Supplementary information

Chiral Phosphoric Acid Catalyzed Intermolecular [4+2] Cycloaddition for Chiral Azomethine imines: Mechanism and Stereochemical Model

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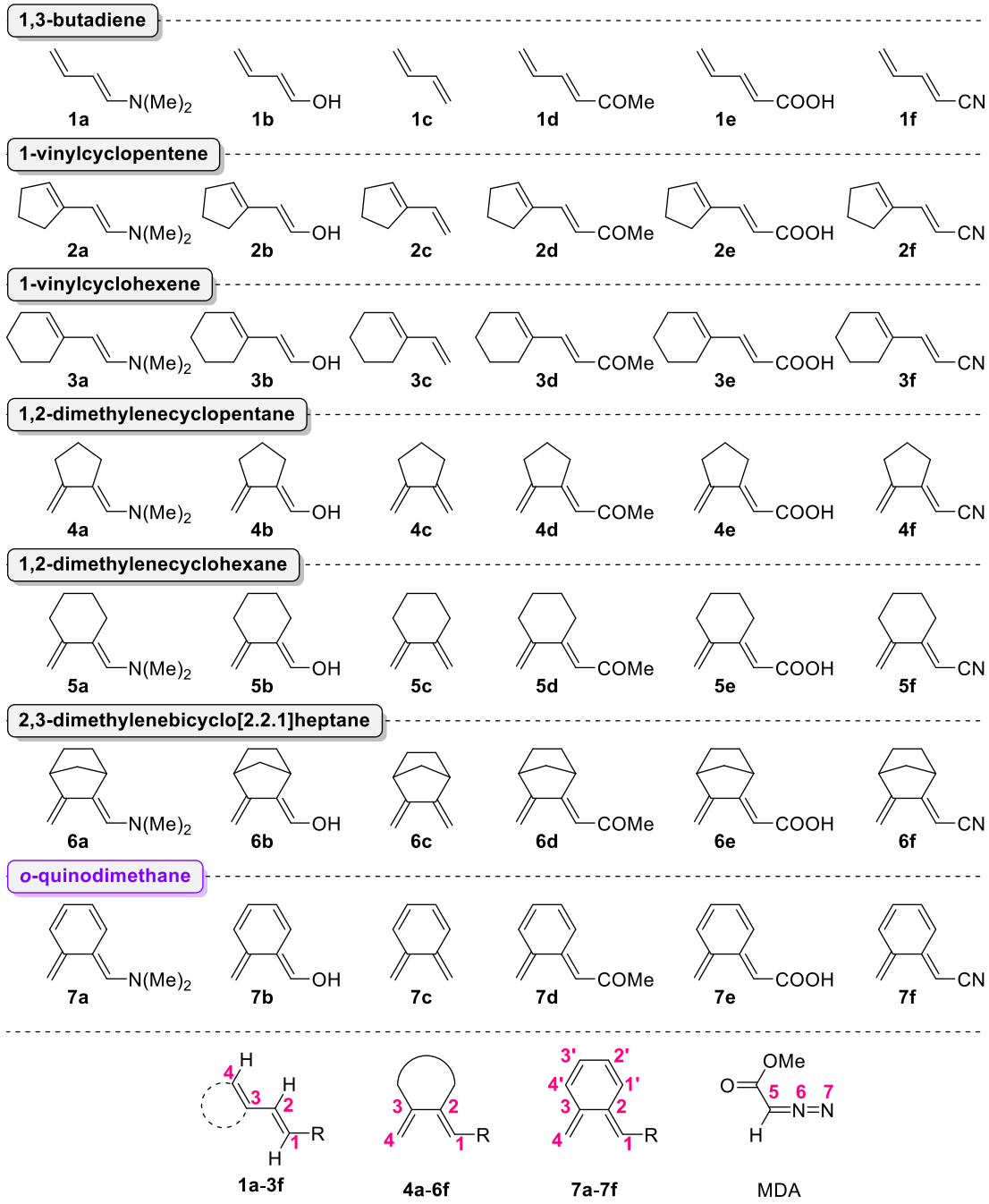
Table of Contents

1. Reactivity of (3+2) Cycloaddition Between Dienes 1a−7f and MDA.....3
2. Free Energy Profiles for (3+2) and [4+2] Cycloadditions.....5
3. Details in Nucleus-Independent Chemical Shifts (NICS).....7
4. Benchmark for Various Atomic Charges.....8
5. Activation Strain Model of Intermolecular (3+2) Cycloaddition.....15
6. Activation Strain and Compete Energy Decomposition Diagrams of (3+2) and [4+2] Cycloadditions.....16
7. Free Energy Profile of Light Excitation of 2-Methylbenzophenone to Afford Hydroxy-*o*-quinodimethane.....17
8. Equation of Calculation *ee* Values.....17
9. Buried Volumes of CPA Catalysts.....17
10. Space-Filling Models of Transition States for 7bb Enantiomers.....18
11. Possible transition states of CPA-catalyzed (3+2) and [4+2] cycloadditions.....19
12. Benchmark for Various DFT Methods.....21
13. Conformation Analysis of Possible (3+2) and [4+2] Cycloaddition Transition States.....22
14. Table of Energies.....37
15. Cartesian Coordinates of the Structures.....44
16. Refrences.....155

1. Reactivity of (3+2) Cycloaddition Between Dienes 1a−7f and MDA



Scheme S1. Schematic structures of dienes involved in (3+2) and [4+2] cycloadditions.

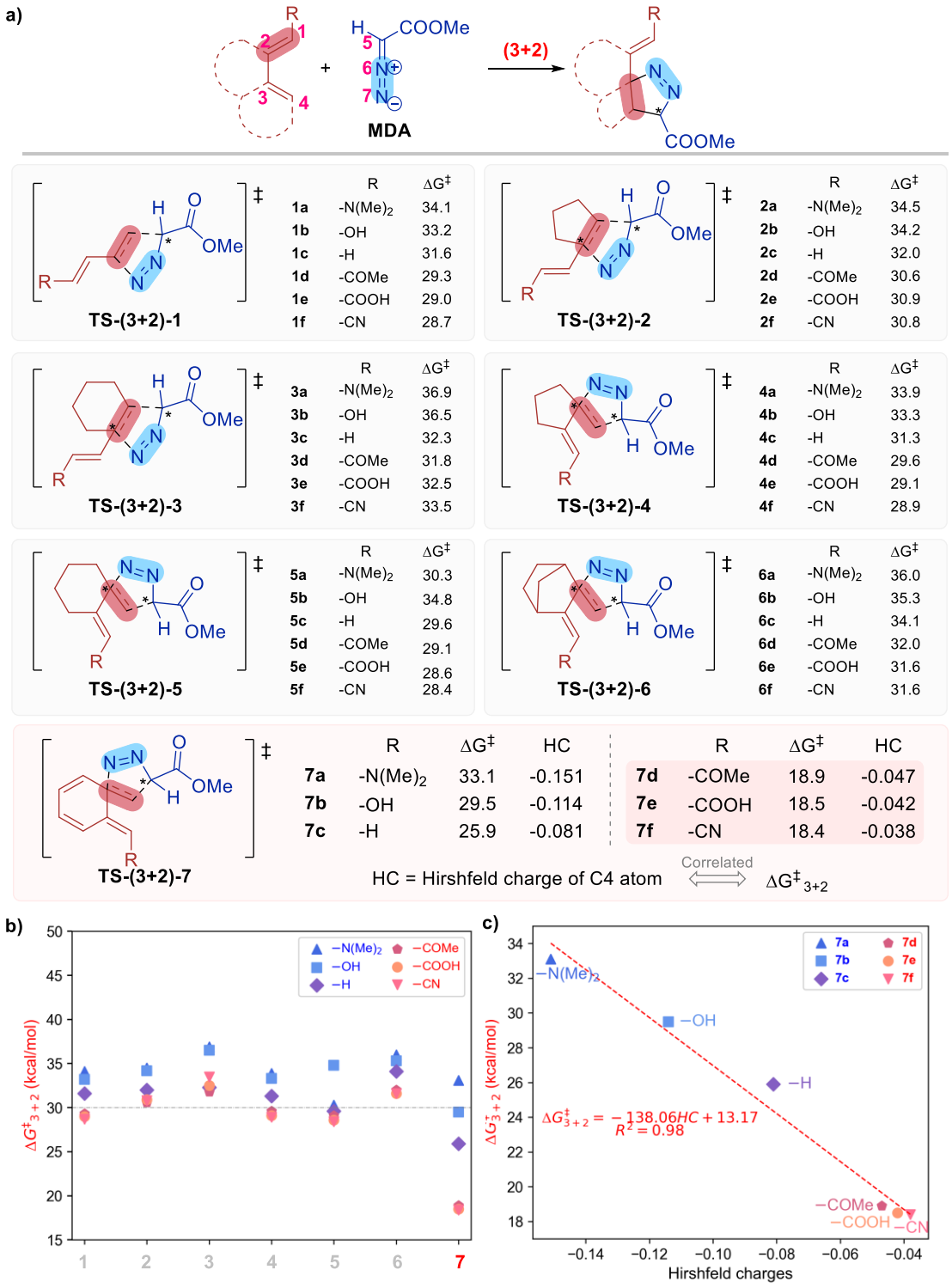


Figure S1. (a) Schematic structures of dienes involved in (3+2) cycloadditions and atom numbering. (b) Activation barriers for (3+2) cycloadditions between **MDA** and dienes. (c) Linear correlations between Hirshfeld charges on the C4 atom of dienes and activation barriers for (3+2) cycloadditions.

2. Free Energy Profiles for (3+2) and [4+2] Cycloadditions

Table S1. Free activation energies and reaction energies for (3+2) cycloadditions (energies in kcal/mol).

Free energy profile for (3+2) cycloaddition					
diene	$\Delta G^{\ddagger}$	ΔG_{rxn}	diene	$\Delta G^{\ddagger}$	ΔG_{rxn}
1a	34.1	−12.8	**2a**	34.5	−12.0
1b	33.2	−13.3	**2b**	34.2	−12.0
1c	31.6	−13.3	**2c**	32.0	−13.5
1d	29.3	−12.3	**2d**	30.6	−6.0
1e	29.0	−12.0	**2e**	30.9	−10.1
1f	28.7	−11.5	**2f**	30.8	−9.4
3a	36.9	−4.9	**4a**	33.9	−4.6
3b	36.5	−8.2	**4b**	33.3	−14.6
3c	32.3	−14.2	**4c**	31.3	−15.0
3d	31.8	−5.4	**4d**	29.6	−14.6
3e	32.5	−3.5	**4e**	29.1	−14.5
3f	33.5	−2.5	**4f**	28.9	−13.9
5a	30.3	−18.3	**6a**	36.0	−9.1
5b	34.8	−13.3	**6b**	35.3	−14.9
5c	29.6	−17.7	**6c**	34.1	−15.1
5d	29.1	−15.6	**6d**	32.0	−14.8
5e	28.6	−15.6	**6e**	31.6	−14.8
5f	28.4	−14.8	**6f**	31.6	−13.9
7a	33.1	−4.9			
7b	29.5	−8.6	7**ba**	31.0	−8.3
7c	25.9	−9.4			
7d	18.9	−8.0			
7e	18.5	−7.9			
7f	18.4	−7.5			

Table S2. Free activation energies and reaction energies for [4+2] cycloadditions. (energies in kcal/mol).

Free energy profile for [4+2] cycloaddition					
diene	$\Delta G^{\ddagger}$	ΔG_{rxn}	diene	$\Delta G^{\ddagger}$	ΔG_{rxn}
1a	29.2	15.6	**2a**	25.3	15.0
1b	35.8	11.0	**2b**	32.0	17.0
1c	39.9	6.1	**2c**	36.6	6.8
1d	42.3	18.1	**2d**	39.1	19.0
1e	42.9	19.2	**2e**	40.0	20.3
1f	43.0	20.9	**2f**	40.2	21.9
3a	28.1	12.9	**4a**	23.2	6.9
3b	34.9	10.2	**4b**	31.0	9.0
3c	39.6	8.1	**4c**	35.8	4.3
3d	43.1	20.4	**4d**	38.2	18.4
3e	44.0	17.3	**4e**	39.0	13.4
3f	44.4	20.7	**4f**	39.5	19.3
5a	22.6	1.5	**6a**	23.9	15.0
5b	31.6	5.0	**6b**	31.6	13.7
5c	33.3	−2.1	**6c**	36.6	10.7
5d	37.1	11.0	**6d**	38.7	22.4
5e	38.0	11.4	**6e**	39.7	19.8
5f	37.4	14.5	**6f**	40.5	26.0
7a	17.7	−13.8			
7b	22.4	−17.6	**7ba**	23.7	−16.5
7c	25.6	−23.2			
7d	28.1	−10.8			
7e	29.1	−9.6			
7f	29.0	−.67			

3. Details in Nucleus-Independent Chemical Shifts (NICS)

All the density functional theory (DFT) calculations (at 298K) were carried out by using the Gaussian 16 package[1]. Nucleus-independent chemical shifts (NMR=GIAO) calculations, performed at the M06-2X/6-311+G(d,p)//M06-2X/6-31G(d,p) level of theory. Each six-member (C2-C1'-C2'-C3'-C4'-C3) in **7a−7f** is denoted as ring A. Since ring A is a twisted ring, we first need to calculate the most representative plane based on the cartesian coordination using the least square method. Then coordinates of the points below and above 1 Angstrom of the plane can be obtained for the NMR jobs. Subsequently, with the aid of a powerful tool Multiwfn 3.8 program[2], we attain the values of NICS(+1)zz (above the plane) and NICS(−1)zz (below the plane), and take the average values of NICS(+1)zz and NICS(−1)zz to afford the final NICS(1)zz value.

Table S3. NICS values of ring A in ground states, transition state, and cycloadduct.

	ground state	TS-[4+2]	[4+2]-product
7a	−0.3	−16.1	−29.4
7b	3.0	−17.6	−30.0
7c	3.6	−17.0	−29.8
7d	1.8	−17.7	−29.9
7e	1.9	−18.5	−30.0
7f	2.2	−17.0	−29.9

4. Benchmark for Various Atomic Charges

Table S4. ADCH charges of C1-C4 atoms

dienes	ADCH charges				dienes	ADCH charges			
	C1	C2	C3	C4		C1	C2	C3	C4
1a	0.001	−0.113	−0.060	−0.133	**2a**	−0.006	−0.114	−0.029	−0.079
1b	0.042	−0.096	−0.052	−0.115	**2b**	0.034	−0.099	−0.024	−0.068
1c	−0.089	−0.049	−0.049	−0.089	**2c**	−0.098	−0.053	−0.023	−0.048
1d	−0.064	−0.014	−0.043	−0.062	**2d**	−0.072	−0.017	−0.019	−0.025
1e	−0.063	−0.006	−0.041	−0.057	**2e**	−0.072	−0.010	−0.017	−0.021
1f	−0.025	0.007	−0.038	−0.052	**2f**	−0.034	0.002	−0.016	−0.017
3a	−0.012	−0.113	−0.028	−0.072	**4a**	−0.006	−0.054	−0.015	−0.139
3b	0.027	−0.100	−0.023	−0.063	**4b**	0.029	−0.059	−0.012	−0.129
3c	−0.105	−0.054	−0.022	−0.045	**4c**	−0.106	−0.011	−0.011	−0.106
3d	−0.077	−0.018	−0.018	−0.023	**4d**	−0.077	0.028	−0.007	−0.085
3e	−0.077	−0.011	−0.016	−0.019	**4e**	−0.078	0.033	−0.006	−0.080
3f	−0.039	0.001	−0.015	−0.016	**4f**	−0.043	0.037	−0.005	−0.074
5a	−0.012	−0.026	−0.006	−0.118	**6a**	−0.008	−0.048	−0.013	−0.134
5b	0.022	−0.050	−0.006	−0.118	**6b**	0.028	−0.056	−0.010	−0.127
5c	−0.108	−0.002	−0.002	−0.108	**6c**	−0.106	−0.010	−0.010	−0.106
5d	−0.078	0.036	0.001	−0.090	**6d**	−0.077	0.026	−0.007	−0.086
5e	−0.079	0.041	0.002	−0.086	**6e**	−0.078	0.032	−0.006	−0.081
5f	−0.044	0.044	0.003	−0.081	**6f**	−0.042	0.036	−0.004	−0.075
7a	0.030	−0.067	−0.026	−0.151					
7b	0.058	−0.053	−0.016	−0.114					
7c	−0.081	−0.014	−0.014	−0.081					
7d	−0.069	0.018	−0.008	−0.047					
7e	−0.072	0.022	−0.006	−0.042					
7f	−0.037	0.027	−0.005	−0.038					

Table S5. Chelpg charges of C1-C4 atoms

dienes	Chelpg charge				dienes	Chelpg charge			
	C1	C2	C3	C4		C1	C2	C3	C4
1a	0.009	−0.285	−0.069	−0.437	**2a**	0.061	−0.377	−0.005	−0.364
1b	0.126	−0.342	0.005	−0.451	**2b**	0.182	−0.444	0.048	−0.329
1c	−0.438	−0.033	−0.025	−0.447	**2c**	−0.385	−0.131	0.015	−0.365
1d	−0.469	0.071	−0.083	−0.376	**2d**	−0.388	−0.054	−0.032	−0.284
1e	−0.429	0.022	−0.058	−0.364	**2e**	−0.360	−0.079	−0.004	−0.282
1f	−0.401	0.068	−0.095	−0.333	**2f**	−0.316	−0.068	−0.016	−0.274
3a	0.056	−0.351	−0.029	−0.334	**4a**	0.018	−0.236	0.098	−0.592
3b	0.181	−0.443	0.082	−0.353	**4b**	0.075	−0.236	0.077	−0.589
3c	−0.402	−0.107	0.016	−0.343	**4c**	−0.536	0.095	0.091	−0.532
3d	−0.393	−0.030	−0.038	−0.267	**4d**	−0.566	0.198	0.043	−0.482
3e	−0.356	−0.078	−0.000	−0.281	**4e**	−0.539	0.171	0.050	−0.474
3f	−0.314	−0.067	−0.006	−0.281	**4f**	−0.458	0.145	0.067	−0.483
5a	0.054	−0.222	0.136	−0.541	**6a**	0.047	−0.273	0.161	−0.623
5b	0.082	−0.244	0.098	−0.528	**6b**	0.086	−0.242	0.125	−0.574
5c	−0.491	0.092	0.112	−0.511	**6c**	−0.542	0.124	0.111	−0.542
5d	−0.561	0.220	0.065	−0.462	**6d**	−0.568	0.193	0.076	−0.498
5e	−0.524	0.183	0.070	−0.444	**6e**	−0.535	0.168	0.094	−0.493
5f	−0.472	0.173	0.031	−0.428	**6f**	−0.466	0.181	0.068	−0.459
7a	−0.164	−0.028	0.323	−0.713					
7b	0.046	−0.036	0.256	−0.642					
7c	−0.548	0.236	0.216	−0.548					
7d	−0.620	0.348	0.147	−0.453					
7e	−0.593	0.320	0.157	−0.445					
7f	−0.574	0.356	0.140	−0.435					

Table S6. Hirshfeld charges of C1-C4 atoms

dienes	Hirshfeld charges				dienes	Hirshfeld charges			
	C1	C2	C3	C4		C1	C2	C3	C4
1a	0.001	−0.113	−0.060	−0.133	**2a**	−0.006	−0.114	−0.029	−0.079
1b	0.042	−0.096	−0.052	−0.115	**2b**	0.034	−0.099	−0.024	−0.068
1c	−0.089	−0.049	−0.049	−0.089	**2c**	−0.098	−0.053	−0.023	−0.048
1d	−0.064	−0.014	−0.043	−0.062	**2d**	−0.072	−0.017	−0.019	−0.025
1e	−0.063	−0.006	−0.041	−0.057	**2e**	−0.072	−0.010	−0.017	−0.021
1f	−0.025	0.007	−0.038	−0.052	**2f**	−0.034	0.002	−0.016	−0.017
3a	−0.012	−0.113	−0.028	−0.072	**4a**	−0.006	−0.054	−0.015	−0.139
3b	0.027	−0.100	−0.023	−0.063	**4b**	0.029	−0.059	−0.012	−0.129
3c	−0.105	−0.054	−0.022	−0.045	**4c**	−0.106	−0.011	−0.011	−0.106
3d	−0.077	−0.018	−0.018	−0.023	**4d**	−0.077	0.028	−0.007	−0.085
3e	−0.077	−0.011	−0.016	−0.019	**4e**	−0.078	0.033	−0.006	−0.080
3f	−0.039	0.001	−0.015	−0.016	**4f**	−0.043	0.037	−0.005	−0.074
5a	−0.012	−0.026	−0.006	−0.118	**6a**	−0.008	−0.048	−0.013	−0.134
5b	0.022	−0.050	−0.006	−0.118	**6b**	0.028	−0.056	−0.010	−0.127
5c	−0.108	−0.002	−0.002	−0.108	**6c**	−0.106	−0.010	−0.010	−0.106
5d	−0.078	0.036	0.001	−0.090	**6d**	−0.077	0.026	−0.007	−0.086
5e	−0.079	0.041	0.002	−0.086	**6e**	−0.078	0.032	−0.006	−0.081
5f	−0.044	0.044	0.003	−0.081	**6f**	−0.042	0.036	−0.004	−0.075
7a	0.030	−0.067	−0.026	−0.151					
7b	0.058	−0.053	−0.016	−0.114					
7c	−0.081	−0.014	−0.014	−0.081					
7d	−0.069	0.018	−0.008	−0.047					
7e	−0.072	0.022	−0.006	−0.042					
7f	−0.037	0.027	−0.005	−0.038					

Table S7. NPA charges of C1-C4 atoms

dienes	NPA charges				dienes	NPA charges			
	C1	C2	C3	C4		C1	C2	C3	C4
1a	0.067	−0.381	−0.212	−0.452	**2a**	0.053	−0.363	−0.047	−0.232
1b	0.199	−0.376	−0.219	−0.424	**2b**	0.187	−0.361	−0.054	−0.212
1c	−0.377	−0.240	−0.240	−0.377	**2c**	−0.394	−0.224	−0.076	−0.172
1d	−0.320	−0.138	−0.253	−0.330	**2d**	−0.335	−0.122	−0.091	−0.125
1e	−0.335	−0.131	−0.257	−0.323	**2e**	−0.351	−0.115	−0.095	−0.120
1f	−0.348	−0.116	−0.260	−0.317	**2f**	−0.364	−0.101	−0.098	−0.113
3a	0.039	−0.349	−0.051	−0.217	**4a**	0.055	−0.142	−0.022	−0.449
3b	0.173	−0.351	−0.058	−0.200	**4b**	0.195	−0.187	−0.024	−0.431
3c	−0.409	−0.215	−0.080	−0.163	**4c**	−0.389	−0.049	−0.049	−0.389
3d	−0.350	−0.112	−0.093	−0.119	**4d**	−0.336	0.071	−0.060	−0.355
3e	−0.365	−0.106	−0.096	−0.114	**4e**	−0.352	0.076	−0.063	−0.347
3f	−0.378	−0.093	−0.099	−0.108	**4f**	−0.368	0.082	−0.068	−0.336
5a	0.021	−0.084	−0.025	−0.414	**6a**	0.048	−0.130	−0.020	−0.443
5b	0.181	−0.178	−0.020	−0.419	**6b**	0.193	−0.183	−0.018	−0.432
5c	−0.399	−0.040	−0.040	−0.399	**6c**	−0.392	−0.045	−0.045	−0.392
5d	−0.343	0.079	−0.051	−0.370	**6d**	−0.339	0.072	−0.055	−0.358
5e	−0.359	0.084	−0.054	−0.364	**6e**	−0.355	0.078	−0.058	−0.351
5f	−0.374	0.090	−0.060	−0.354	**6f**	−0.369	0.083	−0.064	−0.340
7a	0.134	−0.231	−0.065	−0.477					
7b	0.234	−0.207	−0.075	−0.404					
7c	−0.341	−0.100	−0.100	−0.341					
7d	−0.309	0.006	−0.111	−0.284					
7e	−0.329	0.012	−0.114	−0.276					
7f	−0.344	0.020	−0.118	−0.269					

Table S8. VDD charges of C1-C4 atoms

dienes	VDD charge				dienes	VDD charge			
	C1	C2	C3	C4		C1	C2	C3	C4
1a	0.008	−0.133	−0.055	−0.114	**2a**	−0.000	−0.132	−0.041	−0.091
1b	0.043	−0.125	−0.052	−0.099	**2b**	0.035	−0.122	−0.038	−0.080
1c	−0.077	−0.058	−0.058	−0.077	**2c**	−0.084	−0.057	−0.044	−0.061
1d	−0.095	−0.020	−0.058	−0.059	**2d**	−0.101	−0.019	−0.044	−0.039
1e	−0.092	−0.011	−0.058	−0.054	**2e**	−0.098	−0.011	−0.046	−0.035
1f	−0.065	−0.004	−0.057	−0.051	**2f**	−0.071	−0.007	−0.045	−0.032
3a	−0.008	−0.133	−0.044	−0.082	**4a**	−0.002	−0.089	−0.022	−0.123
3b	0.025	−0.123	−0.042	−0.074	**4b**	0.028	−0.096	−0.021	−0.118
3c	−0.094	−0.059	−0.048	−0.056	**4c**	−0.098	−0.024	−0.024	−0.098
3d	−0.109	−0.019	−0.045	−0.035	**4d**	−0.109	0.022	−0.028	−0.080
3e	−0.106	−0.012	−0.046	−0.031	**4e**	−0.106	0.031	−0.028	−0.079
3f	−0.081	−0.005	−0.047	−0.026	**4f**	−0.080	0.029	−0.029	−0.073
5a	−0.013	−0.054	−0.026	−0.108	**6a**	−0.006	−0.079	−0.020	−0.119
5b	0.023	−0.092	−0.019	−0.103	**6b**	0.024	−0.094	−0.017	−0.115
5c	−0.098	−0.021	−0.020	−0.098	**6c**	−0.098	−0.020	−0.020	−0.098
5d	−0.108	0.024	−0.021	−0.083	**6d**	−0.110	0.022	−0.026	−0.082
5e	−0.108	0.033	−0.021	−0.079	**6e**	−0.109	0.030	−0.023	−0.079
5f	−0.083	0.034	−0.021	−0.076	**6f**	−0.081	0.033	−0.024	−0.076
7a	0.035	−0.103	−0.021	−0.125					
7b	0.057	−0.079	−0.017	−0.100					
7c	−0.073	−0.020	−0.020	−0.073					
7d	−0.096	0.018	−0.019	−0.044					
7e	−0.096	0.027	−0.018	−0.041					
7f	−0.071	0.029	−0.016	−0.038					

Table S9. Benchmark for linear correlations between various atomic charges of C4 atm of dienes and activation barriers for (3+2) cycloaddition.

CHG	dienes	Linear regression equation	R^2	CHG	dienes	Linear regression equation	R^2
ADCH	**1a–1f**	$\Delta G^{\ddagger}_{3+2} = -75.48CHG + 11.99$	1.00	NPA	**1a–1f**	$\Delta G^{\ddagger}_{3+2} = -40.55CHG + 15.96$	0.99
	2a–2f	$\Delta G^{\ddagger}_{3+2} = -72.06CHG + 19.06$	0.74		**2a–2f**	$\Delta G^{\ddagger}_{3+2} = -33.87CHG + 26.67$	0.96
	3a–3f	$\Delta G^{\ddagger}_{3+2} = -18.41CHG + 31.65$	0.01		**3a–3f**	$\Delta G^{\ddagger}_{3+2} = -39.81CHG + 27.81$	0.71
	4a–4f	$\Delta G^{\ddagger}_{3+2} = -27.13CHG + 26.48$	0.71		**4a–4f**	$\Delta G^{\ddagger}_{3+2} = -46.46CHG + 13.15$	1.00
	5a–5f	$\Delta G^{\ddagger}_{3+2} = -12.97CHG + 29.89$	0.64		**5a–5f**	$\Delta G^{\ddagger}_{3+2} = -67.70CHG + 3.96$	0.61
	6a–6f	$\Delta G^{\ddagger}_{3+2} = -8.06CHG + 32.17$	0.55		**6a–6f**	$\Delta G^{\ddagger}_{3+2} = -44.59CHG + 16.22$	0.98
	7a–7f	$\Delta G^{\ddagger}_{3+2} = -66.84CHG + 12.41$	0.89		**7a–7f**	$\Delta G^{\ddagger}_{3+2} = -75.04CHG - 1.60$	0.97
ChelpG	**1a–1f**	$\Delta G^{\ddagger}_{3+2} = -41.67CHG + 14.26$	0.81	VDD	**1a–1f**	$\Delta G^{\ddagger}_{3+2} = -88.80CHG + 24.26$	0.98
	2a–2f	$\Delta G^{\ddagger}_{3+2} = -31.85CHG + 22.09$	0.58		**2a–2f**	$\Delta G^{\ddagger}_{3+2} = -68.87CHG + 28.29$	0.96
	3a–3f	$\Delta G^{\ddagger}_{3+2} = -66.84CHG + 12.4$	0.43		**3a–3f**	$\Delta G^{\ddagger}_{3+2} = -77.43CHG + 29.99$	0.71
	4a–4f	$\Delta G^{\ddagger}_{3+2} = -66.84CHG + 12.4$	0.98		**4a–4f**	$\Delta G^{\ddagger}_{3+2} = -101.71CHG + 21.34$	1.00
	5a–5f	$\Delta G^{\ddagger}_{3+2} = -34.32CHG + 13.46$	0.46		**5a–5f**	$\Delta G^{\ddagger}_{3+2} = -117.80CHG + 19.39$	0.45
	6a–6f	$\Delta G^{\ddagger}_{3+2} = -31.55CHG + 16.66$	0.94		**6a–6f**	$\Delta G^{\ddagger}_{3+2} = -103.76CHG + 23.59$	0.99
	7a–7f	$\Delta G^{\ddagger}_{3+2} = -54.47CHG - 5.32$	0.99		**7a–7f**	$\Delta G^{\ddagger}_{3+2} = -176.44CHG + 11.67$	0.99
Hirshfeld	**1a–1f**	$\Delta G^{\ddagger}_{3+2} = -69.05CHG + 25.14$	0.99				
	2a–2f	$\Delta G^{\ddagger}_{3+2} = -65.77CHG + 29.34$	0.96				
	3a–3f	$\Delta G^{\ddagger}_{3+2} = -77.18CHG + 30.86$	0.69				
	4a–4f	$\Delta G^{\ddagger}_{3+2} = -80.36CHG + 22.81$	1.00				
	5a–5f	$\Delta G^{\ddagger}_{3+2} = -107.73CHG + 8.68$	0.56				
	6a–6f	$\Delta G^{\ddagger}_{3+2} = -78.46CHG + 25.47$	0.99				
	7a–7f	$\Delta G^{\ddagger}_{3+2} = -138.06CHG + 13.17$	0.98				

Table S10. Benchmark for linear correlations between various atomic charges of C4 atm of dienes and activation barriers for (3+2) cycloaddition.

CHG	dienes	Linear regression equation	R^2	CHG	dienes	Linear regression equation	R^2
ADCH	**1a–1f**	$\Delta G^{\ddagger}_{4+2}$ = 167.83CHG + 81.09	0.89	NPA	**1a–1f**	$\Delta G^{\ddagger}_{4+2}$ = 91.81CHG + 72.86	0.92
	2a–2f	$\Delta G^{\ddagger}_{4+2}$ = 198.61CHG + 71.10	0.49		**2a–2f**	$\Delta G^{\ddagger}_{4+2}$ = 109.76CHG + 53.35	0.91
	3a–3f	$\Delta G^{\ddagger}_{4+2}$ = 45.47CHG + 44.62	0.01		**3a–3f**	$\Delta G^{\ddagger}_{4+2}$ = 131.62CHG + 59.22	0.93
	4a–4f	$\Delta G^{\ddagger}_{4+2}$ = 80.88CHG + 47.98	0.75		**4a–4f**	$\Delta G^{\ddagger}_{4+2}$ = 128.16CHG + 83.73	0.90
	5a–5f	$\Delta G^{\ddagger}_{4+2}$ = 28.05CHG + 33.86	0.50		**5a–5f**	$\Delta G^{\ddagger}_{4+2}$ = 171.23CHG + 99.54	0.65
	6a–6f	$\Delta G^{\ddagger}_{4+2}$ = 21.25CHG + 38.49	0.36		**6a–6f**	$\Delta G^{\ddagger}_{4+2}$ = 136.53CHG + 87.87	0.87
	7a–7f	$\Delta G^{\ddagger}_{4+2}$ = 49.59CHG + 33.95	0.98		**7a–7f**	$\Delta G^{\ddagger}_{4+2}$ = 167.83CHG + 43.71	0.99
Chelpg	**1a–1f**	$\Delta G^{\ddagger}_{4+2}$ = 77.41CHG + 69.92	0.50	VDD	**1a–1f**	$\Delta G^{\ddagger}_{4+2}$ = 203.87CHG + 54.28	0.94
	2a–2f	$\Delta G^{\ddagger}_{4+2}$ = 107.39CHG + 69.50	0.59		**2a–2f**	$\Delta G^{\ddagger}_{4+2}$ = 224.85CHG + 48.20	0.92
	3a–3f	$\Delta G^{\ddagger}_{4+2}$ = 127.18CHG + 78.42	0.55		**3a–3f**	$\Delta G^{\ddagger}_{4+2}$ = 261.07CHG + 52.24	0.92
	4a–4f	$\Delta G^{\ddagger}_{4+2}$ = 105.78CHG + 90.02	0.83		**4a–4f**	$\Delta G^{\ddagger}_{4+2}$ = 275.69CHG + 60.69	0.87
	5a–5f	$\Delta G^{\ddagger}_{4+2}$ = 106.70CHG + 85.15	0.74		**5a–5f**	$\Delta G^{\ddagger}_{4+2}$ = 383.28CHG + 68.28	0.79
	6a–6f	$\Delta G^{\ddagger}_{4+2}$ = 101.77CHG + 89.26	0.93		**6a–6f**	$\Delta G^{\ddagger}_{4+2}$ = 314.67CHG + 65.01	0.86
	7a–7f	$\Delta G^{\ddagger}_{4+2}$ = 38.25CHG + 45.94	0.97		**7a–7f**	$\Delta G^{\ddagger}_{4+2}$ = 124.41CHG + 34.05	0.98
Hirshfeld	**1a–1f**	$\Delta G^{\ddagger}_{4+2}$ = 156.58CHG + 52.11	0.92				
	2a–2f	$\Delta G^{\ddagger}_{4+2}$ = 214.34CHG + 44.75	0.91				
	3a–3f	$\Delta G^{\ddagger}_{4+2}$ = 258.163CHG + 49.28	0.93				
	4a–4f	$\Delta G^{\ddagger}_{4+2}$ = 220.45CHG + 56.97	0.89				
	5a–5f	$\Delta G^{\ddagger}_{4+2}$ = 295.82CHG + 62.97	0.70				
	6a–6f	$\Delta G^{\ddagger}_{4+2}$ = 239.42CHG + 59.47	0.87				
	7a–7f	$\Delta G^{\ddagger}_{4+2}$ = 98.22CHG + 33.06	0.99				

To compare the performance of predicting cycloaddition reactivity with atomic charge, various population analysis approaches to calculate atomic charges have been employed, including atomic dipole moment corrected Hirshfeld atomic charges (ADCH)[3], Chelpg ESP fitting[4], Hirshfeld, natural population analysis (NPA)[5] and Voronoi deformation density (VDD)[6]. The atomic charges are obtained from Multiwfn at the M06-2X/6-311+G(d,p)-SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level of theory. As shown in Tables S4 and S5, the Hirshfeld and NPA charges have good and consistent performance in predicting (3+2) and [4+2] cycloaddition reactivity, and here we chose the Hirshfeld charge.

5. Activation Strain Model of Intermolecular (3+2) Cycloaddition

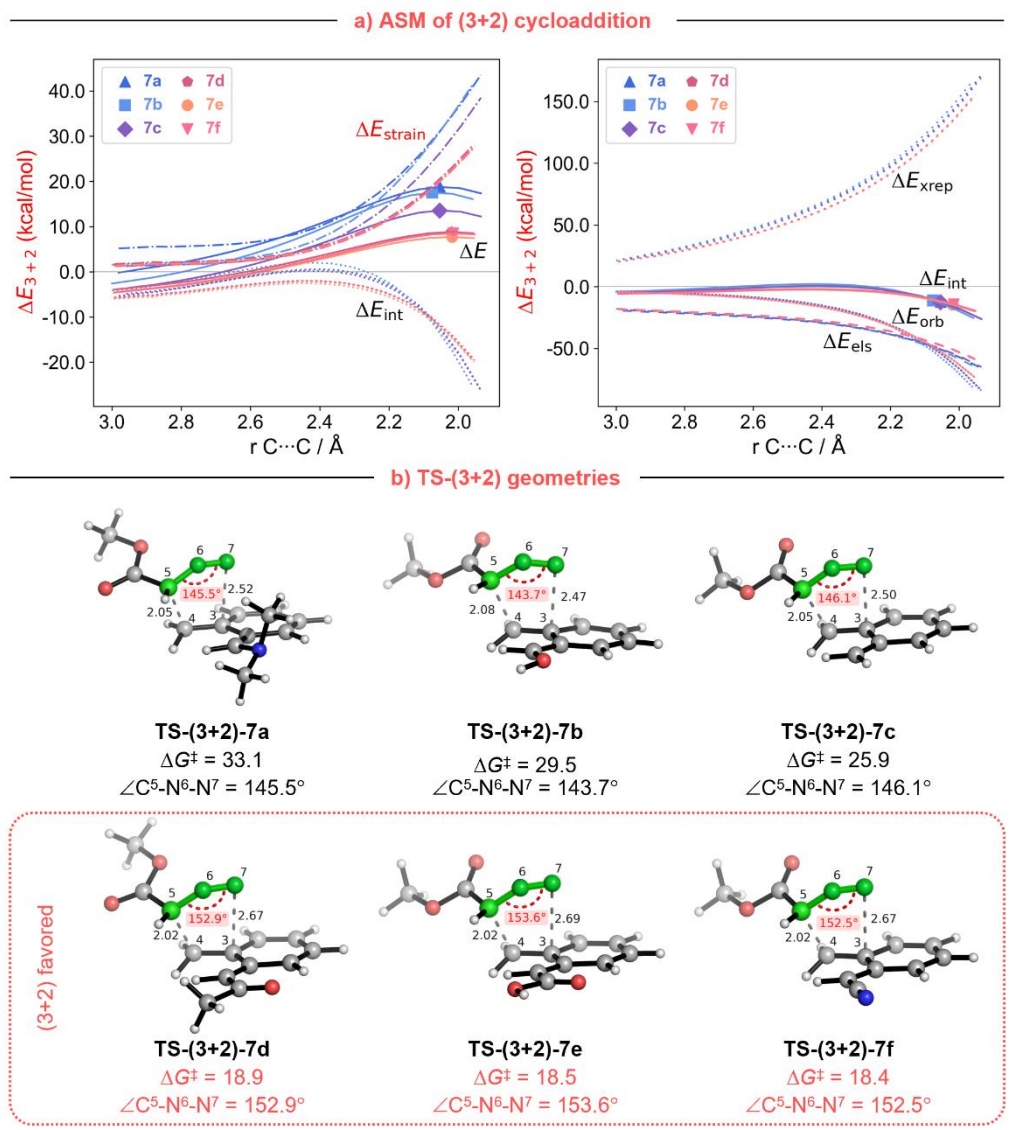


Figure S2. (a) Activation strain analysis and energy decomposition analysis of [4+2] cycloaddition between **MDA** and dienes (**7a**–**7f**) along the reaction coordinate projected onto the N···C bond stretch. (b) Transition geometries and free energy of activation ($\Delta G^{\ddagger}_{298}$) (in kcal/mol) for (4+2) cycloadditions between **MDA** and dienes (**7a**–**7f**). Bond lengths in Å.

6. Activation Strain and Compete Energy Decomposition Diagrams of (3+2) and [4+2] Cycloadditions

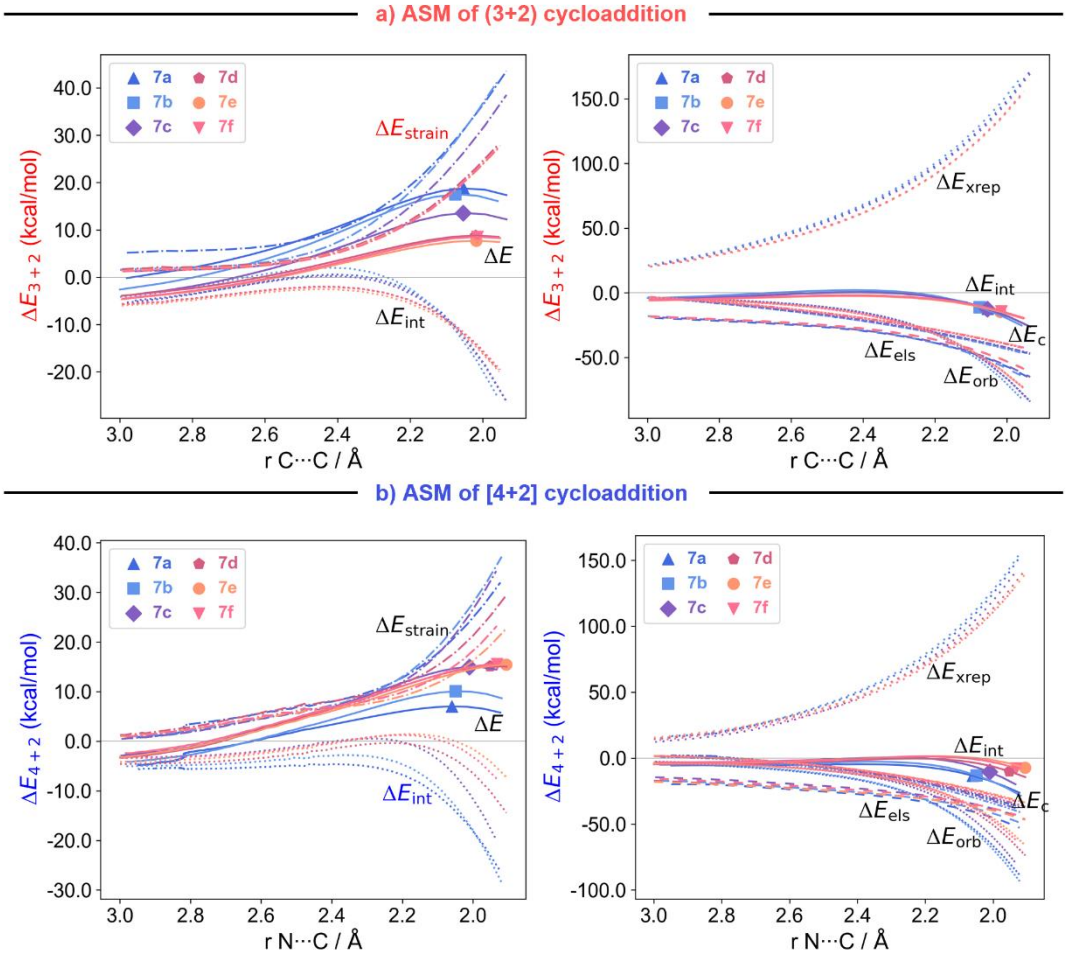


Figure S3. (a) Activation strain analysis and energy decomposition analysis of (3+2) cycloaddition between **MDA** and dienes (**7a**−**7f**) along the reaction coordinate projected onto the C···C bond stretch. (b) Activation strain analysis and energy decomposition analysis of [4+2] cycloaddition between **MDA** and dienes (**7a**−**7f**) along the reaction coordinate projected onto the N···C bond stretch.

7. Free Energy Profile of Light Excitation of 2-Methylbenzophenone to Afford Hydroxy-*o*-quinodimethane

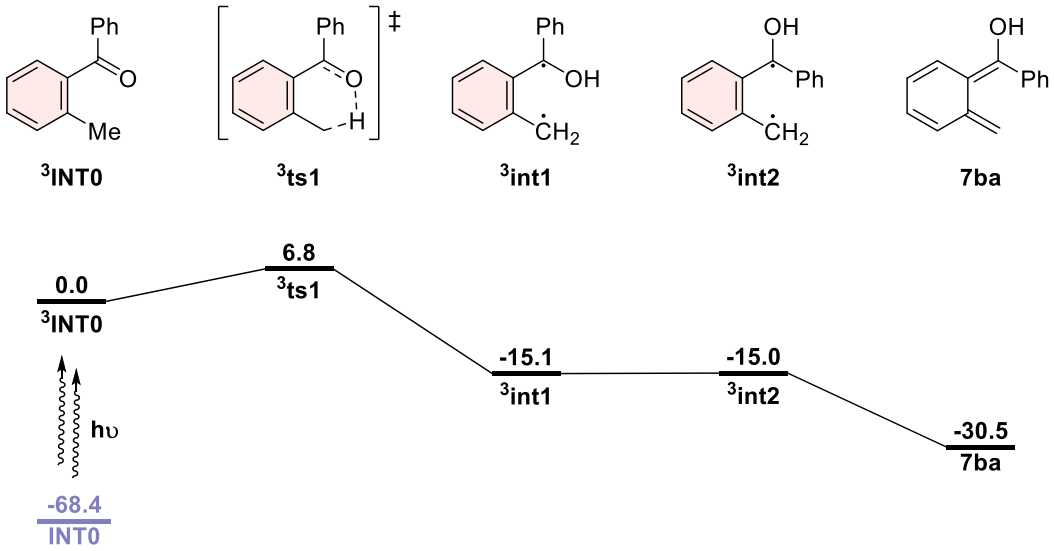


Figure S4. Free energy profile (ΔG in kcal/mol) of light excitation of 2-methylbenzophenone. Computed at M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p).

8. Equation of Calculation *ee* Values

The enantiomeric excess (*ee* %) can be computed using the following equation, where $\Delta G^{\ddagger}$ is the difference in the Gibbs free energies (in kcal/mol) between the enantiomeric transition states; R is the gas constant (1.987 cal/(mol•K)); T is the temperature in K.

$$ee = \frac{1 - e^{\frac{-\Delta G^{\ddagger}_{R/S}}{RT}}}{1 + e^{\frac{-\Delta G^{\ddagger}_{R/S}}{RT}}} \times 100\%$$

9. Buried Volumes of CPA Catalysts

For the consistent quantification of the CPA pocket size, $\%V_{bur}$ is used. To define the xyz axes, first the phosphorus atom defines as the center of the sphere, the middle point between the oxygen atom of the hydroxy group and the phosphoryl group oxygen atom defins the z axis, the oxgen atoms that connecting the backbone defines the xz-plane and teh y axis is determined automatically. All the other parameters are set to default. Based on teh definitin above, the $\%V_{bur}$ is visualized by SambVca 2.1[7].

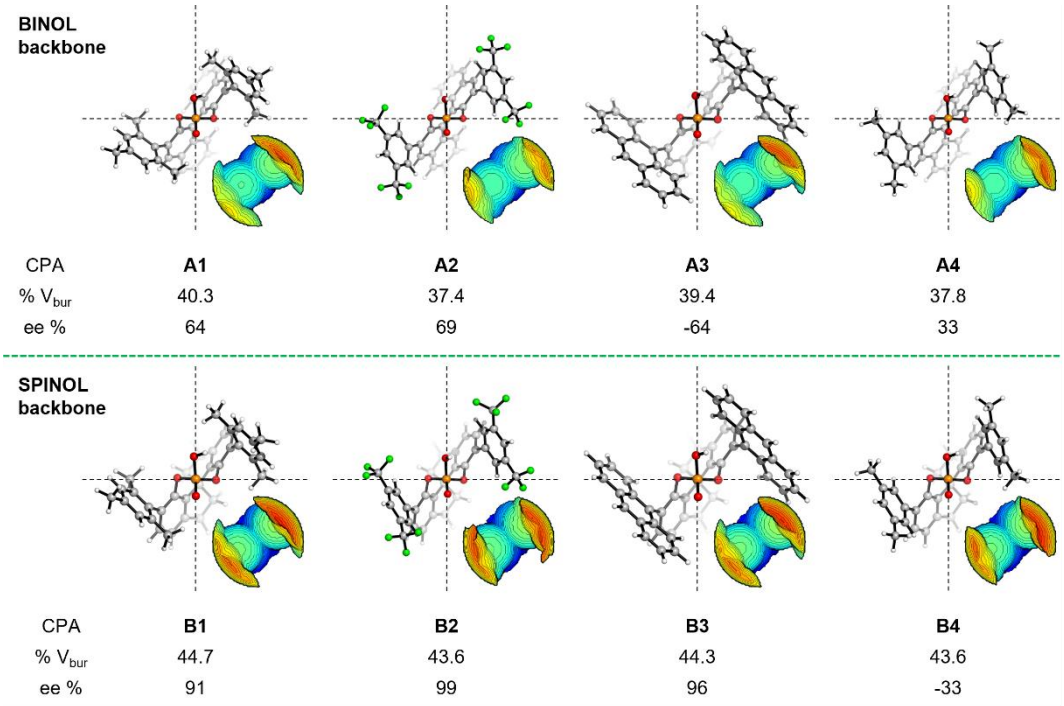


Figure S5. Buried volumes of CPA **A1**−**B4** and the predicted *ee* values for (*S*)-**7bb**.

