	0.701061000	2.904829000
8	-0.006703000	-1.739332000	3.633770000	6	4.791685000	-0.016209000	0.649824000
1	-0.009277000	-2.295118000	1.685928000	1	5.230840000	-0.930050000	1.063774000
6	-3.270871000	0.005293000	0.884298000	1	5.022239000	0.033880000	-0.418271000
6	-0.002072000	-2.763065000	-1.761439000	1	5.264109000	0.832463000	1.155564000
6	-1.244871000	-2.447090000	-0.966066000	6	-0.003227000	-4.238028000	-2.167695000
6	-2.385940000	-3.209476000	-0.801364000	1	-0.002543000	-4.881796000	-1.282427000
7	-1.405459000	-1.219489000	-0.373736000	1	-0.892370000	-4.465111000	-2.766299000
6	-3.299677000	-2.408593000	-0.073441000	1	0.884320000	-4.466053000	-2.768293000
1	-2.548606000	-4.214624000	-1.170691000	6	-0.002526000	-1.910234000	-3.050112000
6	-2.674638000	-1.195427000	0.165373000	1	0.892877000	-2.121937000	-3.647858000
1	-4.302699000	-2.685731000	0.226136000	1	-0.898858000	-2.121089000	-3.646779000
6	1.242227000	-2.448465000	-0.967776000	1	-0.001934000	-0.844972000	-2.801334000
6	2.384267000	-3.210554000	-0.808626000	6	0.005445000	4.775419000	-1.211408000
7	1.403469000	-1.222686000	-0.371778000	1	0.004665000	5.219181000	-0.211004000
6	3.299314000	-2.411502000	-0.080361000	1	0.892365000	5.124577000	-1.750957000
1	2.546639000	-4.214399000	-1.181609000	1	-0.879610000	5.126126000	-1.753008000
6	2.673967000	-1.199678000	0.164280000	6	0.005265000	2.691735000	-2.570965000
1	4.303219000	-2.688976000	0.215869000	1	-0.890594000	3.026791000	-3.108446000
6	3.270430000	-0.001480000	0.887077000	1	0.902879000	3.025376000	-3.106397000
6	2.711792000	1.302533000	0.354801000	1	0.004415000	1.597333000	-2.557640000
6	3.386736000	2.502163000	0.214207000	6	-3.070151000	-0.074281000	2.417554000
7	1.396827000	1.462468000	-0.029028000	1	-3.664926000	0.712915000	2.899684000
6	2.456032000	3.440765000	-0.294667000	1	-3.403203000	-1.051187000	2.789945000
1	4.428477000	2.685705000	0.444877000	1	-2.026459000	0.067936000	2.694902000
6	1.256945000	2.768365000	-0.434768000	6	-4.791701000	-0.008126000	0.643949000
1	2.647615000	4.476498000	-0.546514000	1	-5.264203000	0.842198000	1.146856000
6	0.004041000	3.246474000	-1.125586000	1	-5.019902000	0.039933000	-0.424738000
6	-1.251221000	2.770536000	-0.437603000	1	-5.232839000	-0.920561000	1.058878000
6	-2.449737000	3.444679000	-0.300842000	12-IM1 (in THF solvent)			
7	-1.393703000	1.465292000	-0.030824000	8	-0.001057000	-0.238854000	1.922998000

6	5.769771000	0.275899000	-2.240710000	6	0.935800000	-0.248527000	2.706769000
6	3.589708000	1.754033000	-1.006242000	6	0.738352000	-1.465532000	1.838639000
6	4.834128000	1.042626000	1.024807000	6	1.265411000	-2.724681000	2.047460000
1	5.085008000	0.780607000	-2.925247000	7	-0.207960000	-1.507674000	0.841989000
1	6.473803000	1.013018000	-1.834272000	6	0.609087000	-3.591982000	1.144344000
1	6.338342000	-0.468165000	-2.809999000	1	2.024879000	-2.994245000	2.769566000
1	6.778047000	-0.695754000	0.133314000	6	-0.286731000	-2.824322000	0.425097000