10. Space-Filling Models of Transition States for 7bb Enantiomers

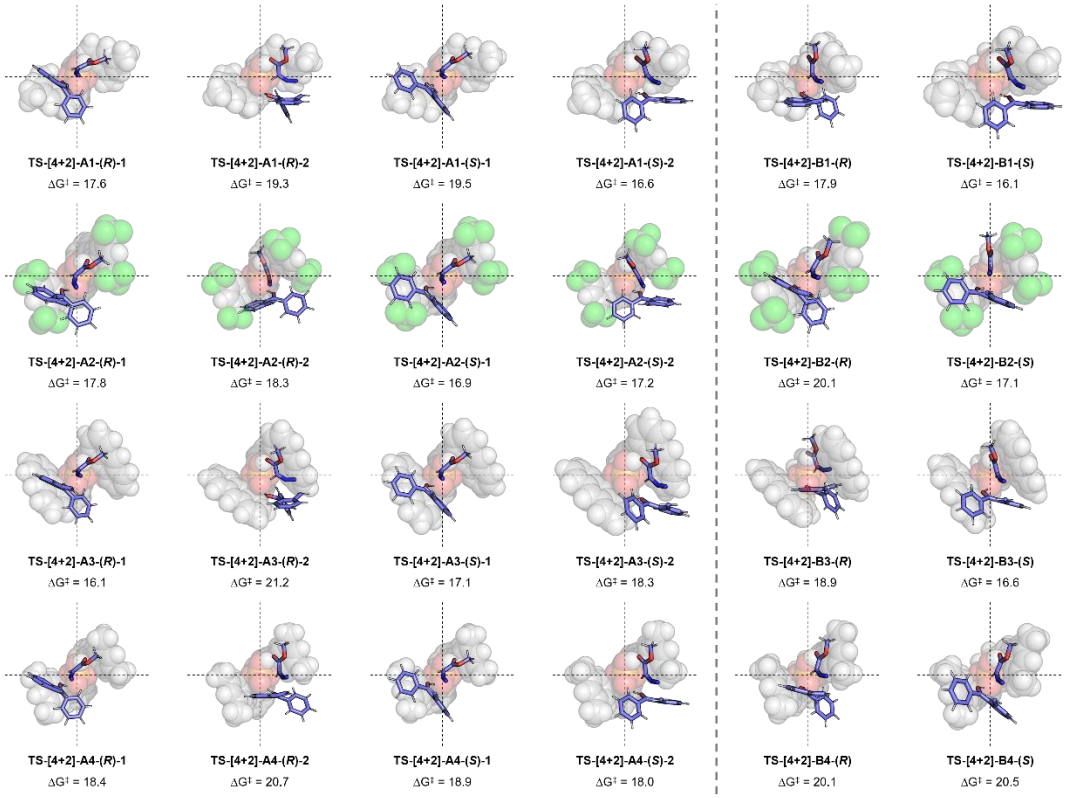
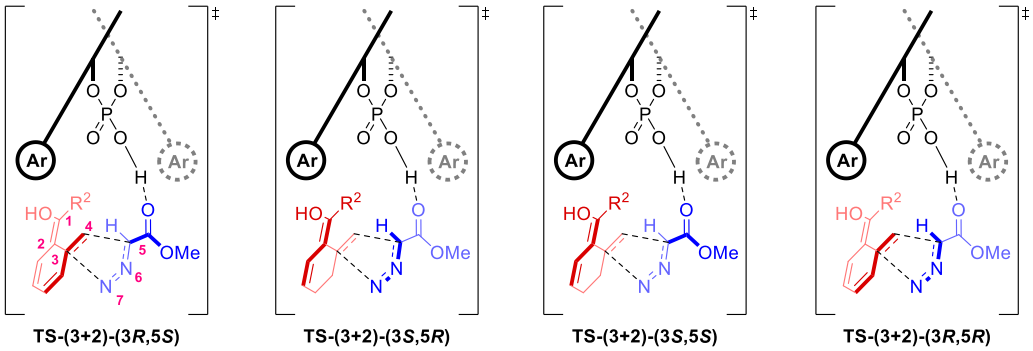


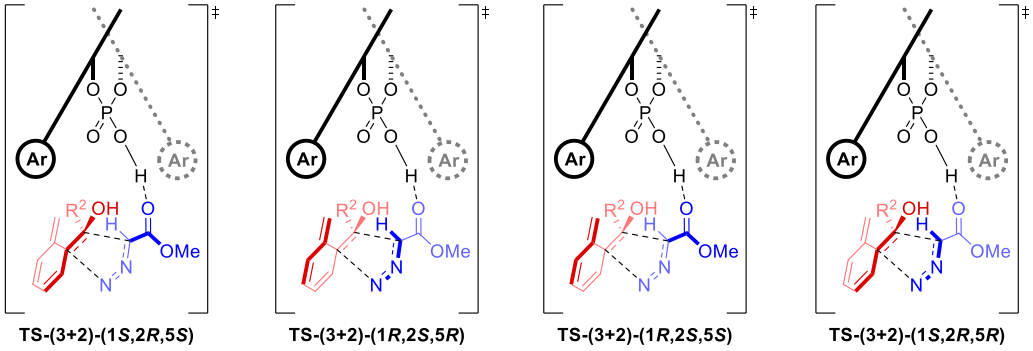
Figure S6. Space-filling models of transition states for **7bb** enantiomers and the relative Gibbs free energy barriers for the **7bb** enantiomers (in kcal/mol).

11. Possible transition states of CPA-catalyzed (3+2) and [4+2] cycloadditions

Table S11. Relative Gibbs free energy barrier for the (3+2) cycloaddition catalyzed by CPA **B2** and **B4**.



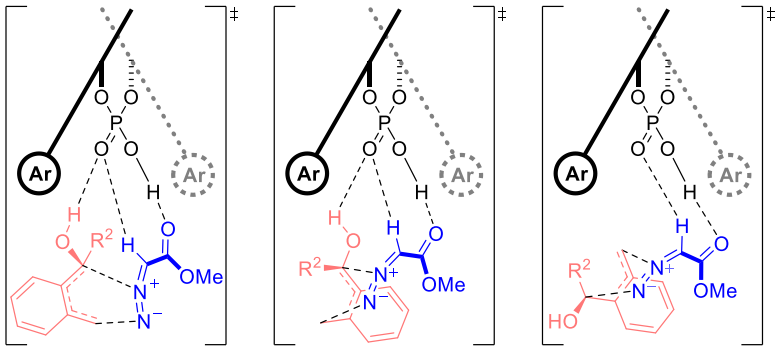
TS-(3+2)-(3*R*,5*S*) TS-(3+2)-(3*S*,5*R*) TS-(3+2)-(3*S*,5*S*) TS-(3+2)-(3*R*,5*R*)



TS-(3+2)-(1*S*,2*R*,5*S*) TS-(3+2)-(1*R*,2*S*,5*R*) TS-(3+2)-(1*R*,2*S*,5*S*) TS-(3+2)-(1*S*,2*R*,5*R*)

TS-(3+2)	$\Delta G^{\ddagger}$ (kcal/mol)		
	No CPA	**B2**	**B4**
(3*R*,5*S*)	31.2	38.8	38.9
(3*S*,5*R*)	31.2	37.6	40.0
(3*S*,5*S*)	31.0	34.7	37.2
(3*R*,5*R*)	31.0	37.2	38.0
(1*S*,2*R*,5*S*)	36.2	42.8	41.3
(1*R*,2*S*,5*R*)	36.2	41.7	42.9
(1*R*,2*S*,5*S*)	37.7	49.2	39.3
(1*S*,2*R*,5*R*)	37.7	40.1	41.3

Table S12. Relative Gibbs free energy barrier for the [4+2] cycloaddition catalyzed by CPA **B2** and **B4**.



TS-[4+2]	$\Delta G^{\ddagger}$ (kcal/mol)		
	No CPA	**B2**	**B4**
(*R*)	23.7	20.1	20.1
(*S*)	23.7	17.1	20.5
(*R*)-2	25.9	26.4	29.3
(*R*)-3	25.2	26.2	27.8
(*S*)-2	25.9	25.9	31.2
(*S*)-3	25.2	24.7	27.9

12. Benchmark for Various DFT Methods

A variety of density functional methods were surveyed to confirm that our conclusions were not sensitive to the method used. The single-point energies were evaluated with the higher accuracy density functionals: ωB97X-D3[8], ωB97M-V[9], ωB97M-D3BJ[10], ωB97M-D4[11], and PWPB95-D3BJ[12] using the ORCA 5.0.3 program[13] for a comparison of the stereoselectivities (Table S13). The trends in enantioselectivities are consistent with each of the five DFT methods.

Table S13. Benchmark for various DFT methods using the def2-TZVP basis set. All numbers are given in kcal/mol.

	ωB97X-D3	ωB97M-V	ωB97M-D3BJ	ωB97M-D4	PWPB95-D3BJ
A1	0.9	1.0	0.6	0.2	0.9
A2	0.1	0.3	0.0	0.3	0.7
A3	-1.6	-1.4	-1.6	-1.7	-0.9
A4	0.4	0.6	0.3	0.1	1.0
B1	1.4	2.0	1.7	1.6	2.2
B2	2.7	2.8	2.2	2.6	2.5
B3	2.0	2.2	1.8	2.1	2.0
B4	-1.2	-1.4	-1.7	-1.6	-1.2

13. Conformation Analysis of Possible (3+2) and [4+2] Cycloaddition Transition States

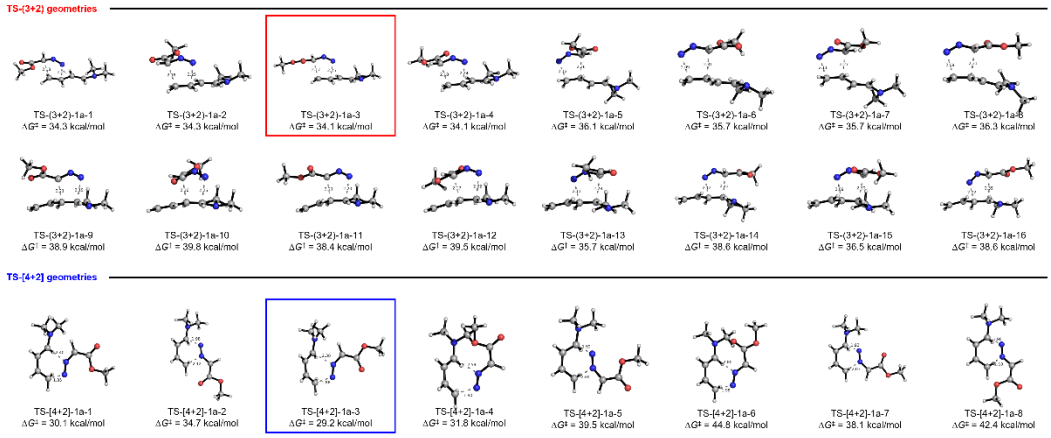


Figure S7. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **1a** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

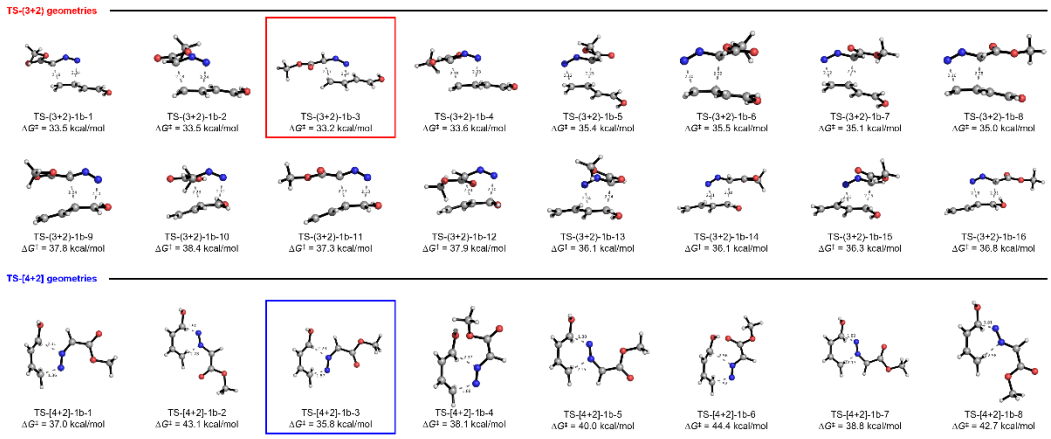


Figure S8. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **1b** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

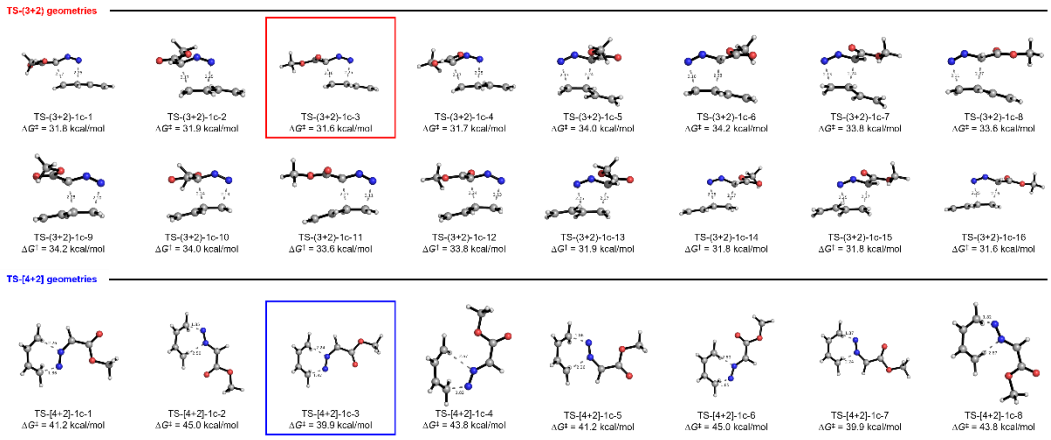


Figure S9. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **1c** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

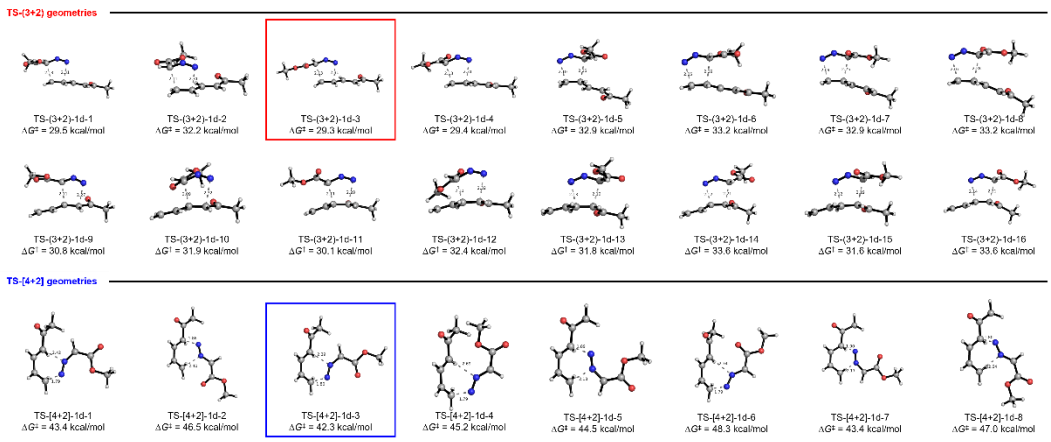


Figure S10. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **1d** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

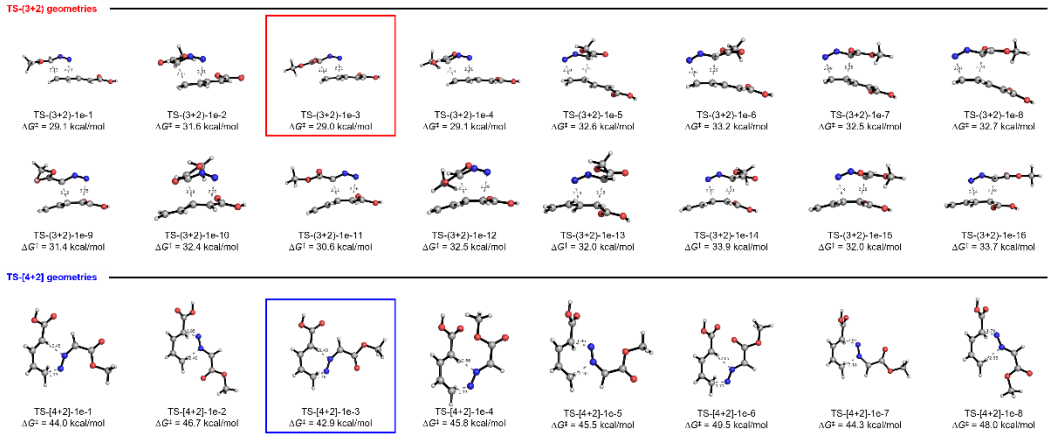


Figure S11. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **1e** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

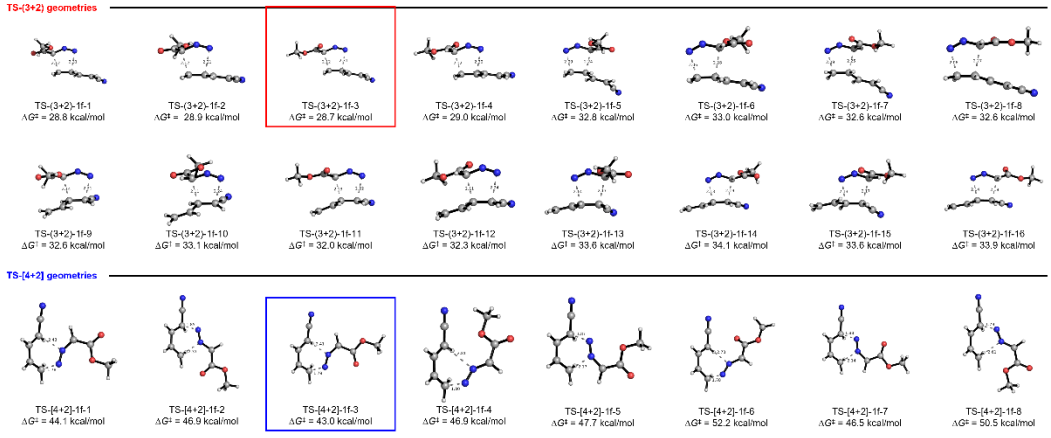


Figure S12. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **1f** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

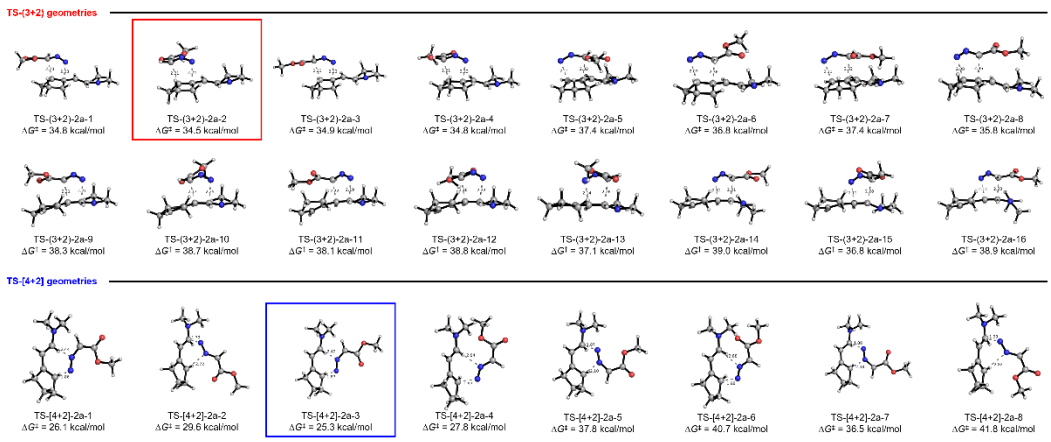


Figure S13. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **2a** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

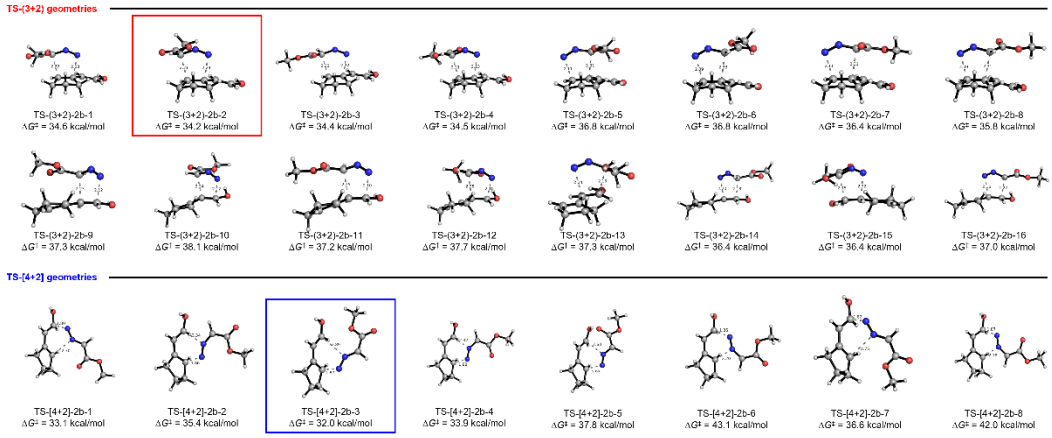


Figure S14. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **2b** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

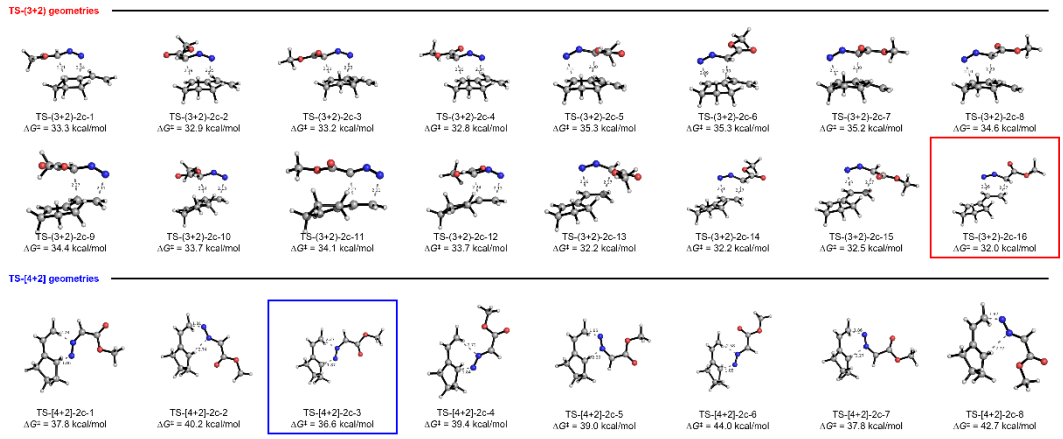


Figure S15. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **2c** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

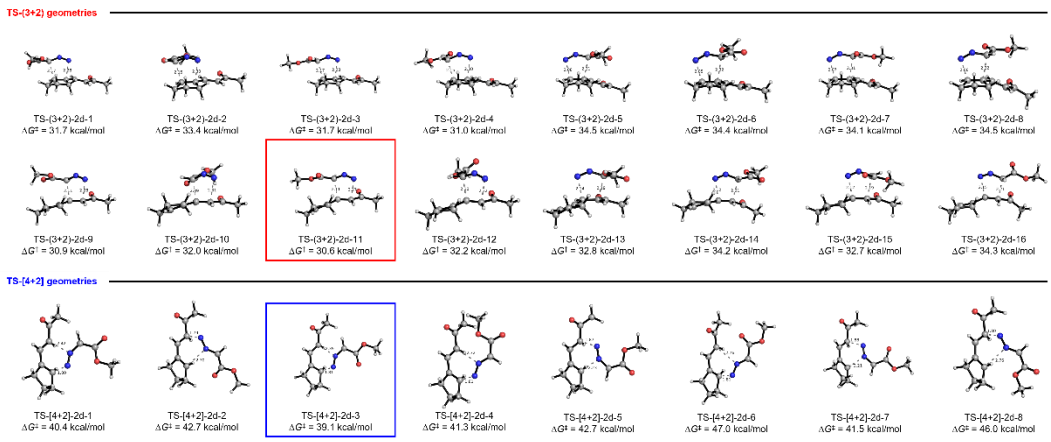


Figure S16. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **2d** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

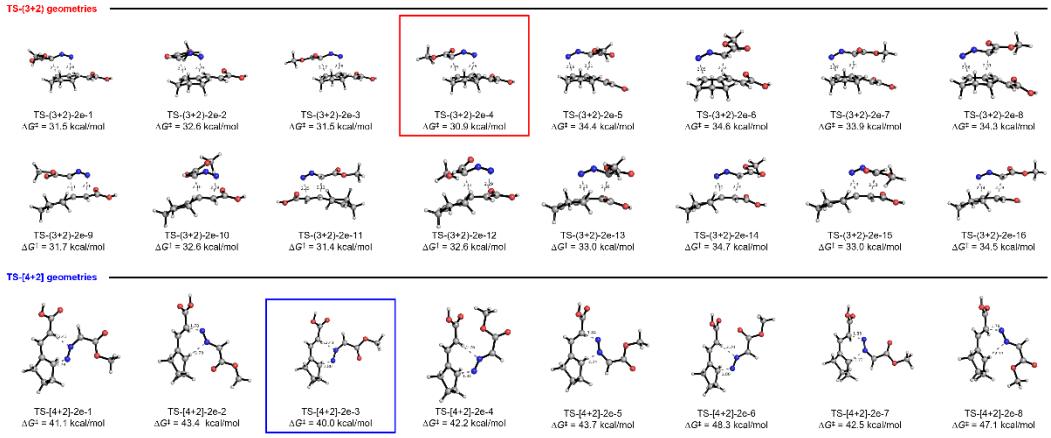


Figure S17. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **2e** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

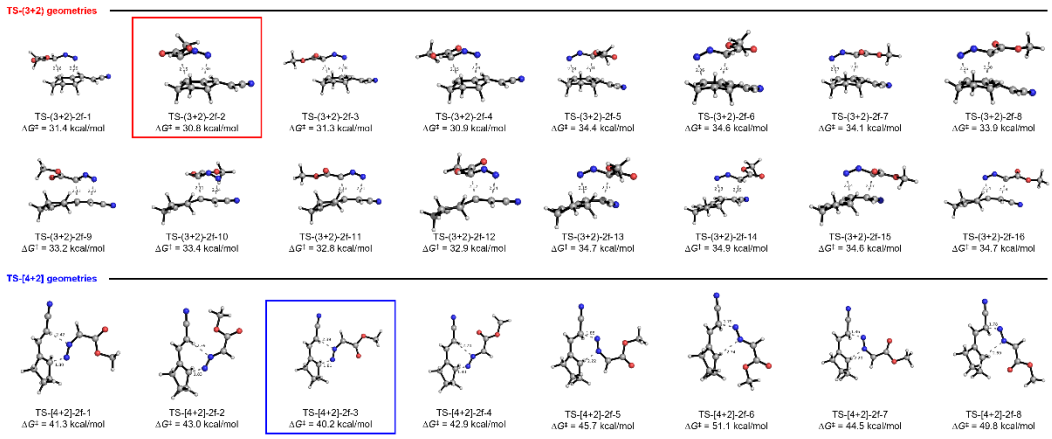


Figure S18. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **2f** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

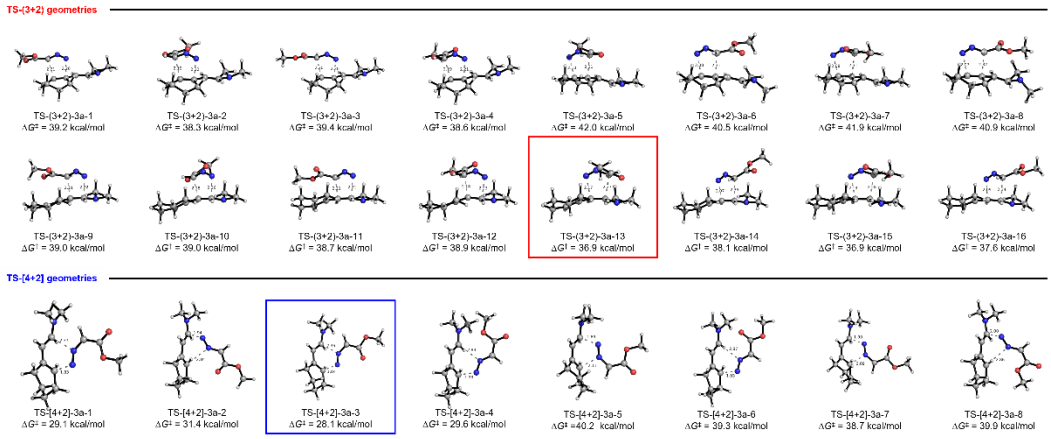


Figure S19. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **3a** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

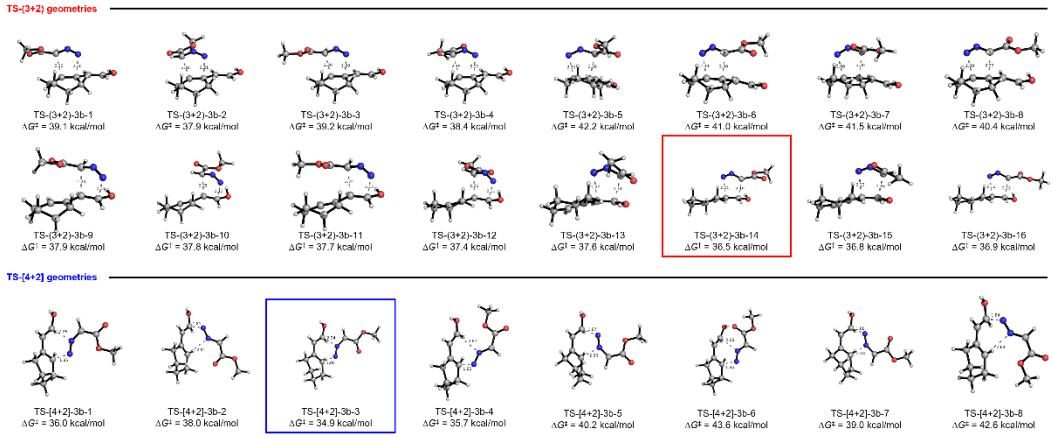


Figure S20. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **3b** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

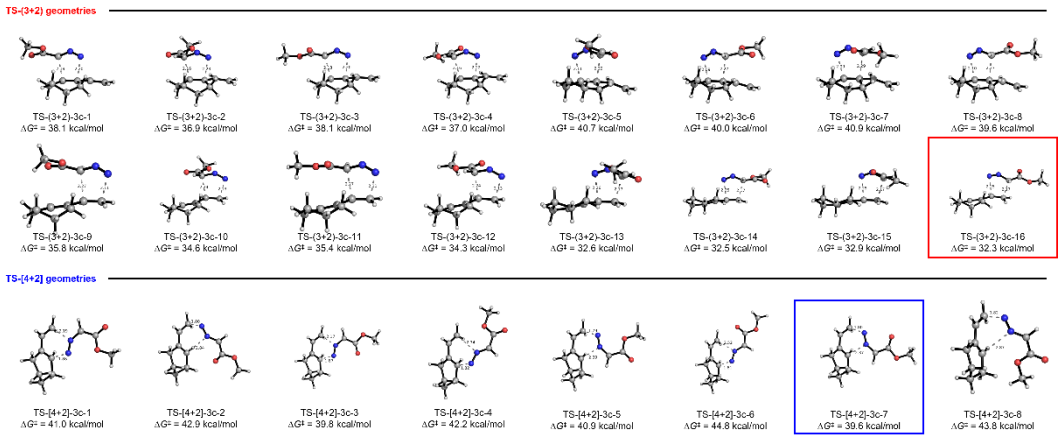


Figure S21. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **3c** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

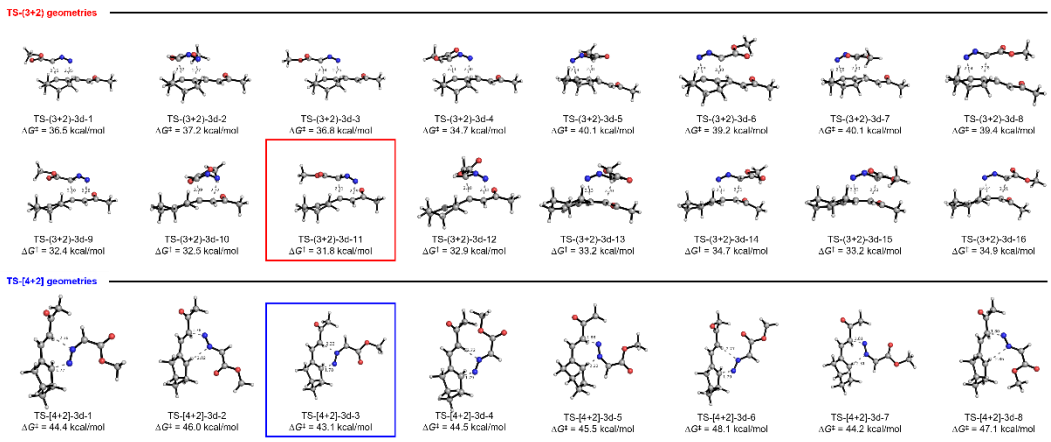


Figure S22. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **3d** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

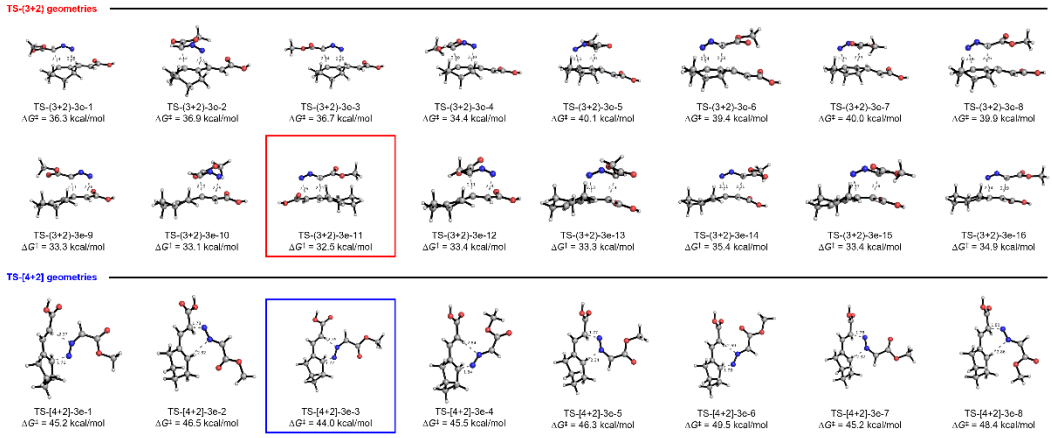


Figure S23. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **3e** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

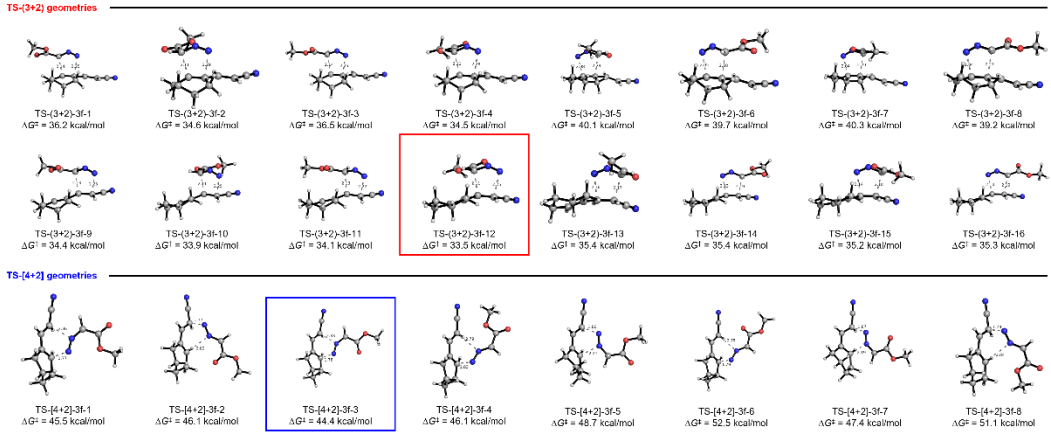


Figure S24. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **3f** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

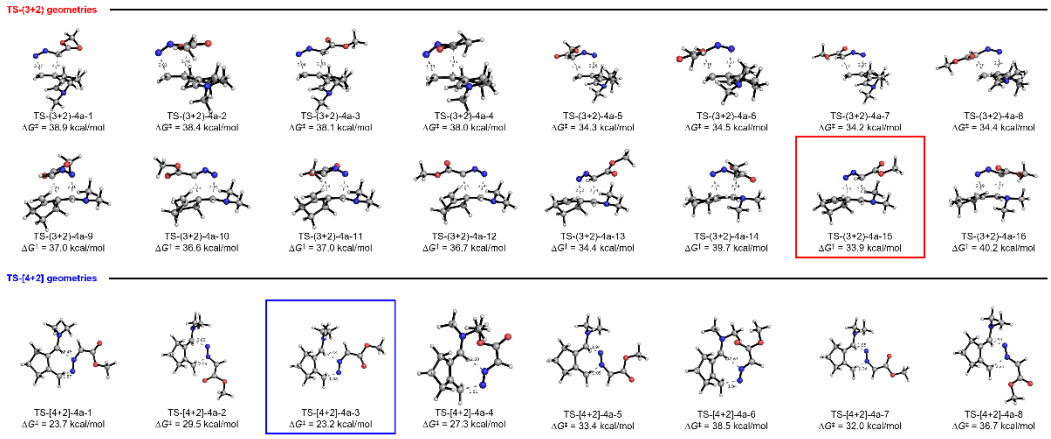


Figure S25. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **4a** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

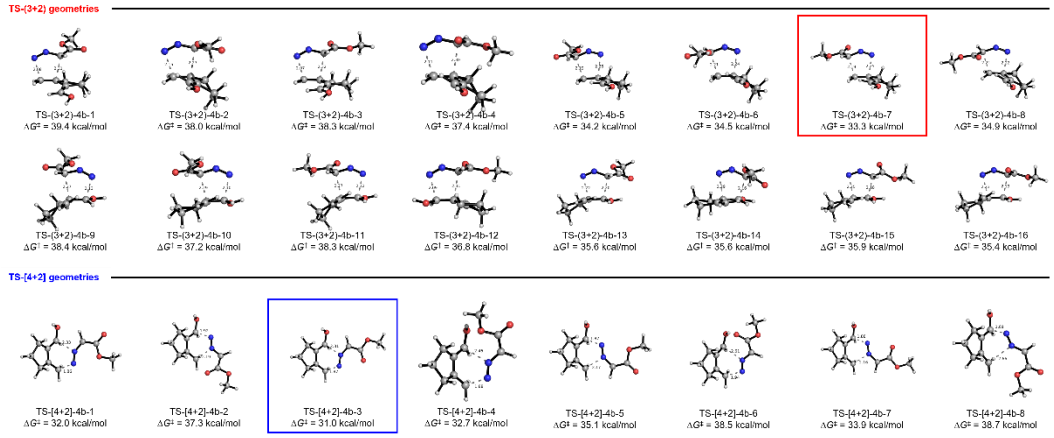


Figure S26. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **4b** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

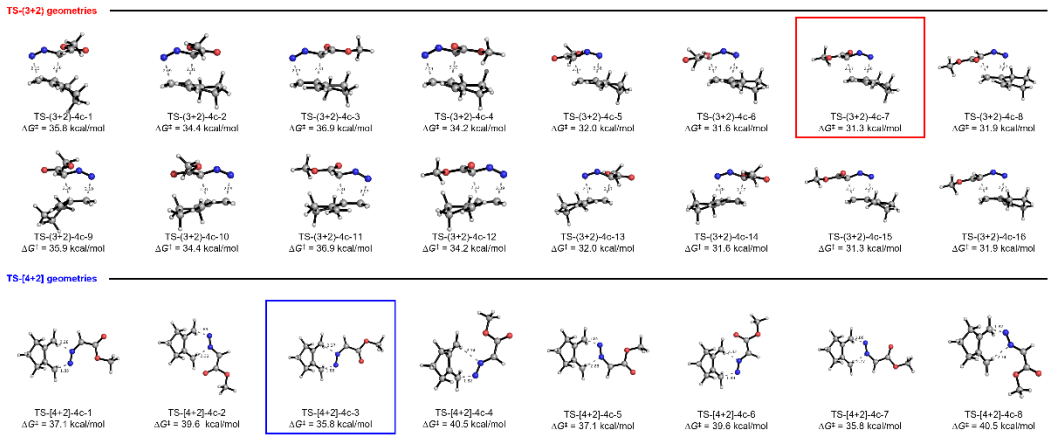


Figure S27. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **4c** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

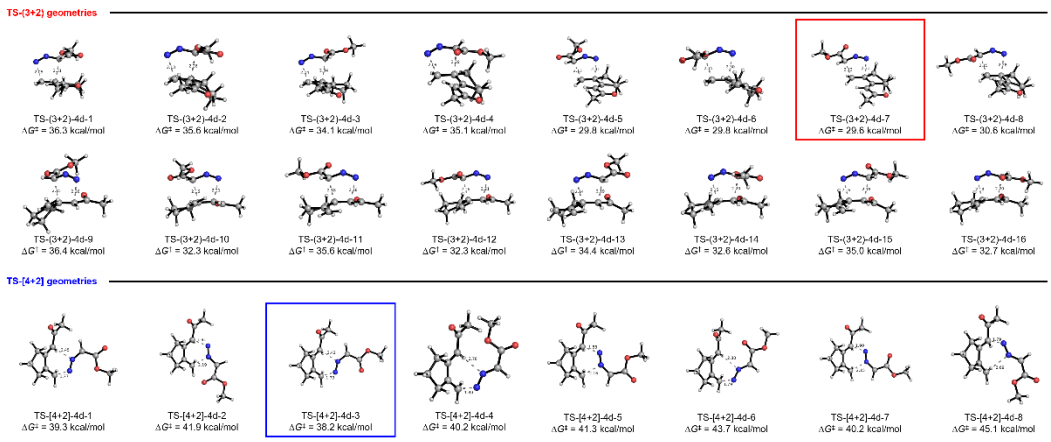


Figure S28. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **4d** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

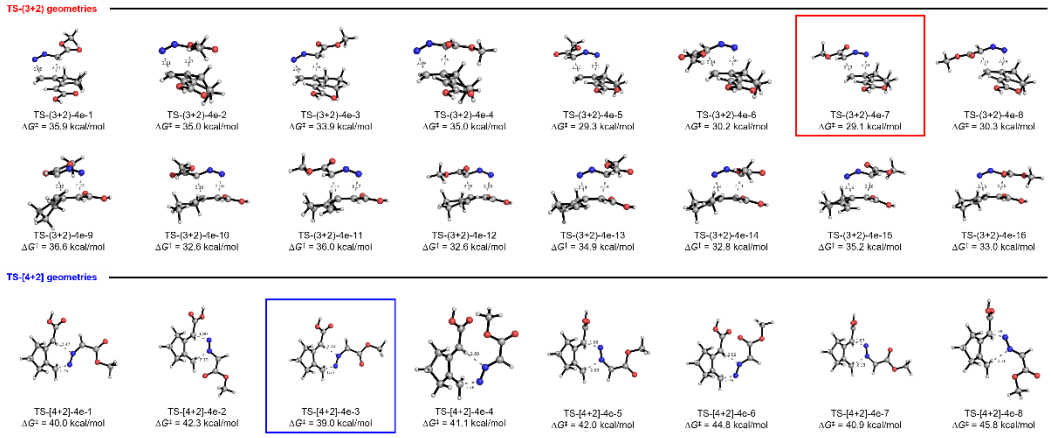


Figure S29. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **4e** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

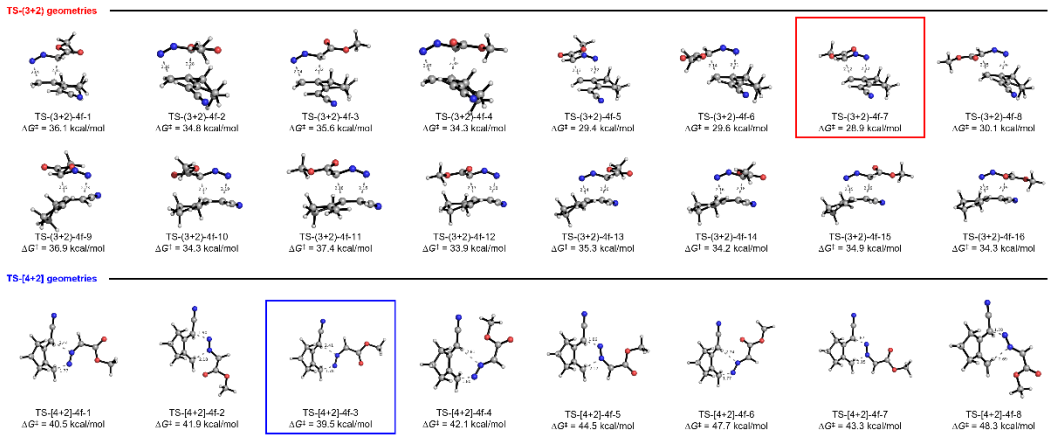


Figure S30. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **4f** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

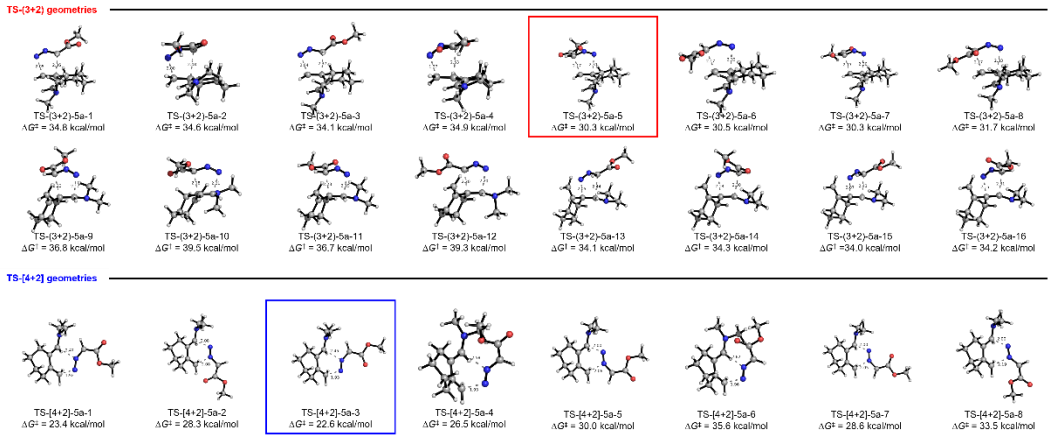


Figure S31. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **5a** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

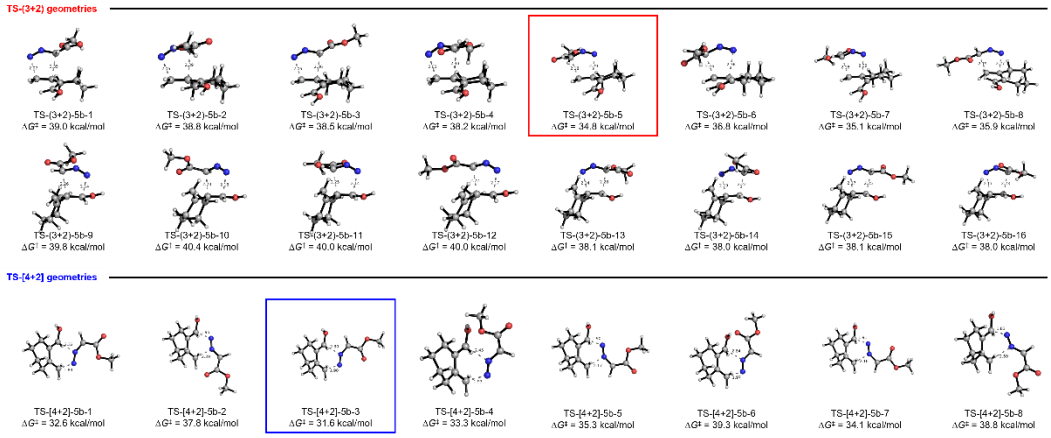


Figure S32. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **5b** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

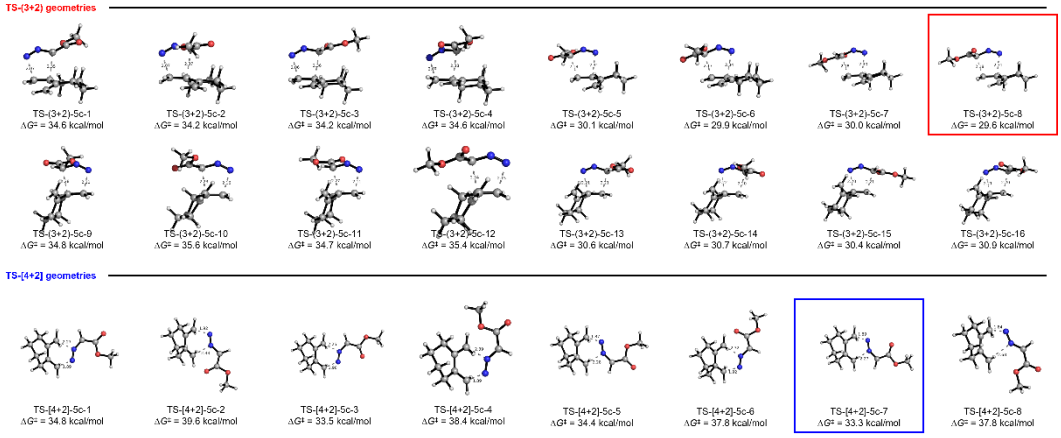


Figure S33. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **5c** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

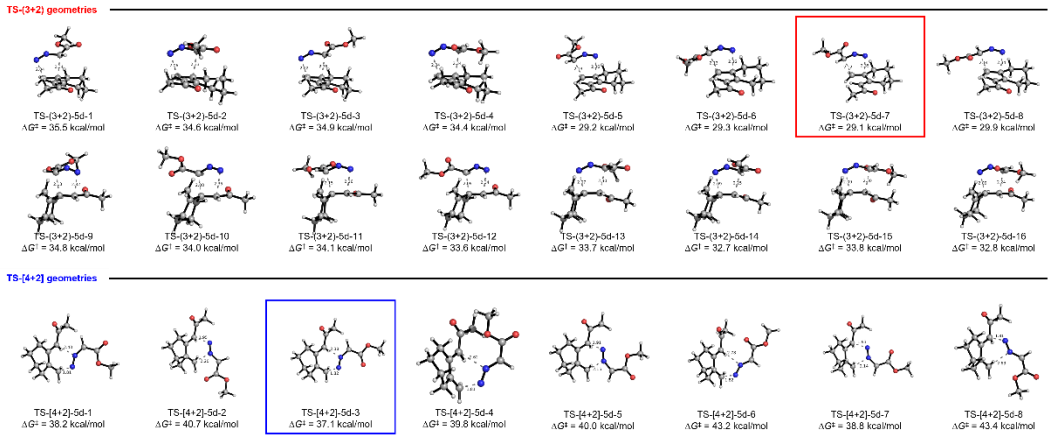


Figure S34. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **5d** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

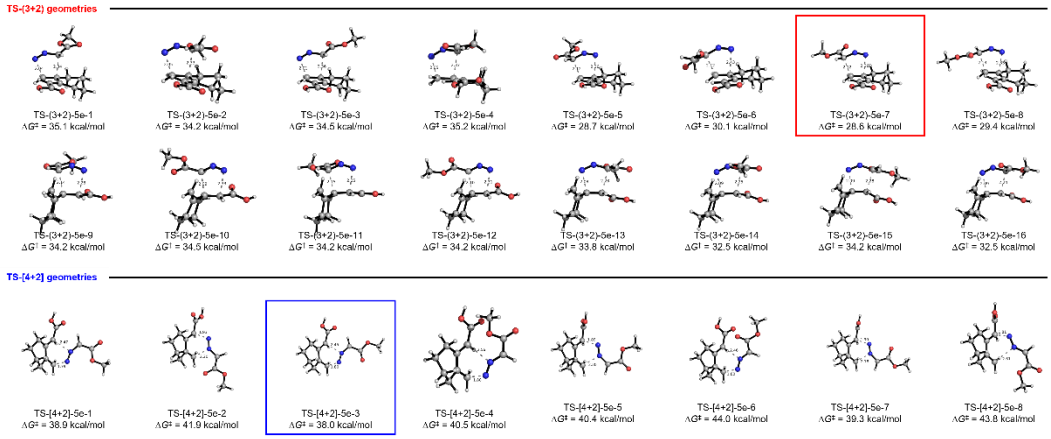


Figure S35. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **5e** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

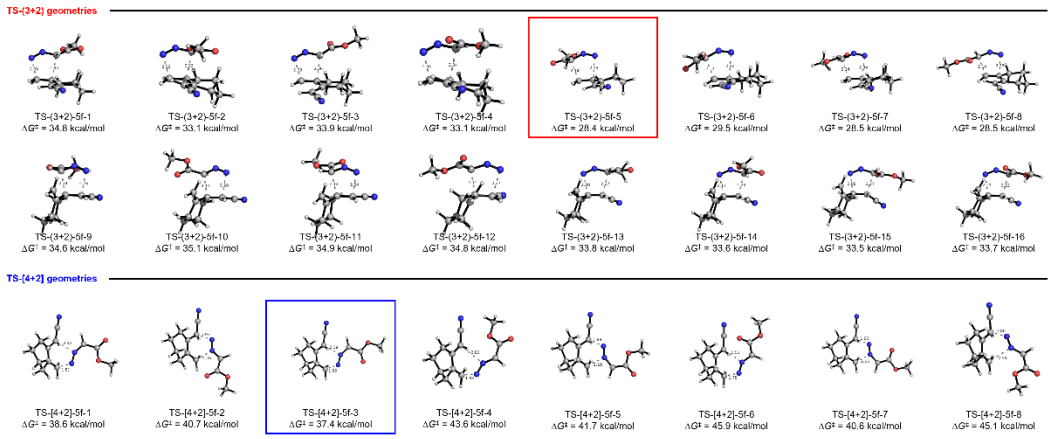


Figure S36. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **5f** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

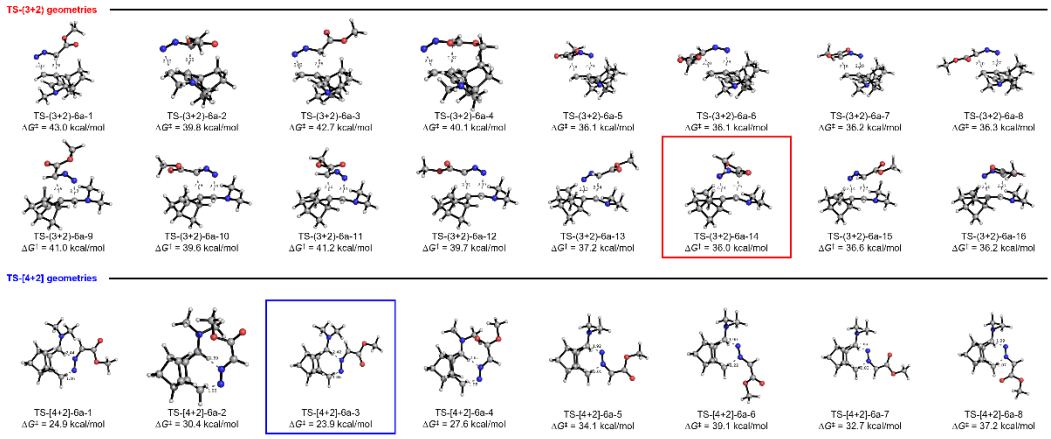


Figure S37. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **6a** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

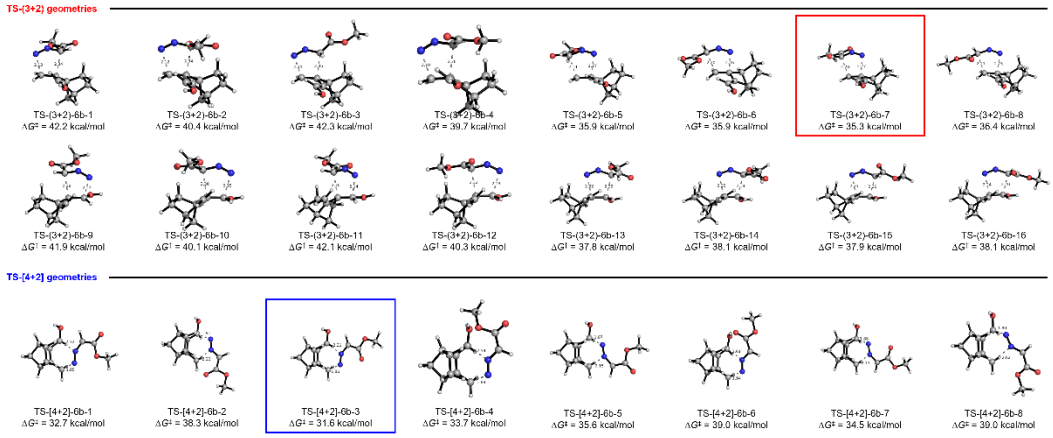


Figure S38. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **6b** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

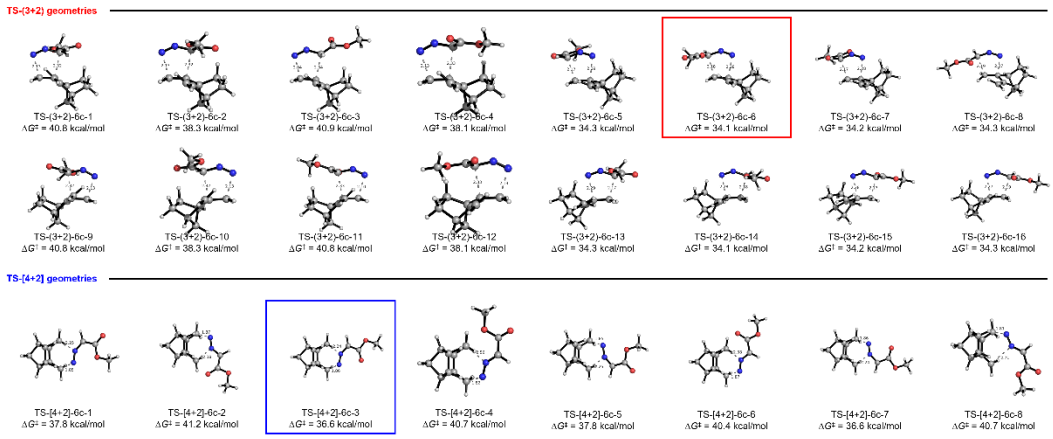


Figure S39. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **6c** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

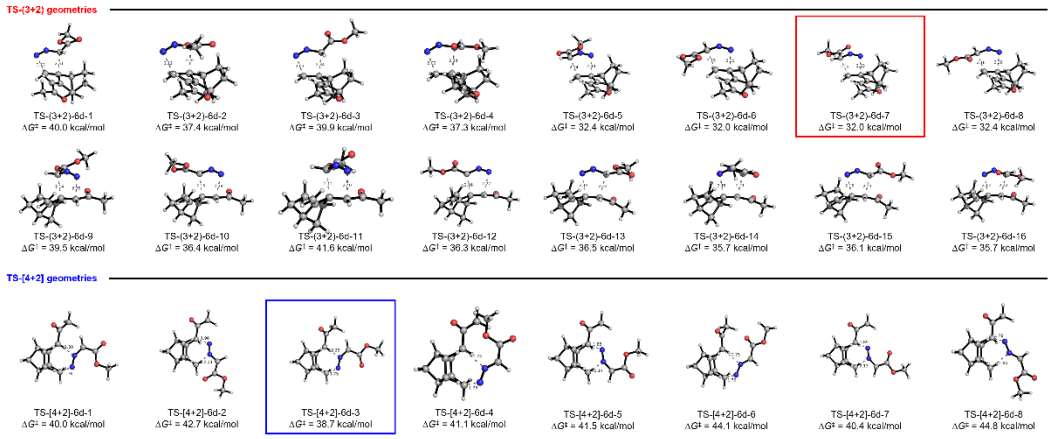


Figure S40. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **6d** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

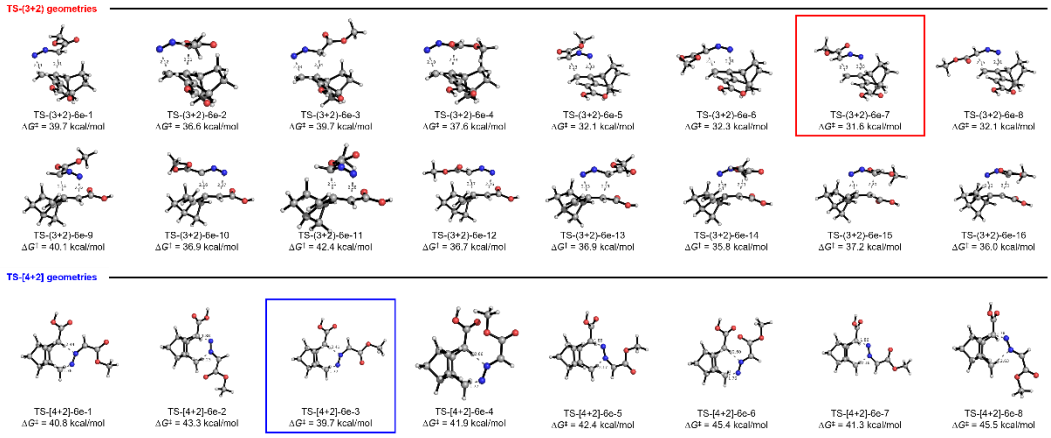


Figure S41. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **6e** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

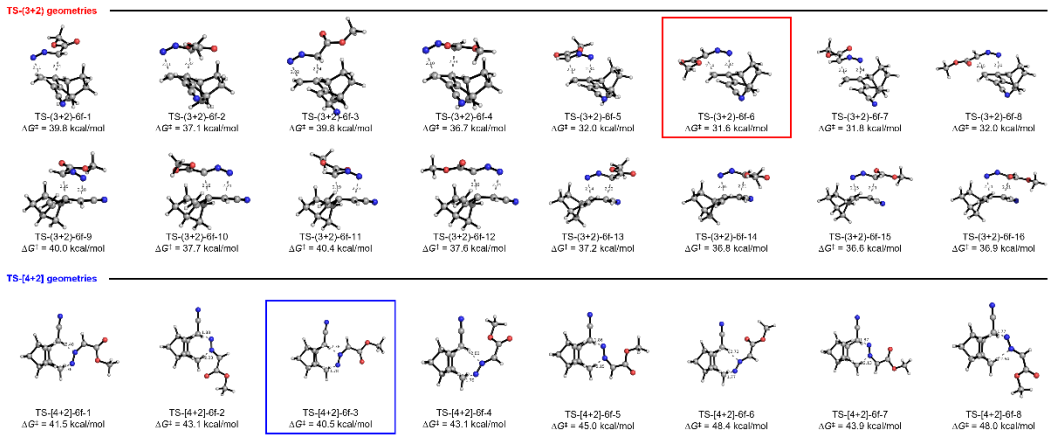


Figure S42. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **6f** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

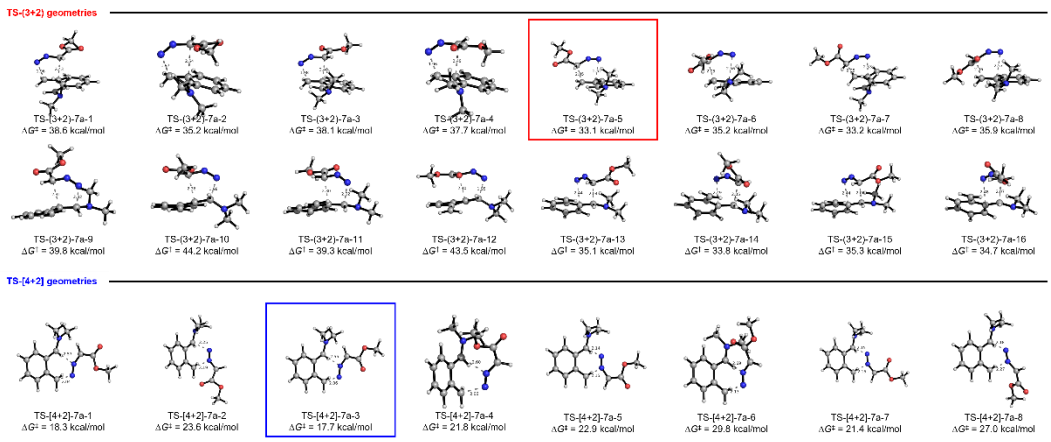


Figure S43. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **7a** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

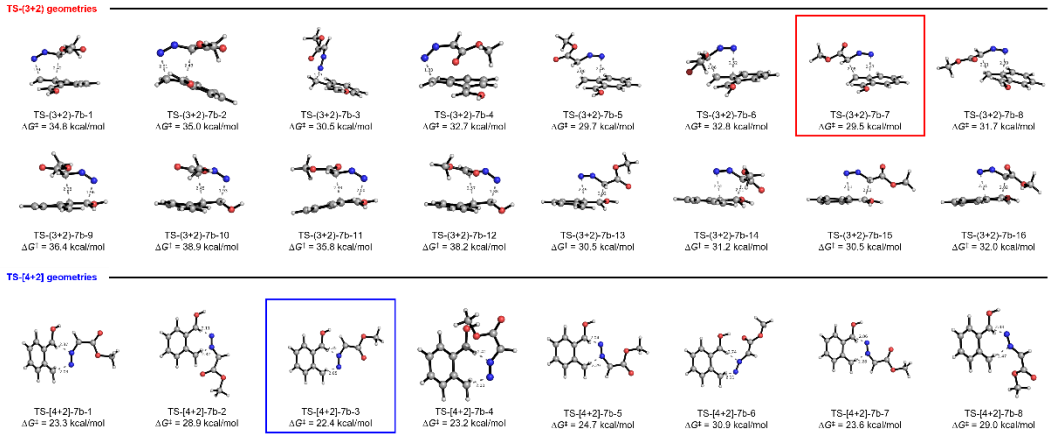


Figure S44. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **7b** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

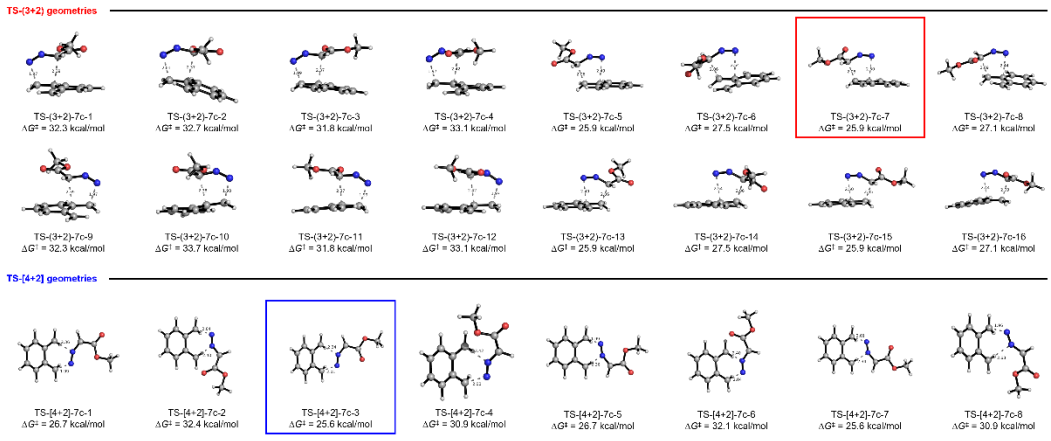


Figure S45. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **7c** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

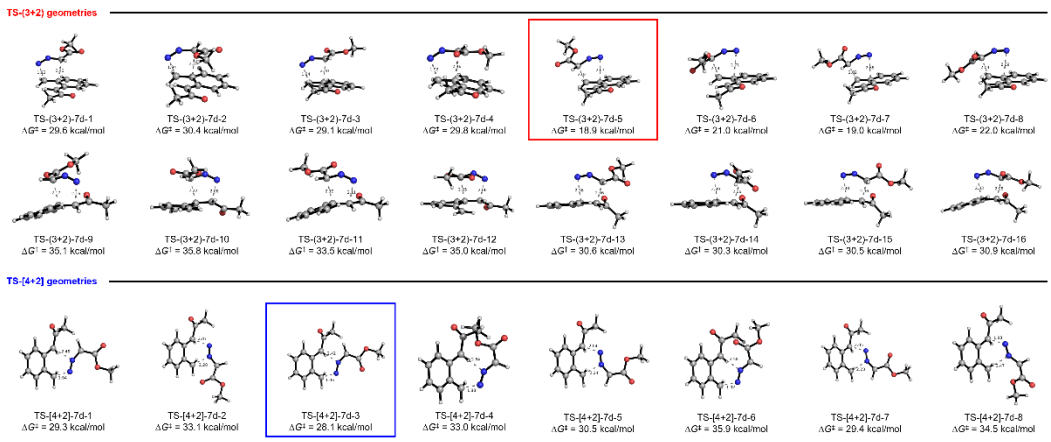


Figure S46. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **7d** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

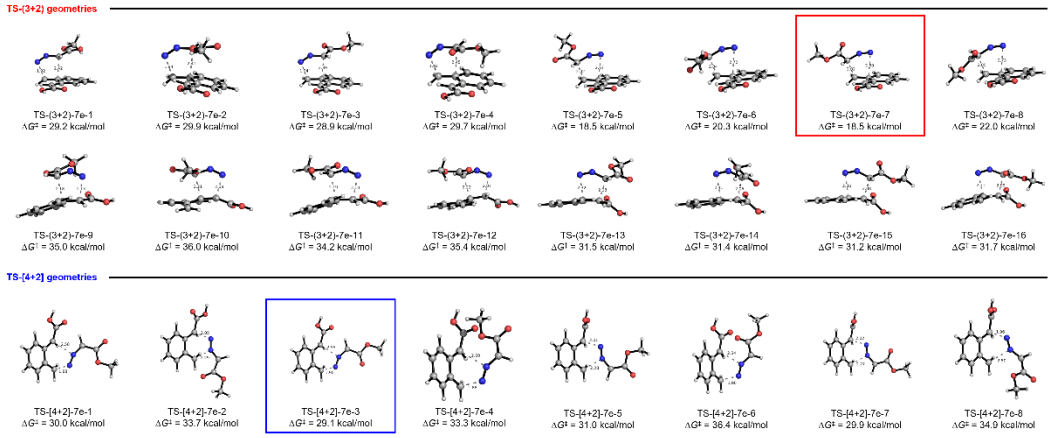


Figure S47. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **7e** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

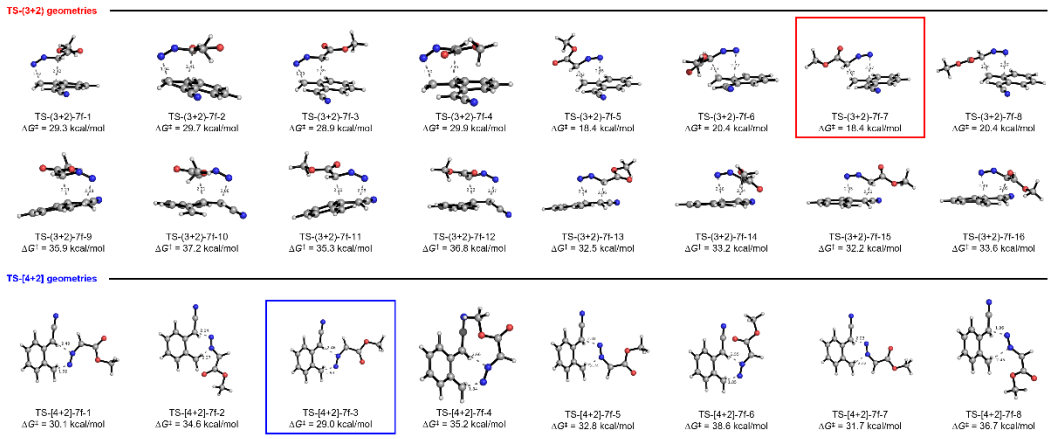


Figure S48. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **7f** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

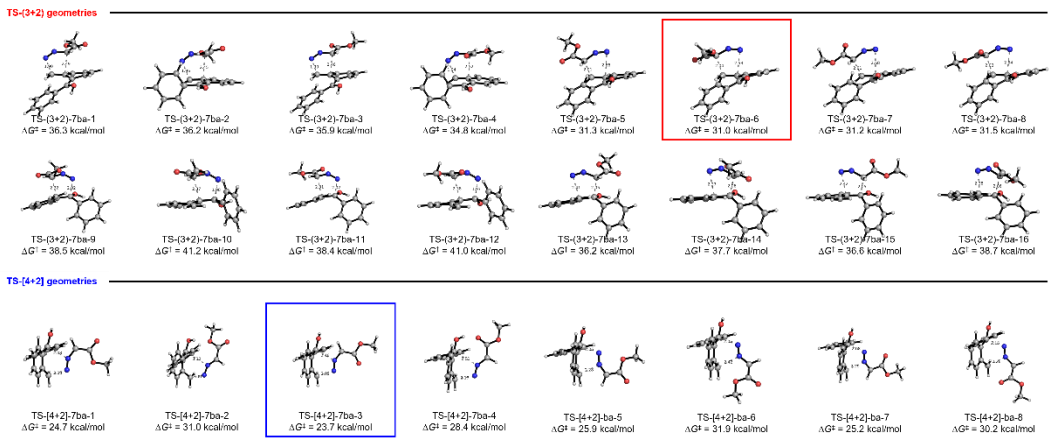


Figure S49. Free energies (ΔG_{298}) (in kcal/mol) of possible transition states of intermolecular (3+2) and [4+2] cycloadditions reactions between **7ba** and **MDA** were calculated at the M06-2X/6-311+G(d,p)/SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level.

14. Table of Energies

Zero-point correction (*ZPE*), thermal correction to enthalpy (*TCH*), thermal correction to Gibbs free energy (*TCG*), energies (*E*), enthalpies (*H*), and Gibbs free energies (*G*) (in Hartree) of the structures calculated at the M06-2X/6-311+G(d,p)-SMD(CH_2Cl_2)//M06-2X/6-31G(d,p) level of theory.

Table S9. Energies for all calculated species

Structures	ZPE	tcH	tcG	E(gas phase)	E(solvent)	Imaginary Frequency
1a	0.160857	0.170252	0.128334	-289.828458	-289.913183	
1b	0.091529	0.098060	0.063282	-231.109156	-231.186979	
1c	0.086097	0.091687	0.059630	-155.911244	-155.957111	
1d	0.124465	0.133348	0.091970	-308.500463	-308.595487	
1e	0.102452	0.110516	0.070888	-344.426434	-344.539366	
1f	0.085469	0.092601	0.055852	-248.127852	-248.204784	
2a	0.226306	0.238014	0.189888	-406.520784	-406.631689	
2b	0.157089	0.165836	0.124815	-347.801972	-347.906463	
2c	0.151767	0.159469	0.121176	-272.604476	-272.677381	
2d	0.189904	0.201085	0.153522	-425.194434	-425.316800	
2e	0.167910	0.178276	0.132440	-461.120562	-461.260956	
2f	0.150990	0.160369	0.117381	-364.822266	-364.926522	
3a	0.256067	0.268644	0.218617	-445.822478	-445.942385	
3b	0.186833	0.196461	0.153483	-387.104010	-387.217722	
3c	0.181572	0.190111	0.149911	-311.907384	-311.989593	
3d	0.219621	0.231696	0.182145	-464.497710	-464.629401	
3e	0.197665	0.208911	0.161146	-500.423939	-500.573756	
3f	0.180770	0.191015	0.146118	-404.125649	-404.239422	
4a	0.225466	0.237241	0.189159	-406.511605	-406.620926	
4b	0.156592	0.165352	0.124188	-347.798435	-347.902156	
4c	0.151150	0.158779	0.120386	-272.601084	-272.673369	
4d	0.189328	0.200413	0.153372	-425.192196	-425.312431	
4e	0.167347	0.177618	0.132293	-461.118295	-461.256669	
4f	0.150389	0.159729	0.116747	-364.820977	-364.924165	
5a	0.255034	0.267715	0.217440	-445.804508	-445.922012	
5b	0.186681	0.196217	0.153617	-387.099951	-387.212398	
5c	0.180731	0.189440	0.148453	-311.896498	-311.977719	
5d	0.219004	0.231097	0.181669	-464.487218	-464.616146	
5e	0.196972	0.208268	0.160538	-500.413432	-500.560568	
5f	0.179999	0.190379	0.144946	-404.117131	-404.229029	
6a	0.261959	0.274622	0.224435	-483.894394	-484.021105	
6b	0.193137	0.202717	0.159673	-425.181369	-425.302599	
6c	0.187833	0.196274	0.156087	-349.985420	-350.075179	
6d	0.226043	0.238053	0.188651	-502.575319	-502.713098	
6e	0.204027	0.215226	0.167552	-538.501645	-538.657516	

6f	0.187139	0.197312	0.152484	-442.204987	-442.325509	
7a	0.208561	0.220244	0.172430	-443.380490	-443.504082	
7b	0.138927	0.147807	0.106577	-384.662894	-384.779703	
7c	0.133789	0.141453	0.103660	-309.466484	-309.550385	
7d	0.172211	0.183353	0.136064	-462.054681	-462.186004	
7e	0.150092	0.160438	0.114824	-497.980869	-498.130186	
7f	0.133089	0.142439	0.099550	-401.685562	-401.799336	
7ba	0.220933	0.234158	0.182109	-615.629765	-615.801443	
MDA	0.078143	0.086235	0.046603	-376.474472	-376.590023	
TS-(3+2)-1a	0.240677	0.257437	0.195866	-666.272431	-666.469809	550.11i
TS-(3+2)-1a-product	0.245982	0.261854	0.201883	-666.352119	-666.550480	
TS-(3+2)-1b	0.171311	0.185193	0.130484	-607.553296	-607.744620	546.55i
TS-(3+2)-1b-product	0.176729	0.189624	0.136729	-607.632848	-607.825029	
TS-(3+2)-1c	0.166088	0.178872	0.127109	-532.357632	-532.517682	535.98i
TS-(3+2)-1c-product	0.171398	0.183215	0.133370	-532.436102	-532.595462	
TS-(3+2)-1d	0.204396	0.220652	0.159679	-684.950216	-685.159912	528.49i
TS-(3+2)-1d-product	0.209429	0.224789	0.165392	-685.023277	-685.231854	
TS-(3+2)-1e	0.182378	0.197810	0.138606	-720.876235	-721.104245	526.97i
TS-(3+2)-1e-product	0.187478	0.202010	0.144441	-720.949143	-721.175502	
TS-(3+2)-1f	0.165451	0.179909	0.123455	-624.577847	-624.770026	526.59i
TS-(3+2)-1f-product	0.170594	0.184109	0.129613	-624.650129	-624.840346	
TS-(3+2)-2a	0.305743	0.324815	0.258342	-782.965552	-783.188643	550.48i
TS-(3+2)-2a-product	0.311062	0.329111	0.265184	-783.045243	-783.269502	
TS-(3+2)-2b	0.236482	0.252627	0.193290	-724.246653	-724.463899	547.58i
TS-(3+2)-2b-product	0.241949	0.256958	0.200352	-724.326495	-724.544512	
TS-(3+2)-2c	0.231576	0.246650	0.188922	-649.050979	-649.237515	536.56i
TS-(3+2)-2c-product	0.236963	0.251067	0.195531	-649.129756	-649.316635	
TS-(3+2)-2d	0.269877	0.288114	0.224537	-801.652430	-801.882476	519.10i
TS-(3+2)-2d-product	0.274417	0.291909	0.229271	-801.713328	-801.945500	
TS-(3+2)-2e	0.247391	0.265154	0.201007	-837.568667	-837.823754	537.86i
TS-(3+2)-2e-product	0.252529	0.269276	0.207329	-837.643193	-837.895304	
TS-(3+2)-2f	0.230615	0.247340	0.186238	-741.271759	-741.489767	538.45i
TS-(3+2)-2f-product	0.235741	0.251434	0.192848	-741.343810	-741.560389	
TS-(3+2)-3a	0.335124	0.355218	0.287095	-822.265075	-822.495437	489.64i
TS-(3+2)-3a-product	0.340858	0.359565	0.295151	-822.337787	-822.570117	
TS-(3+2)-3b	0.266182	0.283130	0.222292	-763.546059	-763.771725	557.31i
TS-(3+2)-3b-product	0.271433	0.287484	0.227866	-763.621909	-763.848514	
TS-(3+2)-3c	0.261156	0.277216	0.216970	-688.352706	-688.548635	539.11i
TS-(3+2)-3c-product	0.266605	0.281657	0.223725	-688.433266	-688.629403	
TS-(3+2)-3d	0.299570	0.318777	0.253242	-840.954455	-841.193202	522.97i
TS-(3+2)-3d-product	0.304149	0.322558	0.258098	-841.016062	-841.257345	
TS-(3+2)-3e	0.277467	0.295873	0.231951	-876.878458	-877.136132	522.77i
TS-(3+2)-3e-product	0.282140	0.299785	0.236719	-876.938684	-877.198351	
TS-(3+2)-3f	0.260186	0.277971	0.213812	-780.569343	-780.797159	529.32i

TS-(3+2)-3f-product	0.265026	0.281898	0.219614	-780.635430	-780.860308	
TS-(3+2)-4a	0.305514	0.324317	0.260283	-782.961889	-783.181493	471.81i
TS-(3+2)-4a-product	0.310858	0.328449	0.267567	-783.029962	-783.250030	
TS-(3+2)-4b	0.235658	0.252322	0.190302	-724.239821	-724.458675	551.08i
TS-(3+2)-4b-product	0.241270	0.256649	0.198699	-724.326479	-724.543347	
TS-(3+2)-4c	0.230961	0.246052	0.188161	-649.048517	-649.234674	546.32i
TS-(3+2)-4c-product	0.236286	0.250271	0.195662	-649.131622	-649.316044	
TS-(3+2)-4d	0.269166	0.287814	0.221399	-801.641397	-801.876629	542.15i
TS-(3+2)-4d-product	0.274406	0.291936	0.228623	-801.722182	-801.954401	
TS-(3+2)-4e	0.247187	0.265008	0.200380	-837.568208	-837.821747	541.06i
TS-(3+2)-4e-product	0.252366	0.269098	0.207463	-837.647986	-837.898428	
TS-(3+2)-4f	0.230316	0.247149	0.184935	-741.271403	-741.489731	544.16i
TS-(3+2)-4f-product	0.235411	0.251188	0.191939	-741.349745	-741.564912	
TS-(3+2)-5a	0.335223	0.355230	0.287303	-822.257991	-822.487029	542.34i
TS-(3+2)-5a-product	0.340270	0.359297	0.293480	-822.339753	-822.570686	
TS-(3+2)-5b	0.266277	0.283381	0.222160	-763.543417	-763.768847	541.32i
TS-(3+2)-5b-product	0.271353	0.287676	0.227908	-763.624410	-763.851234	
TS-(3+2)-5c	0.260995	0.276931	0.217613	-688.348071	-688.543177	531.77i
TS-(3+2)-5c-product	0.266449	0.281087	0.225964	-688.431263	-688.626871	
TS-(3+2)-5d	0.298980	0.318534	0.250429	-840.938741	-841.181945	539.89i
TS-(3+2)-5d-product	0.304327	0.322849	0.256773	-841.017538	-841.259492	
TS-(3+2)-5e	0.276938	0.295688	0.229360	-876.865856	-877.127259	537.98i
TS-(3+2)-5e-product	0.282343	0.300035	0.235986	-876.944596	-877.204372	
TS-(3+2)-5f	0.260366	0.278032	0.214629	-780.571319	-780.796810	531.33i
TS-(3+2)-5f-product	0.265750	0.282348	0.221843	-780.648514	-780.872932	
TS-(3+2)-6a	0.341723	0.361518	0.295133	-860.340236	-860.577910	493.39i
TS-(3+2)-6a-product	0.347304	0.365779	0.302620	-860.419953	-860.657160	
TS-(3+2)-6b	0.272360	0.289731	0.226591	-801.620524	-801.856657	535.86i
TS-(3+2)-6b-product	0.277711	0.294038	0.234135	-801.710403	-801.944233	
TS-(3+2)-6c	0.267735	0.283470	0.225451	-726.431142	-726.633614	522.53i
TS-(3+2)-6c-product	0.272897	0.287796	0.231251	-726.515328	-726.717799	
TS-(3+2)-6d	0.305895	0.325311	0.257203	-879.022161	-879.274117	535.74i
TS-(3+2)-6d-product	0.311025	0.329530	0.263901	-879.106140	-879.355369	
TS-(3+2)-6e	0.283958	0.302514	0.236424	-914.949073	-915.219389	535.46i
TS-(3+2)-6e-product	0.288983	0.306679	0.242799	-915.032327	-915.299721	
TS-(3+2)-6f	0.267024	0.284548	0.222002	-818.654072	-818.888060	522.78i
TS-(3+2)-6f-product	0.272123	0.288791	0.227909	-818.733742	-818.966451	
TS-(3+2)-7a	0.287085	0.306488	0.239189	-819.826506	-820.061459	572.95i
TS-(3+2)-7a-product	0.292154	0.310820	0.244679	-819.893578	-820.127631	
TS-(3+2)-7b	0.217792	0.234655	0.172951	-761.109964	-761.342488	578.55i
TS-(3+2)-7b-product	0.223215	0.238843	0.179957	-761.180927	-761.410140	
TS-(3+2)-7c	0.213276	0.228478	0.171176	-685.919859	-686.120007	549.98i
TS-(3+2)-7c-product	0.218285	0.232544	0.176959	-685.985502	-686.182066	
TS-(3+2)-7d	0.251738	0.270579	0.203938	-838.515084	-838.767193	480.76i

TS-(3+2)-7d-product	0.256406	0.274332	0.209588	-838.570933	-838.815622	
TS-(3+2)-7e	0.229759	0.247706	0.183429	-874.442591	-874.712787	469.83i
TS-(3+2)-7e-product	0.234392	0.251454	0.188606	-874.498753	-874.759974	
TS-(3+2)-7f	0.212638	0.229626	0.167741	-778.146458	-778.381613	479.01i
TS-(3+2)-7f-product	0.217426	0.233467	0.173342	-778.202865	-778.428478	
TS-(3+2)-7ba	0.300550	0.321306	0.250905	-992.078596	-992.364186	570.21i
TS-(3+2)-7ba-product	0.305590	0.325181	0.259038	-992.151383	-992.435062	
TS-[4+2]-1a	0.241655	0.258101	0.198456	-666.274083	-666.480229	434.97i
TS-[4+2]-1a-product	0.245743	0.261321	0.203930	-666.305891	-666.507327	
TS-[4+2]-1b	0.172868	0.185877	0.134321	-607.548116	-607.744328	466.03i
TS-[4+2]-1b-product	0.176917	0.189339	0.138786	-607.593047	-607.788384	
TS-[4+2]-1c	0.167474	0.179534	0.130120	-532.343453	-532.507436	491.94i
TS-[4+2]-1c-product	0.172234	0.183631	0.135501	-532.399153	-532.566684	
TS-[4+2]-1d	0.205418	0.221011	0.162774	-684.931723	-685.142294	463.46i
TS-[4+2]-1d-product	0.209531	0.224355	0.168167	-684.972858	-685.186255	
TS-[4+2]-1e	0.183553	0.198288	0.142021	-720.858925	-721.085479	461.17i
TS-[4+2]-1e-product	0.187329	0.201499	0.146346	-720.897017	-721.127594	
TS-[4+2]-1f	0.166453	0.180266	0.126255	-624.559132	-624.750106	470.52i
TS-[4+2]-1f-product	0.170416	0.183538	0.131116	-624.596666	-624.790191	
TS-[4+2]-2a	0.306316	0.325308	0.259826	-782.972514	-783.204778	391.37i
TS-[4+2]-2a-product	0.310586	0.328562	0.265778	-782.999823	-783.227127	
TS-[4+2]-2b	0.237621	0.253133	0.195779	-724.247127	-724.469833	420.94i
TS-[4+2]-2b-product	0.241893	0.256608	0.200842	-724.287467	-724.508786	
TS-[4+2]-2c	0.232283	0.246773	0.191625	-649.042349	-649.232964	449.34i
TS-[4+2]-2c-product	0.237320	0.250949	0.197596	-649.093408	-649.286363	
TS-[4+2]-2d	0.270018	0.288150	0.224085	-801.631007	-801.868475	425.17i
TS-[4+2]-2d-product	0.274468	0.291694	0.229976	-801.667434	-801.906371	
TS-[4+2]-2e	0.248225	0.265470	0.203530	-837.558092	-837.811719	429.00i
TS-[4+2]-2e-product	0.252279	0.268827	0.208273	-837.591716	-837.847917	
TS-[4+2]-2f	0.231201	0.247493	0.187820	-741.258484	-741.476282	437.05i
TS-[4+2]-2f-product	0.235426	0.250887	0.193110	-741.291971	-741.510850	
TS-[4+2]-3a	0.336063	0.356107	0.288053	-822.268878	-822.510489	400.97i
TS-[4+2]-3a-product	0.341295	0.359803	0.295929	-822.307680	-822.542582	
TS-[4+2]-3b	0.267391	0.283938	0.224003	-763.543998	-763.776086	440.66i
TS-[4+2]-3b-product	0.271680	0.287608	0.228110	-763.590164	-763.819591	
TS-[4+2]-3c	0.262012	0.277568	0.219479	-688.339288	-688.539462	454.69i
TS-[4+2]-3c-product	0.266928	0.281814	0.225510	-688.394321	-688.595702	
TS-[4+2]-3d	0.299773	0.318985	0.252145	-840.927519	-841.174085	422.59i
TS-[4+2]-3d-product	0.303821	0.322247	0.257456	-840.967353	-841.215696	
TS-[4+2]-3e	0.277863	0.296222	0.231415	-876.854435	-877.117288	419.27i
TS-[4+2]-3e-product	0.282424	0.300108	0.236298	-876.899206	-877.164748	
TS-[4+2]-3f	0.260935	0.278310	0.215880	-780.554925	-780.781872	432.97i
TS-[4+2]-3f-product	0.265442	0.282088	0.220826	-780.595288	-780.824509	
TS-[4+2]-4a	0.306030	0.325226	0.258797	-782.965105	-783.197001	417.86i

TS-[4+2]-4a-product	0.311288	0.329232	0.266339	-783.004528	-783.230537	
TS-[4+2]-4b	0.237482	0.253102	0.195385	-724.244635	-724.467450	445.96i
TS-[4+2]-4b-product	0.241656	0.257032	0.198535	-724.285045	-724.505540	
TS-[4+2]-4c	0.232013	0.246610	0.190988	-649.039359	-649.230277	475.81i
TS-[4+2]-4c-product	0.236787	0.251215	0.193106	-649.090767	-649.282734	
TS-[4+2]-4d	0.269840	0.288012	0.223943	-801.628999	-801.865616	446.30i
TS-[4+2]-4d-product	0.274325	0.291944	0.229035	-801.663339	-801.902259	
TS-[4+2]-4e	0.248014	0.265333	0.203198	-837.556031	-837.808904	447.00i
TS-[4+2]-4e-product	0.252351	0.269350	0.207408	-837.595597	-837.853785	
TS-[4+2]-4f	0.230870	0.247310	0.187079	-741.257018	-741.474972	456.77i
TS-[4+2]-4f-product	0.235470	0.251509	0.191406	-741.291199	-741.511508	
TS-[4+2]-5a	0.336083	0.355990	0.288671	-822.261193	-822.500612	392.30i
TS-[4+2]-5a-product	0.340293	0.359388	0.294056	-822.303322	-822.539580	
TS-[4+2]-5b	0.267235	0.283808	0.223868	-763.544164	-763.775770	436.98i
TS-[4+2]-5b-product	0.271490	0.287457	0.228810	-763.592436	-763.823002	
TS-[4+2]-5c	0.261849	0.277394	0.219475	-688.339037	-688.539121	473.25i
TS-[4+2]-5c-product	0.266703	0.281644	0.225177	-688.398531	-688.601274	
TS-[4+2]-5d	0.299728	0.318849	0.252590	-840.926154	-841.171310	451.32i
TS-[4+2]-5d-product	0.304064	0.322523	0.257946	-840.969785	-841.218293	
TS-[4+2]-5e	0.277738	0.296058	0.231568	-876.852783	-877.114539	452.16i
TS-[4+2]-5e-product	0.281815	0.299667	0.235510	-876.894437	-877.160846	
TS-[4+2]-5f	0.260633	0.278063	0.215581	-780.556437	-780.783465	460.57i
TS-[4+2]-5f-product	0.264933	0.281638	0.221038	-780.597087	-780.825503	
TS-[4+2]-6a	0.343115	0.362891	0.295840	-860.349752	-860.597922	420.90i
TS-[4+2]-6a-product	0.347119	0.366196	0.300694	-860.372059	-860.616932	
TS-[4+2]-6b	0.274243	0.290579	0.231436	-801.628598	-801.867410	444.09i
TS-[4+2]-6b-product	0.278232	0.294132	0.235265	-801.660988	-801.899763	
TS-[4+2]-6c	0.268797	0.284106	0.227064	-726.423633	-726.631231	478.80i
TS-[4+2]-6c-product	0.273609	0.288398	0.231996	-726.467058	-726.677386	
TS-[4+2]-6d	0.306652	0.325605	0.259905	-879.012755	-879.266057	448.12i
TS-[4+2]-6d-product	0.310896	0.329228	0.264854	-879.041396	-879.296954	
TS-[4+2]-6e	0.284708	0.302850	0.238914	-914.939279	-915.209111	445.01i
TS-[4+2]-6e-product	0.288933	0.306768	0.242303	-914.970818	-915.244190	
TS-[4+2]-6f	0.267782	0.284926	0.223369	-818.640558	-818.875272	454.60i
TS-[4+2]-6f-product	0.271740	0.288366	0.227516	-818.666470	-818.902491	
TS-[4+2]-7a	0.288884	0.307917	0.242307	-819.846551	-820.089245	328.08i
TS-[4+2]-7a-product	0.293988	0.311926	0.249154	-819.908526	-820.146181	
TS-[4+2]-7b	0.219826	0.235648	0.177348	-761.125226	-761.358259	384.90i
TS-[4+2]-7b-product	0.225114	0.239890	0.183884	-761.195679	-761.428512	
TS-[4+2]-7c	0.214375	0.229131	0.172918	-685.920149	-686.122198	429.83i
TS-[4+2]-7c-product	0.220326	0.234088	0.180123	-686.002544	-686.207242	
TS-[4+2]-7d	0.252566	0.270902	0.206190	-838.508004	-838.754718	417.80i
TS-[4+2]-7d-product	0.257717	0.275037	0.212876	-838.573663	-838.823519	
TS-[4+2]-7e	0.230617	0.248093	0.185370	-874.434662	-874.697772	430.89i

TS-[4+2]-7e-product	0.235573	0.252209	0.191168	-874.498053	-874.765173	
TS-[4+2]-7f	0.213468	0.229999	0.169530	-778.138266	-778.366462	427.41i
TS-[4+2]-7f-product	0.218556	0.234105	0.175972	-778.200621	-778.429814	
TS-[4+2]-7ba	0.301375	0.321736	0.252828	-992.090947	-992.377850	380.67i
TS-[4+2]-7ba-product	0.306500	0.325839	0.258843	-992.163254	-992.447835	
A1	0.616973	0.656146	0.546124	-2109.616141	-2110.103243	
A2	0.470986	0.514580	0.387849	-3221.567094	-3222.463847	
A3	0.638462	0.678306	0.565880	-2488.140558	-2488.728526	
A4	0.560363	0.596941	0.489659	-2031.015071	-2031.488442	
B1	0.623438	0.660452	0.556926	-1996.533449	-1996.990766	
B2	0.476814	0.518607	0.396322	-3108.485585	-3109.352936	
B3	0.644817	0.682515	0.576985	-2375.057970	-2375.615245	
B4	0.566481	0.601092	0.497927	-1917.933579	-1918.376794	
TS-[4+2]-A1-R-1	0.917734	0.976256	0.826517	-3101.771107	-3102.518377	264.76i
TS-[4+2]-A1-R-2	0.918586	0.977432	0.825979	-3101.763249	-3102.515096	316.03i
TS-[4+2]-A1-S-1	0.918196	0.976358	0.827512	-3101.767805	-3102.516325	247.88i
TS-[4+2]-A1-S-2	0.917754	0.976578	0.825007	-3101.770654	-3102.518411	285.50i
TS-[4+2]-A2-R-1	0.773015	0.835806	0.672075	-4213.730536	-4214.882426	235.51i
TS-[4+2]-A2-R-2	0.771891	0.835104	0.669492	-4213.723561	-4214.879153	205.19i
TS-[4+2]-A2-S-1	0.772404	0.835139	0.672519	-4213.733526	-4214.884392	230.29i
TS-[4+2]-A2-S-2	0.771181	0.834386	0.668721	-4213.725048	-4214.880141	214.04i
TS-[4+2]-A3-R-1	0.939168	0.998683	0.845699	-3480.297461	-3481.145363	293.83i
TS-[4+2]-A3-R-2	0.940376	0.999641	0.849014	-3480.294142	-3481.140642	338.33i
TS-[4+2]-A3-S-1	0.939348	0.998472	0.847119	-3480.298781	-3481.145195	240.86i
TS-[4+2]-A3-S-2	0.940611	0.999816	0.849417	-3480.298701	-3481.145652	318.05i
TS-[4+2]-A4-R-1	0.861175	0.917349	0.768373	-3023.166555	-3023.900617	312.88i
TS-[4+2]-A4-R-2	0.861165	0.916852	0.771386	-3023.165519	-3023.899941	289.23i
TS-[4+2]-A4-S-1	0.860553	0.916310	0.770548	-3023.169830	-3023.901988	261.12i
TS-[4+2]-A4-S-2	0.861870	0.917811	0.770038	-3023.168463	-3023.902913	295.60i
TS-[4+2]-B1-R	0.923816	0.980459	0.836343	-2988.683662	-2989.404386	228.25i
TS-[4+2]-B1-S	0.924086	0.980637	0.836154	-2988.689629	-2989.407087	285.74i
TS-[4+2]-B2-R	0.779333	0.840101	0.684244	-4100.650353	-4101.771608	233.79i
TS-[4+2]-B2-S	0.778399	0.839348	0.682408	-4100.652529	-4101.774562	218.61i
TS-[4+2]-B3-R	0.945807	1.003191	0.856523	-3367.208932	-3368.027374	261.06i
TS-[4+2]-B3-S	0.945535	1.002796	0.856641	-3367.212787	-3368.031168	241.60i
TS-[4+2]-B4-R	0.867371	0.921107	0.781355	-2910.085297	-2910.790960	232.85i
TS-[4+2]-B4-S	0.867893	0.921322	0.782539	-2910.088747	-2910.791439	230.86i
TS-(3+2)-B2-1R2S5R	0.778754	0.840609	0.681316	-4100.608767	-4101.734207	542.15i
TS-(3+2)-B2-1R2S5S	0.778870	0.840999	0.677922	-4100.590902	-4101.718897	577.13i
TS-(3+2)-B2-1S2R5R	0.779688	0.841513	0.680285	-4100.607060	-4101.735685	515.77i
TS-(3+2)-B2-1S2R5S	0.779338	0.840899	0.681884	-4100.607988	-4101.732982	555.73i
TS-(3+2)-B2-3R5R	0.779606	0.841595	0.679468	-4100.610432	-4101.739584	584.51i
TS-(3+2)-B2-3R5S	0.779825	0.841632	0.682789	-4100.613369	-4101.740352	594.08i
TS-(3+2)-B2-3S5R	0.779168	0.841422	0.678419	-4100.605985	-4101.737808	595.88i

TS-(3+2)-B2-3S5S	0.779532	0.841525	0.680588	-4100.612346	-4101.744617	585.29i
TS-(3+2)-B4-1R2S5R	0.868552	0.923348	0.780093	-2910.043557	-2910.753310	533.61i
TS-(3+2)-B4-1R2S5S	0.869560	0.923559	0.785147	-2910.059033	-2910.764168	507.39i
TS-(3+2)-B4-1S2R5R	0.869354	0.923890	0.782065	-2910.051520	-2910.757921	501.20i
TS-(3+2)-B4-1S2R5S	0.868778	0.923509	0.780225	-2910.042629	-2910.756033	555.16i
TS-(3+2)-B4-3R5R	0.869781	0.924187	0.783926	-2910.056188	-2910.764979	528.75i
TS-(3+2)-B4-3R5S	0.868829	0.923642	0.781086	-2910.048770	-2910.760694	582.43i
TS-(3+2)-B4-3S5R	0.869278	0.924199	0.780013	-2910.045947	-2910.757872	582.79i
TS-(3+2)-B4-3S5S	0.869357	0.923853	0.783190	-2910.054420	-2910.765464	580.58i
TS-[4+2]-B2-R-2	0.779543	0.840531	0.683994	-4100.632350	-4101.761251	299.16i
TS-[4+2]-B2-R-3	0.778828	0.840820	0.677570	-4100.625438	-4101.755247	254.49i
TS-[4+2]-B2-S-2	0.778330	0.839795	0.680250	-4100.628400	-4101.758360	322.01i
TS-[4+2]-B2-S-3	0.778500	0.840177	0.680235	-4100.632263	-4101.760170	197.51i
TS-[4+2]-B4-R-2	0.869727	0.923693	0.782694	-2910.065212	-2910.777667	364.13i
TS-[4+2]-B4-R-3	0.868342	0.923167	0.779458	-2910.067820	-2910.776756	223.72i
TS-[4+2]-B4-S-2	0.870036	0.922999	0.785333	-2910.064301	-2910.777292	360.18i
TS-[4+2]-B4-S-3	0.868567	0.922775	0.782139	-2910.070951	-2910.779309	220.32i
^{1}INT0	0.221567	0.234757	0.182378	-615.695244	-615.862086	
^{3}INT0	0.218453	0.231942	0.177710	-615.584301	-615.748467	
^{3}TS1	0.213407	0.226132	0.174094	-615.567654	-615.734065	1292.68i
^{3}INT1	0.218135	0.231571	0.178236	-615.601916	-615.773105	
^{3}INT2	0.218297	0.231665	0.178613	-615.601859	-615.773340	