1	6.359909000	-2.064559000	-0.929692000	1	0.779575000	-4.655006000	1.033117000
1	5.397169000	-1.753805000	0.527762000	13	-1.128679000	0.003966000	-0.000019000
1	3.140419000	1.445723000	-1.952929000	6	-0.621849000	-3.227403000	-2.063249000
1	4.376762000	2.494061000	-1.203191000	1	-0.581780000	-2.193958000	-2.395329000
1	2.808612000	2.213577000	-0.389950000	1	0.391178000	-3.645522000	-2.071991000
1	5.725748000	1.631859000	0.771850000	1	-1.251454000	-3.779550000	-2.773512000
1	5.132187000	0.211595000	1.669449000	6	-1.491652000	-4.821328000	-0.396895000
1	4.132855000	1.673695000	1.578976000	1	-1.911572000	-4.985095000	0.599387000
1	2.162317000	-2.173414000	-0.738643000	1	-2.184719000	-5.218570000	-1.145393000
6	-1.234591000	-3.324359000	-0.646743000	1	-0.556242000	-5.383995000	-0.484288000
6	-4.535725000	0.370885000	0.180204000	6	0.188487000	3.178020000	-1.904315000
6	-4.009467000	-0.952527000	-0.306909000	1	0.271921000	2.135035000	-2.194271000
6	-4.739187000	-2.066334000	-0.672126000	1	-0.372841000	3.707172000	-2.684984000
7	-2.666568000	-1.247780000	-0.265532000	1	1.198575000	3.600452000	-1.836373000
6	-3.804826000	-3.112946000	-0.857118000	6	-0.575739000	4.830102000	-0.249320000
1	-5.815660000	-2.126387000	-0.772737000	1	-1.074379000	5.025967000	0.703724000
6	-2.554541000	-2.586398000	-0.589377000	1	0.441541000	5.233625000	-0.208524000
1	-4.025670000	-4.134339000	-1.139569000	1	-1.108042000	5.363310000	-1.043379000
6	-3.734160000	1.521614000	-0.366078000	6	-6.008594000	0.526390000	-0.206089000
6	-4.202425000	2.723722000	-0.858094000	1	-6.128587000	0.506436000	-1.293939000
7	-2.365205000	1.553003000	-0.241351000	1	-6.601981000	-0.285628000	0.227374000
6	-3.068519000	3.552430000	-1.031353000	1	-6.400656000	1.475894000	0.174100000
1	-5.236879000	2.985088000	-1.042580000	6	-4.445646000	0.400153000	1.724472000
6	-1.967530000	2.817360000	-0.629108000	1	-4.825261000	1.354307000	2.110777000
1	-3.065179000	4.576713000	-1.382353000	1	-5.024681000	-0.426633000	2.154036000
6	-0.539285000	3.319445000	-0.549606000	1	-3.405950000	0.292704000	2.048142000
6	0.220755000	2.630032000	0.564673000	6	-0.225568000	-0.199855000	3.730877000
6	1.144713000	3.220932000	1.407073000	1	-1.184755000	-0.097921000	3.212410000
7	0.085497000	1.290867000	0.887508000	1	-0.252949000	-1.125481000	4.318777000
6	1.597232000	2.213655000	2.292071000	1	-0.106528000	0.659815000	4.402115000
1	1.458054000	4.256866000	1.395422000	6	2.251361000	-0.390742000	3.479476000
6	0.932299000	1.052946000	1.942878000	1	2.226625000	-1.288494000	4.106672000
1	2.307294000	2.332956000	3.100477000	1	3.083833000	-0.468435000	2.774797000

1	2.409475000	0.468838000	4.139171000	7	-2.435620000	1.511363000	-0.249300000
				6	-3.216226000	3.562187000	-0.811695000
12-TS2 (in THF solvent)							
8	-0.494712000	-0.076492000	-1.720427000	1	-5.372499000	2.950661000	-0.755751000
6	0.527643000	-0.021710000	-2.478988000	6	-2.081444000	2.815460000	-0.548752000