15. Cartesian Coordinates of the Structures

1a

C	-3.416499	0.178146	0.117920
C	-2.247740	-0.452925	-0.033163
H	-3.461437	1.253450	0.265416
H	-4.358047	-0.357829	0.098145
H	-2.247748	-1.533161	-0.182469
C	-0.943018	0.186959	-0.010913
C	0.193594	-0.519115	-0.174553
H	-0.917073	1.262600	0.139676
H	0.131972	-1.600217	-0.294928
N	1.480582	-0.029720	-0.256541
C	1.670959	1.381470	-0.008295
H	2.714904	1.640986	-0.195785
H	1.042809	1.961936	-0.689047
H	1.414815	1.664040	1.025388
C	2.546312	-0.892422	0.215838
H	2.352323	-1.918703	-0.104621
H	3.496904	-0.572565	-0.219086
H	2.644852	-0.885181	1.312099

1b

C	-2.469416	-0.231109	0.000226
C	-1.288167	0.391194	-0.000243
H	-2.536252	-1.315294	0.000535
H	-3.401336	0.321593	0.000370
H	-1.260651	1.480415	-0.000542
C	0.002717	-0.281199	-0.000307
C	1.159547	0.391382	0.000202
H	0.008375	-1.371035	-0.000701
H	1.196086	1.477300	0.000442
O	2.403486	-0.139063	0.000046
H	2.337796	-1.102083	0.000259

1c

C	-1.839772	0.110555	0.000134
C	-0.608788	-0.403996	0.000006
H	-1.998884	1.185418	0.000240
H	-2.722196	-0.519074	0.000139
H	-0.472039	-1.484584	-0.000099
C	0.608792	0.403888	-0.000006
C	1.839843	-0.110519	-0.000134
H	0.471720	1.484433	0.000099
H	1.998980	-1.185464	-0.000240
H	2.721964	0.519700	-0.000138

1d

C	-3.362063	0.211545	0.000192
C	-2.229105	-0.495984	-0.000098
H	-3.343425	1.297687	0.000495
H	-4.334684	-0.267405	0.000136
H	-2.264351	-1.583876	-0.000406
C	-0.912655	0.123438	-0.000005
C	0.244420	-0.553078	-0.000231
H	-0.859562	1.211873	0.000214
H	0.259970	-1.641137	-0.000483
C	1.544843	0.171469	-0.000064
O	1.601839	1.384926	-0.000158
C	2.790689	-0.686270	0.000261
H	2.797406	-1.336183	0.881137
H	2.797918	-1.336078	-0.880694
H	3.675250	-0.050997	0.000537

1e

C	3.320371	0.274934	0.000298
C	2.208144	-0.464141	-0.000121
H	3.271785	1.360156	0.000548
H	4.305798	-0.176943	0.000330
H	2.271879	-1.550436	-0.000437
C	0.875666	0.120754	-0.000175
C	-0.258361	-0.591057	-0.000232
H	0.794743	1.207156	-0.000116
H	-0.268260	-1.676243	-0.000271
C	-1.560157	0.107485	-0.000254
O	-1.718884	1.306064	-0.000073
O	-2.592462	-0.759650	0.000353
H	-3.399158	-0.222850	0.000601

1f

C	2.836499	-0.401789	0.000176
C	1.747072	0.370161	0.000046
H	2.757664	-1.485202	0.000282
H	3.834131	0.021882	0.000182
H	1.841536	1.454157	-0.000058
C	0.397501	-0.173547	0.000037
C	-0.704528	0.592941	-0.000092
H	0.294067	-1.256752	0.000139
H	-0.639037	1.676914	-0.000198
C	-2.020970	0.030801	-0.000100
N	-3.088829	-0.417486	-0.000106

2a

C	-1.251647	0.305579	0.161084
C	-0.292057	-0.624493	-0.015363
H	-0.555541	-1.667943	-0.162438
C	1.125952	-0.305404	0.002631
C	1.661723	1.100938	0.196843
C	2.137714	-1.181752	-0.096311
C	3.152451	0.970246	-0.173231
H	1.521769	1.412524	1.240817
C	3.488261	-0.523997	0.018607
H	2.007197	-2.255228	-0.195230
H	3.281091	1.230796	-1.227939
H	3.795993	1.632354	0.410595
H	4.211150	-0.885233	-0.720494
H	3.930453	-0.714692	1.006662
H	1.145579	1.839080	-0.426848
H	-0.971034	1.349442	0.288995
N	-2.614023	0.091612	0.253481
C	-3.475926	1.155893	-0.223728
H	-3.568057	1.169859	-1.320756
H	-4.474639	1.039521	0.205548
H	-3.075929	2.120053	0.099024
C	-3.093207	-1.247636	-0.002618

H	-4.168610	-1.285402	0.183302
H	-2.900338	-1.572539	-1.037863
H	-2.600513	-1.950118	0.674784

2b

C	2.165131	-0.335575	0.022670
C	1.215555	0.604796	-0.051762
H	1.507740	1.651237	-0.139117
C	-0.207842	0.309317	-0.007939
C	-0.757335	-1.098599	0.119003
C	-1.203442	1.207025	-0.015276
C	-2.258642	-0.921699	-0.184622
H	-0.583537	-1.476030	1.135683
C	-2.560067	0.563678	0.108527
H	-1.057205	2.282296	-0.054563
H	-2.432023	-1.117160	-1.246767
H	-2.890989	-1.606654	0.384350
H	-3.300993	0.982203	-0.580296
H	-2.961258	0.702530	1.121995
H	-0.275600	-1.802312	-0.568430
H	1.936857	-1.392649	0.118070
O	3.503015	-0.127064	-0.003430
H	3.672740	0.819402	-0.087090

2c

C	2.729053	-0.339569	0.016193
C	1.767419	0.583433	-0.062102
H	2.038190	1.633426	-0.161836
C	0.338774	0.292465	-0.013125
C	-0.225387	-1.107643	0.115332
C	-0.643277	1.204255	-0.016090
C	-1.727091	-0.911018	-0.178801
H	-0.049594	-1.488079	1.130277
C	-2.007486	0.579404	0.113160
H	-0.480984	2.277389	-0.057689
H	-1.911031	-1.106009	-1.239275
H	-2.365790	-1.585140	0.395739
H	-2.745118	1.010165	-0.571296
H	-2.398559	0.727834	1.129056
H	0.246123	-1.814778	-0.574845
H	2.496713	-1.395201	0.121431
H	3.778021	-0.067569	-0.018960

2d

C	-1.329804	0.326171	0.021589
C	-0.337984	-0.576350	-0.029811
H	-0.622515	-1.625943	-0.095147
C	1.077499	-0.260069	0.003432
C	1.634157	1.146929	0.079499
C	2.064883	-1.168781	0.029822
C	3.135490	0.946030	-0.215434
H	1.462967	1.561477	1.081601
C	3.424023	-0.531682	0.129836
H	1.905545	-2.242989	0.025887
H	3.313643	1.102790	-1.283057
H	3.773725	1.642843	0.331336
H	4.161244	-0.986812	-0.538628
H	3.815368	-0.642903	1.150294
H	1.155690	1.826793	-0.632715
H	-1.124196	1.391851	0.092326
C	-2.749913	-0.113965	-0.012176
O	-3.059086	-1.286790	-0.089728
C	-3.792861	0.980423	0.054920
H	-3.669549	1.559467	0.975681
H	-3.662799	1.673360	-0.782506
H	-4.789373	0.542156	0.022694

2e

C	1.335530	-0.375482	0.024796
C	0.367447	0.550330	-0.029661
H	0.670847	1.594154	-0.096904
C	-1.053517	0.259033	0.002923
C	-1.632962	-1.138098	0.082869
C	-2.024224	1.185221	0.024939
C	-3.130708	-0.912446	-0.212945
H	-1.468415	-1.552495	1.086025
C	-3.394186	0.571769	0.125137
H	-1.846431	2.256541	0.017528
H	-3.312009	-1.071635	-1.279618
H	-3.780515	-1.595278	0.337663
H	-4.121918	1.036868	-0.546794
H	-3.785044	0.694914	1.144345
H	-1.165817	-1.827579	-0.627491
H	1.130656	-1.438214	0.097533
C	2.749374	0.046602	-0.008670
O	3.148140	1.185901	-0.086786
O	3.588458	-1.007956	0.059194
H	4.485323	-0.642412	0.032124

2f

C	1.813803	-0.420648	0.037895
C	0.872884	0.535503	-0.046298
H	1.182536	1.573687	-0.144396
C	-0.552389	0.268976	-0.006420
C	-1.154396	-1.115494	0.115406
C	-1.506264	1.212634	-0.013822
C	-2.648229	-0.872822	-0.187241
H	-0.996965	-1.502916	1.130417
C	-2.886178	0.625737	0.103158
H	-1.311042	2.280268	-0.053826
H	-2.832890	-1.063714	-1.247949
H	-3.308256	-1.526467	0.385796
H	-3.604221	1.082190	-0.584663
H	-3.275530	0.788809	1.117168
H	-0.701837	-1.833921	-0.575714
H	1.553591	-1.469294	0.141470
C	3.210190	-0.110042	0.001246
N	4.342584	0.132614	-0.027407

3a

C	0.790489	0.295968	0.048650
C	1.232757	-1.146871	-0.078667
C	2.708922	-1.346892	0.267951
C	3.568762	-0.273561	-0.394693
C	3.180527	1.103535	0.143072
C	1.687916	1.288990	0.168965

C	-0.642319	0.594780	0.031164
H	2.836531	-1.281917	1.355953
H	4.633009	-0.464544	-0.225177
H	3.589565	1.233573	1.156132
H	1.319909	2.308098	0.279894
H	-0.908781	1.641260	0.153511
H	0.615433	-1.771447	0.578027
H	1.034541	-1.493275	-1.102909
H	3.637643	1.893032	-0.465068
H	3.402372	-0.299438	-1.478971
H	3.030185	-2.349084	-0.032576
C	-1.607650	-0.325117	-0.157120
H	-1.347623	-1.375729	-0.267017
N	-2.967250	-0.090557	-0.287060
C	-3.849334	-1.125776	0.217071
H	-3.944429	-1.108776	1.314116
H	-4.844819	-1.002988	-0.217975
H	-3.466548	-2.105729	-0.078335
C	-3.428874	1.260598	-0.064832
H	-2.911625	1.942674	-0.744645
H	-4.499698	1.312100	-0.273220
H	-3.252089	1.602164	0.968314

3b

C	0.099708	0.305217	-0.057155
C	-0.347486	-1.139778	0.005089
C	-1.832355	-1.310565	-0.318894
C	-2.668403	-0.266725	0.417695
C	-2.280613	1.135207	-0.052773
C	-0.787701	1.311543	-0.103327
C	1.536212	0.587989	-0.050778
H	-1.982340	-1.188902	-1.399013
H	-3.737357	-0.439800	0.260251
H	-2.708653	1.324649	-1.048121
H	-0.412911	2.332076	-0.169238
H	1.825874	1.637531	-0.115990
H	0.252515	-1.732512	-0.695430
H	-0.129870	-1.538058	1.006230
H	-2.716326	1.893939	0.607619
H	-2.480842	-0.352043	1.495368
H	-2.155195	-2.324291	-0.062970
C	2.497668	-0.336342	0.052948
H	2.294454	-1.398987	0.134993
O	3.833125	-0.098168	0.077921
H	3.983462	0.852462	0.006101

3c

C	0.614747	0.298123	-0.040182
C	0.167647	-1.144735	0.019362
C	-1.312840	-1.312544	-0.326624
C	-2.157987	-0.266273	0.397164
C	-1.760398	1.136294	-0.064344
C	-0.267195	1.308102	-0.098380
C	2.053329	0.589819	-0.016747
H	-1.446656	-1.191269	-1.408968
H	-3.224777	-0.435704	0.222598
H	-2.171693	1.331444	-1.065438
H	0.113151	2.326783	-0.163394
H	2.316919	1.644384	-0.089735
H	0.780941	-1.738343	-0.668341
H	0.370495	-1.540034	1.024549
H	-2.200479	1.896434	0.591301
H	-1.988501	-0.353110	1.477654
H	-1.643181	-2.324829	-0.074871
C	3.029007	-0.313300	0.103191
H	2.825532	-1.375994	0.188948
H	4.070388	-0.012681	0.125045

3d

C	0.739650	-0.262141	-0.057521
C	1.194185	1.179446	-0.024871
C	2.682597	1.326610	-0.346192
C	3.505127	0.295151	0.423973
C	3.106656	-1.118132	-0.003558
C	1.615486	-1.282166	-0.068423
C	-0.689202	-0.557779	-0.060418
H	2.836323	1.174263	-1.421847
H	4.576101	0.450920	0.264783
H	3.534743	-1.348135	-0.990030
H	1.227088	-2.298289	-0.117363
H	-0.979926	-1.606914	-0.114065
H	0.598365	1.759350	-0.739065
H	0.975918	1.600436	0.966429
H	3.524749	-1.863720	0.682214
H	3.316848	0.414630	1.498086
H	3.015714	2.342849	-0.116107
C	-1.685505	0.338154	0.014375
H	-1.496065	1.406536	0.080510
C	-3.100594	-0.118332	0.016609
O	-3.401552	-1.293881	-0.054298
C	-4.153069	0.965368	0.111763
H	-4.011828	1.545260	1.029429
H	-4.052147	1.660073	-0.728197
H	-5.145454	0.516706	0.105193

3e

C	-0.717982	0.255894	-0.058419
C	-1.192950	-1.178681	-0.020079
C	-2.683322	-1.304599	-0.341434
C	-3.490528	-0.256863	0.423026
C	-3.070505	1.148293	-0.010839
C	-1.577080	1.289667	-0.074690
C	0.715286	0.529529	-0.060563
H	-2.834223	-1.155726	-1.417944
H	-4.563584	-0.396877	0.263518
H	-3.493432	1.380056	-0.999071
H	-1.173233	2.299610	-0.127310
H	1.022600	1.573371	-0.117315
H	-0.605684	-1.770336	-0.731598
H	-0.981045	-1.598373	0.973057
H	-3.477870	1.903576	0.670711
H	-3.305124	-0.373919	1.497873
H	-3.031687	-2.314399	-0.106085
C	1.689592	-0.387982	0.018878
H	1.502362	-1.453634	0.088591
C	3.097815	0.052454	0.021272

O	3.486440	1.195983	-0.049455
O	3.948359	-0.991673	0.113712
H	4.840573	-0.614099	0.108596

3f

C	-0.223905	0.258236	-0.061968
C	-0.719453	-1.167922	0.010078
C	-2.211137	-1.279126	-0.312069
C	-3.004479	-0.200169	0.422616
C	-2.562197	1.186674	-0.046186
C	-1.066925	1.304364	-0.107706
C	1.213129	0.512181	-0.064918
H	-2.356706	-1.156627	-1.392468
H	-4.078729	-0.328211	0.262357
H	-2.977152	1.399022	-1.042043
H	-0.648974	2.307138	-0.183955
H	1.523321	1.552135	-0.147328
H	-0.142474	-1.785969	-0.687632
H	-0.516566	-1.566972	1.013598
H	-2.959924	1.965939	0.613495
H	-2.824823	-0.292013	1.500794
H	-2.574119	-2.277207	-0.051143
C	2.162968	-0.432483	0.044052
H	1.922635	-1.486060	0.139109
C	3.554394	-0.096838	0.049187
N	4.682734	0.165617	0.053813

4a

C	0.697476	-1.417280	0.018215
C	2.766823	-0.167151	0.026486
C	2.117785	-1.421989	-0.575202
H	2.051022	-1.316388	-1.662767
H	2.670438	-2.338928	-0.357487
H	-0.022729	-1.982324	-0.581681
H	3.597980	0.224517	-0.565312
C	0.363551	0.057239	0.059014
C	1.621863	0.825816	0.153360
C	-0.847501	0.605793	-0.132182
H	-0.915275	1.685846	-0.274457
C	1.770200	2.139950	0.341921
H	0.921880	2.798544	0.498850
N	-2.059138	-0.083738	-0.220599
C	-3.194917	0.730747	-0.610888
H	-4.026231	0.081525	-0.898467
H	-3.541090	1.391341	0.201827
H	-2.931501	1.344930	-1.473896
C	-2.389743	-1.002540	0.858311
H	-2.699898	-0.466997	1.770234
H	-3.212874	-1.649267	0.541281
H	-1.536569	-1.632458	1.104613
H	2.755056	2.595233	0.354397
H	3.155486	-0.394070	1.027541
H	0.715051	-1.858847	1.025304

4b

C	-0.142335	-1.427025	0.059285
C	1.937509	-0.212144	0.283329
C	1.352740	-1.505730	-0.301770
H	1.462767	-1.493737	-1.390760
H	1.834491	-2.409390	0.077703
H	-0.760407	-2.003828	-0.639717
H	2.891081	0.080670	-0.161637
C	-0.434638	0.063479	0.031411
C	0.841384	0.810305	0.049912
C	-1.657042	0.603293	0.018928
H	-1.829356	1.674914	0.019893
C	1.036842	2.116753	-0.137990
H	0.216389	2.801410	-0.328752
H	2.034503	2.541473	-0.107556
H	2.094188	-0.335555	1.363098
H	-0.312670	-1.838258	1.063584
O	-2.825658	-0.085063	0.009776
H	-2.632480	-1.030782	0.007302

4c

C	0.095280	0.987476	-1.203314
C	-0.478903	1.751211	-0.000000
C	0.095280	0.987476	1.203314
H	1.128912	1.311398	-1.382891
H	-0.462891	1.136638	-2.130297
H	-0.218808	2.811772	-0.000000
H	-1.570803	1.669249	-0.000000
H	1.128912	1.311398	1.382891
H	-0.462891	1.136638	2.130297
C	0.095280	-0.459024	0.744888
C	0.095280	-0.459024	-0.744888
C	0.068336	-1.525972	1.542646
H	0.065989	-2.536579	1.146322
H	0.046122	-1.420475	2.622462
C	0.068336	-1.525972	-1.542646
H	0.065989	-2.536579	-1.146322
H	0.046122	-1.420475	-2.622462

4d

C	-0.616066	-1.375319	0.018238
C	-2.679788	-0.149689	-0.320557
C	-2.125868	-1.437366	0.307160
H	-2.294655	-1.415320	1.388681
H	-2.594925	-2.341480	-0.085967
H	0.003790	-1.908489	0.740159
H	-3.642267	0.166625	0.087161
C	-0.294449	0.103694	-0.022676
C	-1.576080	0.854208	-0.065657
C	0.927612	0.663658	-0.054301
H	1.021128	1.745978	-0.111533
C	-1.733507	2.159877	0.154570
H	-0.892525	2.807626	0.381936
H	-2.716117	2.619480	0.125424
H	-2.801808	-0.288581	-1.402735
H	-0.375524	-1.813709	-0.958398
C	2.184418	-0.115162	-0.026578
O	2.208541	-1.332871	-0.058248
C	3.464421	0.693639	0.035281
H	3.532573	1.354954	-0.834342
H	3.466793	1.329280	0.926309
H	4.321052	0.021361	0.056408

4e

C	-0.545592	-1.373061	0.003644
C	-2.649812	-0.214623	-0.315810
C	-2.049873	-1.484856	0.305120
H	-2.209891	-1.470240	1.388036
H	-2.491882	-2.403190	-0.086213
H	0.096973	-1.894297	0.713969
H	-3.619476	0.068518	0.099054
C	-0.273430	0.116621	-0.023796
C	-1.578637	0.824959	-0.064754
C	0.925601	0.720018	-0.045737
H	1.010992	1.800356	-0.094707
C	-1.775071	2.125297	0.154266
H	-0.953467	2.798929	0.376899
H	-2.771543	2.554176	0.128009
H	-2.774467	-0.354847	-1.397485
H	-0.304808	-1.790693	-0.981985
C	2.186952	-0.034580	-0.020040
O	2.311016	-1.240089	-0.044305
O	3.256415	0.789628	0.027196
H	4.037284	0.216329	0.033933

4f

C	-0.041874	-1.334870	0.120561
C	2.202455	-0.451528	0.226178
C	1.399276	-1.644124	-0.316596
H	1.456207	-1.658224	-1.409531
H	1.757085	-2.606669	0.053102
H	-0.811242	-1.821865	-0.483064
H	3.157942	-0.295002	-0.278652
C	-0.124854	0.173602	0.055605
C	1.253915	0.718800	0.056658
C	-1.258967	0.890708	0.006627
H	-1.255775	1.975248	-0.019856
C	1.597152	1.995892	-0.113005
H	0.856541	2.776972	-0.254406
C	-2.536389	0.248354	-0.006305
N	-3.564705	-0.286021	-0.017082
H	2.638566	2.300179	-0.121064
H	2.408414	-0.600306	1.293989
H	-0.199082	-1.649188	1.160713

5a

C	-1.400313	-1.855587	0.268261
C	-0.483517	-0.925415	1.100658
C	-2.634310	0.317638	-0.143853
C	-2.285802	-1.062048	-0.711787
H	-0.797968	-2.578339	-0.291816
H	-2.027849	-2.437652	0.951194
H	-1.747663	-0.916042	-1.655429
H	-3.192665	-1.626742	-0.946540
H	0.438158	-1.428021	1.400454
H	-3.350820	0.845246	-0.779998
C	-0.173002	0.343792	0.347526
C	-1.374330	1.149926	0.015924
C	1.054702	0.678228	-0.070225
H	1.196089	1.592130	-0.654858
C	-1.372982	2.478871	-0.112084
H	-0.478771	3.067006	0.067763
N	2.215246	-0.104971	0.169467
C	3.423095	0.701948	0.162732
H	4.279118	0.078670	0.434856
H	3.626520	1.155343	-0.824298
H	3.335111	1.503036	0.899882
C	2.333098	-1.236902	-0.744566
H	2.495985	-0.922123	-1.789581
H	3.176597	-1.862244	-0.436980
H	1.423532	-1.839459	-0.705912
H	-3.115886	0.190660	0.836210
H	-1.011067	-0.645994	2.021294
H	-2.274973	3.016628	-0.388023

5b

C	-0.640029	0.054175	0.086011
C	0.386357	1.121052	0.015819
C	1.720794	0.698327	-0.557988
C	2.201768	-0.616546	0.066950
C	1.147674	-1.709815	-0.107657
C	-0.175555	-1.307077	0.557413
H	1.606515	0.543294	-1.639959
H	3.148217	-0.924104	-0.388801
H	0.974816	-1.875821	-1.178300
H	-0.925149	-2.082126	0.353938
C	-1.900720	0.324757	-0.278658
C	0.156653	2.368403	0.435841
H	-2.177171	1.295091	-0.678920
H	0.911040	3.143087	0.335754
H	-0.788039	2.645539	0.892399
H	2.459428	1.492687	-0.416885
H	2.392998	-0.461741	1.136567
H	1.500626	-2.656086	0.314553
H	-0.029055	-1.288672	1.646246
O	-2.967551	-0.512462	-0.236210
H	-2.715472	-1.331100	0.206696

5c

C	0.710268	-0.739596	-0.070897
C	0.710109	0.739642	0.070749
C	-0.544441	1.463379	-0.398253
C	-1.737269	0.512631	-0.566136
C	-1.737022	-0.512867	0.566381
C	-0.544231	-1.463523	0.397949
H	-0.795914	2.243959	0.328295
H	-2.669283	1.084404	-0.590222
H	-1.661616	0.017009	1.524442
H	-0.332580	-1.972248	1.345334
C	1.751824	-1.391724	-0.591820
C	1.751354	1.392046	0.591951
H	2.628755	-0.858285	-0.943404
H	1.749048	2.474545	0.687365
H	2.628327	0.859013	0.943982
H	-0.332831	1.971632	-1.345897
H	-1.662287	-0.017265	-1.524218
H	-2.669003	-1.084676	0.590850
H	-0.795892	-2.243750	-0.328930

H	1.749726	-2.474257	-0.687137

5d

C	0.060841	0.175914	-0.110983
C	1.215715	1.109817	-0.078711
C	2.483084	0.632714	0.613103
C	2.566278	-0.899089	0.707124
C	1.884985	-1.530766	-0.505321
C	0.379557	-1.271739	-0.426966
H	3.344594	1.019565	0.059277
H	3.611500	-1.208923	0.791172
H	2.301023	-1.096766	-1.423580
H	-0.133218	-1.550379	-1.353462
C	-1.183971	0.637978	0.127116
C	1.149611	2.301147	-0.680043
H	-1.309304	1.685287	0.391042
H	2.000216	2.976955	-0.682457
H	0.254057	2.621990	-1.201611
H	2.530061	1.073902	1.615210
H	2.057385	-1.248763	1.613893
H	2.068568	-2.607865	-0.547235
H	-0.074647	-1.907687	0.340603
C	-2.410561	-0.185682	0.071465
O	-2.406379	-1.371193	-0.211618
C	-3.703853	0.536658	0.394047
H	-3.852439	1.371302	-0.298304
H	-4.538773	-0.158853	0.320232
H	-3.658099	0.958067	1.403176

5e

C	0.042146	0.194465	-0.100743
C	1.221732	1.096560	-0.072081
C	2.482749	0.578119	0.601066
C	2.522825	-0.956007	0.683681
C	1.812860	-1.559603	-0.526655
C	0.315956	-1.259897	-0.432232
H	3.348315	0.943780	0.039299
H	3.559422	-1.296245	0.755225
H	2.231688	-1.130508	-1.445843
H	-0.210684	-1.514963	-1.357593
C	-1.182961	0.692329	0.152776
C	1.179621	2.294952	-0.660992
H	-1.304257	1.734108	0.427728
H	2.047758	2.948025	-0.666061
H	0.286805	2.645065	-1.168147
H	2.554384	1.010617	1.605404
H	2.013004	-1.297575	1.593012
H	1.965699	-2.641035	-0.578091
H	-0.146967	-1.889055	0.335400
C	-2.410894	-0.114493	0.093296
O	-2.497818	-1.291812	-0.183156
O	-3.501075	0.624983	0.395396
H	-4.258224	0.023868	0.333063

5f

C	0.337004	0.260883	0.063729
C	-0.916475	1.049610	0.035990
C	-2.157229	0.361002	-0.514467
C	-1.999133	-1.162684	-0.604296
C	-1.205667	-1.673215	0.597454
C	0.243594	-1.192601	0.486420
H	-3.005429	0.605210	0.133671
H	-2.984063	-1.633295	-0.663390
H	-1.660888	-1.292391	1.520173
H	0.775502	-1.316801	1.436804
C	1.510206	0.826426	-0.275917
C	-0.951330	2.297568	0.511982
H	1.567318	1.853280	-0.619176
H	-1.871497	2.874777	0.504340
H	-0.071528	2.765905	0.940543
C	2.732782	0.084628	-0.215819
N	3.711238	-0.534190	-0.164233
H	-2.386534	0.775131	-1.502457
H	-1.461789	-1.432307	-1.522175
H	-1.226370	-2.764517	0.655587
H	0.784096	-1.805361	-0.244748

6a

C	-1.273285	-1.640700	-0.616476
C	-0.556481	-0.987021	0.592031
C	-2.355820	0.350422	0.287132
C	-2.508333	-0.713427	-0.830551
H	-0.629722	-1.685273	-1.499076
H	-1.583692	-2.661780	-0.374339
H	-2.525559	-0.254200	-1.821390
H	-3.442648	-1.267249	-0.698660
C	-1.764075	-0.502823	1.423809
H	-1.469519	0.084442	2.296938
H	-2.422785	-1.322087	1.730481
H	0.158120	-1.626262	1.113189
H	-3.268310	0.909404	0.501580
C	0.010533	0.346009	0.142072
C	-1.166942	1.218196	-0.087318
C	1.294936	0.718946	0.050877
H	1.518804	1.768247	-0.152020
C	-1.222403	2.467240	-0.553555
H	-0.332443	3.010759	-0.855457
N	2.413003	-0.106541	0.227858
C	3.678872	0.602730	0.256462
H	4.463915	-0.069334	0.613005
H	3.975943	0.981293	-0.736545
H	3.615909	1.445326	0.947674
C	2.481056	-1.305270	-0.595769
H	2.717970	-1.068519	-1.646232
H	3.261056	-1.966016	-0.206696
H	1.534842	-1.843799	-0.571852
H	-2.171235	2.985017	-0.647878

6b

C	-0.761521	-1.547031	-0.827999
C	0.038254	-1.122001	0.427644
C	-1.599342	0.432022	0.329510
C	-1.877266	-0.461544	-0.906899
H	-0.132419	-1.570479	-1.720649
H	-1.190714	-2.544102	-0.689272
H	-1.839491	0.115392	-1.833388

H	-2.870620	-0.913137	-0.831015
C	-1.092873	-0.611792	1.344330
H	-0.723505	-0.166599	2.271325
H	-1.835480	-1.383780	1.570075
H	0.668214	-1.911090	0.849565
H	-2.443043	1.053398	0.633966
C	0.743512	0.183808	0.098878
C	-0.326278	1.210334	0.047666
C	2.047388	0.373599	-0.116736
H	2.463492	1.350560	-0.343109
C	-0.240825	2.519002	-0.192174
H	0.706352	3.008681	-0.396016
H	-1.127480	3.144037	-0.188271
O	3.016111	-0.576328	-0.082060
H	2.609505	-1.430639	0.107947

6c

C	-1.459107	-0.778773	-0.856773
C	-0.593835	-1.132124	0.378596
C	-0.594202	1.131606	0.379555
C	-1.459449	0.779036	-0.856062
H	-1.042842	-1.201545	-1.773788
H	-2.471871	-1.173372	-0.733186
H	-1.043478	1.202850	-1.772727
H	-2.472374	1.173064	-0.731961
C	-0.986701	-0.000724	1.351175
H	-0.396032	-0.001041	2.270945
H	-2.053707	-0.000997	1.595776
H	-0.710185	-2.157357	0.733670
H	-0.710840	2.156512	0.735479
C	0.835416	-0.746034	0.048288
C	0.835113	0.746249	0.048634
C	1.856886	-1.568295	-0.181410
H	2.849670	-1.194088	-0.412395
C	1.856043	1.569047	-0.181552
H	2.848812	1.195375	-0.413462
H	1.731572	-2.645550	-0.140726
H	1.730289	2.646231	-0.140329

6d

C	-1.117926	-1.559285	-0.814528
C	-0.481980	-1.022055	0.494832
C	-2.328205	0.273958	0.239412
C	-2.378174	-0.661516	-0.995397
H	-0.420596	-1.500369	-1.652547
H	-1.394627	-2.608750	-0.682441
H	-2.365231	-0.095784	-1.929848
H	-3.294573	-1.258087	-0.977803
C	-1.743282	-0.667343	1.309372
H	-1.522435	-0.160190	2.252347
H	-2.373403	-1.541406	1.500693
H	0.247931	-1.689928	0.942419
H	-3.270234	0.772919	0.471648
C	0.050350	0.353706	0.151650
C	-1.159526	1.218348	0.045455
C	1.318317	0.734770	-0.073347
H	1.525295	1.774609	-0.319341
C	-1.206767	2.535482	-0.148188
H	-0.305700	3.133064	-0.248239
H	-2.155273	3.059784	-0.203871
C	2.487120	-0.173702	-0.013443
O	2.388993	-1.382716	0.092487
C	3.843537	0.495422	-0.110047
H	3.924154	1.045075	-1.053300
H	3.964235	1.222358	0.699242
H	4.627722	-0.258272	-0.053476

6e

C	-1.063489	-1.562325	-0.833308
C	-0.429335	-1.024966	0.477086
C	-2.310132	0.226882	0.251244
C	-2.349565	-0.697756	-0.991698
H	-0.377108	-1.473767	-1.677857
H	-1.309570	-2.620599	-0.711864
H	-2.362541	-0.123437	-1.920800
H	-3.248997	-1.319420	-0.969375
C	-1.691707	-0.709995	1.306548
H	-1.474497	-0.207105	2.252553
H	-2.297537	-1.601705	1.494444
H	0.320618	-1.678957	0.912597
H	-3.261706	0.700106	0.497668
C	0.064533	0.368407	0.148708
C	-1.167526	1.201818	0.053616
C	1.318385	0.790186	-0.071057
H	1.522820	1.828086	-0.313492
C	-1.246695	2.518028	-0.134123
H	-0.360464	3.136362	-0.239477
H	-2.207616	3.020222	-0.179543
C	2.489354	-0.100162	-0.011703
O	2.488789	-1.303334	0.131413
O	3.638679	0.595382	-0.156391
H	4.353908	-0.056878	-0.116902

6f

C	-0.590578	-1.607539	-0.832135
C	0.079035	-1.006761	0.432140
C	-1.912659	0.072832	0.331772
C	-1.959570	-0.867672	-0.898406
H	0.020889	-1.456697	-1.724263
H	-0.726547	-2.683825	-0.697647
H	-2.094521	-0.310405	-1.827901
H	-2.792452	-1.569695	-0.803399
C	-1.145780	-0.798230	1.347951
H	-0.906924	-0.270558	2.274704
H	-1.658958	-1.736466	1.578447
H	0.913499	-1.589330	0.823521
H	-2.882019	0.464891	0.642271
C	0.423784	0.423568	0.088461
C	-0.876799	1.141349	0.039982
C	1.643202	0.932198	-0.143356
H	1.790135	1.976091	-0.401065
C	-1.082787	2.437189	-0.188935
H	-0.263073	3.124084	-0.376677
C	2.815658	0.116218	-0.063269
N	3.760502	-0.551558	0.002273
H	-2.084586	2.853901	-0.189131

7a

C	-0.239895	0.076519	0.057184
C	-1.373499	1.026140	0.123877
C	-2.689758	0.485908	-0.205569
C	-2.903071	-0.842115	-0.296960
C	-1.814594	-1.782682	-0.132877
C	-0.548017	-1.342418	0.040680
H	-3.510926	1.190255	-0.307262
H	-3.901100	-1.222016	-0.493545
H	-2.017949	-2.846196	-0.198258
H	0.256995	-2.066931	0.073719
C	1.009748	0.604954	-0.146043
C	-1.240525	2.315729	0.507185
H	1.054506	1.646169	-0.468003
H	-2.083410	2.996671	0.454278
H	-0.313799	2.703603	0.913358
N	2.239501	0.043020	0.011373
C	2.469427	-1.175995	0.750652
H	1.709581	-1.274177	1.528163
H	2.449910	-2.073897	0.117475
H	3.454954	-1.119465	1.223989
C	3.367763	0.570296	-0.726240
H	4.256832	0.589219	-0.087610
H	3.595116	-0.031539	-1.616159
H	3.147305	1.589141	-1.051096

7b

C	0.531673	0.009801	0.048719
C	-0.528451	1.045666	0.016502
C	-1.886554	0.553076	-0.222177
C	-2.183501	-0.757820	-0.150316
C	-1.154216	-1.748833	0.126731
C	0.137490	-1.382554	0.227443
H	-2.664001	1.292259	-0.393677
H	-3.207709	-1.091529	-0.285105
H	-1.440056	-2.790703	0.225928
H	0.921840	-2.113974	0.388633
C	1.823095	0.334303	-0.164773
C	-0.308996	2.355757	0.239609
H	2.118718	1.347061	-0.428194
H	-1.116153	3.074120	0.144523
H	0.658522	2.738182	0.545088
O	2.813601	-0.586886	-0.066253
H	3.636797	-0.216703	-0.397599

7c

C	0.007869	0.745490	0.620891
C	-0.007869	-0.745490	0.620891
C	-0.183506	-1.404673	-0.675197
C	-0.113635	-0.719588	-1.829859
C	0.113635	0.719588	-1.829859
C	0.183506	1.404673	-0.675197
H	-0.320394	-2.482376	-0.672839
H	-0.209146	-1.234819	-2.780152
H	0.209146	1.234819	-2.780152
H	0.320394	2.482376	-0.672839
C	-0.183506	1.480838	1.729845
C	0.183506	-1.480838	1.729845
H	-0.412047	1.030828	2.689350
H	-0.135323	2.564133	1.689561
H	0.135323	-2.564133	1.689561
H	0.412047	-1.030828	2.689350

7d

C	0.178721	0.104183	-0.059991
C	1.336048	1.043234	-0.026035
C	2.658140	0.481372	0.249142
C	2.864373	-0.846808	0.223658
C	1.762655	-1.752356	-0.054947
C	0.495974	-1.313068	-0.206605
H	3.476477	1.177175	0.409740
H	3.855861	-1.255909	0.386832
H	1.970799	-2.815795	-0.120928
H	-0.324748	-1.996946	-0.371755
C	-1.088148	0.573289	0.099060
C	1.220556	2.351194	-0.322455
H	-1.218394	1.628212	0.325309
H	2.084868	3.005557	-0.270595
H	0.286837	2.790872	-0.653652
C	-2.343964	-0.204368	0.022343
O	-2.404938	-1.401857	-0.196242
C	-3.609006	0.604728	0.239482
H	-3.680619	1.404063	-0.504808
H	-4.475435	-0.050548	0.162516
H	-3.588239	1.079778	1.225371

7e

C	-0.157021	0.122440	0.053764
C	-1.342724	1.025073	0.022210
C	-2.648491	0.419985	-0.238836
C	-2.812868	-0.913703	-0.206205
C	-1.680700	-1.783043	0.067170
C	-0.427690	-1.304056	0.207376
H	-3.489188	1.089163	-0.396659
H	-3.792012	-1.354743	-0.359815
H	-1.854663	-2.852152	0.139588
H	0.413731	-1.963446	0.370547
C	1.089409	0.634633	-0.111250
C	-1.263522	2.337965	0.306986
H	1.215361	1.686738	-0.338282
H	-2.147602	2.965486	0.257126
H	-0.340190	2.808641	0.624485
C	2.344890	-0.126758	-0.035782
O	2.494766	-1.311800	0.173168
O	3.404765	0.689160	-0.237565
H	4.190616	0.126227	-0.174406

7f

C	0.250167	0.193576	0.023132
C	-1.023917	0.958290	-0.003226
C	-2.257510	0.193261	-0.188236
C	-2.264729	-1.149387	-0.120940
C	-1.030122	-1.881870	0.112813
C	0.157073	-1.250607	0.194899
H	-3.176999	0.754319	-0.325679

H	-3.192593	-1.701959	-0.221579
H	-1.073861	-2.962324	0.203542
H	1.079360	-1.805728	0.332999
C	1.448020	0.807461	-0.154585
C	-1.082691	2.285928	0.207745
H	1.516429	1.864253	-0.384710
H	-2.032370	2.808557	0.160959
H	-0.208257	2.875354	0.459168
C	2.683541	0.097947	-0.082089
N	3.687043	-0.480009	-0.023111

7ba

C	-1.233002	0.455319	-0.118608
C	-1.456369	-0.968647	-0.476289
C	-2.746013	-1.534053	-0.067885
C	-3.772456	-0.749705	0.307640
C	-3.619637	0.694664	0.360598
C	-2.418371	1.266069	0.146283
H	-2.867578	-2.610330	-0.153249
H	-4.733881	-1.187929	0.556690
H	-4.480150	1.308018	0.606551
H	-2.287345	2.337773	0.235456
C	-0.006407	1.035752	-0.015594
C	-0.614179	-1.712415	-1.219046
H	-0.848631	-2.750572	-1.432113
H	0.301475	-1.313697	-1.638299
O	0.053815	2.399233	0.069603
H	0.903372	2.644699	0.456060
C	1.316773	0.371435	0.050841
C	2.390256	0.897944	-0.675249
C	1.541161	-0.708943	0.914692
C	3.661099	0.336732	-0.563978
H	2.219512	1.735545	-1.346156
C	2.807971	-1.261496	1.027178
H	0.708851	-1.105727	1.487003
C	3.871873	-0.743074	0.285300
H	4.483196	0.744965	-1.142801
H	2.973233	-2.094967	1.702102
H	4.861236	-1.179137	0.376630

MDA

C	0.327610	0.048808	-0.000425
O	0.305130	1.258792	-0.000227
C	-0.841533	-0.817774	-0.000201
H	-0.828198	-1.895025	0.001022
N	-2.003263	-0.218234	-0.000299
N	-2.991948	0.321471	0.000576
O	1.452675	-0.689763	-0.000221
C	2.656128	0.076704	0.000417
H	3.468321	-0.647827	-0.001844
H	2.704600	0.712817	-0.885639
H	2.706088	0.708715	0.889360

TS-(3+2)-1a

C	-3.080352	0.287457	-0.249602
O	-3.433387	1.254522	0.380024
C	-1.729992	0.058583	-0.800377
H	-1.631898	-0.576467	-1.673810
N	-0.930412	1.148133	-0.806252
N	-0.009901	1.574545	-0.262980
O	-3.845385	-0.797450	-0.466155
C	-5.136985	-0.738232	0.138734
H	-5.623602	-1.680131	-0.106956
H	-5.046011	-0.621131	1.220571
H	-5.705096	0.104948	-0.259060
C	1.730113	-0.568033	0.390978
C	0.466633	-0.204946	1.028070
C	2.883253	0.078271	0.646389
C	-0.693375	-0.938211	0.830636
H	2.874172	0.926045	1.330563
H	-1.507391	-0.847319	1.542684
H	-0.643366	-1.886804	0.303441
H	0.512586	0.484891	1.865859
H	1.702273	-1.391493	-0.318860
N	4.146219	-0.232114	0.168498
C	5.039557	0.889648	-0.053375
H	4.971787	1.580700	0.790206
H	6.069696	0.529535	-0.118879
H	4.804314	1.445578	-0.974290
C	4.228561	-1.277455	-0.825270
H	5.278002	-1.471605	-1.056825
H	3.786081	-2.195478	-0.429284
H	3.702813	-1.014297	-1.758283

TS-(3+2)-1a-product

C	-3.046606	0.066037	0.296529
O	-3.472999	1.124644	0.684821
C	-1.575902	-0.288538	0.174966
H	-1.458513	-1.354788	0.393385
N	-1.195781	-0.115738	-1.277682
N	-0.146788	0.511778	-1.401614
O	-3.818108	-0.942875	-0.120554
C	-5.218666	-0.662614	-0.128049
H	-5.700865	-1.566504	-0.494550
H	-5.562773	-0.421185	0.879650
H	-5.430998	0.182324	-0.785813
C	1.700028	0.020033	0.093582
C	0.483158	0.875394	-0.085898
C	2.939177	0.534127	0.101101
C	-0.638845	0.632321	0.938981
H	3.069447	1.605044	-0.051062
H	-1.166891	1.556787	1.181945
H	-0.260087	0.185159	1.858135
H	0.776003	1.927010	-0.156138
H	1.528457	-1.047592	0.207224
N	4.124374	-0.135330	0.331891
C	5.309117	0.387704	-0.323353
H	5.305145	1.478639	-0.265530
H	6.202109	0.021929	0.190054
H	5.371827	0.097384	-1.382781
C	4.057625	-1.576683	0.425429
H	5.045125	-1.965625	0.681505
H	3.359462	-1.861474	1.217236
H	3.724254	-2.042911	-0.515296

TS-(3+2)-1b

C	-2.249609	0.319178	-0.107385
O	-2.535766	1.050553	0.808328
C	-0.948687	0.278832	-0.806986
H	-0.928999	-0.065977	-1.834912
N	-0.140984	1.331381	-0.551567
N	0.817966	1.597299	0.024344
O	-3.044039	-0.657627	-0.577673
C	-4.285184	-0.794200	0.115538
H	-4.803060	-1.622716	-0.363483
H	-4.109364	-1.007093	1.171941
H	-4.868607	0.124912	0.034331
C	2.597615	-0.610359	-0.036115
C	1.360269	-0.462282	0.729154
C	3.768264	-0.087885	0.344794
C	0.199948	-1.134200	0.379052
H	3.873776	0.489406	1.258844
H	-0.572325	-1.284600	1.126338
H	0.229816	-1.878819	-0.411394
H	1.446236	-0.048605	1.729560
H	2.542867	-1.174205	-0.968747
O	4.951556	-0.190561	-0.311176
H	4.821076	-0.706485	-1.116062

TS-(3+2)-1b-product

C	-2.185235	-0.297722	-0.139222
O	-2.522305	-1.326076	0.391463
C	-0.746935	0.112809	-0.403541
H	-0.715830	0.672792	-1.343648
N	-0.359224	1.092632	0.677770
N	0.728413	0.816404	1.177310
O	-3.034135	0.651636	-0.541803
C	-4.408266	0.391529	-0.248178
H	-4.960229	1.249795	-0.625465
H	-4.733859	-0.526408	-0.741508
H	-4.549711	0.284031	0.828813
C	2.559230	0.104318	-0.248590
C	1.382239	-0.378341	0.542561
C	3.815563	-0.193517	0.080741
C	0.261398	-1.019979	-0.293033
H	4.053515	-0.816543	0.938652
H	-0.198715	-1.858519	0.233366
H	0.620778	-1.363243	-1.263352
H	1.728188	-1.019101	1.358746
H	2.350768	0.734910	-1.113539
O	4.937998	0.197999	-0.562634
H	4.700345	0.775968	-1.298265

TS-(3+2)-1c

C	-1.759481	0.339529	-0.054824
O	-1.971799	1.017019	0.920143
C	-0.499021	0.311344	-0.828043
H	-0.545419	0.039473	-1.876779
N	0.348260	1.326003	-0.548422
N	1.338653	1.548524	-0.013962
O	-2.606354	-0.581564	-0.542637
C	-3.813560	-0.730470	0.206756
H	-4.379977	-1.511710	-0.295992
H	-3.588822	-1.016787	1.236127
H	-4.372294	0.207258	0.215908
C	3.065956	-0.667595	-0.216156
C	1.840327	-0.567670	0.577297
C	4.269408	-0.243553	0.176175
C	0.671163	-1.200508	0.186540
H	4.412007	0.221537	1.147480
H	-0.089867	-1.423460	0.927571
H	0.688589	-1.867069	-0.671444
H	1.943500	-0.225932	1.603373
H	2.957098	-1.126295	-1.199895
H	5.143263	-0.348820	-0.456169

TS-(3+2)-1c-product

C	-1.542590	-0.237449	-0.184569
O	-1.347117	-1.354805	0.227881
C	-0.445820	0.677685	-0.701319
H	-0.862319	1.387561	-1.417067
N	0.018205	1.457018	0.510787
N	1.092297	1.035928	0.933825
O	-2.734424	0.361922	-0.196753
C	-3.799438	-0.407996	0.366913
H	-4.688734	0.213550	0.288035
H	-3.926705	-1.339818	-0.187382
H	-3.582210	-0.642899	1.410453
C	3.106320	0.044076	-0.080102
C	1.631688	-0.110001	0.129907
C	4.007051	-0.862266	0.281064
C	0.786125	-0.092471	-1.151625
H	3.712535	-1.781768	0.779433
H	0.549005	-1.099104	-1.494202
H	1.307689	0.447310	-1.946681
H	1.426389	-1.005445	0.728133
H	3.417581	0.962400	-0.577272
H	5.065566	-0.718814	0.093621

TS-(3+2)-1d

C	-3.033818	0.273912	-0.194192
O	-3.335599	1.231845	0.472315
C	-1.713048	0.049965	-0.830243
H	-1.675446	-0.549557	-1.733456
N	-0.925891	1.149721	-0.862244
N	0.009361	1.616431	-0.399826
O	-3.811588	-0.799827	-0.390845
C	-5.073637	-0.749431	0.279839
H	-5.574015	-1.684752	0.038472
H	-4.926396	-0.655173	1.357418
H	-5.655437	0.103619	-0.073817
C	1.791417	-0.462415	0.301221
C	0.515734	-0.198417	0.935644
C	2.966257	0.113972	0.609746
C	-0.597897	-0.981288	0.657985
H	3.039722	0.856888	1.400801
H	-1.410222	-1.022756	1.377075
H	-0.471548	-1.877647	0.056948
H	0.504944	0.462539	1.797422
H	1.808116	-1.195731	-0.507132
C	4.194288	-0.253815	-0.131386
O	4.190320	-1.071881	-1.033246

C	5.468186	0.447500	0.291759
H	5.672434	0.248675	1.348623
H	6.300115	0.099181	-0.318910
H	5.353488	1.530661	0.183024

TS-(3+2)-1d-product

C	-2.802054	0.264347	0.236250
O	-2.510511	1.422875	0.063439
C	-1.785141	-0.826834	0.528231
H	-2.257696	-1.636677	1.085343
N	-1.386611	-1.363550	-0.827158
N	-0.282969	-0.948919	-1.172904
O	-4.039381	-0.223063	0.146550
C	-5.037913	0.733305	-0.220381
H	-5.975441	0.183007	-0.257772
H	-5.085973	1.532410	0.521694
H	-4.803421	1.166354	-1.194382
C	1.796525	-0.352005	-0.001693
C	0.343467	-0.040604	-0.154180
C	2.781243	0.531931	-0.158641
C	-0.493939	-0.270925	1.112025
H	2.574984	1.561079	-0.446099
H	-0.649436	0.652726	1.668311
H	-0.015610	-1.009812	1.760293
H	0.203603	0.974318	-0.543353
H	2.062470	-1.371317	0.279561
C	4.205554	0.126587	0.049283
O	4.500522	-0.991509	0.415446
C	5.248922	1.185194	-0.223417
H	5.076497	2.054304	0.419586
H	6.242847	0.779118	-0.041550
H	5.169201	1.529377	-1.259539

TS-(3+2)-1e

C	-3.018429	0.267320	-0.193151
O	-3.323844	1.209761	0.493238
C	-1.696619	0.063091	-0.834587
H	-1.657220	-0.516954	-1.750385
N	-0.915926	1.167948	-0.844680
N	0.015355	1.632653	-0.373026
O	-3.790904	-0.805717	-0.411945
C	-5.053067	-0.775441	0.260147
H	-5.549817	-1.707021	-0.002209
H	-4.905625	-0.705075	1.339503
H	-5.638162	0.083159	-0.074010
C	1.810786	-0.443393	0.301831
C	0.528646	-0.202314	0.932375
C	2.974927	0.136862	0.636999
C	-0.575401	-0.989931	0.631460
H	3.058397	0.862247	1.439151
H	-1.389820	-1.056316	1.346189
H	-0.437257	-1.871611	0.011542
H	0.507641	0.440121	1.807604
H	1.837470	-1.158928	-0.521521
C	4.194907	-0.214973	-0.104152
O	4.269490	-0.995147	-1.028351
O	5.277784	0.444549	0.362551
H	6.023693	0.151276	-0.181396

TS-(3+2)-1e-product

C	-2.786662	0.261672	0.229736
O	-2.504437	1.412963	0.002307
C	-1.759068	-0.807408	0.564129
H	-2.221254	-1.595195	1.160167
N	-1.363728	-1.400968	-0.767808
N	-0.266576	-0.991610	-1.139720
O	-4.020475	-0.238474	0.171236
C	-5.029016	0.692755	-0.232040
H	-5.962467	0.134392	-0.237000
H	-5.077755	1.524754	0.472874
H	-4.804574	1.081994	-1.226659
C	1.813033	-0.323245	-0.012446
C	0.356078	-0.032006	-0.167230
C	2.780784	0.573078	-0.192791
C	-0.469312	-0.214856	1.114482
H	2.583670	1.595385	-0.499723
H	-0.629387	0.730776	1.631066
H	0.020109	-0.920678	1.790776
H	0.204001	0.963615	-0.598921
H	2.091329	-1.332581	0.290638
C	4.194134	0.180037	0.025901
O	4.572838	-0.907587	0.388492
O	5.036694	1.198405	-0.229560
H	5.931669	0.862957	-0.068761

TS-(3+2)-1f

C	-2.527583	0.297511	-0.129348
O	-2.814950	1.033784	0.780169
C	-1.213312	0.258142	-0.819074
H	-1.190287	-0.066701	-1.853916
N	-0.427541	1.327931	-0.556630
N	0.507518	1.658389	0.010094
O	-3.310662	-0.678314	-0.606769
C	-4.567228	-0.813978	0.064308
H	-5.072835	-1.645672	-0.421336
H	-4.409279	-1.021119	1.124346
H	-5.148373	0.104430	-0.034866
C	2.304584	-0.533393	0.134697
C	1.022169	-0.452533	0.804327
C	3.460143	-0.041772	0.620407
C	-0.086137	-1.133293	0.316170
H	3.500809	0.465384	1.579276
H	-0.896102	-1.378794	0.995726
H	0.045791	-1.830576	-0.506832
H	1.006451	-0.052616	1.813702
H	2.320927	-1.030275	-0.835206
C	4.688151	-0.162323	-0.099904
N	5.686175	-0.257460	-0.681691

TS-(3+2)-1f-product

C	-2.297857	-0.265349	-0.185311
O	-2.023353	-1.364569	0.231143
C	-1.258298	0.723717	-0.689159
H	-1.713420	1.418220	-1.396086
N	-0.838713	1.505561	0.532626
N	0.251277	1.132836	0.959522

O	-3.526351	0.246948	-0.215804
C	-4.544873	-0.596258	0.332648
H	-5.473168	-0.037200	0.239562
H	-4.597891	-1.533615	-0.223991
H	-4.326697	-0.815139	1.379303
C	2.307392	0.247154	-0.050483
C	0.843238	0.019971	0.141478
C	3.240239	-0.639925	0.302514
C	0.015862	0.028952	-1.151075
H	2.977685	-1.581838	0.775420
H	-0.166504	-0.978752	-1.522487
H	0.514739	0.617059	-1.926025
H	0.668519	-0.894832	0.718869
H	2.600526	1.185482	-0.518216
C	4.637731	-0.404918	0.075697
N	5.766470	-0.226749	-0.107422

TS-(3+2)-2a

C	-2.367043	1.433671	0.099719
O	-3.223966	1.844313	-0.646144
C	-2.355064	0.065798	0.648337
H	-3.318105	-0.420668	0.751247
N	-1.464547	-0.183576	1.633598
N	-0.420742	-0.647688	1.780930
O	-1.257597	2.120693	0.425063
C	-1.152903	3.403624	-0.190620
H	-0.216883	3.827853	0.168057
H	-1.140136	3.303115	-1.278144
H	-1.997169	4.034350	0.094380
C	1.159799	-0.215246	-0.470961
C	2.435907	-0.513612	-0.163719
H	2.679075	-1.501689	0.223090
H	0.892608	0.777856	-0.822324
N	3.546951	0.301231	-0.328059
C	3.296386	1.667646	-0.724839
H	4.249634	2.179644	-0.872661
H	2.746571	1.681154	-1.669886
H	2.707457	2.222022	0.025445
C	4.603196	0.140465	0.653956
H	4.779507	-0.923918	0.827020
H	5.527768	0.582168	0.272791
H	4.362721	0.611724	1.619788
C	-1.162204	-3.200884	-0.041686
C	-1.899937	-2.314427	-1.059901
C	-1.192649	-0.979511	-0.914264
C	0.063631	-1.170320	-0.339369
C	0.271309	-2.645890	-0.044216
H	-1.213416	-4.264898	-0.282809
H	-2.981239	-2.277209	-0.898023
H	-1.741500	-2.695809	-2.078107
H	-1.380311	-0.178032	-1.624032
H	0.802272	-2.833755	0.894538
H	0.863317	-3.097140	-0.854003
H	-1.603853	-3.064480	0.952384

TS-(3+2)-2a-product

C	-2.604993	1.078503	-0.009616
O	-3.728975	1.456350	-0.215186
C	-2.186802	-0.358688	0.232888
H	-3.103114	-0.954410	0.244296
N	-1.575917	-0.441370	1.598972
N	-0.395976	-0.781947	1.563589
O	-1.538868	1.896064	0.024687
C	-1.834318	3.278058	-0.179816
H	-0.881051	3.799301	-0.113796
H	-2.290739	3.427998	-1.160314
H	-2.522727	3.634166	0.588695
C	1.206524	0.024199	-0.055274
C	2.517946	-0.255876	-0.082374
H	2.861170	-1.277096	0.072355
H	0.845292	1.043604	-0.150206
N	3.549896	0.629587	-0.339490
C	3.203576	2.029807	-0.436307
H	4.093190	2.600888	-0.709876
H	2.450388	2.168331	-1.216784
H	2.800157	2.428948	0.508239
C	4.817380	0.354297	0.311337
H	5.028949	-0.716290	0.257632
H	5.618440	0.886777	-0.208134
H	4.827121	0.655881	1.369707
C	-0.746299	-3.214270	-0.210640
C	-1.398232	-2.300980	-1.255883
C	-1.119259	-0.875966	-0.740940
C	0.138658	-1.003440	0.173932
C	0.560988	-2.479859	0.095424
H	-0.593562	-4.235588	-0.566659
H	-2.464187	-2.494506	-1.405254
H	-0.899537	-2.442365	-2.220777
H	-0.948596	-0.166332	-1.552330
H	1.052385	-2.803942	1.016312
H	1.259490	-2.608593	-0.738959
H	-1.367354	-3.264688	0.691956

TS-(3+2)-2b

C	-2.396386	-0.238234	0.008653
O	-3.252392	-0.618513	-0.753452
C	-1.377783	-1.129414	0.593179
H	-1.653582	-2.173296	0.690045
N	-0.636617	-0.628980	1.605085
N	0.402793	-0.176841	1.803309
O	-2.187478	1.051635	0.326990
C	-3.090794	1.966654	-0.293745
H	-2.818699	2.951419	0.081143
H	-2.988679	1.923548	-1.380220
H	-4.121359	1.724261	-0.027881
C	1.338997	1.227742	-0.413653
C	2.437175	1.917923	-0.087071
H	3.331100	1.443415	0.305789
H	0.464879	1.758718	-0.792345
C	1.800846	-2.519489	0.037335
C	0.709538	-2.417154	-1.041824
C	0.238667	-0.980567	-0.902486
C	1.225328	-0.221957	-0.275523
C	2.407711	-1.107823	0.076670
H	2.536659	-3.299552	-0.168909
H	-0.079125	-3.167443	-0.934902

H	1.150419	-2.554710	-2.038657
H	-0.435854	-0.548274	-1.636974
H	2.863635	-0.863242	1.041479
H	3.185424	-0.997025	-0.693250
H	1.340405	-2.745875	1.006310
O	2.603950	3.261017	-0.196371
H	1.789113	3.649610	-0.536927

TS-(3+2)-2b-product

C	-2.368708	-0.139062	-0.050831
O	-3.499884	-0.487274	-0.266180
C	-1.198835	-1.063601	0.225531
H	-1.600012	-2.080012	0.246165
N	-0.677318	-0.754070	1.595364
N	0.480828	-0.345233	1.574494
O	-1.974569	1.146337	-0.034219
C	-3.018093	2.094333	-0.267383
H	-2.549967	3.074963	-0.207558
H	-3.461177	1.936083	-1.252573
H	-3.796087	1.991747	0.491065
C	1.359149	1.203915	-0.058527
C	2.583847	1.728347	-0.086210
H	3.483754	1.135464	0.044328
H	0.485242	1.845253	-0.169530
C	1.633853	-2.563539	-0.146366
C	0.594151	-2.210807	-1.216984
C	-0.012950	-0.880502	-0.731788
C	1.069337	-0.244899	0.193711
C	2.270679	-1.204305	0.151630
H	2.355938	-3.312920	-0.477672
H	-0.160782	-2.986968	-1.369794
H	1.100763	-2.051047	-2.174782
H	-0.272184	-0.215635	-1.557611
H	2.841798	-1.168875	1.082571
H	2.929522	-0.918889	-0.676013
H	1.139740	-2.950620	0.752969
O	2.890799	3.033014	-0.279646
H	2.073529	3.540671	-0.356924

TS-(3+2)-2c

C	-1.370683	-0.073990	-0.785102
N	-0.651987	1.035602	-1.062592
N	0.222200	1.663249	-0.663134
C	-2.729342	0.194170	-0.266645
O	-3.134315	1.258994	0.129451
O	-3.422878	-0.954738	-0.208021
C	-4.711940	-0.836196	0.396057
H	-5.335542	-0.144323	-0.173228
H	-5.137849	-1.837428	0.384721
H	-4.619592	-0.466678	1.419318
H	-1.240336	-0.885732	-1.492225
C	-0.254214	-0.585319	0.999466
C	0.787194	0.327213	1.065810
H	0.701601	1.175199	1.739131
C	2.123738	0.020629	0.559202
C	3.257816	0.683311	0.825356
C	2.396690	-1.160546	-0.352531
C	4.457079	0.059688	0.158518
H	3.322540	1.544663	1.483015
C	3.812160	-0.872141	-0.889799
H	1.654724	-1.255213	-1.155271
H	2.359951	-2.096717	0.221352
H	5.129915	0.794375	-0.295350
H	5.055293	-0.505361	0.886846
H	3.728978	-0.333815	-1.838580
H	4.392660	-1.779024	-1.073315
H	-0.061556	-1.599987	0.663759
H	-1.095729	-0.476874	1.676487

TS-(3+2)-2c-product

C	-1.116052	-0.139198	0.177601
N	-0.783061	-0.125589	-1.293952
N	0.210782	0.557358	-1.531477
C	-2.607595	0.115600	0.306986
O	-3.102839	1.173060	0.605888
O	-3.306903	-0.983607	0.012557
C	-4.725590	-0.812811	0.021597
H	-5.018760	-0.055226	-0.707546
H	-5.143077	-1.782439	-0.241399
H	-5.063344	-0.500764	1.011802
H	-0.906032	-1.156940	0.523628
C	-0.235992	0.938366	0.791385
C	0.833752	1.136553	-0.295771
H	1.052220	2.186994	-0.503768
C	2.112470	0.393744	-0.041113
C	3.337048	0.917277	0.021525
C	2.131705	-1.094472	0.244577
C	4.379559	-0.117537	0.363592
H	3.562910	1.970653	-0.114827
C	3.629315	-1.446731	0.125708
H	1.510291	-1.665064	-0.454550
H	1.745950	-1.293305	1.255033
H	5.283386	-0.031909	-0.246917
H	4.693856	-0.008205	1.410105
H	3.830699	-1.790905	-0.892434
H	3.936453	-2.239302	0.810921
H	0.194451	0.638658	1.747582
H	-0.826840	1.844985	0.936286

TS-(3+2)-2d

C	-1.107654	-1.567664	-0.307658
O	-1.619294	-1.298075	-1.367759
C	0.342041	-1.512716	-0.017023
H	0.749387	-2.139298	0.771239
N	1.146954	-1.457409	-1.107439
N	1.943841	-0.796464	-1.597342
O	-1.777498	-1.863683	0.811924
C	-3.196716	-1.744407	0.698762
H	-3.592831	-1.972090	1.686313
H	-3.460723	-0.727048	0.399835
H	-3.578521	-2.447374	-0.043828
C	0.684944	0.450749	0.677057
H	0.797279	0.056212	1.685025
C	1.867456	0.797640	0.015621
H	1.885932	1.597442	-0.717141
C	-2.374597	2.004145	-0.941056

C	-2.731578	2.087240	0.558339
C	-1.613295	1.304226	1.200607
C	-0.572725	1.148994	0.371499
C	-0.849535	1.790455	-0.973851
H	-2.700347	2.878068	-1.509004
H	-3.725935	1.684625	0.780494
H	-2.727943	3.124389	0.920788
H	-1.637627	0.949477	2.227112
H	-0.534595	1.156651	-1.809209
H	-0.305047	2.741193	-1.056437
H	-2.850803	1.118662	-1.373738
C	3.131452	0.264859	0.544453
O	3.133780	-0.667451	1.336995
C	4.415913	0.865721	0.019605
H	4.449981	1.937365	0.237025
H	5.269300	0.365747	0.476034
H	4.456786	0.751306	-1.068464

TS-(3+2)-2d-product

C	1.132689	-1.520064	0.399767
O	1.753546	-1.299197	1.406937
C	-0.335942	-1.229445	0.183805
H	-0.802920	-2.062615	-0.352335
N	-1.054334	-1.082944	1.472353
N	-1.852069	-0.145518	1.453305
O	1.673028	-1.987915	-0.733408
C	3.096385	-2.101976	-0.707438
H	3.382466	-2.492096	-1.682079
H	3.542366	-1.118239	-0.538551
H	3.411553	-2.777899	0.089222
C	-0.564602	0.107884	-0.571460
H	-0.742769	-0.092338	-1.628874
C	-1.847639	0.561280	0.121565
H	-1.910590	1.635740	0.319525
C	2.365188	2.152772	0.763036
C	2.534957	2.325994	-0.761176
C	1.478748	1.397855	-1.310153
C	0.583917	1.055266	-0.380059
C	0.903719	1.706178	0.953985
H	2.620878	3.049788	1.330721
H	3.544225	2.077526	-1.103825
H	2.339279	3.359035	-1.079269
H	1.440291	1.075129	-2.346694
H	0.784530	1.024520	1.801177
H	0.236427	2.563185	1.124570
H	3.013131	1.338731	1.103484
C	-3.126285	0.079084	-0.578186
O	-3.067700	-0.703563	-1.497816
C	-4.421124	0.591882	-0.005428
H	-4.487303	1.674115	-0.155700
H	-5.262645	0.098624	-0.489904
H	-4.435154	0.411170	1.073677

TS-(3+2)-2e

C	2.397953	-1.049831	0.414314
O	1.746370	-2.016766	0.720625
C	2.068600	0.349312	0.772531
H	2.868551	1.079994	0.823526
N	1.138910	0.446982	1.748094
N	0.022611	0.631850	1.919110
O	3.466343	-1.069563	-0.395917
C	3.791449	-2.362920	-0.913741
H	4.653435	-2.213907	-1.560547
H	4.032874	-3.046440	-0.097853
H	2.948607	-2.768281	-1.476790
C	-1.455492	-0.098297	-0.321994
C	-2.777546	0.017454	-0.110859
H	-3.254073	0.963766	0.121111
H	-1.064776	-1.093727	-0.535542
C	0.422439	3.196627	-0.206326
C	1.250069	2.328932	-1.169539
C	0.767490	0.926281	-0.842764
C	-0.510385	0.998004	-0.282095
C	-0.917992	2.449101	-0.102970
H	0.316866	4.229864	-0.542704
H	2.330021	2.471858	-1.073550
H	0.985147	2.560155	-2.209802
H	1.065028	0.080921	-1.458192
H	-1.447140	2.639095	0.836036
H	-1.590179	2.742958	-0.921906
H	0.907612	3.217659	0.777346
C	-3.633149	-1.175360	-0.194544
O	-3.270802	-2.299571	-0.461314
O	-4.928751	-0.885168	0.062994
H	-5.408517	-1.723010	-0.014749

TS-(3+2)-2e-product

C	2.310828	-0.905837	-0.200671
O	1.545938	-1.744410	-0.610207
C	1.923024	0.542234	0.054339
H	2.814948	1.171664	-0.003934
N	1.442170	0.575068	1.477870
N	0.232389	0.771240	1.552294
O	3.580575	-1.142938	0.128114
C	3.987312	-2.509594	0.006852
H	5.028908	-2.537072	0.319172
H	3.372329	-3.142513	0.648930
H	3.882496	-2.843844	-1.026953
C	-1.370383	-0.200876	0.031901
C	-2.698148	-0.123883	0.108276
H	-3.229105	0.800894	0.308133
H	-0.905938	-1.168658	-0.158351
C	0.120915	3.270046	-0.135676
C	0.830839	2.481800	-1.245076
C	0.744420	1.008464	-0.798714
C	-0.435127	0.958609	0.214383
C	-1.058617	2.360930	0.217007
H	-0.186874	4.269527	-0.449957
H	1.860333	2.807173	-1.419228
H	0.284725	2.606529	-2.185805
H	0.588682	0.321621	-1.632066
H	-1.530259	2.587261	1.176246
H	-1.820524	2.415542	-0.568663
H	0.778608	3.381377	0.734360
C	-3.516235	-1.346565	-0.076280
O	-3.094466	-2.451336	-0.317522

O	-4.832070	-1.083713	0.057117
H	-5.293020	-1.926436	-0.071092

TS-(3+2)-2f

C	2.382349	-0.804502	-0.010787
O	3.316966	-0.868133	-0.769566
C	1.886646	0.473529	0.553959
H	2.615895	1.271835	0.637236
N	1.029223	0.370772	1.594311
N	-0.082782	0.413816	1.861656
O	1.595144	-1.835354	0.325065
C	1.956428	-3.085527	-0.271586
H	1.236847	-3.809332	0.104299
H	1.902511	-3.013031	-1.359402
H	2.972210	-3.360965	0.016838
C	-1.612897	-0.294076	-0.351930
C	-2.918405	-0.377949	-0.029838
H	-3.472967	0.482343	0.330630
H	-1.101650	-1.190148	-0.700815
C	-0.166683	3.193139	0.003386
C	0.697906	2.541793	-1.089261
C	0.415261	1.061822	-0.895280
C	-0.819696	0.912097	-0.257806
C	-1.394397	2.270666	0.097482
H	-0.423191	4.231340	-0.215318
H	1.755496	2.812935	-1.033594
H	0.340578	2.839861	-2.083641
H	0.770165	0.334714	-1.621721
H	-1.876862	2.296483	1.079696
H	-2.151232	2.555047	-0.647777
H	0.374773	3.180598	0.957119
C	-3.639211	-1.606124	-0.147697
N	-4.226908	-2.600729	-0.243308

TS-(3+2)-2f-product

C	2.358858	-0.751928	-0.081852
O	3.519285	-0.935976	-0.334862
C	1.716798	0.601757	0.171624
H	2.516840	1.344682	0.128787
N	1.171457	0.594739	1.562252
N	-0.051916	0.694780	1.593175
O	1.442921	-1.730130	0.004149
C	1.950163	-3.052909	-0.202147
H	1.097528	-3.719329	-0.090339
H	2.382523	-3.138947	-1.200581
H	2.717913	-3.278208	0.539665
C	-1.536944	-0.405061	0.049776
C	-2.871768	-0.398238	0.010033
H	-3.450816	0.514927	0.103192
H	-0.995757	-1.345905	-0.025538
C	-0.261390	3.141874	-0.198604
C	0.504603	2.359411	-1.272745
C	0.525343	0.909786	-0.749953
C	-0.681329	0.814033	0.229671
C	-1.388865	2.175381	0.172659
H	-0.625550	4.109308	-0.549923
H	1.507925	2.747566	-1.466922
H	-0.050904	2.397063	-2.215588
H	0.455242	0.176385	-1.555763
H	-1.888320	2.405346	1.116865
H	-2.137855	2.162420	-0.627300
H	0.378468	3.322462	0.673240
C	-3.620094	-1.611418	-0.157693
N	-4.230559	-2.584526	-0.299526

TS-(3+2)-3a

C	-1.540005	1.822053	0.185905
O	-2.166146	2.155283	-0.797509
C	-1.776990	0.553071	0.875069
H	-2.816360	0.299387	1.055017
N	-0.942646	0.193649	1.899069
N	-0.117236	-0.591577	2.083363
O	-0.508803	2.525077	0.690354
C	-0.120407	3.654075	-0.091440
H	0.700084	4.120684	0.450612
H	0.208595	3.332590	-1.083064
H	-0.955599	4.347472	-0.203163
C	1.442383	-1.000569	-0.118719
C	1.618242	0.428034	-0.589462
C	3.032697	0.708786	-1.097620
C	4.067321	0.174675	-0.109999
C	3.940014	-1.344212	0.006920
C	2.505331	-1.777193	0.145016
C	0.079575	-1.502808	0.129146
H	3.175634	0.217649	-2.068385
H	5.081048	0.450468	-0.416620
H	4.386966	-1.822755	-0.876903
H	2.330469	-2.795736	0.488573
H	0.034111	-2.502921	0.549622
H	0.894294	0.665597	-1.379345
H	1.381076	1.101139	0.245813
H	4.516773	-1.708447	0.865160
H	3.889716	0.629472	0.872594
H	3.162804	1.784071	-1.258657
C	-1.037236	-1.030284	-0.569928
H	-0.898100	-0.266811	-1.329410
N	-2.188734	-1.787073	-0.793561
C	-2.593638	-2.704920	0.248482
H	-2.833381	-2.185325	1.193715
H	-3.483497	-3.245471	-0.080725
H	-1.811499	-3.439053	0.448715
C	-3.294281	-1.065717	-1.391349
H	-3.994935	-1.776668	-1.836561
H	-3.843401	-0.445621	-0.663330
H	-2.922937	-0.397556	-2.170651

TS-(3+2)-3a-product

C	-1.303721	1.741528	-0.160303
O	-1.473798	1.981301	-1.331701
C	-1.659813	0.402139	0.454665
H	-2.753064	0.395788	0.542388
N	-1.098410	0.226836	1.822069
N	-0.242367	-0.659770	1.860985
O	-0.784994	2.606130	0.712331
C	-0.392034	3.859090	0.148568
H	-0.013198	4.450470	0.979317

H	0.386081	3.703734	-0.603005
H	-1.245508	4.349781	-0.322391
C	1.414310	-0.909262	0.093125
C	1.683643	0.548617	-0.204516
C	3.067197	0.776905	-0.819975
C	4.128646	-0.053486	-0.102463
C	3.818054	-1.541927	-0.260460
C	2.373923	-1.837503	0.044432
C	0.015644	-1.286751	0.523071
H	3.042877	0.484102	-1.877016
H	5.126371	0.170841	-0.491305
H	4.053806	-1.869637	-1.282700
H	2.113543	-2.872369	0.260055
H	-0.030525	-2.371532	0.655253
H	0.924065	0.931069	-0.898926
H	1.570480	1.127772	0.723299
H	4.454739	-2.139591	0.401113
H	4.128670	0.203567	0.963826
H	3.314812	1.842381	-0.789677
C	-1.135258	-0.796389	-0.371210
H	-0.771406	-0.453517	-1.342743
N	-2.114479	-1.843244	-0.624975
C	-2.782634	-2.342930	0.565913
H	-3.451290	-1.602557	1.041110
H	-3.391136	-3.208641	0.291962
H	-2.055290	-2.666428	1.314261
C	-3.082612	-1.433906	-1.628678
H	-3.724889	-2.283000	-1.877482
H	-3.731459	-0.602805	-1.297529
H	-2.562621	-1.112360	-2.534417

TS-(3+2)-3b

C	2.787460	-0.813127	0.142818
O	3.398694	-1.574960	-0.563964
C	1.346336	-0.948615	0.426366
H	0.949623	-1.956788	0.363666
N	0.842978	-0.218190	1.460273
N	0.154455	0.691528	1.623376
O	3.300735	0.317034	0.664994
C	4.638503	0.593229	0.245847
H	4.927500	1.509467	0.757537
H	5.302361	-0.227819	0.521328
H	4.665635	0.725032	-0.838173
C	-1.828384	0.488008	-0.307240
C	-2.019515	-1.012831	-0.391208
C	-3.491408	-1.410493	-0.508549
C	-4.332266	-0.653112	0.516331
C	-4.264805	0.848519	0.238172
C	-2.855982	1.305113	-0.026308
C	-0.471121	1.024719	-0.471663
H	-3.850400	-1.168107	-1.516544
H	-5.370539	-0.997951	0.501122
H	-4.900673	1.095311	-0.624577
H	-2.667016	2.376401	0.023058
H	-0.360618	2.100933	-0.355051
H	-1.461477	-1.419998	-1.242227
H	-1.583545	-1.475606	0.507724
H	-4.678692	1.411119	1.082984
H	-3.938607	-0.853781	1.520702
H	-3.596088	-2.492230	-0.381134
C	0.548194	0.357867	-1.143136
H	0.367401	-0.503305	-1.775774
O	1.678741	1.025825	-1.543277
H	1.845679	1.745117	-0.920802

TS-(3+2)-3b-product

C	-2.826284	0.710580	-0.203993
O	-3.441718	1.517676	-0.846796
C	-1.324697	0.710402	-0.006959
H	-0.968939	1.712174	-0.258954
N	-0.988289	0.461358	1.429067
N	-0.091468	-0.373056	1.560642
O	-3.391315	-0.338733	0.422289
C	-4.811487	-0.430858	0.270208
H	-5.116334	-1.300998	0.847708
H	-5.286895	0.473355	0.653050
H	-5.069428	-0.551436	-0.783646
C	1.843142	-0.411339	0.072297
C	2.068889	1.083835	0.066443
C	3.461734	1.457524	-0.444526
C	4.524091	0.563023	0.191541
C	4.290259	-0.895364	-0.204415
C	2.843755	-1.285877	-0.060998
C	0.424298	-0.889536	0.256324
H	3.492731	1.329703	-1.533795
H	5.528007	0.880376	-0.105185
H	4.609272	-1.060194	-1.243106
H	2.614633	-2.350221	-0.057510
H	0.410103	-1.983061	0.301475
H	1.308166	1.573237	-0.556116
H	1.917793	1.469042	1.084327
H	4.906799	-1.562657	0.407869
H	4.464062	0.655159	1.282850
H	3.663611	2.512665	-0.238784
C	-0.595113	-0.400021	-0.795100
H	-0.102556	0.000256	-1.682986
O	-1.441342	-1.427811	-1.247579
H	-2.009248	-1.698791	-0.513399

TS-(3+2)-3c

C	3.049820	-0.143284	-0.322678
O	3.474702	-1.259096	-0.150847
C	1.675331	0.202896	-0.741040
H	1.517682	1.134529	-1.273471
N	0.951023	-0.838254	-1.206190
N	0.079273	-1.524809	-0.909187
O	3.737017	0.981767	-0.062714
C	5.043872	0.765425	0.471399
H	5.462701	1.755378	0.640664
H	4.984356	0.205587	1.406953
H	5.655164	0.203099	-0.236984
C	-1.813585	-0.144786	0.606090
C	-1.979068	1.157878	-0.146060
C	-3.444789	1.561222	-0.318031
C	-4.289444	0.363691	-0.746230
C	-4.256409	-0.709325	0.341853

C	-2.854511	-0.962740	0.825509
C	-0.458679	-0.529727	1.037920
H	-3.826434	1.941304	0.637981
H	-5.320143	0.667292	-0.953474
H	-4.892423	-0.403104	1.185301
H	-2.679085	-1.886668	1.374686
H	-0.379151	-1.494184	1.532654
H	-1.442242	1.959368	0.373675
H	-1.496810	1.060369	-1.131315
H	-4.687599	-1.645070	-0.032004
H	-3.879530	-0.051533	-1.675477
H	-3.524400	2.378221	-1.041803
C	0.608272	0.347880	1.143063
H	0.463456	1.417534	1.036365
H	1.453784	0.063166	1.761607

TS-(3+2)-3c-product

C	2.976534	-0.125032	0.313595
O	3.370925	-1.235877	0.565291
C	1.513625	0.282566	0.236515
H	1.422823	1.304621	0.616682
N	1.159810	0.349754	-1.228181
N	0.169703	-0.326242	-1.495831
O	3.774840	0.907359	0.029732
C	5.168730	0.595202	-0.009502
H	5.674439	1.525786	-0.258353
H	5.500677	0.220849	0.960904
H	5.363592	-0.165316	-0.767876
C	-1.826121	-0.439477	-0.102157
C	-1.935379	1.062142	0.031424
C	-3.281565	1.490628	0.616293
C	-4.422199	0.751431	-0.082344
C	-4.302411	-0.755449	0.152325
C	-2.891007	-1.242370	-0.041601
C	-0.438573	-0.997762	-0.306034
H	-3.303424	1.253415	1.687530
H	-5.393397	1.112917	0.268411
H	-4.633883	-1.005653	1.169984
H	-2.745309	-2.317315	-0.138092
H	-0.510779	-2.060599	-0.554185
H	-1.114721	1.440544	0.656176
H	-1.787924	1.514157	-0.958789
H	-4.971023	-1.301565	-0.522418
H	-4.371180	0.954213	-1.159093
H	-3.403988	2.573755	0.523536
C	0.549539	-0.725493	0.846623
H	0.043260	-0.333231	1.729838
H	1.091091	-1.631337	1.122812

TS-(3+2)-3d

C	0.745251	1.756452	-0.471824
O	1.360652	1.471385	-1.471372
C	-0.690103	1.496811	-0.235979
H	-1.235332	2.128905	0.460215
N	-1.431708	1.197186	-1.332588
N	-2.156096	0.400126	-1.723102
O	1.288514	2.276891	0.635716
C	2.709617	2.410663	0.591004
H	3.003571	2.781948	1.570792
H	3.170186	1.441098	0.388504
H	2.999737	3.113721	-0.192177
C	-0.805352	-0.384415	0.702280
H	-0.926497	0.138178	1.650140
C	-1.977316	-0.905804	0.143932
H	-1.976676	-1.810594	-0.451497
C	0.526297	-0.986088	0.459044
C	0.753829	-1.708778	-0.850419
C	1.509002	-0.810072	1.355906
C	2.096825	-2.440965	-0.895128
H	-0.057416	-2.423330	-1.026342
H	0.698473	-0.971575	-1.663292
C	2.922143	-1.289232	1.159016
H	1.283443	-0.273587	2.276773
C	3.207817	-1.567027	-0.316899
H	2.028478	-3.364970	-0.306964
H	2.324025	-2.732449	-1.924600
H	3.091908	-2.199711	1.751340
H	3.620132	-0.543793	1.559112
H	4.184707	-2.045478	-0.434111
H	3.233140	-0.617933	-0.868612
C	-3.257337	-0.362152	0.615365
O	-3.301397	0.686896	1.246118
C	-4.515971	-1.108035	0.231852
H	-4.483562	-2.131057	0.618124
H	-5.386796	-0.587636	0.628594
H	-4.587270	-1.172439	-0.858754

TS-(3+2)-3d-product

C	-0.709673	1.757531	0.551578
O	-1.381247	1.591934	1.536397
C	0.684506	1.221825	0.320112
H	1.303742	2.004578	-0.132407
N	1.351135	0.819431	1.582847
N	2.021610	-0.204101	1.438395
O	-1.131563	2.396722	-0.549030
C	-2.508143	2.774840	-0.523888
H	-2.696605	3.279419	-1.469376
H	-3.134670	1.883841	-0.429428
H	-2.707260	3.440370	0.317791
C	0.699651	-0.051492	-0.565251
H	0.868025	0.231987	-1.605244
C	1.937068	-0.721139	0.021619
H	1.900683	-1.813702	0.066076
C	-0.577234	-0.850510	-0.422865
C	-0.841067	-1.552403	0.893410
C	-1.479134	-0.828573	-1.411069
C	-2.064482	-2.468205	0.825351
H	0.040444	-2.132387	1.193918
H	-0.979921	-0.796442	1.677744
C	-2.847142	-1.451092	-1.319580
H	-1.229795	-0.306242	-2.334054
C	-3.223075	-1.755670	0.130576
H	-1.813722	-3.376118	0.261906
H	-2.346449	-2.782966	1.834097
H	-2.875155	-2.372165	-1.918658
H	-3.581127	-0.776340	-1.775530

H	-4.136000	-2.357155	0.170231
H	-3.425602	-0.814111	0.657418
C	3.248031	-0.273190	-0.639085
O	3.257720	0.620231	-1.454120
C	4.493950	-0.972956	-0.162637
H	4.455607	-2.028733	-0.449136
H	5.373750	-0.502688	-0.599698
H	4.536042	-0.933362	0.930057

TS-(3+2)-3e

C	0.731675	1.764212	-0.461044
O	1.355109	1.485791	-1.457226
C	-0.704625	1.498775	-0.236491
H	-1.251686	2.132415	0.456662
N	-1.438936	1.201531	-1.339133
N	-2.153705	0.397545	-1.734295
O	1.264809	2.281428	0.653008
C	2.685678	2.422364	0.618783
H	2.971192	2.788772	1.602880
H	3.152400	1.456479	0.413082
H	2.977440	3.131930	-0.157884
C	-0.825989	-0.398548	0.681744
H	-0.961884	0.108739	1.635316
C	-1.979902	-0.926058	0.094366
H	-1.980484	-1.825746	-0.504553
C	0.513016	-0.987228	0.446518
C	0.757683	-1.699472	-0.865449
C	1.484837	-0.810446	1.354741
C	2.106369	-2.421599	-0.901628
H	-0.046355	-2.419025	-1.053075
H	0.704524	-0.957688	-1.674246
C	2.903208	-1.278050	1.168343
H	1.246304	-0.282781	2.277459
C	3.205309	-1.543742	-0.306548
H	2.038631	-3.350084	-0.320610
H	2.345538	-2.704248	-1.930789
H	3.073328	-2.191351	1.756128
H	3.591762	-0.530476	1.580598
H	4.186657	-2.014525	-0.417121
H	3.229355	-0.590830	-0.851682
C	-3.260850	-0.420568	0.584436
O	-3.397730	0.611087	1.217301
O	-4.312948	-1.180171	0.221500
H	-5.100616	-0.728044	0.558539

TS-(3+2)-3e-product

C	-0.686597	1.768593	0.527608
O	-1.378047	1.625050	1.501866
C	0.706993	1.217300	0.330565
H	1.345537	1.985934	-0.117606
N	1.342446	0.818579	1.608266
N	2.007576	-0.210878	1.493492
O	-1.081513	2.393297	-0.591357
C	-2.454548	2.785326	-0.597932
H	-2.620393	3.276613	-1.554591
H	-3.091650	1.902092	-0.501031
H	-2.662309	3.466075	0.229300
C	0.723884	-0.067663	-0.539669
H	0.905935	0.201172	-1.581375
C	1.941355	-0.751602	0.078915
H	1.901060	-1.840651	0.130198
C	-0.562478	-0.852945	-0.407008
C	-0.852386	-1.534914	0.914151
C	-1.448646	-0.834323	-1.409315
C	-2.083174	-2.440122	0.838216
H	0.018624	-2.119050	1.236112
H	-0.996631	-0.767321	1.686106
C	-2.823809	-1.442412	-1.330779
H	-1.180606	-0.326010	-2.334964
C	-3.224324	-1.725522	0.117194
H	-1.832123	-3.357267	0.290204
H	-2.383126	-2.739411	1.846390
H	-2.851269	-2.370410	-1.919015
H	-3.544059	-0.766308	-1.806194
H	-4.143259	-2.318115	0.150027
H	-3.426175	-0.775705	0.629229
C	3.240405	-0.318315	-0.574967
O	3.383085	0.709207	-1.190337
O	4.228464	-1.191073	-0.349775
H	5.034330	-0.817793	-0.740145

TS-(3+2)-3f

C	1.925955	1.184449	0.571877
O	3.098195	0.916235	0.522520
C	0.858243	0.296607	1.099165
H	0.001817	0.756005	1.582727
N	1.323518	-0.820587	1.707391
N	1.436981	-1.947699	1.534723
O	1.366510	2.295473	0.069918
C	2.288074	3.177877	-0.578900
H	1.691463	4.011541	-0.943085
H	3.042959	3.522199	0.130102
H	2.785135	2.664886	-1.404310
C	0.065818	-0.644310	-0.619225
H	0.610731	0.001972	-1.305238
C	0.523577	-1.963516	-0.516648
H	-0.137611	-2.773353	-0.235353
C	-1.358656	-0.274503	-0.429152
C	-2.206256	-1.132776	0.481786
C	-1.839180	0.831425	-1.013958
C	-3.694245	-0.783543	0.401256
H	-2.069920	-2.190348	0.231966
H	-1.845807	-1.023213	1.516996
C	-3.237207	1.351655	-0.819130
H	-1.177753	1.408112	-1.658798
C	-3.900353	0.729266	0.409628
H	-4.107178	-1.192995	-0.528736
H	-4.231834	-1.258971	1.226679
H	-3.836742	1.140369	-1.715741
H	-3.208294	2.443243	-0.729085
H	-4.965392	0.977055	0.435308
H	-3.448814	1.150533	1.317191
C	1.726587	-2.345280	-1.190243
N	2.705995	-2.645257	-1.733379

TS-(3+2)-3f-product

C	2.165961	0.853211	-0.278621
O	2.537716	0.299013	-1.280989
C	0.834330	0.577247	0.413471
H	0.374741	1.532723	0.679030
N	1.153086	-0.140474	1.689480
N	0.850997	-1.330405	1.646644
O	2.866976	1.768654	0.388463
C	4.165534	2.040505	-0.149771
H	4.608531	2.783043	0.510023
H	4.763634	1.127885	-0.165257
H	4.078200	2.426611	-1.166980
C	-0.073709	-0.366466	-0.383821
H	0.252366	-0.401245	-1.424570
C	0.231439	-1.707009	0.324736
H	-0.669255	-2.291272	0.536626
C	-1.532770	0.007268	-0.289813
C	-2.136550	0.123425	1.094182
C	-2.246579	0.229607	-1.397430
C	-3.665531	0.158551	1.055684
H	-1.798873	-0.707983	1.726639
H	-1.755500	1.031409	1.584442
C	-3.691727	0.649652	-1.402320
H	-1.762404	0.108656	-2.365417
C	-4.151217	1.124535	-0.023241
H	-4.043155	-0.847103	0.832630
H	-4.056751	0.438174	2.037921
H	-4.310083	-0.195508	-1.735404
H	-3.837577	1.438296	-2.148740
H	-5.240510	1.220007	0.001104
H	-3.735667	2.120557	0.174293
C	1.176521	-2.568381	-0.392848
N	1.915997	-3.251757	-0.958607

TS-(3+2)-4a

C	2.398677	-0.666141	0.497372
O	2.896280	-0.067496	1.425972
C	0.984473	-1.008852	0.330510
H	0.745975	-1.880232	-0.272279
N	0.205414	-0.952342	1.453107
N	-0.880582	-0.641533	1.695807
O	3.096981	-1.050039	-0.594408
C	4.467176	-0.658562	-0.584885
H	4.893621	-1.042315	-1.509979
H	4.554199	0.430691	-0.545029
H	4.980811	-1.079901	0.281297
C	-2.589816	1.142831	0.409112
C	-3.707359	-0.961375	-0.026469
C	-3.952708	0.553106	-0.003806
H	-4.210386	0.893314	-1.012037
H	-4.760383	0.849130	0.669645
H	-2.427340	2.146115	0.002198
H	-4.441177	-1.523604	-0.608271
C	-1.581286	0.145434	-0.154330
C	-2.305560	-1.071604	-0.587472
C	-0.381567	0.517736	-0.779273
H	-0.098847	0.014077	-1.700657
C	-1.855801	-2.085012	-1.335817
H	-0.848055	-2.113378	-1.738717
N	0.206540	1.755086	-0.601762
C	0.381117	2.228240	0.766649
H	-0.533700	2.092522	1.342698
H	1.195670	1.687724	1.271278
H	0.621012	3.294095	0.746113
C	1.373127	2.006987	-1.427586
H	1.625048	3.068944	-1.383993
H	2.247299	1.426286	-1.092314
H	1.157588	1.745721	-2.465382
H	-2.505248	-2.914279	-1.594087
H	-3.714780	-1.351380	1.000090
H	-2.529849	1.211530	1.502815

TS-(3+2)-4a-product

C	2.230248	-0.561360	0.509961
O	2.828885	0.008030	1.384263
C	0.738166	-0.777073	0.420762
H	0.584584	-1.816137	0.108886
N	0.052436	-0.643247	1.727476
N	-1.103657	-0.243920	1.578593
O	2.824060	-1.097068	-0.573006
C	4.238299	-0.910108	-0.631127
H	4.567577	-1.403645	-1.543352
H	4.479859	0.155526	-0.661085
H	4.716362	-1.353116	0.244396
C	-2.414215	1.236337	0.055900
C	-3.709939	-0.811409	-0.000679
C	-3.776954	0.670327	-0.394237
H	-3.879145	0.750172	-1.481040
H	-4.617397	1.198746	0.060702
H	-2.024936	2.004621	-0.614685
H	-4.431893	-1.447791	-0.516848
C	-1.439392	0.038199	0.126925
C	-2.282329	-1.147584	-0.343457
C	-0.050408	0.165014	-0.535542
H	-0.068826	-0.249944	-1.545888
C	-1.880373	-2.211073	-1.034013
H	-0.851085	-2.369358	-1.338775
N	0.404233	1.534628	-0.635168
C	0.552128	2.257353	0.623992
H	-0.384419	2.244958	1.184867
H	1.342483	1.855232	1.273257
H	0.789510	3.299442	0.392008
C	1.545757	1.737120	-1.511727
H	1.599388	2.795778	-1.783816
H	2.512624	1.464136	-1.058177
H	1.419417	1.152936	-2.426927
H	-2.595630	-2.968197	-1.339670
H	-3.860251	-0.915324	1.081280
H	-2.498796	1.667577	1.057943

TS-(3+2)-4b

C	-2.701647	-0.151275	0.323355
O	-2.930378	0.903588	0.862181
C	-1.468373	-0.949223	0.478865
H	-1.518104	-2.019846	0.315955
N	-0.685496	-0.561663	1.506875
N	0.279144	0.022843	1.723828

O	-3.500208	-0.727147	-0.591921
C	-4.666926	0.030004	-0.915717
H	-5.197249	-0.549391	-1.668873
H	-5.287282	0.170151	-0.028448
H	-4.387675	1.010060	-1.307880
C	3.256474	0.804687	0.126238
C	1.141311	1.946890	-0.188042
C	2.654125	2.108195	-0.423950
H	2.852304	2.172107	-1.499154
H	3.064485	3.003513	0.049111
H	4.241575	0.564309	-0.279922
H	0.535742	2.549553	-0.870173
C	2.216899	-0.230372	-0.234570
C	0.909754	0.450468	-0.390334
C	2.453216	-1.534425	-0.374569
H	1.668010	-2.245504	-0.627271
C	-0.178537	-0.078921	-1.061067
H	-0.082328	-1.020963	-1.593255
H	-0.930804	0.596672	-1.458364
H	0.892434	2.257134	0.833180
H	3.353931	0.864981	1.218357
O	3.708008	-2.049972	-0.180120
H	3.722273	-2.968957	-0.460558

TS-(3+2)-4b-product

C	-2.494925	-0.007848	-0.310087
O	-2.481312	1.198963	-0.296046
C	-1.270102	-0.887140	-0.501788
H	-1.572094	-1.794757	-1.028641
N	-0.839852	-1.300199	0.886952
N	0.222630	-0.771238	1.208790
O	-3.592042	-0.743711	-0.118305
C	-4.777435	0.004706	0.160185
H	-5.567313	-0.730795	0.296901
H	-4.642958	0.600632	1.064749
H	-5.008434	0.671770	-0.672599
C	3.019102	1.220279	-0.034858
C	0.734417	1.583445	0.656931
C	1.887546	2.260809	-0.092636
H	1.595992	2.439249	-1.134091
H	2.165405	3.223534	0.341818
H	3.722408	1.293176	-0.868946
H	-0.248362	2.026761	0.481599
C	2.282909	-0.100376	-0.015448
C	0.795357	0.123828	0.161538
C	2.838525	-1.305031	-0.089320
H	2.246314	-2.216902	-0.026198
C	-0.071644	-0.154452	-1.086323
H	0.466915	-0.791548	-1.789744
H	-0.364850	0.768757	-1.589579
H	0.936408	1.584358	1.734102
H	3.603327	1.334441	0.886617
O	4.186701	-1.449779	-0.242392
H	4.418526	-2.381730	-0.201388

TS-(3+2)-4c

C	2.382033	0.060317	0.334974
O	2.408391	-0.967208	0.966343
C	1.287977	1.055665	0.361866
H	1.510425	2.085686	0.108288
N	0.431762	0.887251	1.390547
N	-0.600700	0.456796	1.642229
O	3.300188	0.419760	-0.576292
C	4.338986	-0.540097	-0.778216
H	4.987352	-0.118462	-1.543577
H	4.890711	-0.702613	0.149543
H	3.917845	-1.491574	-1.109131
C	-3.501023	-0.274621	0.201279
C	-1.506445	-1.605383	-0.126849
C	-3.040825	-1.671126	-0.244088
H	-3.322065	-1.828876	-1.290706
H	-3.479405	-2.477174	0.348608
H	-4.508008	-0.011239	-0.130446
H	-1.000557	-2.298670	-0.804521
C	-2.437499	0.646475	-0.359124
C	-1.188570	-0.150474	-0.459148
C	-2.608375	1.928548	-0.687383
H	-1.794177	2.536445	-1.071870
C	-0.058555	0.259088	-1.141840
H	-0.082096	1.184041	-1.710985
H	0.635729	-0.490186	-1.512169
H	-1.195478	-1.864612	0.892018
H	-3.479050	-0.213865	1.297551
H	-3.573507	2.411997	-0.581270

TS-(3+2)-4c-product

C	-2.170844	0.122418	-0.298369
O	-2.018173	1.319844	-0.293610
C	-1.056622	-0.891725	-0.500501
H	-1.464696	-1.762090	-1.018484
N	-0.656684	-1.342259	0.883738
N	0.462845	-0.935367	1.188178
O	-3.341198	-0.481775	-0.085119
C	-4.429069	0.398355	0.206911
H	-5.294533	-0.241882	0.363552
H	-4.211514	0.981281	1.103708
H	-4.597815	1.081399	-0.627834
C	3.453529	0.686206	0.012243
C	1.226135	1.344579	0.617324
C	2.475920	1.864704	-0.101906
H	2.245038	2.061334	-1.155327
H	2.861900	2.789274	0.332508
H	4.244327	0.688262	-0.742013
H	0.312747	1.908380	0.416582
C	2.562820	-0.536229	-0.083465
C	1.113516	-0.112682	0.128379
C	2.938209	-1.790052	-0.310316
H	2.212487	-2.599004	-0.332560
C	0.208604	-0.301111	-1.106918
H	0.662105	-1.000780	-1.810777
H	0.013070	0.645571	-1.613706
H	1.399331	1.330422	1.699560
H	3.936821	0.704297	0.997117
H	3.979377	-2.054395	-0.466211

TS-(3+2)-4d

C	-3.105862	-0.440572	0.338891
O	-3.461060	0.582524	0.868227
C	-1.757121	-1.044989	0.464558
H	-1.652975	-2.115313	0.326039
N	-1.036747	-0.528807	1.484746
N	-0.199898	0.212208	1.724657
O	-3.837586	-1.147714	-0.533504
C	-5.117117	-0.581532	-0.829515
H	-5.576066	-1.250958	-1.553907
H	-5.721368	-0.518949	0.077217
H	-5.000357	0.420472	-1.246809
C	2.388664	1.707152	0.085926
C	0.052798	2.276457	-0.300129
C	1.481969	2.823826	-0.456318
H	1.698060	2.979266	-1.518545
H	1.631463	3.776326	0.056540
H	3.405121	1.716489	-0.305450
H	-0.643320	2.689034	-1.035626
C	1.653670	0.430563	-0.255272
C	0.237483	0.774680	-0.471002
C	2.177561	-0.813180	-0.322554
H	1.531263	-1.652734	-0.574680
C	-0.680321	-0.059591	-1.089220
H	-0.335993	-0.980835	-1.550808
H	-1.555060	0.383809	-1.557560
H	-0.343240	2.522011	0.692344
H	2.477716	1.766210	1.179058
C	3.593538	-1.128010	-0.076816
O	4.412127	-0.308737	0.307540
C	4.000912	-2.569552	-0.325965
H	3.415290	-3.242627	0.308333
H	3.799444	-2.845837	-1.365705
H	5.061654	-2.690268	-0.109869

TS-(3+2)-4d-product

C	-3.043931	-0.215560	-0.326593
O	-3.205404	0.980264	-0.305775
C	-1.696559	-0.901978	-0.493442
H	-1.844794	-1.840598	-1.031288
N	-1.240808	-1.252999	0.899968
N	-0.274276	-0.576689	1.247350
O	-4.022495	-1.106511	-0.165199
C	-5.312921	-0.545195	0.090021
H	-5.986158	-1.391603	0.206524
H	-5.287488	0.057666	0.999475
H	-5.622684	0.085091	-0.745679
C	2.195761	1.786209	-0.077923
C	-0.093029	1.835740	0.705570
C	0.930043	2.660128	-0.084346
H	0.575842	2.804404	-1.111250
H	1.095675	3.649708	0.345917
H	2.841271	1.912985	-0.949330
H	-1.133755	2.126390	0.547138
C	1.682538	0.369969	0.040975
C	0.173600	0.400826	0.218712
C	2.385770	-0.769824	0.037197
H	1.867987	-1.718135	0.171959
C	-0.611581	0.009515	-1.052786
H	0.026143	-0.533732	-1.752185
H	-1.034491	0.883371	-1.551192
H	0.129516	1.881033	1.777573
H	2.831796	2.000097	0.789248
C	3.860371	-0.807676	-0.110884
O	4.528019	0.201926	-0.240897
C	4.498519	-2.179961	-0.082247
H	4.270974	-2.677709	0.865656
H	4.086469	-2.803902	-0.881641
H	5.576842	-2.085851	-0.202705