8	1.725246000	-0.109477000	-2.200019000	1	-3.249873000	4.610826000	-1.078239000
1	0.274201000	0.121880000	-3.544870000	6	-0.647722000	3.301765000	-0.613368000
5	2.850213000	-1.044692000	-0.899433000	6	0.188363000	2.628536000	0.459594000
8	3.995337000	-1.223137000	-1.700991000	6	1.146575000	3.240795000	1.249106000
8	3.109774000	-0.126494000	0.116404000	7	0.027250000	1.314660000	0.866744000
6	5.058581000	-0.477211000	-1.101539000	6	1.590079000	2.274893000	2.187359000
6	4.293520000	0.586511000	-0.252137000	1	1.475050000	4.269891000	1.179961000
6	5.859065000	-1.446891000	-0.229032000	6	0.886570000	1.115584000	1.921543000
6	5.952264000	0.097564000	-2.191489000	1	2.322699000	2.421244000	2.970663000
6	3.891052000	1.813912000	-1.072343000	6	0.867011000	-0.142256000	2.755706000
6	5.013998000	1.030946000	1.012588000	6	0.690801000	-1.395648000	1.934384000
1	5.375310000	0.682202000	-2.911696000	6	1.245223000	-2.638375000	2.177640000
1	6.731390000	0.738527000	-1.762705000	7	-0.239697000	-1.483370000	0.924984000
1	6.445132000	-0.716696000	-2.733601000	6	0.624345000	-3.542957000	1.280549000
1	6.739563000	-0.971381000	0.216580000	1	1.990824000	-2.877546000	2.924844000
1	6.194972000	-2.285699000	-0.847130000	6	-0.278443000	-2.810474000	0.529814000
1	5.230562000	-1.846561000	0.573728000	1	0.825934000	-4.602855000	1.192627000
1	3.437362000	1.517624000	-2.021315000	13	-1.150880000	-0.004020000	0.003363000
1	4.750929000	2.464001000	-1.271418000	6	-0.379438000	-3.305685000	-1.944726000
1	3.144504000	2.377629000	-0.502757000	1	-0.132680000	-2.288624000	-2.239072000
1	5.975776000	1.499753000	0.771998000	1	0.552556000	-3.877600000	-1.867458000
1	5.194133000	0.190636000	1.687844000	1	-0.997204000	-3.748175000	-2.736140000
1	4.395849000	1.764878000	1.539438000	6	-1.432034000	-4.832254000	-0.327842000
1	2.084878000	-1.946804000	-0.737531000	1	-1.967491000	-4.968736000	0.616623000
6	-1.139284000	-3.344032000	-0.599525000	1	-2.035967000	-5.258512000	-1.134648000
6	-4.576350000	0.243225000	0.150996000	1	-0.501394000	-5.406297000	-0.286559000
6	-3.983970000	-1.021205000	-0.415339000	6	-0.082450000	3.102127000	-2.039226000
6	-4.648112000	-2.120553000	-0.926021000	1	-0.304271000	2.106084000	-2.411080000
7	-2.641602000	-1.293712000	-0.283884000	1	-0.553715000	3.815915000	-2.726191000
6	-3.672290000	-3.134156000	-1.098409000	1	1.001948000	3.262705000	-2.057578000
1	-5.710594000	-2.199825000	-1.118746000	6	-0.620216000	4.820313000	-0.362688000
6	-2.462123000	-2.605473000	-0.680740000	1	-0.988435000	5.072582000	0.636001000
1	-3.845684000	-4.140063000	-1.459442000	1	0.400573000	5.202969000	-0.465026000
6	-3.811785000	1.460282000	-0.303363000	1	-1.233673000	5.341168000	-1.103410000
6	-4.325614000	2.694927000	-0.651649000	6	-6.048708000	0.363553000	-0.250133000
				1	-6.162462000	0.428460000	-1.337134000

1	-6.613568000	-0.503861000	0.106153000	1	-5.082985000	2.707629000	-0.747079000
1	-6.496523000	1.256127000	0.198137000	1	-2.604207000	-1.326437000	-1.926832000