TS-(3+2)-4e

C	-3.104905	-0.421782	0.338230
O	-3.453834	0.595555	0.882615
C	-1.758208	-1.033940	0.451652
H	-1.659169	-2.103209	0.300926
N	-1.031685	-0.534012	1.475602
N	-0.186475	0.193970	1.723940
O	-3.841906	-1.114059	-0.541091
C	-5.120387	-0.539529	-0.825580
H	-5.583841	-1.197815	-1.557237
H	-5.721506	-0.486841	0.083847
H	-5.001305	0.467431	-1.230085
C	2.417920	1.650796	0.109478
C	0.097965	2.274515	-0.285561
C	1.539801	2.792741	-0.426950
H	1.766501	2.954420	-1.485949
H	1.706988	3.735912	0.097463
H	3.439171	1.646389	-0.268999
H	-0.583433	2.710177	-1.021484
C	1.659372	0.396300	-0.261818
C	0.251580	0.771196	-0.472312
C	2.152449	-0.856195	-0.353560
H	1.511210	-1.691519	-0.617668
C	-0.682609	-0.042118	-1.093780
H	-0.354733	-0.962536	-1.568724
H	-1.552849	0.420385	-1.551959
H	-0.299690	2.518288	0.706709
H	2.488059	1.692237	1.204754
C	3.556386	-1.182305	-0.105323
O	4.436399	-0.429915	0.259168
O	3.805498	-2.496669	-0.326041
H	4.746280	-2.620388	-0.132454

TS-(3+2)-4e-product

C	-3.038199	-0.197368	-0.329246
O	-3.180887	1.001111	-0.330494
C	-1.700776	-0.907304	-0.477238
H	-1.860368	-1.852743	-0.999597
N	-1.256679	-1.240925	0.923741
N	-0.281182	-0.574367	1.264372
O	-4.031027	-1.069919	-0.157120
C	-5.314066	-0.484576	0.081140
H	-6.000668	-1.318482	0.209075
H	-5.284011	0.133969	0.979853
H	-5.609797	0.135232	-0.767375
C	2.229049	1.737248	-0.063947
C	-0.068177	1.826223	0.684522

C	0.974590	2.625606	-0.104956
H	0.637347	2.755021	-1.139493
H	1.146241	3.620534	0.310221
H	2.896639	1.850660	-0.920224
H	-1.103077	2.128008	0.510121
C	1.692934	0.328674	0.052016
C	0.183968	0.380606	0.221478
C	2.374289	-0.822013	0.047617
H	1.867135	-1.773730	0.175327
C	-0.599111	-0.022390	-1.047245
H	0.033989	-0.588417	-1.732577
H	-1.006185	0.848185	-1.564213
H	0.142837	1.884280	1.758254
H	2.842354	1.949248	0.819788
C	3.839178	-0.855797	-0.105179
O	4.569560	0.104560	-0.212380
O	4.310851	-2.119301	-0.112708
H	5.272541	-2.049803	-0.208112

TS-(3+2)-4f

C	-2.805564	-0.314800	0.319277
O	-2.987786	0.737542	0.878052
C	-1.560102	-1.120163	0.406052
H	-1.618568	-2.188263	0.229370
N	-0.771987	-0.750317	1.439634
N	0.144358	-0.121781	1.706863
O	-3.649819	-0.879945	-0.552469
C	-4.834882	-0.120007	-0.809482
H	-5.400978	-0.694194	-1.539608
H	-5.407005	0.008415	0.110930
H	-4.574864	0.863335	-1.205760
C	2.780211	1.238319	0.248487
C	0.526770	2.008612	-0.231844
C	1.999854	2.457219	-0.269537
H	2.294277	2.661236	-1.303880
H	2.186312	3.358996	0.316868
H	3.828940	1.211092	-0.054876
H	-0.085405	2.510724	-0.986236
C	1.991520	0.061699	-0.275130
C	0.606459	0.506362	-0.476889
C	2.484866	-1.173392	-0.497529
H	1.864167	-1.983841	-0.865870
C	-0.372983	-0.235672	-1.117162
H	-0.105712	-1.176499	-1.590881
H	-1.198536	0.288435	-1.591035
H	0.079946	2.232919	0.743862
H	2.750743	1.207103	1.345783
C	3.858393	-1.478226	-0.259630
N	4.976239	-1.719323	-0.065496

TS-(3+2)-4f-product

C	-2.695581	-0.099254	-0.325871
O	-2.733898	1.107109	-0.330639
C	-1.422957	-0.920470	-0.476424
H	-1.664017	-1.851856	-0.992633
N	-1.000452	-1.281110	0.923674
N	0.024084	-0.689777	1.259286
O	-3.757072	-0.883647	-0.148061
C	-4.986436	-0.191950	0.092255
H	-5.740116	-0.965336	0.222011
H	-4.902201	0.421938	0.990658
H	-5.230034	0.449807	-0.756404
C	2.716066	1.410556	-0.027400
C	0.420418	1.686987	0.657965
C	1.538585	2.395101	-0.117045
H	1.239737	2.530499	-1.162296
H	1.776596	3.379820	0.288843
H	3.429599	1.481742	-0.852610
H	-0.582882	2.071797	0.464687
C	2.057128	0.053232	0.043411
C	0.558275	0.220659	0.207699
C	2.663363	-1.138177	0.002835
H	2.107719	-2.065469	0.107109
C	-0.254098	-0.133483	-1.056755
H	0.331000	-0.756443	-1.735443
H	-0.589357	0.760676	-1.584861
H	0.617894	1.735680	1.734750
H	3.282649	1.570713	0.898391
C	4.082914	-1.235300	-0.161702
N	5.231382	-1.291780	-0.301019

TS-(3+2)-5a

C	-3.192925	-1.178177	0.095374
O	-3.803280	-2.002673	-0.540407
C	-1.843335	-1.420153	0.646784
H	-1.603754	-2.450169	0.882416
N	-1.366824	-0.507427	1.515432
N	-0.631525	0.375388	1.581546
O	-3.604156	0.085477	0.290656
C	-4.855407	0.402987	-0.321135
H	-5.057005	1.439783	-0.060026
H	-4.788341	0.282838	-1.404293
H	-5.641209	-0.252147	0.059278
C	1.557121	0.298853	-0.217874
C	0.122186	0.304334	-0.596674
C	-0.481118	1.649235	-0.982751
C	0.037033	2.823952	-0.150946
C	1.562589	2.809087	-0.091856
C	2.078807	1.505251	0.529650
H	-0.236222	1.841085	-2.037971
H	-0.320575	3.763803	-0.584614
H	1.967873	2.904874	-1.107573
H	3.172115	1.485965	0.512527
C	2.380373	-0.704416	-0.572648
C	-0.547930	-0.843507	-0.997416
H	2.024643	-1.494061	-1.238336
H	-1.375030	-0.755060	-1.697614
H	-0.036529	-1.800096	-1.015184
H	-1.573305	1.583421	-0.916911
H	-0.364037	2.766554	0.866881
H	1.932930	3.663722	0.483628
H	1.760649	1.468848	1.580853
N	3.723205	-0.819192	-0.150757
C	4.506589	-1.712889	-0.982937
H	5.559457	-1.651895	-0.694697
H	4.186909	-2.766584	-0.893918

H	4.421768	-1.412210	-2.029294
C	3.894980	-1.112801	1.266591
H	3.567658	-2.134146	1.525019
H	4.951955	-1.013107	1.531446
H	3.321783	-0.405764	1.867870

TS-(3+2)-5a-product

C	-3.042531	-0.977296	0.059783
O	-3.570377	-2.059780	0.073324
C	-1.553528	-0.731595	0.174399
H	-1.078480	-1.698749	0.366283
N	-1.287773	0.134576	1.373382
N	-0.423895	0.977665	1.142263
O	-3.710166	0.178853	-0.065372
C	-5.129209	0.044537	-0.150901
H	-5.519968	1.056678	-0.233590
H	-5.402533	-0.549067	-1.025666
H	-5.515872	-0.447016	0.743723
C	1.502941	0.267445	-0.096916
C	0.125430	0.894541	-0.263404
C	0.213946	2.319319	-0.825740
C	1.228989	3.190872	-0.088289
C	2.604817	2.530805	-0.091466
C	2.545119	1.142761	0.557566
H	0.491447	2.240037	-1.885036
H	1.272713	4.179319	-0.556667
H	2.959977	2.428185	-1.124859
H	3.516173	0.645894	0.487428
C	1.765253	-0.999573	-0.446139
C	-0.926428	0.040537	-0.982419
H	1.015043	-1.606981	-0.958364
H	-1.675906	0.699763	-1.429352
H	-0.517004	-0.595832	-1.765562
H	-0.785789	2.766492	-0.782060
H	0.893706	3.333320	0.945124
H	3.332326	3.153673	0.438261
H	2.303171	1.262869	1.622989
N	2.992655	-1.651058	-0.184389
C	3.226948	-2.777498	-1.070694
H	4.232107	-3.171415	-0.900187
H	2.504604	-3.598309	-0.914336
H	3.161291	-2.449861	-2.110450
C	3.172453	-2.023749	1.215742
H	2.475670	-2.818485	1.529848
H	4.195133	-2.382500	1.363677
H	3.014415	-1.155520	1.857265

TS-(3+2)-5b

C	-2.879877	-0.743940	0.104291
O	-3.651958	-1.434065	-0.515790
C	-1.636452	-1.265114	0.708571
H	-1.645601	-2.311481	0.989362
N	-0.980412	-0.448646	1.554950
N	-0.063366	0.245243	1.605517
O	-2.988506	0.588778	0.231565
C	-4.118068	1.157579	-0.432465
H	-4.077633	2.224371	-0.222430
H	-4.058550	0.972348	-1.506881
H	-5.042821	0.722232	-0.049456
C	2.094381	-0.408398	-0.126599
C	0.703158	-0.084269	-0.530083
C	0.460051	1.352661	-0.975237
C	1.225256	2.394821	-0.154450
C	2.700718	2.017233	-0.024428
C	2.859291	0.644152	0.641077
H	0.778936	1.440025	-2.024631
H	1.122597	3.376545	-0.628827
H	3.159442	1.987485	-1.021516
H	3.912364	0.360807	0.698624
C	2.683542	-1.550275	-0.499716
C	-0.208512	-1.055538	-0.919021
H	2.186164	-2.275160	-1.139970
H	-0.978982	-0.800322	-1.642320
H	0.065409	-2.105614	-0.897884
H	-0.616246	1.559150	-0.950554
H	0.786342	2.474682	0.845912
H	3.237584	2.775992	0.554359
H	2.478620	0.704169	1.668250
O	3.942814	-1.884295	-0.080487
H	4.279093	-2.598224	-0.629255

TS-(3+2)-5b-product

C	-2.870302	-0.670524	0.062790
O	-3.892684	-1.305194	0.076142
C	-1.500799	-1.210769	0.429704
H	-1.656806	-2.238116	0.763331
N	-0.985334	-0.432972	1.602432
N	0.075302	0.133173	1.356527
O	-2.799192	0.622351	-0.290574
C	-4.050132	1.221596	-0.633978
H	-3.826104	2.257381	-0.880788
H	-4.495127	0.706994	-1.487876
H	-4.738498	1.165406	0.211088
C	2.023349	-0.462874	0.024272
C	0.564151	-0.057708	-0.051393
C	0.468974	1.332791	-0.723213
C	1.369868	2.375239	-0.057659
C	2.822475	1.901497	-0.003279
C	2.925142	0.541273	0.701339
H	0.767874	1.198347	-1.770854
H	1.295339	3.320082	-0.606055
H	3.215172	1.803795	-1.023521
H	3.953772	0.176664	0.694976
C	2.516113	-1.558388	-0.553630
C	-0.434481	-1.061803	-0.663063
H	1.904550	-2.270673	-1.098935
H	-0.851075	-0.676547	-1.595798
H	0.011023	-2.034470	-0.864290
H	-0.578462	1.651314	-0.711168
H	1.010042	2.562136	0.959951
H	3.443948	2.639675	0.513743
H	2.612774	0.657334	1.745753
O	3.852187	-1.847305	-0.509962
H	4.013160	-2.681531	-0.958458

TS-(3+2)-5c

C	2.535379	-0.250534	0.392840
O	2.512862	0.559662	1.284883
C	1.483349	-1.249793	0.102966
H	1.770404	-2.186325	-0.361360
N	0.540994	-1.354093	1.057692
N	-0.548855	-1.080871	1.293607
O	3.490821	-0.321993	-0.549461
C	4.505704	0.676957	-0.436485
H	5.187805	0.501792	-1.265995
H	4.065771	1.674203	-0.500840
H	5.026209	0.582905	0.518494
C	-1.444016	1.219906	-0.108437
C	-1.024820	-0.067304	-0.732413
C	-2.133612	-1.041481	-1.112330
C	-3.306388	-1.079480	-0.130629
C	-3.786362	0.335464	0.189157
C	-2.648310	1.154002	0.807324
H	-2.523521	-0.740122	-2.095810
H	-4.119830	-1.674547	-0.558546
H	-4.128480	0.824703	-0.732284
H	-2.983522	2.168330	1.042136
C	-0.834542	2.386885	-0.340706
C	0.214529	-0.217825	-1.331032
H	0.006074	2.484899	-1.018847
H	0.340416	-0.979317	-2.095954
H	0.893484	0.624806	-1.411691
H	-1.708907	-2.044034	-1.243775
H	-3.001071	-1.571916	0.799216
H	-4.639586	0.304900	0.874302
H	-2.356273	0.679236	1.752760
H	-1.168882	3.293104	0.154202

TS-(3+2)-5c-product

C	-2.254150	-0.328982	-0.352233
O	-2.430720	0.088055	-1.464084
C	-1.248508	-1.397134	0.054603
H	-1.811085	-2.307478	0.280651
N	-0.358185	-1.671343	-1.114707
N	0.763363	-1.195438	-0.948575
O	-2.949193	0.088317	0.723471
C	-3.911472	1.106919	0.442174
H	-4.392047	1.333689	1.391874
H	-3.414114	1.991614	0.037677
H	-4.641346	0.749907	-0.286654
C	0.908835	1.010920	0.027230
C	0.911678	-0.474158	0.373871
C	2.262013	-0.876825	0.985744
C	3.456003	-0.432357	0.139392
C	3.408222	1.070275	-0.134776
C	2.084852	1.447099	-0.813711
H	2.320186	-0.423405	1.983792
H	4.385884	-0.700797	0.650663
H	3.497391	1.621332	0.810324
H	2.029216	2.524373	-0.993762
C	-0.026353	1.870165	0.430868
C	-0.291742	-0.979358	1.171053
H	-0.877808	1.585198	1.040195
H	0.002098	-1.858219	1.751625
H	-0.717878	-0.248869	1.855447
H	2.270227	-1.964742	1.120059
H	3.437912	-0.974709	-0.812093
H	4.250680	1.370504	-0.765442
H	2.031612	0.942946	-1.786657
H	0.035852	2.915772	0.144895

TS-(3+2)-5d

C	-3.126393	-0.415919	0.360299
O	-3.518133	0.637542	0.797434
C	-1.752682	-0.951101	0.523332
H	-1.604358	-2.024559	0.477674
N	-1.045401	-0.326800	1.489409
N	-0.213080	0.432153	1.681229
O	-3.837103	-1.229968	-0.431075
C	-5.141617	-0.745557	-0.762214
H	-5.579971	-1.499012	-1.413013
H	-5.738677	-0.620133	0.142699
H	-5.069250	0.215439	-1.275059
C	1.604761	0.220689	-0.358678
C	0.244859	0.737637	-0.608116
C	-0.054995	2.230664	-0.562220
C	1.001657	3.039558	0.180230
C	2.373398	2.669078	-0.371325
C	2.709998	1.213338	-0.054712
H	-0.115764	2.610965	-1.591760
H	0.801187	4.108601	0.061275
H	2.376237	2.827943	-1.457812
H	3.620414	0.895655	-0.566144
C	1.843568	-1.118472	-0.321991
C	-0.745319	-0.084915	-1.134128
H	1.025901	-1.810692	-0.508593
H	-1.621892	0.397631	-1.561128
H	-0.492101	-1.035816	-1.590053
H	-1.048674	2.375355	-0.120963
H	0.965575	2.817168	1.253515
H	3.155281	3.311950	0.043655
H	2.950962	1.113708	1.012048
C	3.133381	-1.759699	-0.033111
O	4.146347	-1.162867	0.298235
C	3.147230	-3.274781	-0.162607
H	2.419905	-3.721248	0.523049
H	2.864321	-3.573286	-1.176865
H	4.144315	-3.647919	0.067704

TS-(3+2)-5d-product

C	-3.159230	-0.226421	-0.237271
O	-3.668356	0.452915	-1.092983
C	-1.666859	-0.316210	0.021306
H	-1.420377	-1.339752	0.324802
N	-1.354867	0.555386	1.212655
N	-0.330024	1.208533	1.036206
O	-3.840684	-0.978381	0.630219
C	-5.262731	-0.887605	0.516890
H	-5.664173	-1.541352	1.288212
H	-5.588233	0.142171	0.674912
H	-5.584941	-1.213128	-0.474113
C	1.544616	0.071087	0.051870

C	0.326064	0.928899	-0.299324
C	0.761787	2.264711	-0.922273
C	1.823310	2.997261	-0.103976
C	3.022708	2.092190	0.160227
C	2.582392	0.801562	0.867464
H	1.147971	2.045956	-1.926367
H	2.129917	3.904227	-0.634490
H	3.514199	1.835835	-0.786808
H	3.429187	0.151556	1.069521
C	1.632401	-1.215449	-0.329026
C	-0.797661	0.249212	-1.085223
H	0.819708	-1.656938	-0.898762
H	-1.376144	1.002935	-1.627145
H	-0.454853	-0.491585	-1.805334
H	-0.131433	2.886637	-1.047193
H	1.386280	3.309391	0.850850
H	3.765379	2.606041	0.777480
H	2.114931	1.075062	1.822638
C	2.744582	-2.170873	-0.053449
O	3.788492	-1.884704	0.498362
C	2.486628	-3.586566	-0.532616
H	1.581710	-3.985085	-0.062892
H	2.320737	-3.593769	-1.614672
H	3.340702	-4.215061	-0.285055

TS-(3+2)-5e

C	-3.125724	-0.394685	0.362479
O	-3.512516	0.656496	0.809418
C	-1.752602	-0.934955	0.516110
H	-1.605986	-2.008533	0.464068
N	-1.039578	-0.318735	1.483051
N	-0.200780	0.430903	1.680221
O	-3.841375	-1.200792	-0.431945
C	-5.146354	-0.711480	-0.753877
H	-5.588672	-1.459109	-1.408666
H	-5.739364	-0.592104	0.154514
H	-5.074325	0.253335	-1.259547
C	1.600638	0.186055	-0.367534
C	0.255154	0.735836	-0.616807
C	-0.008550	2.235100	-0.568593
C	1.061667	3.017844	0.182830
C	2.430058	2.612037	-0.352226
C	2.724189	1.148271	-0.030832
H	-0.053803	2.619252	-1.597514
H	0.890315	4.091410	0.059242
H	2.451180	2.769447	-1.438649
H	3.638901	0.810998	-0.520543
C	1.802928	-1.157092	-0.352782
C	-0.753613	-0.065806	-1.139665
H	0.990752	-1.846029	-0.554611
H	-1.624449	0.435689	-1.556484
H	-0.521584	-1.017827	-1.604438
H	-1.001114	2.402742	-0.133093
H	1.008605	2.799544	1.256198
H	3.222979	3.234462	0.072820
H	2.929283	1.043715	1.043065
C	3.075819	-1.808836	-0.052415
O	4.127563	-1.296413	0.274465
O	2.968138	-3.157811	-0.168394
H	3.843650	-3.507747	0.052265

TS-(3+2)-5e-product

C	-3.165730	-0.228433	-0.238122
O	-3.671325	0.462634	-1.086540
C	-1.673237	-0.330363	0.017200
H	-1.432647	-1.358679	0.309028
N	-1.354527	0.526769	1.216249
N	-0.327830	1.178324	1.044958
O	-3.850548	-0.983875	0.623163
C	-5.272161	-0.885026	0.511235
H	-5.676463	-1.544225	1.276371
H	-5.592562	0.144791	0.679182
H	-5.596090	-1.199592	-0.482721
C	1.538832	0.047346	0.043026
C	0.322996	0.911430	-0.296355
C	0.761922	2.252618	-0.904807
C	1.827051	2.971659	-0.079010
C	3.024332	2.059942	0.172241
C	2.582187	0.761955	0.864745
H	1.145391	2.044808	-1.912203
H	2.136253	3.883915	-0.598695
H	3.513370	1.813651	-0.778711
H	3.428286	0.107440	1.058097
C	1.615712	-1.231664	-0.357322
C	-0.803359	0.241191	-1.086111
H	0.820059	-1.684716	-0.936174
H	-1.379844	1.000911	-1.621670
H	-0.464346	-0.495682	-1.811940
H	-0.129598	2.878640	-1.020249
H	1.392454	3.273465	0.880190
H	3.769556	2.563991	0.794405
H	2.118752	1.023354	1.825024
C	2.732207	-2.165526	-0.082727
O	3.774126	-1.953238	0.493616
O	2.444655	-3.384164	-0.591205
H	3.204154	-3.949354	-0.384611

TS-(3+2)-5f

C	-2.959559	-0.928144	0.056251
O	-3.696442	-1.606879	-0.613577
C	-1.628389	-1.395875	0.512383
H	-1.523860	-2.465890	0.650159
N	-1.011124	-0.642058	1.443467
N	-0.174489	0.123320	1.602714
O	-3.185354	0.351798	0.384806
C	-4.414703	0.886890	-0.115178
H	-4.459896	1.910598	0.249678
H	-4.419743	0.863102	-1.206521
H	-5.258972	0.304409	0.257265
C	1.898626	-0.137489	-0.257677
C	0.500578	0.145532	-0.645844
C	0.095111	1.594365	-0.891783
C	0.835947	2.613025	-0.026726
C	2.337686	2.344200	-0.061759
C	2.640776	0.948448	0.489687
H	0.293994	1.829502	-1.947352

H	0.614957	3.623598	-0.384096
H	2.703183	2.419112	-1.093856
H	3.713927	0.745263	0.470479
C	2.502669	-1.314184	-0.538810
C	-0.349673	-0.845808	-1.115711
H	2.012940	-2.092906	-1.111298
H	-1.174756	-0.558622	-1.762818
H	0.002706	-1.859996	-1.268343
H	-0.988001	1.684501	-0.749745
H	0.484099	2.552858	1.009454
H	2.879748	3.091323	0.525296
H	2.325407	0.912953	1.540792
C	3.833644	-1.613809	-0.113776
N	4.913091	-1.867272	0.225923

TS-(3+2)-5f-product

C	-3.013093	-0.808860	0.060256
O	-3.996910	-1.499425	0.089288
C	-1.625816	-1.249631	0.494747
H	-1.735004	-2.263395	0.883446
N	-1.189859	-0.380593	1.631699
N	-0.161136	0.239745	1.383195
O	-3.000759	0.461325	-0.371617
C	-4.273268	0.968340	-0.784461
H	-4.097914	1.997131	-1.091831
H	-4.664251	0.376341	-1.614009
H	-4.980195	0.927027	0.045769
C	1.852847	-0.263550	0.095773
C	0.363685	0.010049	-0.006965
C	0.192126	1.356917	-0.756168
C	0.977439	2.496452	-0.103376
C	2.456411	2.141009	0.046735
C	2.627710	0.813334	0.807328
H	0.543483	1.197883	-1.783570
H	0.864907	3.402589	-0.706763
H	2.918036	2.041632	-0.943571
H	3.682810	0.540787	0.879488
C	2.444152	-1.298531	-0.521099
C	-0.534933	-1.102964	-0.574750
H	1.893542	-2.034112	-1.094925
H	-0.942366	-0.821832	-1.547625
H	-0.008659	-2.050447	-0.682370
H	-0.877281	1.584207	-0.797869
H	0.550882	2.707940	0.882544
H	2.991248	2.935666	0.574587
H	2.228114	0.926541	1.820483
C	3.864890	-1.492215	-0.487566
N	5.011153	-1.657047	-0.470305

TS-(3+2)-6a

C	2.760283	-0.193579	0.238149
O	3.530164	0.407195	-0.478297
C	1.640675	0.467473	0.917846
H	1.880299	1.438941	1.338670
N	0.812364	-0.272602	1.709499
N	-0.289425	-0.603019	1.749738
O	2.792344	-1.523924	0.427598
C	3.787991	-2.209038	-0.333455
H	3.684988	-3.260715	-0.073890
H	3.619761	-2.056995	-1.401929
H	4.782953	-1.841390	-0.076159
C	-3.134943	-0.124502	1.109380
C	-2.446947	0.609900	-0.058651
C	-2.617557	-1.504199	-0.841902
C	-3.148183	-1.601115	0.616213
H	-2.614401	-0.002522	2.060412
H	-4.154426	0.254458	1.232316
H	-2.510856	-2.247258	1.225123
H	-4.160561	-2.015138	0.628012
C	-3.112121	-0.106898	-1.257072
H	-2.717973	0.219370	-2.222932
H	-4.203271	-0.012478	-1.247499
H	-2.556235	1.694848	-0.053832
H	-2.895992	-2.346499	-1.477654
C	-1.001082	0.123656	-0.230769
C	-1.124408	-1.255603	-0.769764
C	0.057024	0.960338	-0.601249
H	0.732504	0.608935	-1.379265
C	-0.158529	-2.111733	-1.109342
H	0.892165	-1.873138	-0.978564
N	-0.009302	2.357301	-0.506763
C	-0.358517	2.925833	0.784460
H	0.540321	3.123298	1.393726
H	-0.882679	3.876743	0.649760
H	-1.004486	2.247371	1.342729
C	1.116563	3.045101	-1.110648
H	0.920548	4.120135	-1.120384
H	2.057113	2.859421	-0.562991
H	1.251777	2.709475	-2.140589
H	-0.398562	-3.088595	-1.515975

TS-(3+2)-6a-product

C	2.462546	-0.169525	-0.188780
O	2.732931	-0.030048	-1.355701
C	1.416512	0.669023	0.523349
H	1.936246	1.588230	0.820700
N	0.893563	0.035542	1.772121
N	-0.291307	-0.291866	1.652667
O	3.071306	-1.040801	0.621069
C	4.062784	-1.850909	-0.014819
H	4.460199	-2.496858	0.765100
H	3.608225	-2.440711	-0.814071
H	4.849176	-1.225069	-0.440498
C	-3.164763	-0.667449	0.983595
C	-2.313916	0.369858	0.217699
C	-2.235477	-1.462495	-1.107088
C	-3.190274	-1.898515	0.029837
H	-2.727959	-0.901625	1.955906
H	-4.171212	-0.274965	1.149892
H	-2.852568	-2.817522	0.512903
H	-4.194501	-2.070203	-0.370402
C	-2.617992	0.020843	-1.251115
H	-2.000790	0.580682	-1.958658
H	-3.673559	0.159589	-1.502983
H	-2.498260	1.405711	0.495505
H	-2.276359	-2.087190	-2.000978

C	-0.828990	-0.042686	0.290258
C	-0.866576	-1.382075	-0.464664
C	0.175601	0.952836	-0.343582
H	0.384071	0.685862	-1.380988
C	0.074368	-2.319992	-0.443711
H	0.969965	-2.226013	0.164389
N	-0.282031	2.333365	-0.328436
C	-0.384516	2.928623	0.995606
H	0.594771	3.122660	1.467494
H	-0.906508	3.886174	0.914187
H	-0.954878	2.284478	1.668317
C	0.518763	3.169211	-1.207723
H	0.084769	4.172108	-1.245674
H	1.569339	3.265676	-0.878310
H	0.518969	2.752104	-2.217775
H	-0.043031	-3.236089	-1.014642

TS-(3+2)-6b

C	2.939255	0.151781	0.334524
O	2.960924	-0.946943	0.832317
C	1.846530	1.136393	0.477645
H	2.061673	2.188618	0.337305
N	0.978930	0.838088	1.462477
N	-0.025630	0.310239	1.644038
O	3.864475	0.619841	-0.520183
C	4.901250	-0.310924	-0.834457
H	5.555051	0.199863	-1.538560
H	5.447996	-0.589516	0.068407
H	4.479397	-1.212780	-1.282785
C	-2.815451	-1.301296	0.944920
C	-2.948560	-0.537620	-0.401193
C	-0.932439	-1.559676	-0.562245
C	-1.473886	-2.074452	0.787088
H	-2.800710	-0.608954	1.790070
H	-3.656159	-1.987695	1.083211
H	-0.784028	-1.912579	1.615484
H	-1.653743	-3.151456	0.711192
C	-2.249522	-1.511872	-1.374473
H	-2.123095	-1.097285	-2.377984
H	-2.744377	-2.487031	-1.432606
H	-3.963258	-0.223956	-0.646487
H	-0.119476	-2.158930	-0.977989
C	-1.940861	0.591993	-0.374845
C	-0.612837	-0.063257	-0.514534
C	-2.194922	1.889997	-0.227195
H	-1.397898	2.631622	-0.185883
C	0.492090	0.496915	-1.128834
H	0.422865	1.495963	-1.550258
H	1.225026	-0.153468	-1.598107
O	-3.478786	2.360813	-0.127883
H	-3.459148	3.311705	0.006966

TS-(3+2)-6b-product

C	2.781252	0.109731	-0.300081
O	2.673213	-1.024797	-0.697360
C	1.639907	1.109584	-0.217759
H	2.041158	2.114262	-0.365250
N	1.138067	1.031355	1.205812
N	0.023357	0.515220	1.264803
O	3.917815	0.632285	0.166128
C	5.021570	-0.274603	0.213465
H	5.855169	0.293598	0.620690
H	4.783085	-1.125170	0.854647
H	5.254282	-0.640443	-0.788470
C	-2.881472	-1.502371	0.845558
C	-2.793214	-0.711272	-0.481210
C	-0.665036	-1.422777	-0.168649
C	-1.412286	-1.971111	1.066223
H	-3.252334	-0.875965	1.659379
H	-3.558411	-2.355592	0.736885
H	-0.988850	-1.601220	2.000655
H	-1.345463	-3.062522	1.073401
C	-1.749836	-1.541403	-1.255834
H	-1.465552	-1.094622	-2.213167
H	-2.062622	-2.577557	-1.417783
H	-3.751345	-0.525603	-0.967311
H	0.298155	-1.895363	-0.370831
C	-1.993566	0.536095	-0.191636
C	-0.536043	0.121992	-0.060113
C	-2.443663	1.771904	-0.008570
H	-1.771283	2.592698	0.239750
C	0.442532	0.742203	-1.080251
H	0.004717	1.629922	-1.540388
H	0.710710	0.029809	-1.862427
O	-3.770974	2.073690	-0.115605
H	-3.902677	3.010490	0.053743

TS-(3+2)-6c

C	2.850695	-0.556001	-0.122259
O	3.698578	-0.841260	-0.931931
C	1.686008	-1.417915	0.163230
H	1.833133	-2.480434	0.006501
N	0.926681	-1.105885	1.231351
N	-0.104732	-0.699131	1.527687
O	2.794897	0.610460	0.540171
C	3.835296	1.533341	0.210787
H	3.652649	2.413207	0.824272
H	4.811558	1.099772	0.434962
H	3.794223	1.786136	-0.850569
C	-3.148767	0.462710	1.085194
C	-2.711564	1.184959	-0.219364
C	-2.251871	-0.994491	-0.628681
C	-2.923828	-1.041661	0.758588
H	-2.553592	0.796736	1.938562
H	-4.200653	0.669371	1.302844
H	-2.323516	-1.553835	1.511183
H	-3.879606	-1.569226	0.679557
C	-3.081830	0.134745	-1.287863
H	-2.729538	0.398183	-2.288495
H	-4.153418	-0.088890	-1.316123
H	-3.125875	2.187620	-0.337766
H	-2.232215	-1.951174	-1.155558
C	-1.197637	1.128247	-0.271768
C	-0.890614	-0.298550	-0.573661
C	-0.337422	2.125460	-0.066700
H	0.735540	1.951937	-0.071253

C	0.217268	-0.711705	-1.289386
H	0.895070	0.038037	-1.689994
H	0.182824	-1.646918	-1.840639
H	-0.682435	3.136153	0.124649

TS-(3+2)-6c-product

C	2.820356	-0.539202	-0.164662
O	3.863312	-1.064183	-0.455303
C	1.470839	-1.229536	-0.119496
H	1.654916	-2.292305	-0.290965
N	0.919397	-1.091737	1.266036
N	-0.218088	-0.625516	1.273184
O	2.700581	0.758410	0.158422
C	3.925435	1.494069	0.157950
H	3.661850	2.511006	0.441669
H	4.624379	1.061081	0.875734
H	4.379068	1.473991	-0.834885
C	-3.479744	0.534729	0.733402
C	-2.713627	1.067423	-0.502486
C	-2.053550	-1.092987	-0.371989
C	-3.028452	-0.952612	0.814421
H	-3.226459	1.099473	1.632943
H	-4.559017	0.614726	0.573407
H	-2.556568	-1.197705	1.765961
H	-3.876109	-1.627882	0.668847
C	-2.711735	-0.173461	-1.418797
H	-2.113652	-0.039251	-2.325401
H	-3.717739	-0.505314	-1.692602
H	-3.111520	1.994607	-0.918185
H	-1.861229	-2.125114	-0.675771
C	-1.254836	1.138884	-0.118868
C	-0.750789	-0.307016	-0.077368
C	-0.509394	2.204890	0.145799
H	0.535591	2.096992	0.426050
C	0.414321	-0.612781	-1.044228
H	0.778904	0.305203	-1.507153
H	0.112961	-1.305937	-1.832228
H	-0.918621	3.208973	0.091011

TS-(3+2)-6d

C	-3.200335	-0.585576	0.323522
O	-3.342599	0.487176	0.855718
C	-1.972574	-1.415289	0.402137
H	-2.042170	-2.482435	0.230387
N	-1.159217	-1.026134	1.405676
N	-0.294279	-0.313421	1.640706
O	-4.080892	-1.149696	-0.514509
C	-5.246288	-0.360207	-0.768169
H	-5.846911	-0.936497	-1.468636
H	-5.793746	-0.186129	0.159794
H	-4.964826	0.602623	-1.198999
C	1.732866	2.099029	1.008368
C	2.146516	1.479247	-0.359766
C	-0.080760	1.855321	-0.574049
C	0.229379	2.448185	0.815467
H	1.903155	1.397598	1.828396
H	2.330094	2.993585	1.203039
H	-0.416077	2.047710	1.598721
H	0.081175	3.532082	0.788534
C	1.211737	2.236962	-1.328306
H	1.246395	1.850092	-2.350386
H	1.400191	3.315372	-1.334175
H	3.214669	1.498063	-0.553607
H	-1.026927	2.186898	-1.006825
C	1.533456	0.095186	-0.396103
C	0.081990	0.337597	-0.561446
C	2.138063	-1.104141	-0.278750
H	1.527847	-2.006470	-0.311396
C	-0.804580	-0.542564	-1.158434
H	-0.431455	-1.490642	-1.537819
H	-1.666229	-0.145247	-1.688591
C	3.587987	-1.302377	-0.101229
O	4.386723	-0.393562	0.050361
C	4.054735	-2.747257	-0.105617
H	3.561378	-3.304952	0.696800
H	3.784215	-3.229705	-1.050141
H	5.134690	-2.781112	0.031927

TS-(3+2)-6d-product

C	-3.211650	-0.409878	-0.303015
O	-3.318713	0.741076	-0.649677
C	-1.898079	-1.175280	-0.254474
H	-2.096467	-2.231959	-0.444140
N	-1.416874	-1.056206	1.168979
N	-0.419775	-0.341406	1.253954
O	-4.225758	-1.160109	0.129067
C	-5.484641	-0.485724	0.205191
H	-6.193013	-1.222159	0.578216
H	-5.415136	0.364517	0.886004
H	-5.781329	-0.127010	-0.782179
C	2.093512	2.156369	0.859264
C	2.109086	1.407003	-0.499851
C	-0.102994	1.745885	-0.107743
C	0.575174	2.372539	1.128755
H	2.592344	1.578251	1.639423
H	2.621006	3.108702	0.755554
H	0.242930	1.908619	2.058295
H	0.332032	3.437234	1.176596
C	0.914866	2.069861	-1.215263
H	0.676465	1.614897	-2.181336
H	1.056454	3.145976	-1.351651
H	3.075301	1.402231	-0.996550
H	-1.138092	2.049171	-0.275083
C	1.555076	0.038304	-0.196592
C	0.042992	0.204476	-0.051382
C	2.185467	-1.125194	0.003009
H	1.598267	-2.008564	0.253042
C	-0.798981	-0.548841	-1.102013
H	-0.204612	-1.318165	-1.598363
H	-1.207089	0.131495	-1.851091
C	3.658824	-1.296252	-0.070458
O	4.425186	-0.363304	-0.218595
C	4.164470	-2.716909	0.067189
H	3.850111	-3.133022	1.029612
H	3.731781	-3.348735	-0.714913
H	5.251139	-2.727661	-0.004037

TS-(3+2)-6e

C	-3.205457	-0.556504	0.321251
O	-3.335784	0.517063	0.854857
C	-1.986032	-1.399234	0.398171
H	-2.066674	-2.465480	0.225237
N	-1.169983	-1.020984	1.403850
N	-0.296322	-0.321190	1.643220
O	-4.092076	-1.110375	-0.516730
C	-5.249883	-0.309130	-0.768583
H	-5.856592	-0.878705	-1.469264
H	-5.794840	-0.130886	0.160051
H	-4.959233	0.651374	-1.198487
C	1.766212	2.052493	1.017768
C	2.175484	1.428086	-0.349490
C	-0.043303	1.846296	-0.573690
C	0.271025	2.431716	0.817939
H	1.917878	1.346255	1.837350
H	2.380050	2.934577	1.217525
H	-0.385781	2.042573	1.597421
H	0.144398	3.518348	0.792055
C	1.259860	2.204789	-1.321512
H	1.292357	1.818658	-2.343866
H	1.469202	3.279304	-1.324572
H	3.244889	1.428298	-0.539837
H	-0.980783	2.196174	-1.010813
C	1.535777	0.056551	-0.395480
C	0.090387	0.325693	-0.561485
C	2.112955	-1.154859	-0.286231
H	1.510444	-2.058196	-0.317747
C	-0.810091	-0.540644	-1.158123
H	-0.450832	-1.493256	-1.539454
H	-1.664960	-0.129067	-1.688401
C	3.553928	-1.353265	-0.111674
O	4.410252	-0.503619	0.018542
O	3.868986	-2.671438	-0.097743
H	4.828417	-2.709733	0.028732

TS-(3+2)-6e-product

C	-3.209120	-0.391020	-0.305208
O	-3.296833	0.755473	-0.671857
C	-1.907229	-1.174759	-0.236178
H	-2.119563	-2.231487	-0.409549
N	-1.431806	-1.039421	1.187370
N	-0.424630	-0.338426	1.266647
O	-4.236571	-1.118712	0.132980
C	-5.486043	-0.425074	0.189459
H	-6.207244	-1.144790	0.570391
H	-5.408420	0.435563	0.856171
H	-5.771280	-0.079151	-0.805809
C	2.108421	2.122556	0.861485
C	2.132097	1.359273	-0.489819
C	-0.080630	1.724182	-0.124853
C	0.590120	2.361630	1.109775
H	2.589060	1.546149	1.654327
H	2.650194	3.066440	0.754907
H	0.241587	1.916729	2.042533
H	0.360013	3.429901	1.137731
C	0.951532	2.024361	-1.225985
H	0.719025	1.559153	-2.188556
H	1.105328	3.097155	-1.374365
H	3.103201	1.340288	-0.977309
H	-1.111084	2.034343	-0.307119
C	1.560267	-0.000798	-0.182320
C	0.050034	0.182122	-0.045238
C	2.172381	-1.171538	0.019210
H	1.600690	-2.060106	0.273098
C	-0.794278	-0.578899	-1.087962
H	-0.207480	-1.365445	-1.565898
H	-1.188146	0.092989	-1.852121
C	3.636400	-1.332490	-0.064249
O	4.453976	-0.454452	-0.226343
O	3.995947	-2.625475	0.075385
H	4.963305	-2.644762	0.023438

TS-(3+2)-6f

C	3.017715	-0.620624	-0.089278
O	3.916484	-0.891546	-0.844682
C	1.932304	-1.571996	0.246457
H	2.192707	-2.622335	0.174227
N	1.149192	-1.264487	1.300947
N	0.090862	-0.945035	1.597650
O	2.814626	0.587569	0.456559
C	3.778811	1.581653	0.090762
H	3.475139	2.489005	0.608354
H	4.776565	1.270553	0.404318
H	3.774110	1.730540	-0.990491
C	-3.047619	-0.175098	1.041117
C	-2.688752	0.505511	-0.311814
C	-2.007818	-1.639290	-0.583388
C	-2.671895	-1.666431	0.809088
H	-2.495550	0.273880	1.870248
H	-4.115114	-0.057859	1.244633
H	-2.021252	-2.066017	1.587808
H	-3.568534	-2.292330	0.771682
C	-2.946084	-0.644668	-1.309119
H	-2.623253	-0.411934	-2.326930
H	-3.990461	-0.971803	-1.315206
H	-3.193817	1.456100	-0.486085
H	-1.885235	-2.619195	-1.049370
C	-1.180777	0.585238	-0.358776
C	-0.726836	-0.803539	-0.570241
C	-0.410452	1.677288	-0.200658
H	0.673344	1.604709	-0.183034
C	0.443319	-1.139228	-1.231168
H	1.033727	-0.345718	-1.683526
H	0.512506	-2.101971	-1.729233
C	-0.981933	2.974181	-0.022305
N	-1.447720	4.026407	0.121908

TS-(3+2)-6f-product

C	3.008033	-0.511762	-0.155347
O	4.125446	-0.860352	-0.428685
C	1.794943	-1.422693	-0.091765
H	2.159027	-2.441667	-0.237121
N	1.225938	-1.343644	1.288475

N	0.036040	-1.035523	1.292663
O	2.664299	0.755202	0.127198
C	3.744264	1.694195	0.101873
H	3.304982	2.659606	0.344856
H	4.499254	1.415472	0.838715
H	4.202339	1.714728	-0.888493
C	-3.346513	-0.205145	0.682083
C	-2.611897	0.351920	-0.565650
C	-1.752516	-1.732222	-0.336618
C	-2.750379	-1.634496	0.835186
H	-3.178787	0.421819	1.560024
H	-4.422362	-0.237958	0.490066
H	-2.265883	-1.786616	1.799805
H	-3.524646	-2.397032	0.718034
C	-2.474269	-0.919560	-1.428785
H	-1.878366	-0.768072	-2.333855
H	-3.442526	-1.348944	-1.700614
H	-3.080326	1.227638	-1.016324
H	-1.457857	-2.751787	-0.595734
C	-1.184629	0.562871	-0.139305
C	-0.533575	-0.816273	-0.063564
C	-0.558042	1.702602	0.168522
H	0.478023	1.702682	0.496799
C	0.652032	-1.018521	-1.034087
H	0.882817	-0.097311	-1.570916
H	0.438452	-1.801828	-1.763899
C	-1.227712	2.965906	0.073400
N	-1.774914	3.983383	-0.010438

TS-(3+2)-7a

C	-2.910157	-1.002902	-0.091610
O	-3.444993	-1.734006	-0.887444
C	-1.445047	-1.003811	0.136263
H	-0.951634	-1.963116	0.012227
N	-0.998931	-0.320026	1.220006
N	-0.382128	0.567837	1.582640
O	-3.532891	-0.042307	0.604236
C	-4.935871	0.062397	0.348700
H	-5.292590	0.867004	0.988014
H	-5.112034	0.295581	-0.703071
H	-5.435884	-0.876713	0.592170
C	0.246588	1.011651	-0.813632
C	1.576864	0.476622	-0.466532
C	2.532211	1.428386	0.088478
C	2.237214	2.740754	0.219833
C	0.949724	3.268556	-0.169805
C	0.005627	2.430959	-0.653263
H	3.515529	1.047230	0.342927
H	2.988069	3.422932	0.607413
H	0.751981	4.330169	-0.071834
H	-0.969734	2.807029	-0.953231
C	-0.742887	0.196120	-1.374673
C	1.887056	-0.843002	-0.559979
H	-0.464824	-0.668954	-1.969042
H	1.202514	-1.555024	-1.029539
H	-1.656828	0.682404	-1.709763
N	3.084452	-1.386648	-0.031189
C	3.494414	-2.593129	-0.724339
H	2.763317	-3.415422	-0.610677
H	3.613945	-2.382833	-1.789263
H	4.454539	-2.936457	-0.329693
C	3.016993	-1.595214	1.412377
H	3.999026	-1.904258	1.783437
H	2.736720	-0.660997	1.904006
H	2.280825	-2.370529	1.690478

TS-(3+2)-7a-product

C	-3.131075	-1.004696	-0.252739
O	-3.993065	-1.752258	-0.634379
C	-1.641601	-1.295418	-0.280174
H	-1.532906	-2.324696	-0.626734
N	-1.131858	-1.230635	1.126713
N	-0.295057	-0.347203	1.291653
O	-3.369313	0.217538	0.249126
C	-4.750053	0.578612	0.322141
H	-4.774293	1.578064	0.751709
H	-5.195636	0.574224	-0.674508
H	-5.290337	-0.127531	0.955050
C	0.010306	0.448886	0.044790
C	1.513818	0.415500	-0.192985
C	2.191985	1.644325	-0.577885
C	1.587535	2.842394	-0.490271
C	0.224046	2.940299	0.024702
C	-0.502989	1.849724	0.288746
H	3.200122	1.549442	-0.971161
H	2.098329	3.745961	-0.805304
H	-0.207817	3.925337	0.174189
H	-1.526557	1.914354	0.646225
C	-0.815044	-0.268318	-1.061689
C	2.169150	-0.759348	-0.077280
H	-0.146015	-0.756952	-1.771202
H	1.596895	-1.672401	0.111499
H	-1.440412	0.441737	-1.605636
N	3.553893	-0.922135	-0.178908
C	3.973895	-2.300148	-0.365848
H	3.824630	-2.911016	0.540035
H	3.417447	-2.750320	-1.190124
H	5.036179	-2.322380	-0.621983
C	4.368770	-0.240873	0.825416
H	5.398682	-0.164661	0.464852
H	3.986428	0.762359	1.007168
H	4.372987	-0.789597	1.780205

TS-(3+2)-7b

C	2.728489	-0.046650	0.378977
O	3.073754	-1.113215	0.821590
C	1.401511	0.584483	0.571114
H	1.358555	1.669174	0.595778
N	0.643260	-0.002730	1.530843
N	-0.309648	-0.606697	1.710504
O	3.463983	0.711836	-0.449509
C	4.726585	0.144712	-0.806156
H	5.192910	0.860089	-1.480380
H	5.339811	-0.004315	0.084435
H	4.583580	-0.817587	-1.301506
C	-0.913788	-0.421063	-0.675326

C	-1.960492	0.561569	-0.328765
C	-3.264264	0.034512	0.060372
C	-3.530804	-1.287293	0.018421
C	-2.530867	-2.245157	-0.408408
C	-1.287948	-1.823908	-0.721633
H	-4.020119	0.747806	0.368984
H	-4.514898	-1.647365	0.302287
H	-2.787093	-3.297479	-0.462781
H	-0.522109	-2.530852	-1.031414
C	0.352760	-0.022855	-1.114161
C	-1.724776	1.892116	-0.293341
H	0.486657	0.940558	-1.597400
H	-0.770035	2.329729	-0.572584
H	1.014647	-0.799460	-1.490872
O	-2.694765	2.767258	0.114661
H	-2.419398	3.665869	-0.084469

TS-(3+2)-7b-product

C	2.608567	0.011401	-0.288758
O	2.581173	-1.190604	-0.390988
C	1.383309	0.909470	-0.345154
H	1.690464	1.898066	-0.692747
N	0.931790	1.062149	1.086270
N	-0.144036	0.509199	1.296119
O	3.718302	0.717793	-0.064385
C	4.904776	-0.063066	0.100215
H	5.706015	0.649815	0.282570
H	4.792443	-0.744170	0.945656
H	5.101743	-0.646104	-0.801414
C	-0.741709	-0.159068	0.073661
C	-2.181618	0.312817	-0.064592
C	-3.263546	-0.653805	-0.179477
C	-3.038950	-1.971756	-0.047871
C	-1.690130	-2.469525	0.210339
C	-0.636371	-1.650507	0.288198
H	-4.260871	-0.264110	-0.352763
H	-3.855806	-2.681406	-0.121501
H	-1.545425	-3.538934	0.330921
H	0.370203	-2.025101	0.451038
C	0.197971	0.295537	-1.076871
C	-2.429027	1.632828	-0.046549
H	-0.306383	1.034476	-1.701712
H	-1.627757	2.359301	0.083321
H	0.498201	-0.550034	-1.697061
O	-3.684773	2.130367	-0.181330
H	-3.674370	3.082355	-0.048257

TS-(3+2)-7c

C	2.515942	-0.124841	0.374850
O	2.732977	-1.224603	0.817242
C	1.264422	0.650807	0.559456
H	1.334684	1.733698	0.597667
N	0.439787	0.144675	1.510595
N	-0.569821	-0.330933	1.728049
O	3.337717	0.550901	-0.440365
C	4.536862	-0.147444	-0.786220
H	5.084778	0.517316	-1.450522
H	5.119231	-0.365165	0.110805
H	4.296384	-1.086108	-1.288947
C	-1.131547	-0.069262	-0.697902
C	-2.035223	1.024478	-0.286004
C	-3.382613	0.616720	0.104211
C	-3.798777	-0.665391	0.026078
C	-2.922923	-1.717443	-0.439392
C	-1.645306	-1.422075	-0.765340
H	-4.057730	1.395142	0.448727
H	-4.814298	-0.918838	0.315622
H	-3.294791	-2.733221	-0.511539
H	-0.964671	-2.198511	-1.106669
C	0.171064	0.209699	-1.122558
C	-1.653159	2.319842	-0.194771
H	0.395515	1.173719	-1.569334
H	-0.667463	2.665923	-0.484817
H	0.752576	-0.615621	-1.528592
H	-2.351987	3.074547	0.147639

TS-(3+2)-7c-product

C	2.344729	-0.123142	-0.270468
O	2.166586	-1.311440	-0.384661
C	1.239775	0.920147	-0.327623
H	1.668802	1.871062	-0.650191
N	0.783532	1.096583	1.095853
N	-0.358087	0.683721	1.275852
O	3.531386	0.436189	-0.031511
C	4.610415	-0.487928	0.133120
H	5.492811	0.118335	0.325863
H	4.408277	-1.155899	0.972302
H	4.738763	-1.083811	-0.772435
C	-1.007719	0.123365	0.026747
C	-2.359218	0.816688	-0.128307
C	-3.570981	0.002144	-0.160346
C	-3.535762	-1.329893	-0.000002
C	-2.266589	-2.027281	0.199870
C	-1.103850	-1.369911	0.222731
H	-4.512793	0.523630	-0.306337
H	-4.452846	-1.909440	-0.016658
H	-2.280182	-3.106235	0.318078
H	-0.154143	-1.883606	0.344457
C	0.004005	0.467004	-1.096255
C	-2.420833	2.152831	-0.200368
H	-0.386149	1.268815	-1.724320
H	-1.529823	2.772114	-0.145681
H	0.214075	-0.404605	-1.717497
H	-3.372525	2.665373	-0.294731

TS-(3+2)-7d

C	-2.874612	-1.010545	-0.047002
O	-3.421994	-1.775956	-0.797699
C	-1.404238	-1.029071	0.176983
H	-0.925513	-2.001063	0.112147
N	-0.956344	-0.308008	1.236542
N	-0.371517	0.537137	1.699420
O	-3.467882	-0.001157	0.599110
C	-4.873997	0.121669	0.353866
H	-5.203636	0.966996	0.953381
H	-5.055627	0.302577	-0.706946

H	-5.389051	-0.792230	0.653895
C	0.286134	0.937270	-0.854176
C	1.580346	0.436558	-0.385274
C	2.474827	1.431873	0.171179
C	2.138327	2.749693	0.207402
C	0.878831	3.231441	-0.272452
C	-0.020383	2.338513	-0.760624
H	3.429049	1.087511	0.545109
H	2.848519	3.461351	0.618682
H	0.648467	4.290020	-0.231932
H	-0.991225	2.668423	-1.123332
C	-0.684912	0.058944	-1.365326
C	1.883315	-0.913017	-0.417569
H	-0.381829	-0.832916	-1.905111
H	1.189239	-1.595672	-0.899248
H	-1.602630	0.505536	-1.743696
C	3.100141	-1.544586	0.075834
O	4.013899	-0.974604	0.661681
C	3.196840	-3.044165	-0.180085
H	2.324154	-3.566441	0.224835
H	3.225605	-3.243069	-1.256163
H	4.103601	-3.428659	0.285382

TS-(3+2)-7d-product

C	-3.017099	-1.045424	-0.309170
O	-3.827059	-1.839608	-0.707462
C	-1.518663	-1.285543	-0.231493
H	-1.353377	-2.321663	-0.532267
N	-1.104183	-1.152904	1.196752
N	-0.299667	-0.244917	1.383520
O	-3.323087	0.188466	0.121084
C	-4.718210	0.503805	0.100264
H	-4.799661	1.518782	0.483520
H	-5.104133	0.441510	-0.918898
H	-5.269500	-0.194015	0.732609
C	0.062903	0.511340	0.126021
C	1.584035	0.459794	-0.030465
C	2.296314	1.705414	-0.280000
C	1.662170	2.891692	-0.215202
C	0.241349	2.994426	0.099172
C	-0.501600	1.899235	0.278645
H	3.355033	1.639016	-0.489150
H	2.220332	3.806961	-0.385401
H	-0.206542	3.979631	0.179729
H	-1.563454	1.946844	0.501896
C	-0.676009	-0.259524	-1.003212
C	2.180861	-0.751424	0.064138
H	0.039198	-0.752492	-1.661899
H	1.556317	-1.614676	0.290669
H	-1.292783	0.414471	-1.599911
C	3.627728	-1.050133	-0.074162
O	4.471657	-0.224512	-0.370666
C	4.008823	-2.493954	0.183320
H	3.715606	-2.784273	1.197052
H	3.478184	-3.154888	-0.509335
H	5.084022	-2.613463	0.058701

TS-(3+2)-7e

C	-2.972384	-0.277790	0.397806
O	-3.491316	0.625209	1.002699
C	-1.523245	-0.616355	0.436481
H	-1.229554	-1.657831	0.343561
N	-0.858102	0.013408	1.438325
N	-0.095501	0.734577	1.844018
O	-3.585636	-1.080127	-0.476662
C	-4.974587	-0.793234	-0.678024
H	-5.320892	-1.518195	-1.410970
H	-5.519704	-0.899237	0.261260
H	-5.098470	0.225401	-1.049691
C	0.395693	1.003709	-0.784243
C	1.609878	0.267731	-0.429692
C	2.731365	1.074209	0.006746
C	2.656071	2.432075	0.045158
C	1.467814	3.143740	-0.315093
C	0.370372	2.437166	-0.690869
H	3.639215	0.558288	0.288788
H	3.527258	2.996469	0.365218
H	1.447428	4.226743	-0.274465
H	-0.552642	2.944953	-0.960680
C	-0.765995	0.320023	-1.183425
C	1.632172	-1.113430	-0.450255
H	-0.682514	-0.611984	-1.734414
H	0.786434	-1.672913	-0.829393
H	-1.617289	0.930187	-1.479914
C	2.751800	-1.942362	-0.052374
O	3.838010	-1.609006	0.388303
O	2.459583	-3.265580	-0.212013
H	3.257089	-3.734631	0.072383

TS-(3+2)-7e-product

C	-3.049960	-0.314899	-0.288991
O	-3.263553	0.864520	-0.430673
C	-1.661349	-0.937914	-0.282541
H	-1.741857	-1.985330	-0.580574
N	-1.220077	-0.914875	1.152553
N	-0.281410	-0.148393	1.345332
O	-3.994848	-1.228393	-0.072783
C	-5.324048	-0.708586	0.031090
H	-5.964321	-1.568588	0.214114
H	-5.384944	0.003149	0.856166
H	-5.605052	-0.204762	-0.895525
C	0.186899	0.562826	0.090891
C	1.696114	0.344275	-0.019950
C	2.564278	1.507380	-0.132977
C	2.065926	2.754617	-0.037410
C	0.643996	3.009693	0.162563
C	-0.230785	2.003040	0.234317
H	3.622337	1.330389	-0.270794
H	2.737424	3.604683	-0.106966
H	0.302429	4.036942	0.236832
H	-1.298354	2.167851	0.349878
C	-0.618639	-0.123390	-1.043378
C	2.135622	-0.933672	0.010463
H	0.030452	-0.769250	-1.635605
H	1.424787	-1.746126	0.131857
H	-1.085044	0.614185	-1.697579

C	3.541948	-1.362405	-0.085425
O	4.525956	-0.669464	-0.224625
O	3.632088	-2.707560	-0.003263
H	4.575392	-2.918894	-0.068158

TS-(3+2)-7f

C	2.795362	0.155766	0.385381
O	3.197731	-0.800168	0.996970
C	1.398688	0.673155	0.422755
H	1.245172	1.743543	0.321099
N	0.664286	0.146308	1.436845
N	-0.186120	-0.475252	1.836033
O	3.500849	0.867866	-0.497070
C	4.843210	0.408626	-0.698960
H	5.274435	1.078404	-1.439242
H	5.399974	0.454697	0.238264
H	4.837919	-0.620753	-1.061391
C	-0.707289	-0.714886	-0.769070
C	-1.820041	0.172847	-0.442569
C	-3.033498	-0.466714	0.020431
C	-3.141038	-1.818228	0.097065
C	-2.053493	-2.685318	-0.251897
C	-0.874685	-2.137930	-0.644158
H	-3.869749	0.170694	0.289691
H	-4.075372	-2.256286	0.434999
H	-2.174540	-3.760268	-0.186664
H	-0.027405	-2.769186	-0.900882
C	0.528614	-0.186736	-1.178741
C	-1.703016	1.545042	-0.497915
H	0.556427	0.737673	-1.748731
H	-0.817624	2.033038	-0.885828
H	1.297051	-0.901197	-1.467984
C	-2.762770	2.405127	-0.112596
N	-3.628907	3.106593	0.216994

TS-(3+2)-7f-product

C	2.779896	0.170160	-0.281956
O	2.847192	-1.030905	-0.379096
C	1.475364	0.955211	-0.300093
H	1.681512	1.976958	-0.624972
N	1.029250	1.021091	1.131522
N	0.012415	0.366462	1.340229
O	3.827481	0.970816	-0.100888
C	5.086711	0.300686	0.021266
H	5.825548	1.085146	0.168110
H	5.067689	-0.379527	0.874432
H	5.299065	-0.269142	-0.885033
C	-0.527734	-0.321702	0.102476
C	-1.999925	0.047656	-0.021424
C	-2.986315	-1.008125	-0.177590
C	-2.637238	-2.303332	-0.078918
C	-1.256072	-2.705054	0.169815
C	-0.279586	-1.798926	0.271960
H	-4.017647	-0.713572	-0.344267
H	-3.393486	-3.075360	-0.176433
H	-1.029345	-3.762334	0.257843
H	0.758295	-2.080788	0.423390
C	0.345331	0.250412	-1.045798
C	-2.342228	1.354417	0.027270
H	-0.230001	0.956678	-1.645972
H	-1.596599	2.128332	0.184093
H	0.721418	-0.545022	-1.690181
C	-3.695185	1.794881	-0.102079
N	-4.793372	2.146967	-0.216140

TS-(3+2)-7ba

C	1.670086	-0.200606	-0.879744
C	1.446963	-0.980916	0.359398
C	2.648104	-1.265981	1.140552
C	3.889123	-1.121263	0.624286
C	4.087377	-0.622094	-0.714110
C	3.021654	-0.171524	-1.412767
H	2.510793	-1.673573	2.134352
H	4.753257	-1.402016	1.218564
H	5.085964	-0.581773	-1.135464
H	3.154106	0.257450	-2.403735
C	0.673625	0.482808	-1.595623
C	0.241303	-1.373218	0.865745
H	-0.372923	0.224416	-1.497844
C	-1.005622	2.394553	-0.295039
O	-1.930050	2.585581	-1.045632
C	0.400093	2.327686	-0.776884
H	0.612289	3.005113	-1.597787
N	1.371335	2.338599	0.175012
N	2.218122	1.737255	0.648611
O	-1.120337	2.156194	1.016285
C	-2.459589	2.229473	1.513351
H	-2.397982	1.952633	2.564225
H	-2.842228	3.246831	1.405957
H	-3.104267	1.542263	0.963711
H	0.944853	0.810901	-2.596419
O	0.203001	-1.747955	2.195014
H	-0.473491	-2.428810	2.296144
C	-1.064532	-1.467907	0.188977
C	-2.230631	-1.114504	0.881426
C	-1.190238	-2.023179	-1.094313
C	-3.483935	-1.270980	0.293325
H	-2.139598	-0.705069	1.883842
C	-2.438853	-2.175708	-1.679197
H	-0.290820	-2.325689	-1.623038
C	-3.592431	-1.796182	-0.989721
H	-4.376435	-0.982322	0.840675
H	-2.518203	-2.605719	-2.672495
H	-4.567420	-1.918914	-1.449376

TS-(3+2)-7ba-product

C	1.627700	0.846783	-0.012905
C	2.115281	-0.597295	0.037052
C	3.549943	-0.865824	0.016731
C	4.468383	0.112106	-0.053377
C	4.052975	1.506856	-0.129555
C	2.761284	1.844240	-0.109614
H	3.853785	-1.904383	0.068368
H	5.526421	-0.125442	-0.054099
H	4.811762	2.279497	-0.209337
H	2.451542	2.885974	-0.161717

C	0.572635	1.158919	-1.102587
C	1.268824	-1.656536	0.056135
H	0.139374	0.254617	-1.529628
C	-1.906956	1.458704	-0.584994
O	-2.229215	0.736838	-1.495233
C	-0.485671	1.942082	-0.336778
H	-0.483661	3.018835	-0.546379
N	-0.136086	1.810217	1.112835
N	0.928972	1.223767	1.284033
O	-2.764502	1.983970	0.295189
C	-4.130744	1.631340	0.081698
H	-4.691737	2.125445	0.872627
H	-4.463176	1.974731	-0.900438
H	-4.252381	0.547773	0.136102
H	1.012012	1.740721	-1.913543
O	1.800436	-2.911374	-0.076167
H	1.131964	-3.554537	0.187145
C	-0.215183	-1.661314	0.152391
C	-0.889058	-1.164323	1.272224
C	-0.947073	-2.296569	-0.862070
C	-2.276109	-1.270339	1.356061
H	-0.323864	-0.712775	2.079025
C	-2.328630	-2.402179	-0.773766
H	-0.421442	-2.688008	-1.728833
C	-2.994928	-1.889865	0.337706
H	-2.789280	-0.878352	2.228546
H	-2.886801	-2.877424	-1.573294
H	-4.074522	-1.980757	0.410969

TS-[4+2]-1a

C	-2.318773	-0.246606	-0.043681
O	-2.790369	-1.359012	0.065380
C	-0.913646	0.093397	-0.046700
H	-0.563693	1.109881	-0.152146
N	-0.021787	-0.869143	0.078425
N	0.063444	-2.055860	0.163262
O	-3.087261	0.870014	-0.178300
C	-4.484390	0.612310	-0.186865
H	-4.969412	1.581349	-0.301333
H	-4.752618	-0.048354	-1.014926
H	-4.797827	0.136814	0.745831
C	2.612244	-0.523668	-0.612973
C	2.546034	-1.906989	-0.480322
C	2.025388	0.320961	0.330448
C	1.821145	-2.541618	0.535642
H	1.849757	-0.040496	1.338689
H	1.759489	-3.623428	0.519211
H	1.819623	-2.127483	1.539547
H	2.875054	-2.505840	-1.324688
H	3.001896	-0.101115	-1.532934
N	1.796170	1.635357	0.167788
C	1.418207	2.478201	1.287390
H	2.243749	3.129909	1.596503
H	0.560617	3.100836	1.016925
H	1.128483	1.849369	2.130427
C	1.963080	2.252724	-1.134069
H	1.463068	3.222265	-1.133929
H	3.020080	2.403513	-1.384264
H	1.502246	1.620027	-1.899088

TS-[4+2]-1a-product

C	-2.127859	-0.337833	-0.004531
O	-2.480744	-1.495473	0.003199
C	-0.793320	0.212692	0.092165
H	-0.666263	1.276968	0.068915
N	0.306770	-0.537828	0.207684
N	0.300182	-1.812824	0.251905
O	-3.017510	0.694906	-0.115347
C	-4.371878	0.281274	-0.217644
H	-4.960480	1.194621	-0.298379
H	-4.521430	-0.347827	-1.098718
H	-4.672495	-0.289228	0.664764
C	2.666736	-0.464944	-0.514107
C	2.666930	-1.792268	-0.479270
C	1.668740	0.256306	0.343746
C	1.613839	-2.444632	0.364849
H	1.895426	0.086080	1.404270
H	1.466871	-3.490909	0.092868
H	1.940691	-2.440736	1.420141
H	3.365462	-2.392861	-1.052806
H	3.364832	0.133007	-1.089215
N	1.619112	1.642181	0.111792
C	1.230393	2.545658	1.174666
H	1.800461	3.476508	1.082754
H	0.161155	2.803632	1.164751
H	1.462081	2.097847	2.143598
C	1.400204	2.146240	-1.231200
H	0.356274	2.442698	-1.405080
H	2.036818	3.020401	-1.407136
H	1.651467	1.378674	-1.965259

TS-[4+2]-1b

C	2.016739	-0.184624	0.024159
O	2.227476	-1.378277	0.044301
C	0.713328	0.451109	-0.026180
H	0.579819	1.520852	-0.064499
N	-0.348300	-0.324590	-0.072760
N	-0.670371	-1.471500	-0.036632
O	3.003796	0.745221	0.048152
C	4.316021	0.199179	0.099813
H	4.995045	1.050726	0.114862
H	4.446314	-0.410120	0.997308
H	4.508510	-0.428073	-0.773791
C	-2.876307	0.509813	0.547102
C	-3.088335	-0.868106	0.491031
C	-2.077606	1.145579	-0.381429
C	-2.476110	-1.667658	-0.475268
H	-1.943701	0.780146	-1.392691
H	-2.592251	-2.742572	-0.405809
H	-2.364499	-1.306767	-1.492954
H	-3.535892	-1.348040	1.355645
H	-3.170664	1.059368	1.438919
O	-1.631920	2.404944	-0.259490
H	-1.753178	2.710255	0.649674

TS-[4+2]-1b-product

C	1.877733	-0.199411	0.006458
O	2.016622	-1.395900	0.119700
C	0.657849	0.566862	-0.154176
H	0.706005	1.635783	-0.252492
N	-0.548820	0.000064	-0.239486
N	-0.757613	-1.262502	-0.241146
O	2.932768	0.665285	0.030944
C	4.194954	0.034060	0.193589
H	4.933882	0.834434	0.189178
H	4.235079	-0.517687	1.136092
H	4.386352	-0.666970	-0.622544
C	-2.845787	0.485002	0.502680
C	-3.076474	-0.821721	0.525631
C	-1.737890	0.981916	-0.373219
C	-2.156835	-1.678174	-0.292238
H	-1.996694	0.918404	-1.436060
H	-2.171506	-2.717071	0.040944
H	-2.506671	-1.683891	-1.339780
H	-3.862443	-1.268617	1.125495
H	-3.417781	1.226881	1.050543
O	-1.377317	2.289980	-0.125910
H	-1.219077	2.389676	0.822826

TS-[4+2]-1c

C	-1.861641	-0.080003	-0.027057
O	-1.953240	-1.286101	-0.100802
C	-0.626438	0.680617	0.048057
H	-0.605108	1.754141	0.118289
N	0.506770	0.007408	0.045770
N	0.918249	-1.101546	-0.062996
O	-2.932476	0.749382	0.001389
C	-4.187630	0.082619	-0.069594
H	-4.944427	0.865264	-0.042174
H	-4.266255	-0.494185	-0.994001
H	-4.310878	-0.599009	0.775187
C	3.022022	0.982742	-0.440877
C	3.327325	-0.383764	-0.430067
C	2.122379	1.511059	0.452747
C	2.702874	-1.244433	0.472539
H	1.985298	1.092697	1.443552
H	2.855098	-2.312151	0.367331
H	2.517881	-0.924541	1.493205
H	3.835472	-0.809458	-1.289638
H	3.319088	1.573456	-1.302569
H	1.731084	2.513475	0.312219

TS-[4+2]-1c-product

C	-1.749992	-0.091468	-0.005363
O	-1.823184	-1.298075	-0.060735
C	-0.574064	0.742195	0.121330
H	-0.685998	1.811649	0.169717
N	0.670329	0.251496	0.200818
N	0.967405	-0.989744	0.137489
O	-2.851127	0.713279	-0.054598
C	-4.078107	0.007758	-0.176222
H	-4.859181	0.766472	-0.207157
H	-4.092120	-0.592304	-1.089363
H	-4.228345	-0.660165	0.675577
C	2.937725	0.949007	-0.436710
C	3.274703	-0.334425	-0.491570
C	1.749801	1.280879	0.410610
C	2.394634	-1.287753	0.266761
H	1.992183	1.220021	1.478725
H	2.517231	-2.315380	-0.076988
H	2.679305	-1.277746	1.333887
H	4.101500	-0.704044	-1.088637
H	3.448122	1.739132	-0.974889
H	1.329461	2.261318	0.200635

TS-[4+2]-1d

C	-2.369157	-0.133974	-0.068057
O	-2.794930	-1.262278	0.031206
C	-0.957318	0.241053	-0.105667
H	-0.629332	1.262030	-0.211011
N	-0.075010	-0.721413	-0.030553
N	0.020257	-1.907623	-0.043140
O	-3.151335	0.962651	-0.148376
C	-4.549543	0.688070	-0.123807
H	-5.044712	1.654370	-0.202440
H	-4.828121	0.044130	-0.960723
H	-4.825810	0.188747	0.807489
C	2.693507	-0.677791	-0.453886
C	2.472967	-2.048561	-0.293833
C	2.071232	0.256753	0.339656
C	1.557909	-2.521895	0.660588
H	1.715777	0.015102	1.336662
H	1.351121	-3.585576	0.688653
H	1.495020	-2.043035	1.633556
H	2.808398	-2.726929	-1.071265
H	3.213244	-0.310139	-1.335018
C	2.118621	1.700410	-0.023649
O	2.559370	2.071104	-1.092914
C	1.595173	2.668636	1.013040
H	0.612116	2.353664	1.377731
H	2.269364	2.672005	1.876443
H	1.541015	3.670859	0.590143

TS-[4+2]-1d-product

C	-2.121798	-0.282678	-0.004471
O	-2.475902	-1.422732	0.189234
C	-0.781017	0.268473	0.010330
H	-0.651629	1.313627	-0.207977
N	0.313785	-0.482112	0.191775
N	0.300564	-1.748869	0.349676
O	-2.999501	0.725252	-0.271535
C	-4.359557	0.314311	-0.311659
H	-4.937175	1.210615	-0.533631
H	-4.512960	-0.440874	-1.086230
H	-4.664858	-0.109873	0.647985
C	2.601408	-0.491700	-0.663608
C	2.604695	-1.813232	-0.526966
C	1.660760	0.232960	0.247297
C	1.620988	-2.372067	0.463532
H	1.955050	0.085147	1.297122
H	1.458789	-3.441283	0.326981
H	2.012252	-2.239241	1.488387

H	3.215621	-2.472746	-1.133780
H	3.174571	0.078058	-1.384565
C	1.577470	1.741624	-0.024350
O	1.854267	2.176068	-1.115125
C	1.222417	2.620052	1.149811
H	0.423163	2.175805	1.747877
H	2.107031	2.711991	1.790326
H	0.936597	3.610475	0.797272

TS-[4+2]-1e

C	-2.376719	-0.127066	-0.088102
O	-2.800616	-1.255764	-0.179098
C	-0.959639	0.246155	-0.029445
H	-0.624634	1.264937	0.089208
N	-0.090118	-0.721260	-0.051190
N	0.050079	-1.894101	-0.206310
O	-3.155525	0.970084	-0.019678
C	-4.554631	0.700674	-0.072282
H	-5.047091	1.669697	-0.014705
H	-4.811297	0.192868	-1.004397
H	-4.853548	0.066506	0.765091
C	2.731848	-0.654984	-0.333785
C	2.486387	-2.026617	-0.223814
C	2.061453	0.277769	0.418769
C	1.488567	-2.519084	0.637827
H	1.606511	0.062582	1.377729
H	1.288328	-3.584555	0.628558
H	1.343787	-2.060816	1.612487
H	2.882235	-2.688023	-0.986841
H	3.329007	-0.282372	-1.162206
C	2.143708	1.698860	0.033448
O	2.793995	2.152706	-0.878171
O	1.360275	2.472011	0.820350
H	1.456107	3.380155	0.494655

TS-[4+2]-1e-product

C	2.120259	0.287490	-0.021134
O	2.456296	1.449040	-0.011389
C	0.789000	-0.278045	0.081813
H	0.682375	-1.346898	0.071727
N	-0.310499	0.471172	0.219843
N	-0.304791	1.746624	0.293591
O	3.012686	-0.735462	-0.144719
C	4.364384	-0.313482	-0.266187
H	4.955923	-1.223771	-0.354705
H	4.495917	0.315260	-1.150094
H	4.672022	0.258829	0.612324
C	-2.632896	0.438271	-0.575498
C	-2.639727	1.763640	-0.503319
C	-1.651359	-0.253123	0.321028
C	-1.618473	2.379254	0.408638
H	-1.918807	-0.133652	1.378430
H	-1.460700	3.436471	0.194411
H	-1.971590	2.317655	1.453501
H	-3.286273	2.384819	-1.113427
H	-3.237827	-0.162780	-1.242925
C	-1.563037	-1.739430	0.009971
O	-1.823328	-2.225467	-1.057104
O	-1.203292	-2.449991	1.088427
H	-1.171821	-3.382931	0.823131

TS-[4+2]-1f

C	2.140005	-0.192811	0.045553
O	2.409953	-1.370929	0.080197
C	0.781846	0.362998	0.043168
H	0.578093	1.423180	0.010103
N	-0.201380	-0.488072	0.064249
N	-0.497363	-1.632785	0.200207
O	3.052368	0.794015	-0.004475
C	4.406221	0.345149	-0.002872
H	5.017565	1.244759	-0.040403
H	4.617306	-0.227057	0.902905
H	4.599013	-0.288845	-0.870910
C	-2.963050	-0.001529	0.415799
C	-2.935576	-1.397037	0.328584
C	-2.187519	0.784348	-0.406917
C	-2.066186	-2.051973	-0.560881
H	-1.840254	0.439215	-1.373763
H	-2.024921	-3.134557	-0.526674
H	-1.894919	-1.646808	-1.554528
H	-3.393689	-1.973503	1.124440
H	-3.458647	0.464027	1.262447
C	-1.977628	2.172765	-0.152545
N	-1.742226	3.289919	0.050012

TS-[4+2]-1f-product

C	-1.958616	-0.258335	-0.002643
O	-2.170286	-1.448474	-0.007967
C	-0.686203	0.436882	0.097579
H	-0.672048	1.512511	0.090578
N	0.477964	-0.208604	0.195391
N	0.609433	-1.481610	0.200132
O	-2.947967	0.669213	-0.093361
C	-4.254904	0.118244	-0.198256
H	-4.933126	0.967733	-0.262151
H	-4.339512	-0.507678	-1.089729
H	-4.487658	-0.493218	0.676766
C	2.816466	0.105642	-0.541699
C	2.951961	-1.214804	-0.534717
C	1.738740	0.640614	0.363624
C	1.979792	-1.978154	0.316627
H	2.007982	0.480653	1.416418
H	1.938983	-3.032411	0.042625
H	2.308177	-1.940572	1.371099
H	3.676472	-1.731543	-1.154531
H	3.390396	0.797103	-1.145820
C	1.514455	2.072175	0.166187
N	1.404919	3.211345	0.013786

TS-[4+2]-2a

C	-1.522905	-0.053952	-0.005050
C	-2.531401	-1.088906	-0.052927
O	-2.351575	-2.277729	0.110688
O	-3.759771	-0.558598	-0.309865
N	-0.272662	-0.386525	0.241322
N	0.425387	-1.337655	0.422681

H	-1.755834	0.988849	-0.167240
C	-4.802874	-1.520673	-0.374067
H	-5.715092	-0.963446	-0.585769
H	-4.610451	-2.250830	-1.164041
H	-4.895536	-2.057863	0.573135
C	0.850965	1.743947	0.454304
C	1.863124	1.264878	-0.373268
H	2.053209	1.750346	-1.325711
C	2.494201	0.056158	-0.094383
C	3.444229	-0.650833	-1.037419
C	2.139929	-0.810547	0.956001
C	3.294359	-2.131691	-0.643146
H	4.468305	-0.300899	-0.848549
C	2.938594	-2.087529	0.851984
H	1.839256	-0.445515	1.933724
H	2.451350	-2.564344	-1.189058
H	4.185493	-2.724546	-0.859319
H	2.350797	-2.950377	1.176081
H	3.838384	-2.028659	1.476801
H	3.222297	-0.455980	-2.090866
H	0.795274	1.402879	1.483209
N	-0.015504	2.726189	0.149419
C	-0.868923	3.318840	1.162272
H	-0.526896	4.322409	1.441610
H	-1.896740	3.387745	0.794557
H	-0.867977	2.684809	2.050141
C	-0.080009	3.249857	-1.201016
H	-0.084139	2.418733	-1.913369
H	-1.004344	3.817157	-1.318656
H	0.767120	3.908792	-1.426924

TS-[4+2]-2a-product

C	1.479698	0.063021	-0.060276
C	2.298220	-1.127300	0.016364
O	1.980677	-2.284823	-0.142023
O	3.581558	-0.757885	0.311148
N	0.173454	0.039589	-0.338488
N	-0.502743	-1.024992	-0.531353
H	1.934208	1.020207	0.105097
C	4.486777	-1.846850	0.412264
H	5.456915	-1.411196	0.649417
H	4.177027	-2.539041	1.199305
H	4.537410	-2.400183	-0.528898
C	-0.537507	1.470349	-0.458782
C	-1.831449	1.338014	0.286172
H	-2.117964	2.119284	0.982147
C	-2.530280	0.231597	0.057117
C	-3.741036	-0.347253	0.734312
C	-1.914394	-0.794523	-0.865645
C	-3.393305	-1.848383	0.749043
H	-4.634491	-0.180120	0.118552
C	-2.731091	-2.073893	-0.620216
H	-1.983972	-0.469399	-1.917405
H	-2.664002	-2.042212	1.542304
H	-4.261833	-2.488380	0.919193
H	-2.088303	-2.954747	-0.657106
H	-3.501337	-2.171440	-1.392295
H	-3.925526	0.082445	1.721661
H	-0.712467	1.505544	-1.540903
N	0.239229	2.579980	-0.091636
C	1.154496	3.174778	-1.042784
H	1.179752	4.259348	-0.890464
H	2.183964	2.797363	-0.954921
H	0.807686	2.981634	-2.060289
C	0.561697	2.825653	1.301425
H	-0.093862	2.241668	1.948880
H	1.597456	2.549137	1.544246
H	0.430924	3.888433	1.534864

TS-[4+2]-2b

C	1.589673	0.574156	-0.034948
C	2.641820	-0.422223	0.033550
O	2.494318	-1.622928	-0.051287
O	3.851900	0.165576	0.211651
N	0.356314	0.160965	-0.227656
N	-0.291081	-0.836003	-0.332609
H	1.778581	1.634725	0.030537
C	4.937041	-0.749755	0.290269
H	5.831313	-0.144190	0.432138
H	4.803678	-1.437315	1.128931
H	5.015085	-1.337300	-0.627621
C	-0.872243	2.117239	-0.440716
C	-1.890906	1.635511	0.351604
H	-2.095571	2.129925	1.300222
C	-2.456544	0.386442	0.094648
C	-3.364065	-0.368476	1.040897
C	-2.027945	-0.463860	-0.936269
C	-3.103493	-1.841553	0.672677
H	-4.407942	-0.094594	0.837091
C	-2.723610	-1.797470	-0.816781
H	-1.726972	-0.096392	-1.912618
H	-2.244389	-2.206898	1.241714
H	-3.956094	-2.490543	0.881399
H	-2.067699	-2.617958	-1.117515
H	-3.612446	-1.813104	-1.459213
H	-3.166668	-0.142407	2.092753
H	-0.751987	1.834930	-1.479808
O	-0.099404	3.169288	-0.130352
H	-0.208399	3.390828	0.804174

TS-[4+2]-2b-product

C	1.553746	0.698211	-0.079323
C	2.481017	-0.411306	0.015998
O	2.261781	-1.597128	-0.086440
O	3.727963	0.082940	0.265683
N	0.257408	0.535434	-0.352422
N	-0.310087	-0.593292	-0.560421
H	1.914040	1.706374	0.013182
C	4.732500	-0.913854	0.387168
H	5.662539	-0.381148	0.581942
H	4.504574	-1.597437	1.208839
H	4.812898	-1.498312	-0.532712
C	-0.589555	1.846339	-0.419616
C	-1.851602	1.588873	0.342444
H	-2.178919	2.331380	1.064310
C	-2.444917	0.424584	0.106671

C	-3.568820	-0.294702	0.796385
C	-1.745103	-0.507954	-0.856626
C	-3.063117	-1.750258	0.763653
H	-4.489053	-0.208037	0.204247
C	-2.414699	-1.872358	-0.625296
H	-1.876654	-0.165781	-1.896901
H	-2.298508	-1.884636	1.535580
H	-3.855053	-2.482184	0.935769
H	-1.682831	-2.678120	-0.698179
H	-3.188421	-2.033835	-1.382823
H	-3.773048	0.090619	1.797933
H	-0.759051	1.968711	-1.494679
O	0.117022	2.949012	0.007441
H	0.185404	2.913366	0.971171

TS-[4+2]-2c

C	1.608522	0.852580	-0.009783
C	2.636603	-0.171522	0.043185
O	2.457937	-1.368097	-0.033092
O	3.861873	0.390099	0.188810
N	0.359563	0.465810	-0.169144
N	-0.292339	-0.527622	-0.239130
H	1.831011	1.903709	0.058836
C	4.929002	-0.548433	0.251121
H	5.838155	0.038864	0.372568
H	4.796613	-1.228287	1.096005
H	4.976113	-1.141340	-0.665327
C	-0.883782	2.345078	-0.427759
C	-1.943504	1.891680	0.316829
H	-2.188967	2.386890	1.253147
C	-2.500610	0.635019	0.059440
C	-3.426578	-0.129616	0.979835
C	-2.001929	-0.221487	-0.934959
C	-3.106876	-1.601408	0.653646
H	-4.468317	0.107642	0.725211
C	-2.661576	-1.572763	-0.818152
H	-1.663285	0.137305	-1.902061
H	-2.264528	-1.931078	1.267849
H	-3.948276	-2.272634	0.835520
H	-1.975107	-2.380941	-1.080476
H	-3.521190	-1.616263	-1.498165
H	-3.283158	0.121915	2.034282
H	-0.744755	2.049024	-1.461178
H	-0.308989	3.207101	-0.104463

TS-[4+2]-2c-product

C	-1.557158	0.917391	0.013126
C	-2.512502	-0.168669	-0.019417
O	-2.327518	-1.348692	0.177096
O	-3.743485	0.340590	-0.316026
N	-0.258116	0.743505	0.289419
N	0.300754	-0.389381	0.487457
H	-1.892713	1.923633	-0.170211
C	-4.774768	-0.634601	-0.372160
H	-5.686766	-0.093516	-0.621585
H	-4.556677	-1.387089	-1.133983
H	-4.882972	-1.141748	0.589812
C	0.558792	2.015916	0.381253
C	1.856012	1.815648	-0.336843
H	2.192317	2.541034	-1.069366
C	2.452739	0.654949	-0.087481
C	3.600435	-0.051447	-0.752617
C	1.725125	-0.300407	0.836979
C	3.102267	-1.509410	-0.758741
H	4.503031	0.029010	-0.132831
C	2.411755	-1.656117	0.607371
H	1.811394	0.024000	1.887468
H	2.362659	-1.635100	-1.556147
H	3.902403	-2.235704	-0.916832
H	1.686126	-2.469862	0.647416
H	3.163244	-1.821235	1.386275
H	3.832469	0.349328	-1.741964
H	0.699985	2.174920	1.456711
H	-0.041127	2.828758	-0.020279

TS-[4+2]-2d

C	-1.608409	0.147448	-0.068716
C	-2.630649	-0.893995	-0.084563
O	-2.431075	-2.081346	0.043040
O	-3.857048	-0.352869	-0.252788
N	-0.363128	-0.220682	0.096183
N	0.312783	-1.201784	0.156200
H	-1.843485	1.190451	-0.204721
C	-4.917012	-1.303710	-0.284754
H	-5.829964	-0.728676	-0.430539
H	-4.773647	-2.010960	-1.104626
H	-4.960455	-1.862318	0.652928
C	0.999239	1.714761	0.438911
C	2.041465	1.174624	-0.275068
H	2.351937	1.694237	-1.179166
C	2.507449	-0.114679	-0.012590
C	3.443679	-0.917722	-0.887726
C	1.917652	-0.954302	0.958488
C	3.065420	-2.376551	-0.565928
H	4.481153	-0.710804	-0.592533
C	2.552452	-2.321667	0.882671
H	1.565968	-0.578204	1.915073
H	2.245689	-2.689621	-1.217940
H	3.895008	-3.073012	-0.699823
H	1.840791	-3.113809	1.125274
H	3.379412	-2.367746	1.601444
H	3.351110	-0.669211	-1.948263
H	0.766632	1.380264	1.445135
C	0.330489	2.960007	-0.030031
O	0.580567	3.444112	-1.115616
C	-0.662958	3.586082	0.922712
H	-1.363460	2.835966	1.303293
H	-0.126170	3.989552	1.788253
H	-1.200561	4.390194	0.422011

TS-[4+2]-2d-product

C	-1.489813	0.129817	-0.019414
C	-2.319789	-1.058400	-0.022108
O	-2.027026	-2.190237	0.289400
O	-3.571492	-0.710632	-0.435012
N	-0.188583	0.108608	0.297973

N	0.469829	-0.951786	0.566508
H	-1.919798	1.059487	-0.347852
C	-4.491001	-1.793417	-0.474782
H	-5.433717	-1.373663	-0.823272
H	-4.143425	-2.571835	-1.158240
H	-4.612725	-2.235732	0.517034
C	0.548492	1.454956	0.370374
C	1.816326	1.314126	-0.410142
H	2.029680	2.020629	-1.203651
C	2.509153	0.218216	-0.118570
C	3.677793	-0.444465	-0.792877
C	1.886893	-0.731070	0.886151
C	3.295689	-1.932987	-0.683361
H	4.597806	-0.254158	-0.224953
C	2.672404	-2.040617	0.718193
H	1.965974	-0.337933	1.913700
H	2.537801	-2.168267	-1.437496
H	4.143704	-2.605424	-0.829283
H	2.019453	-2.905622	0.843349
H	3.463603	-2.088770	1.473453
H	3.832583	-0.093882	-1.815541
H	0.751387	1.541836	1.447027
C	-0.314685	2.648579	-0.059790
O	-0.222649	3.093478	-1.177584
C	-1.198009	3.257489	1.001104
H	-1.699453	2.481805	1.585310
H	-0.567690	3.835254	1.686676
H	-1.925288	3.924285	0.539264

TS-[4+2]-2e

C	-1.614875	0.172431	0.011354
C	-2.654704	-0.851478	-0.102384
O	-2.463951	-2.044981	-0.159121
O	-3.877889	-0.282826	-0.130966
N	-0.378467	-0.231998	0.087187
N	0.317487	-1.198952	0.011032
H	-1.836589	1.225350	0.091475
C	-4.953175	-1.210706	-0.244348
H	-5.862899	-0.612959	-0.261405
H	-4.859823	-1.795209	-1.162248
H	-4.959348	-1.896081	0.606088
C	0.992451	1.700099	0.517225
C	2.064931	1.175917	-0.160679
H	2.436763	1.734438	-1.017142
C	2.500606	-0.132720	0.053134
C	3.483526	-0.890379	-0.811511
C	1.848069	-1.025498	0.936156
C	3.083945	-2.363062	-0.596973
H	4.503201	-0.707501	-0.446646
C	2.486973	-2.388388	0.819789
H	1.443015	-0.703284	1.891663
H	2.303922	-2.634508	-1.313065
H	3.918800	-3.055062	-0.720929
H	1.763924	-3.191710	0.976730
H	3.270974	-2.475110	1.581655
H	3.452791	-0.581820	-1.859879
H	0.671513	1.348577	1.489886
C	0.375134	2.946902	0.026712
O	0.745349	3.597690	-0.921826
O	-0.707749	3.288091	0.761776
H	-1.062745	4.099028	0.366525

TS-[4+2]-2e-product

C	-1.507802	0.162439	0.043260
C	-2.344295	-1.019157	-0.032308
O	-2.039475	-2.178474	0.130146
O	-3.615598	-0.628913	-0.332094
N	-0.203338	0.110861	0.332764
N	0.446186	-0.970726	0.536936
H	-1.961884	1.123903	-0.111047
C	-4.540547	-1.702171	-0.441583
H	-5.500309	-1.247537	-0.683591
H	-4.237069	-2.396393	-1.228945
H	-4.605713	-2.255320	0.498538
C	0.554140	1.444545	0.444125
C	1.834868	1.314178	-0.319587
H	2.071568	2.050625	-1.078357
C	2.509831	0.197953	-0.070464
C	3.678932	-0.443913	-0.762863
C	1.863070	-0.789747	0.876741
C	3.274111	-1.930354	-0.736732
H	4.592479	-0.296923	-0.172190
C	2.630209	-2.101399	0.649087
H	1.938280	-0.450806	1.923423
H	2.523675	-2.114402	-1.512217
H	4.114691	-2.606416	-0.906676
H	1.961482	-2.960460	0.719831
H	3.410130	-2.202640	1.410762
H	3.853665	-0.042090	-1.763231
H	0.718779	1.540228	1.523661
C	-0.264665	2.635023	-0.027723
O	-0.200565	3.112342	-1.128430
O	-1.041676	3.119689	0.952044
H	-1.528308	3.875746	0.587086

TS-[4+2]-2f

C	1.604105	0.418277	0.001618
C	2.629718	-0.625728	0.057541
O	2.416921	-1.816825	0.041103
O	3.858936	-0.079103	0.123369
N	0.364200	0.029487	-0.091994
N	-0.349536	-0.925173	-0.057567
H	1.836798	1.472706	0.022321
C	4.921670	-1.026846	0.185387
H	5.838574	-0.442871	0.240737
H	4.816342	-1.662562	1.067145
H	4.921780	-1.660499	-0.704202
C	-0.952611	1.981155	-0.509107
C	-2.019700	1.504209	0.219067
H	-2.344996	2.055050	1.097742
C	-2.510490	0.215491	0.002217
C	-3.486858	-0.519742	0.893388
C	-1.924918	-0.683605	-0.917980
C	-3.142045	-2.001331	0.647166
H	-4.512242	-0.299934	0.567529
C	-2.599761	-2.027672	-0.791297

H	-1.543187	-0.366365	-1.884649
H	-2.344870	-2.305626	1.330367
H	-3.993476	-2.667789	0.794896
H	-1.906993	-2.849584	-0.983977
H	-3.413473	-2.082720	-1.524367
H	-3.408564	-0.226778	1.943837
H	-0.719898	1.603077	-1.497646
C	-0.236316	3.154725	-0.124935
N	0.395420	4.076789	0.183290

TS-[4+2]-2f-product

C	-1.542449	0.484295	0.054126
C	-2.440595	-0.656106	-0.010979
O	-2.187918	-1.826799	0.156477
O	-3.690092	-0.204171	-0.297915
N	-0.241606	0.355930	0.321633
N	0.365982	-0.758836	0.486002
H	-1.933530	1.473073	-0.109794
C	-4.673815	-1.227177	-0.385541
H	-5.609579	-0.722765	-0.621518
H	-4.416727	-1.944140	-1.168879
H	-4.757074	-1.765539	0.561590
C	0.580088	1.649630	0.480229
C	1.864455	1.495960	-0.286849
H	2.152850	2.251076	-1.008260
C	2.481314	0.339201	-0.072397
C	3.624084	-0.330875	-0.780855
C	1.785815	-0.646661	0.841724
C	3.154953	-1.798658	-0.799917
H	4.538740	-0.240234	-0.180962
C	2.499048	-1.981919	0.578403
H	1.872014	-0.342828	1.898697
H	2.401046	-1.927907	-1.582953
H	3.967104	-2.503977	-0.986908
H	1.793820	-2.812972	0.622739
H	3.270447	-2.137450	1.339380
H	3.821835	0.093306	-1.767509
H	0.762446	1.690323	1.561574
C	-0.156105	2.853744	0.098691
N	-0.681528	3.838503	-0.196992

TS-[4+2]-3a

C	-2.554509	-1.383991	-0.074779
O	-2.167326	-2.524091	0.075725
C	-1.747976	-0.186009	-0.010856
H	-2.168851	0.798165	-0.161001
N	-0.457724	-0.280286	0.239271
N	0.385682	-1.117076	0.408036
O	-3.857610	-1.078049	-0.332213
C	-4.711534	-2.209892	-0.415274
H	-5.707940	-1.821921	-0.625524
H	-4.388688	-2.883204	-1.213228
H	-4.710547	-2.768114	0.524293
C	2.211417	0.537929	-0.107225
C	3.203074	0.152346	-1.184760
C	3.526354	-1.340631	-1.158166
C	3.989531	-1.727367	0.243614
C	2.850385	-1.543538	1.251589
C	1.958300	-0.349964	0.966141
C	1.380896	1.633185	-0.334353
H	2.628947	-1.914044	-1.419636
H	4.342032	-2.762444	0.270731
H	2.199916	-2.426008	1.242602
H	1.477481	2.161663	-1.278638
H	2.813726	0.451996	-2.163551
H	4.131614	0.720762	-1.031124
H	3.254744	-1.460697	2.265250
H	4.842536	-1.093628	0.518586
H	4.295150	-1.567889	-1.902635
C	0.296498	1.933426	0.492278
H	0.296651	1.611841	1.528503
H	1.538634	0.089435	1.867876
N	-0.709242	2.770742	0.180988
C	-1.649703	3.226417	1.187747
H	-2.675918	3.103125	0.829343
H	-1.531162	2.626103	2.090928
H	-1.489409	4.281319	1.439567
C	-0.871094	3.250019	-1.178056
H	-0.739934	2.416414	-1.875286
H	-1.879430	3.649735	-1.295723
H	-0.150909	4.039272	-1.424911

TS-[4+2]-3a-product

C	2.886368	-0.827022	-0.082366
O	2.644882	-1.940245	0.326144
C	1.973769	0.243689	-0.425322
H	2.377622	1.167094	-0.803144
N	0.637938	0.135735	-0.382565
N	0.043278	-0.886997	0.109039
O	4.162904	-0.394070	-0.308489
C	5.160798	-1.363976	-0.025655
H	6.115641	-0.883313	-0.235788
H	5.112854	-1.677579	1.020141
H	5.033115	-2.248646	-0.654520
C	-2.096670	0.002106	-0.914627
C	-3.538459	-0.297409	-1.220140
C	-4.281672	-0.666207	0.074261
C	-3.572008	-1.809066	0.805207
C	-2.114592	-1.456210	1.108237
C	-1.364036	-1.081028	-0.182432
C	-1.487746	1.146075	-1.206380
H	-4.315256	0.215881	0.726743
H	-4.099171	-2.050567	1.733127
H	-2.069485	-0.607570	1.801316
H	-2.000471	1.961566	-1.709573
H	-4.006859	0.558094	-1.716062
H	-3.591648	-1.149438	-1.911792
H	-1.588011	-2.288626	1.582488
H	-3.603273	-2.711336	0.179647
H	-5.316824	-0.937678	-0.154404
C	-0.087335	1.438915	-0.779041
H	0.499490	1.834586	-1.612732
H	-1.403639	-1.981085	-0.823357
N	-0.062390	2.404734	0.282126
C	1.193546	3.102310	0.506098
H	1.936832	2.496930	1.046480

H	1.623018	3.408175	-0.452392
H	0.990758	4.005086	1.088913
C	-0.669570	1.966927	1.529144
H	-1.682582	1.605692	1.342412
H	-0.091469	1.166962	2.021520
H	-0.729062	2.821368	2.207622

TS-[4+2]-3b

C	2.840035	-0.550054	0.059366
O	2.570377	-1.729995	-0.016798
C	1.900261	0.550388	-0.031067
H	2.202410	1.584795	0.024761
N	0.629296	0.275057	-0.234970
N	-0.103617	-0.667587	-0.332993
O	4.103240	-0.089615	0.248015
C	5.085886	-1.112110	0.346992
H	6.036390	-0.601958	0.498362
H	4.870475	-1.776523	1.187286
H	5.115114	-1.710977	-0.566471
C	-2.157259	0.707016	0.092582
C	-3.098473	0.230012	1.177333
C	-3.223042	-1.292937	1.194204
C	-3.603031	-1.782663	-0.200637
C	-2.479131	-1.483331	-1.197573
C	-1.780525	-0.160469	-0.953999
C	-1.460058	1.901497	0.282243
H	-2.264403	-1.735108	1.490401
H	-3.813928	-2.855674	-0.196821
H	-1.708912	-2.260498	-1.138341
H	-1.606125	2.447108	1.214361
H	-2.759791	0.606438	2.148310
H	-4.090817	0.668751	1.001018
H	-2.865942	-1.501138	-2.221033
H	-4.526434	-1.277960	-0.512070
H	-3.970648	-1.595292	1.933141
C	-0.384763	2.258610	-0.509233
H	-0.293241	1.979011	-1.551937
H	-1.402476	0.302552	-1.861769
O	0.473099	3.245137	-0.202160
H	0.385442	3.474218	0.732824

TS-[4+2]-3b-product

C	2.825833	-0.441130	-0.032752
O	2.562636	-1.620026	-0.115308
C	1.941498	0.703605	-0.105886
H	2.331684	1.693274	0.052136
N	0.624116	0.602690	-0.320466
N	0.044501	-0.503530	-0.601860
O	4.097815	0.008069	0.177230
C	5.066562	-1.024606	0.283674
H	6.022158	-0.525300	0.439619
H	4.840199	-1.685849	1.123971
H	5.094696	-1.626817	-0.627852
C	-2.188628	0.638334	-0.280833
C	-3.678786	0.470266	-0.145719
C	-4.040011	-0.739886	0.724560
C	-3.328063	-1.992895	0.213639
C	-1.815171	-1.784857	0.204170
C	-1.402387	-0.578801	-0.666257
C	-1.557620	1.792714	-0.094880
H	-3.733098	-0.545953	1.759712
H	-3.580664	-2.856409	0.836154
H	-1.459138	-1.592812	1.223701
H	-2.083683	2.704577	0.178040
H	-4.123606	1.391963	0.241831
H	-4.094799	0.309336	-1.150596
H	-1.280976	-2.665255	-0.160167
H	-3.677164	-2.221366	-0.802619
H	-5.125119	-0.879834	0.729752
C	-0.092997	1.962001	-0.312871
H	0.134011	2.386946	-1.295530
H	-1.668938	-0.829289	-1.707916
O	0.478800	2.823918	0.612776
H	0.228734	2.524509	1.497397

TS-[4+2]-3c

C	-2.725568	-0.057279	-0.081197
O	-3.223218	1.029451	-0.279360
C	-1.314349	-0.325316	0.139989
H	-0.944857	-1.323235	0.309095
N	-0.478643	0.686465	0.135711
N	-0.473170	1.857639	-0.102664
O	-3.442579	-1.206937	-0.032028
C	-4.838955	-1.031443	-0.239977
H	-5.278903	-2.025801	-0.177455
H	-5.263756	-0.376143	0.524040
H	-5.030723	-0.588887	-1.220242
C	2.282832	0.650829	-0.026674
C	3.114117	-0.112105	-1.039518
C	2.708986	-1.584577	-1.104604
C	2.746288	-2.190792	0.296739
C	1.727244	-1.503814	1.211485
C	1.616117	-0.024374	0.977226
C	2.005601	2.009942	-0.239940
H	1.693505	-1.664662	-1.512921
H	2.552385	-3.266596	0.266780
H	0.735405	-1.958099	1.080407
H	1.168196	0.540079	1.788442
H	2.372336	2.463588	-1.157525
H	3.014304	0.361117	-2.021309
H	4.174690	-0.040973	-0.763920
H	1.975781	-1.675367	2.265242
H	3.753552	-2.059588	0.710498
H	3.376057	-2.128987	-1.779074
C	1.012552	2.690729	0.476332
H	0.888096	2.511414	1.540245
H	0.793802	3.712496	0.188319