6	-4.510300000	0.164234000	1.694668000	6	1.259510000	-3.202134000	-0.741328000
1	-4.933943000	1.069699000	2.145302000	6	1.846739000	-0.396604000	3.397394000
1	-5.066906000	-0.707302000	2.059992000	6	1.444344000	-1.584690000	2.563142000
1	-3.473875000	0.068873000	2.036370000	6	1.030515000	-2.839037000	2.968336000
6	-0.318967000	-0.040627000	3.745876000	7	1.539628000	-1.535018000	1.193126000
1	-1.268893000	0.047134000	3.206066000	6	0.871809000	-3.607285000	1.788777000
1	-0.371583000	-0.934253000	4.379847000	1	0.880399000	-3.169223000	3.988554000
1	-0.211206000	0.843974000	4.385127000	6	1.205712000	-2.790074000	0.722079000
6	2.159942000	-0.241791000	3.570556000	1	0.570932000	-4.645840000	1.730814000
1	2.134364000	-1.114601000	4.230957000	6	1.056689000	0.821922000	2.989127000
1	3.022474000	-0.326336000	2.902171000	6	0.485988000	1.785057000	3.796040000
1	2.287044000	0.641113000	4.204719000	7	0.909532000	1.162256000	1.663872000
				6	-0.036773000	2.775849000	2.929535000
				1	0.456522000	1.782422000	4.878495000
12-IM2 (in gas phase)				6	0.243499000	2.373375000	1.636028000
8	-0.513194000	-0.323624000	-0.342656000	1	-0.550666000	3.682090000	3.222533000
6	-1.264861000	-0.857863000	0.517306000	6	-0.111021000	3.115526000	0.359400000
8	-2.468304000	-1.186228000	0.332597000	6	0.965162000	2.937162000	-0.689799000
1	-0.865873000	-1.065896000	1.520127000	6	1.401413000	3.877114000	-1.602873000
5	-3.296547000	-0.950479000	-1.010896000	7	1.649040000	1.751665000	-0.880442000
8	-4.538361000	-1.690566000	-0.787577000	6	2.412764000	3.260501000	-2.379762000
8	-3.670551000	0.450974000	-1.078132000	1	1.041669000	4.893082000	-1.700105000
6	-5.610959000	-0.783311000	-0.881366000	6	2.542005000	1.970876000	-1.907473000
6	-4.949186000	0.576953000	-0.495536000	1	2.991543000	3.715897000	-3.173275000
6	-6.115111000	-0.773116000	-2.331870000	6	3.625738000	0.975715000	-2.235357000
6	-6.736281000	-1.231881000	0.047691000	6	3.108486000	-0.438475000	-2.294119000
6	-4.821364000	0.729953000	1.026733000	6	3.535810000	-1.459999000	-3.118302000
6	-5.625689000	1.815046000	-1.076152000	7	2.250378000	-0.929806000	-1.336577000
1	-6.361396000	-1.378837000	1.062988000	6	2.921039000	-2.644520000	-2.645177000
1	-7.551337000	-0.496801000	0.070972000	1	4.222638000	-1.371248000	-3.950421000
1	-7.143436000	-2.186199000	-0.304904000	6	2.152641000	-2.290173000	-1.552652000
1	-7.013171000	-0.155758000	-2.460871000	1	3.026052000	-3.637782000	-3.062162000
1	-6.349258000	-1.801987000	-2.623989000	13	1.299663000	0.071774000	0.057522000
1	-5.326055000	-0.399109000	-2.991050000	6	-0.147630000	-3.263163000	-1.382547000
1	-4.409542000	-0.180716000	1.468733000	1	-0.557249000	-2.268905000	-1.558020000
1	-5.787900000	0.953968000	1.496407000	1	-0.081602000	-3.768070000	-2.354289000
1	-4.128771000	1.550187000	1.237186000	1	-0.841325000	-3.818955000	-0.739564000
1	-6.667573000	1.897158000	-0.739755000	6	1.834469000	-4.631115000	-0.798138000
1	-5.603858000	1.791843000	-2.168394000				

6	3.040892000	-0.509970000	-2.336895000				
6	3.444738000	-1.557065000	-3.142163000				
7	2.200408000	-0.971589000	-1.346784000				
6	2.836521000	-2.727133000	-2.620492000				
1	4.113923000	-1.496069000	-3.990873000				
6	2.092285000	-2.339214000	-1.521459000				
1	2.928587000	-3.732039000	-3.011987000				
13	1.307602000	0.071045000	0.058076000				
6	-0.211929000	-3.279669000	-1.285916000				
1	-0.609691000	-2.282638000	-1.473085000				
1	-0.174142000	-3.806134000	-2.247143000				
1	-0.903473000	-3.815584000	-0.624272000				
6	1.757906000	-4.661958000	-0.703590000				
1	2.768209000	-4.710345000	-0.285610000				
1	1.112201000	-5.332500000	-0.128240000				
1	1.786103000	-5.042727000	-1.729241000				
6	-1.498896000	2.704600000	-0.143785000				
1	-1.552630000	1.655828000	-0.428397000				
1	-2.225399000	2.877736000	0.660130000				
1	-1.801349000	3.300140000	-1.014479000				
6	-0.174595000	4.645932000	0.607584000				
1	0.784051000	5.046200000	0.952363000				
1	-0.476940000	5.188492000	-0.293242000				
1	-0.931385000	4.847457000	1.372091000				
6	1.774652000	-0.585075000	4.879079000				
1	0.722859000	-0.752061000	5.133213000				
1	2.348279000	-1.467882000	5.180683000				
1	2.139032000	0.266755000	5.462176000				
6	3.449984000	-0.076000000	3.107963000				
1	3.807343000	0.784936000	3.684977000				
1	4.043743000	-0.956011000	3.382618000				
1	3.627247000	0.132088000	2.047269000				
6	4.651612000	1.019285000	-1.236346000				
1	4.244589000	0.775464000	-0.248412000				
1	5.474987000	0.324801000	-1.441079000				
1	5.049538000	2.040049000	-1.194303000				
6	4.211415000	1.239097000	-3.674479000				
1	5.028763000	0.542643000	-3.886062000				
1	3.487801000	1.183312000	-4.493781000				
1	4.636625000	2.247568000	-3.654060000				
				12-TS3 (in gas phase)			
				8	-0.957924000	0.215042000	-2.342957000
				6	-0.078380000	0.210901000	-3.186653000
				8	1.206760000	0.133113000	-3.014551000
				1	-0.342813000	0.283054000	-4.257812000
				5	1.825977000	-0.017484000	-1.631151000
				8	2.692202000	-1.176672000	-1.666621000
				8	2.657050000	1.116407000	-1.285897000
				6	3.821117000	-0.854318000	-0.880919000
				6	3.991064000	0.673002000	-1.166661000
				6	3.494245000	-1.127950000	0.588466000
				6	4.993055000	-1.722446000	-1.329355000
				6	4.700910000	0.926241000	-2.503907000
				6	4.669473000	1.456756000	-0.047812000
				1	5.136033000	-1.659059000	-2.411583000
				1	5.921872000	-1.421066000	-0.828125000
				1	4.786245000	-2.766768000	-1.072234000
				1	4.378102000	-1.032614000	1.233780000
				1	3.086460000	-2.140180000	0.678173000
				1	2.726332000	-0.433182000	0.943876000
				1	4.227534000	0.329525000	-3.290149000
				1	5.771305000	0.685774000	-2.463085000
				1	4.587427000	1.984636000	-2.760318000
				1	5.674108000	1.064107000	0.160864000
				1	4.061894000	1.420393000	0.860279000
				1	4.763179000	2.508074000	-0.343662000
				1	0.869385000	-0.120069000	-0.831757000
				6	-0.730852000	-3.267514000	-0.586633000
				6	-4.234217000	0.280339000	-0.030165000
				6	-3.596696000	-0.982107000	-0.549185000
				6	-4.227059000	-2.083315000	-1.091895000
				7	-2.269216000	-1.261822000	-0.315875000
				6	-3.246284000	-3.100731000	-1.194212000
				1	-5.274485000	-2.159669000	-1.355354000
				6	-2.069346000	-2.572280000	-0.701637000
				1	-3.391068000	-4.106283000	-1.568152000
				6	-3.411020000	1.503638000	-0.338039000
				6	-3.867189000	2.758622000	-0.686124000
				7	-2.055613000	1.539409000	-0.100889000

1	0.830570000	-0.141689000	-0.798835000	1	-0.311199000	-3.433357000	-2.694472000
6	-0.638300000	-3.284313000	-0.552508000	6	-0.825836000	-4.806850000	-0.461761000
6	-4.242424000	0.176317000	-0.037215000	1	-1.421051000	-5.089899000	0.411869000
6	-3.569295000	-1.075544000	-0.537868000	1	-1.325707000	-5.182442000	-1.360044000
6	-4.169583000	-2.202951000	-1.063260000	1	0.145860000	-5.306977000	-0.399760000
7	-2.230632000	-1.312866000	-0.311750000	6	0.437762000	3.178176000	-1.562212000
6	-3.159249000	-3.194675000	-1.155517000	1	0.541532000	2.135359000	-1.845307000
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6	-1.994717000	-2.624848000	-0.675498000	1	1.449827000	3.588025000	-1.477721000
1	-3.279604000	-4.210739000	-1.509140000	6	-0.371277000	4.834191000	0.079430000
6	-3.453166000	1.411039000	-0.388277000	1	-0.904671000	5.037173000	1.013158000
6	-3.941577000	2.640484000	-0.784626000	1	0.640799000	5.242672000	0.159814000
7	-2.099664000	1.494515000	-0.143313000	1	-0.870517000	5.373972000	-0.731244000
6	-2.840779000	3.534190000	-0.776806000	6	-5.662982000	0.275815000	-0.600003000
1	-4.971297000	2.879090000	-1.018812000	1	-5.657485000	0.339026000	-1.693021000
6	-1.735638000	2.808893000	-0.369701000	1	-6.251314000	-0.599228000	-0.306338000
1	-2.862269000	4.586462000	-1.029601000	1	-6.169568000	1.161535000	-0.203781000
6	-0.318919000	3.327640000	-0.228207000	6	-4.355202000	0.086516000	1.503261000
6	0.402634000	2.625384000	0.905517000	1	-4.843141000	0.982320000	1.905644000
6	1.338463000	3.178295000	1.761655000	1	-4.936876000	-0.796108000	1.795193000
7	0.179361000	1.306250000	1.249627000	1	-3.365057000	0.004511000	1.964371000
6	1.697990000	2.166003000	2.687827000	6	-0.562390000	-0.074236000	3.959825000
1	1.715041000	4.192787000	1.737865000	1	-1.408341000	0.009623000	3.269093000
6	0.961375000	1.043269000	2.354774000	1	-0.727477000	-0.954860000	4.591989000
1	2.376163000	2.265599000	3.526122000	1	-0.554099000	0.821910000	4.592063000
6	0.770184000	-0.205352000	3.183950000	6	1.899845000	-0.329615000	4.211258000
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7	0.008573000	-1.491973000	1.150719000	1	1.916214000	0.543080000	4.871707000
6	0.801727000	-3.563533000	1.586446000				
1	1.801123000	-2.969031000	3.503184000				
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6	0.201421000	-3.019884000	-1.816576000				
1	0.348664000	-1.956183000	-1.975105000				
1	1.192770000	-3.475707000	-1.727117000				