TS-[4+2]-3c-product

C	-2.749030	-0.037284	0.035205
O	-3.193969	1.028526	-0.328242
C	-1.375930	-0.431719	0.247741
H	-1.161408	-1.438268	0.565940
N	-0.321369	0.384884	0.075044
N	-0.444946	1.605549	-0.275135
O	-3.554701	-1.106500	0.314379

C	-4.939468	-0.847112	0.138848
H	-5.453780	-1.772540	0.396104
H	-5.269124	-0.033939	0.790356
H	-5.155200	-0.565870	-0.895037
C	2.144548	0.631482	0.486614
C	3.424899	-0.052394	0.875541
C	3.782960	-1.090065	-0.202867
C	2.617207	-2.051696	-0.452016
C	1.317246	-1.312668	-0.792374
C	0.993242	-0.312980	0.328977
C	2.026432	1.900927	0.121262
H	4.019336	-0.558342	-1.132331
H	2.864091	-2.746627	-1.259869
H	1.428858	-0.750899	-1.727701
H	0.840738	-0.865619	1.263442
H	2.875648	2.578018	0.175178
H	4.225088	0.683904	0.991751
H	3.301028	-0.563227	1.840421
H	0.494208	-2.019334	-0.923907
H	2.452693	-2.660414	0.447272
H	4.677610	-1.647989	0.089808
C	0.736566	2.433821	-0.406550
H	0.489251	3.385498	0.080760
H	0.852498	2.684534	-1.472942

TS-[4+2]-3d

C	-2.633847	-1.256735	-0.117973
O	-2.201999	-2.380487	0.010372
C	-1.843677	-0.030001	-0.094041
H	-2.289988	0.942361	-0.227762
N	-0.549529	-0.126620	0.078873
N	0.299074	-0.972889	0.128469
O	-3.943483	-0.972564	-0.293574
C	-4.790668	-2.116559	-0.332959
H	-5.799607	-1.736361	-0.484429
H	-4.503250	-2.779317	-1.152209
H	-4.727034	-2.674383	0.604088
C	2.248047	0.455294	-0.029765
C	3.277031	0.023130	-1.049397
C	3.449437	-1.495103	-1.083883
C	3.732407	-2.001407	0.327942
C	2.526077	-1.756969	1.241475
C	1.790332	-0.459360	0.956775
C	1.536815	1.642035	-0.230100
H	2.533685	-1.960669	-1.466856
H	3.976324	-3.067232	0.324058
H	1.797222	-2.566159	1.128590
H	1.733653	2.234333	-1.121999
H	2.999194	0.411238	-2.034464
H	4.240665	0.486426	-0.792741
H	2.837660	-1.758281	2.290301
H	4.611818	-1.475630	0.720498
H	4.263829	-1.759934	-1.763989
C	0.402024	1.959726	0.481458
H	0.230151	1.597967	1.490115
H	1.334426	-0.024225	1.842781
C	-0.483028	3.066196	0.016521
O	-0.320861	3.599309	-1.062327
C	-1.582363	3.485102	0.966351
H	-2.133422	2.612605	1.331523
H	-1.136258	3.970311	1.841428
H	-2.256659	4.181354	0.469478

TS-[4+2]-3d-product

C	-2.500295	-1.251183	-0.062579
O	-2.061643	-2.360361	0.139458
C	-1.825523	0.027980	0.029941
H	-2.373944	0.916230	-0.227729
N	-0.523387	0.148282	0.324145
N	0.245649	-0.837824	0.573069
O	-3.795243	-1.029402	-0.428156
C	-4.571917	-2.212233	-0.557665
H	-5.569655	-1.885675	-0.848001
H	-4.149379	-2.871942	-1.319374
H	-4.608159	-2.758095	0.388304
C	2.187093	0.556336	-0.134750
C	3.599956	0.519894	-0.663542
C	4.135856	-0.893133	-0.897174
C	3.880140	-1.756159	0.337891
C	2.378039	-1.896798	0.564574
C	1.671119	-0.548192	0.767925
C	1.346477	1.565915	-0.348320
H	3.635466	-1.346091	-1.761469
H	4.325997	-2.747434	0.214405
H	1.923403	-2.366032	-0.314608
H	1.543846	2.403288	-1.008594
H	3.666746	1.135692	-1.565923
H	4.240822	1.000891	0.089491
H	2.149576	-2.542756	1.416076
H	4.361488	-1.297641	1.212992
H	5.203605	-0.844014	-1.130664
C	0.057993	1.546846	0.410012
H	0.245423	1.655658	1.489156
H	1.831194	-0.219887	1.813191
C	-0.917319	2.652408	-0.022170
O	-0.859498	3.111936	-1.135848
C	-1.861905	3.170166	1.035386
H	-2.265738	2.354565	1.640038
H	-1.299117	3.832115	1.703523
H	-2.664616	3.739461	0.567872

TS-[4+2]-3e

C	2.672884	-1.189709	0.138236
O	2.254992	-2.324626	0.174703
C	1.854116	0.018436	0.026478
H	2.283391	1.006427	-0.038803
N	0.562416	-0.124088	-0.070367
N	-0.292422	-0.964630	0.000221
O	3.983125	-0.869603	0.189296
C	4.856130	-1.989930	0.299824
H	5.864250	-1.580658	0.337598
H	4.637633	-2.558313	1.206521
H	4.742037	-2.651461	-0.561830
C	-2.249617	0.412988	-0.030827
C	-3.304720	0.013025	0.975322
C	-3.440253	-1.505007	1.092901

C	-3.661054	-2.099250	-0.295589
C	-2.431414	-1.874326	-1.183020
C	-1.730158	-0.548961	-0.941545
C	-1.580791	1.631312	0.122882
H	-2.527619	-1.922849	1.533661
H	-3.877667	-3.169375	-0.237589
H	-1.690657	-2.661592	-1.009364
H	-1.833977	2.265070	0.970862
H	-3.073448	0.464060	1.945579
H	-4.270058	0.433755	0.658557
H	-2.709930	-1.932026	-2.239559
H	-4.539764	-1.621365	-0.746535
H	-4.271854	-1.751642	1.758914
C	-0.429631	1.948082	-0.559366
H	-0.173494	1.556843	-1.535787
H	-1.244067	-0.155799	-1.831509
C	0.390024	3.078960	-0.078542
O	0.134027	3.794687	0.860552
O	1.517500	3.219910	-0.811500
H	2.005009	3.963277	-0.424626

TS-[4+2]-3e-product

C	-2.949021	-0.704576	0.117859
O	-2.767368	-1.876555	-0.123187
C	-1.978602	0.323706	0.422684
H	-2.312337	1.328491	0.624010
N	-0.651428	0.106997	0.461906
N	-0.109094	-1.017356	0.216538
O	-4.193990	-0.145741	0.141531
C	-5.243531	-1.059618	-0.143823
H	-6.166287	-0.483106	-0.090556
H	-5.120940	-1.493118	-1.139426
H	-5.259133	-1.873403	0.585336
C	2.104681	-0.047605	0.947414
C	3.565402	-0.335259	1.138957
C	4.184664	-0.631574	-0.240479
C	3.425005	-1.750268	-0.960822
C	1.931735	-1.434630	-1.088969
C	1.330352	-1.154979	0.304041
C	1.520912	1.118861	1.192203
H	4.139434	0.282623	-0.844626
H	3.855991	-1.916148	-1.952758
H	1.771665	-0.542836	-1.705019
H	2.051308	1.956247	1.637100
H	4.065495	0.509652	1.621736
H	3.690592	-1.213352	1.785958
H	1.385523	-2.264254	-1.545638
H	3.548772	-2.687883	-0.402087
H	5.240426	-0.895581	-0.125242
C	0.115787	1.372329	0.757386
H	-0.456698	1.914284	1.510521
H	1.488911	-2.065843	0.903284
C	0.107845	2.163293	-0.552607
O	0.587871	1.771491	-1.581387
O	-0.481836	3.357566	-0.401068
H	-0.447847	3.804569	-1.261877

TS-[4+2]-3f

C	2.766490	-0.812908	0.090924
O	2.398315	-1.965400	0.070827
C	1.890915	0.359161	0.023110
H	2.267486	1.371521	0.043372
N	0.609364	0.151536	-0.086171
N	-0.210226	-0.723208	-0.046488
O	4.057303	-0.434952	0.171168
C	4.983301	-1.515872	0.242462
H	5.969432	-1.059633	0.307519
H	4.785391	-2.132060	1.122203
H	4.907761	-2.143964	-0.647886
C	-2.217257	0.607538	0.006585
C	-3.236229	0.174389	1.036516
C	-3.327044	-1.347524	1.145927
C	-3.572578	-1.937341	-0.240156
C	-2.377088	-1.671451	-1.162119
C	-1.706028	-0.329142	-0.932226
C	-1.570352	1.837975	0.160053
H	-2.390969	-1.743250	1.556886
H	-3.756291	-3.013567	-0.184223
H	-1.609202	-2.438152	-1.016956
H	-1.819825	2.447359	1.025382
H	-2.992575	0.623843	2.004589
H	-4.220128	0.570589	0.747175
H	-2.685099	-1.730009	-2.210319
H	-4.477691	-1.482008	-0.660920
H	-4.131946	-1.620763	1.833769
C	-0.447275	2.172694	-0.568168
H	-0.254237	1.778157	-1.558514
H	-1.257388	0.080005	-1.834554
C	0.387491	3.269402	-0.191007
N	1.111470	4.122132	0.113389

TS-[4+2]-3f-product

C	-2.970094	-0.464146	0.096807
O	-2.797348	-1.650700	-0.061805
C	-1.982726	0.576045	0.308529
H	-2.304558	1.598636	0.418329
N	-0.661737	0.346737	0.336742
N	-0.131294	-0.799091	0.158267
O	-4.206020	0.106049	0.110251
C	-5.272300	-0.813557	-0.086947
H	-6.186646	-0.222807	-0.055307
H	-5.175176	-1.316982	-1.051738
H	-5.279312	-1.572375	0.699184
C	2.089656	0.165474	0.877597
C	3.538176	-0.144423	1.120528
C	4.184484	-0.525292	-0.225852
C	3.410663	-1.652243	-0.917631
C	1.929551	-1.303700	-1.093362
C	1.303506	-0.956098	0.274201
C	1.534982	1.361028	1.030799
H	4.189429	0.360766	-0.872036
H	3.859002	-1.871112	-1.891142
H	1.814679	-0.434739	-1.753624
H	2.073454	2.217694	1.424332
H	4.046725	0.712468	1.571660
H	3.624272	-0.990071	1.814858

H	1.370803	-2.133006	-1.534459
H	3.492941	-2.568915	-0.318597
H	5.226852	-0.817025	-0.066809
C	0.135248	1.617341	0.558193
H	-0.430725	2.198365	1.290529
H	1.438063	-1.843186	0.912653
C	0.153123	2.367663	-0.710710
N	0.213250	2.976775	-1.690481

TS-[4+2]-4a

C	-2.849998	-0.609386	-0.138930
O	-3.085590	-1.791124	0.003698
C	-1.580782	0.045685	0.080653
H	-1.448186	1.108018	-0.059870
N	-0.552424	-0.669563	0.494307
N	-0.241597	-1.792169	0.747119
O	-3.794563	0.286239	-0.542769
C	-5.070760	-0.289209	-0.783329
H	-5.717139	0.529938	-1.097502
H	-5.013090	-1.050499	-1.565245
H	-5.463108	-0.758241	0.122402
C	2.817124	0.392080	-1.209387
C	3.070186	-1.912045	-0.512174
C	3.814998	-0.779330	-1.232576
H	4.705562	-0.508852	-0.656403
H	4.132103	-1.043565	-2.243351
H	3.310160	1.367019	-1.255196
H	3.733488	-2.656524	-0.064411
C	2.067666	0.158701	0.094529
C	2.236817	-1.171690	0.509639
C	1.197547	1.004085	0.775646
H	0.974624	0.763406	1.811756
C	1.482615	-1.795020	1.503920
H	1.186669	-1.241432	2.389606
N	0.702022	2.194941	0.384360
C	0.665011	2.594161	-1.012692
H	1.586142	3.091788	-1.333398
H	0.484757	1.715932	-1.635093
H	-0.168314	3.286462	-1.154317
C	0.065610	3.084312	1.339003
H	0.029273	2.604998	2.317852
H	0.622316	4.023741	1.432139
H	-0.958655	3.313754	1.026962
H	1.649283	-2.851626	1.686182
H	2.397468	-2.440663	-1.202204
H	2.145656	0.318903	-2.073653

TS-[4+2]-4a-product

C	-2.892523	-0.522823	0.116774
O	-3.060094	-1.462006	-0.628018
C	-1.668066	0.167345	0.460259
H	-1.710152	0.981190	1.163886
N	-0.455139	-0.176019	-0.000998
N	-0.281752	-1.096608	-0.873050
O	-3.923593	0.058961	0.800603
C	-5.188091	-0.539567	0.557941
H	-5.906502	0.022905	1.153360
H	-5.446639	-0.486556	-0.502610
H	-5.185250	-1.590691	0.857204
C	3.186203	0.414374	1.280910
C	3.558281	-1.564748	-0.148513
C	4.094856	-0.825397	1.101229
H	3.984235	-1.476184	1.972802
H	5.151453	-0.565192	1.015568
H	2.996370	0.647973	2.333835
H	3.613294	-2.653726	-0.051888
C	1.946799	0.004702	0.530142
C	2.143410	-1.052753	-0.250166
C	0.670010	0.764386	0.503599
H	0.358035	1.050190	1.512034
C	1.072573	-1.551995	-1.151948
H	1.030674	-2.649190	-1.131152
N	0.766058	1.955146	-0.290652
C	1.041694	1.732902	-1.703389
H	1.232655	2.698512	-2.177359
H	1.934349	1.114461	-1.818015
H	0.200401	1.247070	-2.224770
C	-0.292305	2.934852	-0.095620
H	-0.462000	3.086166	0.974276
H	0.030716	3.886805	-0.525477
H	-1.244494	2.642481	-0.562988
H	1.315446	-1.295319	-2.196502
H	4.119152	-1.297956	-1.054225
H	3.616543	1.316108	0.826926

TS-[4+2]-4b

C	2.762481	-0.211558	0.126186
O	2.938009	-1.408933	0.204352
C	1.516588	0.449728	-0.210135
H	1.421522	1.522108	-0.282698
N	0.468865	-0.299437	-0.481488
N	0.125691	-1.442345	-0.510879
O	3.744013	0.697923	0.355369
C	5.000067	0.124227	0.693574
H	5.680691	0.960582	0.848208
H	4.919469	-0.476336	1.602839
H	5.361768	-0.518665	-0.112473
C	-2.714932	1.098719	0.989809
C	-3.085797	-1.296622	0.789414
C	-3.714677	-0.014228	1.360298
H	-4.666343	0.178856	0.856273
H	-3.906215	-0.070098	2.433069
H	-3.194461	2.077537	0.882373
H	-3.820618	-2.069481	0.549718
C	-2.107606	0.576283	-0.297197
C	-2.322085	-0.803844	-0.419005
C	-1.166687	1.234658	-1.055665
H	-0.876985	0.908779	-2.047889
C	-1.571307	-1.608226	-1.273977
H	-1.295703	-1.239961	-2.257467
H	-1.706785	-2.683550	-1.229221
H	-2.367250	-1.732374	1.497754
H	-1.938384	1.186555	1.763626
O	-0.727162	2.476282	-0.794529
H	-0.987744	2.731516	0.101114

TS-[4+2]-4b-product

C	2.856492	-0.186705	0.016129
O	3.017021	-1.374483	0.186797
C	1.628553	0.555022	-0.176525
H	1.661156	1.625690	-0.274451
N	0.416551	-0.015384	-0.218170
N	0.239266	-1.279929	-0.128930
O	3.901558	0.692367	-0.014901
C	5.172808	0.086304	0.165060
H	5.901144	0.894942	0.114724
H	5.230007	-0.418994	1.132512
H	5.366790	-0.651064	-0.617956
C	-3.288804	1.241886	0.079509
C	-3.656518	-1.190922	0.331335
C	-4.382059	0.146527	0.046241
H	-4.816108	0.108978	-0.956474
H	-5.194302	0.342211	0.748510
H	-3.441139	2.013254	-0.681950
H	-4.060253	-2.021878	-0.255872
C	-2.031711	0.437566	-0.143350
C	-2.224867	-0.870426	-0.016006
C	-0.706923	1.027241	-0.455462
H	-0.602918	1.294744	-1.511531
C	-1.103702	-1.830448	-0.158053
H	-1.216301	-2.400192	-1.094100
H	-1.144704	-2.585002	0.638981
H	-3.727555	-1.485457	1.386380
H	-3.254051	1.761022	1.045630
O	-0.455548	2.192850	0.256203
H	-0.576355	2.006796	1.197221

TS-[4+2]-4c

C	2.739554	0.041702	-0.114655
O	2.857065	1.180470	-0.513012
C	1.521052	-0.570464	0.383311
H	1.482591	-1.588548	0.730886
N	0.431513	0.169758	0.430599
N	0.048201	1.255308	0.128326
O	3.766685	-0.842941	-0.076801
C	5.002119	-0.320470	-0.550122
H	5.722570	-1.133193	-0.468203
H	4.910782	0.006978	-1.588407
H	5.317821	0.532942	0.054576
C	-2.854163	-1.518727	-0.502197
C	-3.232857	0.843104	-0.918618
C	-3.887593	-0.539145	-1.086938
H	-4.804154	-0.579887	-0.490093
H	-4.150753	-0.764235	-2.121867
H	-3.300549	-2.437206	-0.113656
H	-3.954439	1.661371	-0.848744
C	-2.165634	-0.692968	0.567885
C	-2.399220	0.675451	0.330677
C	-1.164488	-1.111490	1.404612
H	-0.862922	-0.522505	2.263769
C	-1.594976	1.658508	0.902760
H	-1.268859	1.553262	1.933122
H	-1.711441	2.687017	0.577678
H	-2.562562	1.065702	-1.760744
H	-2.116863	-1.804617	-1.263314
H	-0.831980	-2.145781	1.400748

TS-[4+2]-4c-product

C	-2.835798	0.052800	-0.008947
O	-2.996955	1.252788	-0.014653
C	-1.606331	-0.705002	0.004339
H	-1.648869	-1.781874	0.010384
N	-0.380867	-0.153497	0.012099
N	-0.187564	1.106950	0.003698
O	-3.884758	-0.824024	-0.013195
C	-5.159670	-0.199345	-0.024545
H	-5.890448	-1.007462	-0.026120
H	-5.291708	0.432383	0.857439
H	-5.279740	0.424806	-0.913558
C	3.340227	-1.439360	0.092008
C	3.754254	0.996571	0.078783
C	4.415726	-0.370293	-0.219166
H	4.669210	-0.419909	-1.281377
H	5.336261	-0.525070	0.346419
H	3.363072	-2.273144	-0.618095
H	4.050461	1.770204	-0.637097
C	2.065935	-0.637219	0.023072
C	2.283552	0.671706	0.015855
C	0.702151	-1.211608	0.034477
H	0.516557	-1.848710	-0.835639
C	1.162437	1.644262	0.015291
H	1.240143	2.316842	-0.851142
H	1.233421	2.304460	0.892477
H	4.014955	1.372053	1.076885
H	3.465873	-1.872462	1.093212
H	0.518626	-1.811469	0.931424

TS-[4+2]-4d

C	-2.935238	-0.490087	-0.155574
O	-3.115375	-1.672005	0.033462
C	-1.660889	0.209613	-0.018054
H	-1.558273	1.264555	-0.215220
N	-0.614575	-0.486659	0.343603
N	-0.272080	-1.616396	0.527299
O	-3.911546	0.369846	-0.519005
C	-5.192180	-0.232664	-0.679790
H	-5.865096	0.570207	-0.976324
H	-5.157667	-1.008254	-1.448046
H	-5.523803	-0.685637	0.257226
C	2.938022	0.272967	-1.075090
C	2.934925	-2.065158	-0.403036
C	3.792683	-1.006232	-1.117603
H	4.716195	-0.847886	-0.551749
H	4.068793	-1.297623	-2.132386
H	3.513521	1.199970	-1.089372
H	3.521171	-2.859770	0.066800
C	2.126593	0.105989	0.191739
C	2.145709	-1.246681	0.589674
C	1.246043	1.002032	0.751099
H	0.850615	0.818856	1.746050
C	1.216023	-1.765903	1.502242
H	0.932912	-1.178217	2.371098

H	1.224999	-2.835337	1.686683
H	2.234470	-2.543662	-1.102394
H	2.248908	0.328595	-1.926311
C	0.973712	2.340719	0.175741
O	1.408715	2.679686	-0.909101
C	0.115828	3.262033	1.016177
H	-0.788019	2.747584	1.357944
H	0.672822	3.559411	1.911272
H	-0.146702	4.148609	0.440421

TS-[4+2]-4d-product

C	-2.786236	-0.564049	-0.125978
O	-2.966604	-1.740341	0.090783
C	-1.575690	0.218299	0.025695
H	-1.603599	1.258984	-0.242406
N	-0.403052	-0.311496	0.402451
N	-0.225076	-1.555066	0.618501
O	-3.780069	0.262573	-0.561572
C	-5.032416	-0.383120	-0.744690
H	-5.719106	0.387324	-1.093062
H	-4.950909	-1.184489	-1.482994
H	-5.387331	-0.815443	0.194117
C	3.041237	0.678112	-0.843903
C	3.405705	-1.733686	-0.428075
C	4.128935	-0.423847	-0.825301
H	4.868689	-0.181779	-0.056692
H	4.656692	-0.506312	-1.777225
H	3.419381	1.647643	-0.506134
H	4.028291	-2.388495	0.189515
C	1.994740	0.082845	0.066226
C	2.188660	-1.214742	0.291332
C	0.755135	0.672208	0.652170
H	0.816910	0.666374	1.749810
C	1.124363	-1.957958	1.030713
H	1.238039	-1.801605	2.117834
H	1.176251	-3.035745	0.864739
H	3.098470	-2.318043	-1.305059
H	2.622540	0.837962	-1.842992
C	0.443903	2.099884	0.181853
O	0.700092	2.437863	-0.947908
C	-0.137051	3.033862	1.213545
H	-0.975221	2.556743	1.729531
H	0.628512	3.255301	1.965557
H	-0.455777	3.959899	0.736846

TS-[4+2]-4e

C	-2.964357	-0.466528	-0.172118
O	-3.123443	-1.665402	-0.194362
C	-1.691642	0.219164	0.063967
H	-1.606998	1.294176	0.107031
N	-0.645687	-0.516559	0.305957
N	-0.251790	-1.645195	0.325623
O	-3.956031	0.428426	-0.360444
C	-5.233812	-0.154876	-0.600210
H	-5.921262	0.677957	-0.737871
H	-5.206773	-0.783042	-1.493233
H	-5.539768	-0.769613	0.249167
C	3.016170	0.348145	-0.954568
C	2.971163	-2.027045	-0.425763
C	3.868197	-0.931325	-1.026553
H	4.759022	-0.811404	-0.402073
H	4.200019	-1.161954	-2.040293
H	3.595818	1.268366	-0.871346
H	3.531313	-2.847941	0.030813
C	2.127272	0.108161	0.248620
C	2.125283	-1.265969	0.565789
C	1.218096	0.977270	0.801135
H	0.744634	0.776240	1.754622
C	1.147526	-1.845235	1.391614
H	0.809931	-1.311554	2.276048
H	1.163165	-2.923434	1.516315
H	2.313522	-2.464248	-1.190649
H	2.382827	0.462855	-1.842613
C	0.984987	2.313667	0.235170
O	1.553969	2.806973	-0.712485
O	-0.005284	2.961880	0.893418
H	-0.110093	3.818283	0.451506

TS-[4+2]-4e-product

C	-2.973980	-0.373248	0.157707
O	-3.180949	-1.304524	-0.586364
C	-1.716363	0.250844	0.506715
H	-1.710564	1.076386	1.197776
N	-0.534355	-0.125245	-0.008070
N	-0.387824	-1.087151	-0.831999
O	-3.976232	0.268012	0.826809
C	-5.271564	-0.252414	0.563910
H	-5.961717	0.345310	1.158173
H	-5.514044	-0.171767	-0.498557
H	-5.333007	-1.305051	0.851048
C	3.073180	0.168996	1.387934
C	3.411301	-1.657077	-0.257646
C	3.921847	-1.094749	1.093940
H	3.738098	-1.834259	1.877525
H	4.992900	-0.885245	1.083522
H	2.817037	0.264430	2.448169
H	3.375547	-2.750811	-0.271248
C	1.873719	-0.059606	0.509708
C	2.048980	-1.027263	-0.384402
C	0.610560	0.735083	0.460882
H	0.346000	1.150922	1.433709
C	0.953870	-1.344880	-1.346675
H	0.965982	-2.401379	-1.629141
H	1.087736	-0.768284	-2.276072
H	4.047257	-1.349344	-1.097557
H	3.588988	1.093845	1.100257
C	0.790627	1.857374	-0.552174
O	0.442447	1.823880	-1.700467
O	1.472517	2.871698	0.004427
H	1.619707	3.531120	-0.691766

TS-[4+2]-4f

C	2.872999	-0.315726	0.133039
O	3.011038	-1.517076	0.167169
C	1.609169	0.385101	-0.109151
H	1.530442	1.462213	-0.126757

N	0.553047	-0.344021	-0.327666
N	0.139176	-1.464252	-0.313225
O	3.876455	0.565392	0.309113
C	5.146879	-0.032035	0.555608
H	5.844804	0.793613	0.682087
H	5.111592	-0.647924	1.456790
H	5.443467	-0.661433	-0.286261
C	-2.961349	0.766411	0.937342
C	-3.085639	-1.637635	0.582521
C	-3.886616	-0.447179	1.141431
H	-4.796645	-0.312929	0.549015
H	-4.181530	-0.584092	2.182867
H	-3.493782	1.713239	0.819120
H	-3.718179	-2.450153	0.214657
C	-2.162973	0.383524	-0.288679
C	-2.244175	-1.004980	-0.500629
C	-1.232443	1.165085	-0.931303
H	-0.814378	0.884993	-1.891272
C	-1.322306	-1.684145	-1.312066
H	-0.993730	-1.231676	-2.244005
H	-1.378037	-2.767128	-1.353527
H	-2.419576	-2.060155	1.347949
H	-2.271874	0.884108	1.783292
C	-0.937305	2.489134	-0.488038
N	-0.655076	3.549055	-0.111204

TS-[4+2]-4f-product

C	-2.877185	-0.291608	0.129763
O	-3.040027	-1.308820	-0.503432
C	-1.642752	0.419755	0.399597
H	-1.670626	1.328782	0.976341
N	-0.449833	0.028312	-0.070817
N	-0.263249	-1.012463	-0.783835
O	-3.900517	0.378438	0.727098
C	-5.176469	-0.218606	0.533660
H	-5.887134	0.416393	1.060688
H	-5.422895	-0.268038	-0.529587
H	-5.194503	-1.232831	0.939693
C	3.177713	0.653751	1.220002
C	3.569749	-1.355221	-0.177536
C	4.077013	-0.600360	1.076870
H	3.938491	-1.237007	1.954401
H	5.136725	-0.348118	1.014928
H	2.945789	0.885962	2.264500
H	3.594202	-2.442203	-0.054341
C	1.970129	0.251145	0.417624
C	2.172470	-0.817520	-0.343798
C	0.673747	0.984145	0.314169
H	0.384118	1.435415	1.265618
C	1.089752	-1.309707	-1.241121
H	1.131252	-2.397223	-1.353527
H	1.224113	-0.894483	-2.253619
H	4.166992	-1.120389	-1.067655
H	3.644706	1.547592	0.786942
C	0.739595	2.041956	-0.708814
N	0.840303	2.873127	-1.504808

TS-[4+2]-5a

C	-3.065924	-0.698719	-0.196167
O	-3.247379	-1.888284	-0.040579
C	-1.840373	0.022308	0.062836
H	-1.751932	1.086958	-0.083337
N	-0.805823	-0.643088	0.542479
N	-0.443138	-1.729133	0.848587
O	-4.034580	0.141739	-0.654571
C	-5.270932	-0.499695	-0.935195
H	-5.942604	0.281721	-1.289606
H	-5.144520	-1.269717	-1.700201
H	-5.676227	-0.972340	-0.037152
C	1.853451	0.313525	0.251693
C	2.055217	-1.000876	0.731019
C	3.012402	-1.949662	0.031930
C	3.562683	-1.432044	-1.293861
C	3.940119	0.038282	-1.147694
C	2.671861	0.854555	-0.910944
H	3.850205	-2.144193	0.715223
H	4.421064	-2.036320	-1.601314
H	4.628693	0.158816	-0.301736
H	2.922681	1.901658	-0.704446
C	0.879111	1.103661	0.862955
C	1.264452	-1.555988	1.736940
H	0.586654	0.878475	1.884446
H	1.462226	-2.583423	2.025546
H	0.845021	-0.953266	2.533866
H	2.501757	-2.909155	-0.106113
H	2.802260	-1.529111	-2.078543
H	4.453112	0.407992	-2.040353
H	2.096089	0.850116	-1.844191
N	0.363376	2.271279	0.410132
C	0.212483	2.560841	-1.009008
H	0.076515	1.625933	-1.556956
H	-0.689570	3.163994	-1.143466
H	1.060742	3.112937	-1.425137
C	-0.349665	3.152794	1.319202
H	0.059688	4.167167	1.267739
H	-1.417238	3.193524	1.073715
H	-0.239166	2.793288	2.342587

TS-[4+2]-5a-product

C	-3.036416	-0.642801	-0.149284
O	-3.171985	-1.843846	-0.081495
C	-1.858840	0.162537	0.086118
H	-1.929413	1.226678	-0.020190
N	-0.675326	-0.348869	0.445459
N	-0.465154	-1.595740	0.609815
O	-4.070363	0.187908	-0.487369
C	-5.292273	-0.487512	-0.743430
H	-6.016605	0.285835	-0.997626
H	-5.181796	-1.192918	-1.570930
H	-5.622292	-1.043865	0.137568
C	1.756670	0.133226	0.141126
C	1.965372	-1.174388	0.317397
C	3.206482	-1.892455	-0.139313
C	4.099216	-1.005897	-1.008952
C	4.178529	0.405092	-0.426043
C	2.797449	1.061934	-0.439982

H	3.758942	-2.236257	0.747128
H	5.095051	-1.448907	-1.100682
H	4.544774	0.349263	0.606755
H	2.798801	1.996980	0.130879
C	0.474771	0.697831	0.717179
C	0.888226	-1.942615	1.026452
H	0.526314	0.666854	1.813783
H	0.989179	-3.017256	0.856176
H	0.992963	-1.791097	2.116563
H	2.915836	-2.800219	-0.681429
H	3.677805	-0.949280	-2.020105
H	4.888840	1.018081	-0.988518
H	2.540052	1.339002	-1.470516
N	0.193664	2.020448	0.327779
C	0.049443	2.345474	-1.080693
H	0.295668	1.475964	-1.693023
H	-0.981635	2.634533	-1.324560
H	0.711577	3.174968	-1.357701
C	-0.478601	2.923723	1.237412
H	-0.105159	3.941292	1.079130
H	-1.571537	2.941323	1.109285
H	-0.261049	2.640763	2.269635

TS-[4+2]-5b

C	2.997534	-0.223596	0.189953
O	3.175976	-1.422415	0.233352
C	1.769639	0.444161	-0.193580
H	1.671297	1.517432	-0.239210
N	0.747598	-0.304077	-0.553555
N	0.398001	-1.436617	-0.655413
O	3.958177	0.680864	0.510091
C	5.196162	0.100031	0.898822
H	5.861427	0.932841	1.123643
H	5.067107	-0.534561	1.778929
H	5.607831	-0.510648	0.091690
C	-1.847687	0.608382	-0.489009
C	-2.077360	-0.771098	-0.666491
C	-2.984030	-1.529092	0.280927
C	-3.257204	-0.790544	1.589293
C	-3.649134	0.654348	1.294491
C	-2.471754	1.387606	0.654342
H	-3.938056	-1.718114	-0.230573
H	-4.045073	-1.302667	2.148801
H	-4.505599	0.667365	0.609228
H	-2.793999	2.374190	0.295980
C	-0.844218	1.221543	-1.217725
C	-1.281706	-1.507824	-1.545174
H	-0.498536	0.868821	-2.180743
H	-1.432459	-2.581073	-1.592176
H	-0.916554	-1.079006	-2.471607
H	-2.538445	-2.510186	0.474991
H	-2.355590	-0.801645	2.214011
H	-3.955674	1.176570	2.205001
H	-1.710510	1.560998	1.431585
O	-0.402236	2.466738	-0.977053
H	-0.693148	2.759525	-0.102994

TS-[4+2]-5b-product

C	3.014467	-0.202249	0.163976
O	3.141458	-1.399983	0.281474
C	1.846655	0.557811	-0.231289
H	1.904103	1.628234	-0.302597
N	0.691191	-0.016766	-0.579136
N	0.498401	-1.279362	-0.648803
O	4.032820	0.669230	0.424045
C	5.239626	0.042762	0.833862
H	5.955165	0.847503	0.998883
H	5.088897	-0.528528	1.753320
H	5.604432	-0.640008	0.062492
C	-1.714210	0.448968	-0.262439
C	-1.925778	-0.867366	-0.314254
C	-3.120230	-1.537592	0.307354
C	-3.883000	-0.587238	1.233628
C	-4.034487	0.792154	0.590334
C	-2.665374	1.437599	0.363973
H	-3.780084	-1.903885	-0.491772
H	-4.861728	-1.007866	1.481043
H	-4.542556	0.685471	-0.375970
H	-2.752430	2.322296	-0.275978
C	-0.463368	0.946909	-0.936082
C	-0.862571	-1.673362	-1.007221
H	-0.529089	0.858665	-2.027138
H	-0.942027	-2.734428	-0.760828
H	-0.999385	-1.595576	-2.100978
H	-2.787897	-2.426622	0.855613
H	-3.330244	-0.483215	2.175313
H	-4.655989	1.443178	1.211585
H	-2.266501	1.793510	1.325808
O	-0.154492	2.264135	-0.665100
H	-0.180487	2.396741	0.292382

TS-[4+2]-5c

C	-2.982992	0.014464	-0.162587
O	-3.104309	1.064023	-0.757126
C	-1.782635	-0.459959	0.500496
H	-1.735120	-1.401894	1.018925
N	-0.719093	0.318814	0.473900
N	-0.332343	1.345333	0.021008
O	-3.988257	-0.886306	-0.030825
C	-5.204806	-0.495691	-0.655757
H	-5.909576	-1.305684	-0.472633
H	-5.576327	0.438646	-0.228441
H	-5.058954	-0.350544	-1.728754
C	2.131563	0.839241	0.414501
C	1.893625	-0.469892	0.899961
C	2.602995	-1.662556	0.286634
C	3.093395	-1.399995	-1.135689
C	3.897229	-0.102717	-1.165585
C	2.999480	1.078463	-0.804162
H	3.466494	-1.911695	0.917902
H	3.697058	-2.243237	-1.483633
H	4.724103	-0.175497	-0.447797
H	3.595124	1.985238	-0.654539
C	1.291515	1.877246	0.817962
C	0.848277	-0.680841	1.768404
H	0.901878	1.925253	1.828408

H	0.533034	-1.695696	1.995804
H	0.484714	0.079200	2.448520
H	1.936438	-2.530150	0.319636
H	2.234324	-1.312654	-1.812441
H	4.342727	0.062826	-2.150636
H	2.322102	1.290688	-1.644446
H	1.416687	2.847868	0.348306

TS-[4+2]-5c-product

C	-3.032811	0.031522	-0.121864
O	-3.189822	1.182351	-0.462416
C	-1.839276	-0.614208	0.377809
H	-1.874231	-1.655595	0.647610
N	-0.671634	0.023174	0.545572
N	-0.466975	1.251060	0.258176
O	-4.041573	-0.888201	-0.163184
C	-5.275799	-0.370847	-0.638627
H	-5.978382	-1.203233	-0.618684
H	-5.629051	0.441989	0.000783
H	-5.169741	0.014744	-1.655677
C	1.971481	0.753680	0.176998
C	1.727796	-0.528963	0.449316
C	2.650896	-1.661084	0.084179
C	3.709259	-1.199414	-0.921391
C	4.304860	0.146880	-0.503760
C	3.226828	1.233116	-0.497431
H	3.136196	-2.052215	0.989692
H	4.492663	-1.956775	-1.015959
H	4.729707	0.054053	0.503504
H	3.590405	2.135930	0.008786
C	0.884715	1.728150	0.542162
C	0.429745	-0.806899	1.146520
H	0.968852	1.989273	1.612491
H	0.134952	-1.853512	1.085993
H	0.464490	-0.510433	2.202184
H	2.067087	-2.492152	-0.330362
H	3.241810	-1.092108	-1.907690
H	5.122453	0.431082	-1.172344
H	2.983862	1.540057	-1.524269
H	0.994185	2.664454	-0.010943

TS-[4+2]-5d

C	-3.087149	-0.628976	-0.206939
O	-3.227205	-1.783772	0.129153
C	-1.856316	0.145965	-0.098133
H	-1.779721	1.166412	-0.437518
N	-0.803918	-0.454155	0.401219
N	-0.413971	-1.522334	0.752137
O	-4.077619	0.124803	-0.733104
C	-5.318570	-0.558562	-0.878433
H	-6.007528	0.162742	-1.314947
H	-5.205306	-1.425759	-1.532778
H	-5.684810	-0.900966	0.092073
C	1.909684	0.338092	0.305448
C	2.012987	-0.978691	0.823029
C	2.897348	-2.023327	0.174473
C	3.394408	-1.633190	-1.214467
C	3.894206	-0.192859	-1.186762
C	2.732318	0.753449	-0.899195
H	3.761845	-2.195265	0.831417
H	4.179881	-2.323512	-1.534796
H	4.665841	-0.090680	-0.412606
H	3.078844	1.780607	-0.759728
C	0.904571	1.151263	0.801013
C	1.089957	-1.428374	1.780716
H	0.493144	0.959366	1.785266
H	1.162509	-2.465029	2.093814
H	0.716276	-0.771985	2.558719
H	2.345832	-2.969544	0.139741
H	2.573400	-1.716323	-1.936993
H	4.357697	0.082501	-2.138187
H	2.064217	0.800055	-1.767144
C	0.484935	2.450165	0.221078
O	0.848810	2.840908	-0.872924
C	-0.467611	3.259991	1.075872
H	-1.335802	2.653400	1.354665
H	0.030267	3.557977	2.004639
H	-0.787846	4.146233	0.529670

TS-[4+2]-5d-product

C	-3.000579	-0.623504	-0.173286
O	-3.161986	-1.782472	0.134041
C	-1.821143	0.205282	-0.026485
H	-1.858182	1.218290	-0.383395
N	-0.658913	-0.261091	0.452945
N	-0.457379	-1.480378	0.772122
O	-3.991529	0.132665	-0.727640
C	-5.214879	-0.564285	-0.917350
H	-5.901348	0.151628	-1.367667
H	-5.072968	-1.424136	-1.576516
H	-5.609074	-0.924003	0.036366
C	1.752254	0.179691	0.137467
C	1.962170	-1.101354	0.456632
C	3.154361	-1.893449	-0.007022
C	3.933927	-1.154125	-1.095955
C	4.089752	0.322563	-0.732550
C	2.724678	1.010166	-0.664882
H	3.804601	-2.099079	0.855258
H	4.910074	-1.624247	-1.245567
H	4.586921	0.401763	0.242628
H	2.825404	2.007184	-0.220779
C	0.466920	0.741366	0.696803
C	0.884828	-1.761200	1.274984
H	0.521512	0.749459	1.795524
H	0.984863	-2.848178	1.274588
H	0.966483	-1.436929	2.329071
H	2.815582	-2.870814	-0.369947
H	3.388461	-1.232210	-2.044095
H	4.724951	0.835262	-1.460449
H	2.322639	1.177667	-1.670217
C	0.095984	2.154534	0.226226
O	0.273681	2.491488	-0.919198
C	-0.480269	3.070426	1.275956
H	-1.320518	2.578037	1.775477
H	0.279096	3.277615	2.037822
H	-0.803795	4.002868	0.815572

TS-[4+2]-5e

C	-3.153149	-0.571460	-0.223243
O	-3.264638	-1.770915	-0.112096
C	-1.919836	0.191067	-0.020791
H	-1.879153	1.266333	-0.094596
N	-0.859953	-0.470611	0.345078
N	-0.416197	-1.563591	0.519311
O	-4.170175	0.252052	-0.551593
C	-5.412798	-0.410115	-0.769812
H	-6.125430	0.370491	-1.030603
H	-5.323137	-1.135732	-1.581160
H	-5.731069	-0.935119	0.133566
C	1.918066	0.306268	0.359664
C	1.948832	-1.044715	0.794937
C	2.828113	-2.079946	0.125918
C	3.408859	-1.622317	-1.208097
C	3.969492	-0.213498	-1.053203
C	2.840165	0.768394	-0.754701
H	3.650589	-2.330817	0.810988
H	4.177990	-2.325471	-1.540008
H	4.703250	-0.203386	-0.236795
H	3.231711	1.756783	-0.504361
C	0.914276	1.126681	0.838406
C	0.963321	-1.528528	1.674324
H	0.396758	0.916871	1.764129
H	1.014679	-2.577903	1.947337
H	0.549831	-0.902352	2.457652
H	2.241914	-2.997554	0.000671
H	2.620467	-1.616881	-1.970713
H	4.494394	0.106001	-1.957819
H	2.235437	0.926241	-1.655792
C	0.595591	2.444947	0.270111
O	1.140650	3.009535	-0.652186
O	-0.468412	2.993617	0.907010
H	-0.630175	3.846939	0.476611

TS-[4+2]-5e-product

C	-3.038811	-0.574974	-0.164116
O	-3.193648	-1.760699	0.018460
C	-1.849754	0.231706	0.023505
H	-1.901704	1.280149	-0.204636
N	-0.682674	-0.277769	0.437390
N	-0.486672	-1.520728	0.658516
O	-4.045525	0.238358	-0.595302
C	-5.278601	-0.432540	-0.813626
H	-5.978337	0.329272	-1.155060
H	-5.166266	-1.214239	-1.568855
H	-5.637675	-0.895139	0.109033
C	1.744456	0.153672	0.169103
C	1.942757	-1.146004	0.402238
C	3.146408	-1.903889	-0.087634
C	3.949885	-1.091023	-1.104569
C	4.099777	0.356457	-0.635575
C	2.733619	1.039520	-0.548306
H	3.776372	-2.168615	0.773452
H	4.928944	-1.551194	-1.265291
H	4.575537	0.366533	0.353146
H	2.825956	1.999630	-0.025378
C	0.452634	0.695522	0.733183
C	0.846702	-1.855742	1.148797
H	0.485595	0.706624	1.829517
H	0.935724	-2.940100	1.059451
H	0.918881	-1.621027	2.226602
H	2.817379	-2.853601	-0.525047
H	3.425483	-1.101411	-2.067579
H	4.750390	0.917235	-1.312509
H	2.353948	1.280399	-1.547798
C	0.137368	2.103184	0.252954
O	0.184841	2.469040	-0.891057
O	-0.180587	2.905278	1.278504
H	-0.364103	3.783802	0.909054

TS-[4+2]-5f

C	3.097161	-0.360453	0.188434
O	3.223006	-1.562348	0.127277
C	1.854987	0.375123	-0.054456
H	1.785885	1.450843	0.010929
N	0.805597	-0.323792	-0.384420
N	0.371445	-1.427382	-0.493872
O	4.099487	0.489076	0.487425
C	5.350418	-0.144547	0.741718
H	6.049499	0.657698	0.971054
H	5.266052	-0.834200	1.584369
H	5.681353	-0.704433	-0.135720
C	-1.910168	0.496272	-0.447561
C	-2.018645	-0.882271	-0.741153
C	-2.931781	-1.786767	0.058257
C	-3.395351	-1.173180	1.377386
C	-3.879606	0.254028	1.138641
C	-2.716027	1.125288	0.672879
H	-3.810502	-2.024697	-0.557756
H	-4.184779	-1.789693	1.816141
H	-4.669457	0.247739	0.377032
H	-3.067105	2.110884	0.351151
C	-0.893097	1.226794	-1.033581
C	-1.075724	-1.485473	-1.590625
H	-0.426679	0.943402	-1.967754
H	-1.154326	-2.556696	-1.745713
H	-0.671539	-0.957591	-2.448061
H	-2.412608	-2.735389	0.233456
H	-2.560398	-1.158547	2.088570
H	-4.313380	0.681307	2.046703
H	-2.035555	1.307729	1.515458
C	-0.565835	2.538729	-0.576773
N	-0.256242	3.586397	-0.186918

TS-[4+2]-5f-product

C	-3.015708	-0.351957	-0.163094
O	-3.157077	-1.551739	-0.110108
C	-1.836154	0.438696	0.140010
H	-1.881881	1.509076	0.045013
N	-0.684752	-0.111814	0.534933
N	-0.486058	-1.367989	0.673530
O	-4.013969	0.492376	-0.539305
C	-5.235084	-0.158994	-0.864326

H	-5.930738	0.631159	-1.143010
H	-5.093111	-0.854697	-1.694796
H	-5.615167	-0.718932	-0.006484
C	1.742695	0.330701	0.253559
C	1.938138	-0.982929	0.385601
C	3.111999	-1.701594	-0.221795
C	3.839174	-0.824879	-1.244329
C	4.029592	0.593207	-0.704083
C	2.678898	1.270490	-0.459112
H	3.799628	-2.005679	0.579687
H	4.802697	-1.271946	-1.504094
H	4.584453	0.546412	0.241055
H	2.812117	2.186427	0.127819
C	0.464158	0.829257	0.891246
C	0.858159	-1.736083	1.114135
H	0.524549	0.743640	1.985081
H	0.941099	-2.812449	0.953927
H	0.958503	-1.571753	2.202517
H	2.760512	-2.628607	-0.688674
H	3.244913	-0.780812	-2.164903
H	4.623998	1.195091	-1.396682
H	2.227447	1.586502	-1.409315
C	0.185818	2.230401	0.573178
N	0.033559	3.351743	0.343283

TS-[4+2]-6a

C	-2.968417	-0.663265	-0.025381
O	-3.156831	-1.801190	0.351550
C	-1.751604	0.101742	0.128103
H	-1.657866	1.115604	-0.233639
N	-0.720706	-0.441203	0.746170
N	-0.382235	-1.471549	1.249230
O	-3.922379	0.066109	-0.669712
C	-5.147550	-0.626420	-0.861954
H	-5.807802	0.066637	-1.382770
H	-4.994925	-1.528828	-1.459154
H	-5.583021	-0.920143	0.096380
C	1.746842	-0.656052	-1.844490
C	2.563868	0.358043	-0.988245
C	2.911609	-1.600754	0.073606
C	1.982607	-2.005512	-1.108143
H	0.685124	-0.397565	-1.887482
H	2.134338	-0.688106	-2.867341
H	1.054374	-2.457756	-0.753190
H	2.493248	-2.725025	-1.754540
C	3.771242	-0.510796	-0.587553
H	4.444367	-0.008103	0.111266
H	4.332680	-0.876784	-1.452778
H	2.798962	1.297721	-1.487999
H	3.429983	-2.435967	0.546865
C	1.852705	0.466870	0.355084
C	2.065803	-0.761666	1.008845
C	0.897570	1.359017	0.829996
H	0.635046	1.272060	1.880461
C	1.284509	-1.260958	2.054095
H	0.945423	-0.589487	2.837730
N	0.349269	2.438070	0.238794
C	0.508812	2.737253	-1.172030
H	1.391322	3.359429	-1.363825
H	0.585343	1.812173	-1.743279
H	-0.376444	3.277633	-1.516824
C	-0.419769	3.392772	1.016166
H	-0.589993	2.997991	2.018245
H	0.105770	4.351718	1.098797
H	-1.392519	3.566440	0.545322
H	1.486613	-2.267871	2.405101

TS-[4+2]-6a-product

C	-2.977206	-0.708889	-0.092687
O	-3.084581	-1.885744	0.169743
C	-1.848835	0.173199	0.109410
H	-1.932037	1.201554	-0.183962
N	-0.691819	-0.220364	0.648788
N	-0.444747	-1.409257	1.032476
O	-3.994496	0.005685	-0.663907
C	-5.166372	-0.756159	-0.911820
H	-5.882691	-0.069523	-1.362082
H	-4.955305	-1.586074	-1.590982
H	-5.566694	-1.169005	0.017615
C	2.481366	-0.210365	-1.849258
C	2.755450	0.695313	-0.601164
C	3.203467	-1.390952	0.155955
C	2.772073	-1.643235	-1.321938
H	1.459618	-0.113139	-2.223565
H	3.162483	0.058308	-2.661810
H	1.898999	-2.297491	-1.379165
H	3.585666	-2.113959	-1.880789
C	3.960785	-0.055718	0.005376
H	4.283063	0.362514	0.961400
H	4.808821	-0.121281	-0.683972
H	2.890546	1.755235	-0.820678
H	3.734141	-2.222033	0.622628
C	1.697720	0.335454	0.425063
C	1.957930	-0.901951	0.862273
C	0.408755	0.951318	0.845723
H	0.390665	1.016780	1.940140
C	0.893568	-1.631451	1.606097
H	0.892518	-1.324323	2.665935
N	0.084868	2.211517	0.327638
C	0.079407	2.466939	-1.099970
H	0.566201	3.426675	-1.309039
H	0.619129	1.682316	-1.627510
H	-0.939029	2.506873	-1.511443
C	-0.749424	3.110730	1.098979
H	-0.635965	2.900909	2.164656
H	-0.429420	4.142524	0.917886
H	-1.817478	3.037340	0.846995
H	1.049169	-2.712400	1.596504

TS-[4+2]-6b

C	2.955317	-0.215419	0.025584
O	3.108591	-1.407378	-0.137767
C	1.743172	0.534670	-0.239648
H	1.667516	1.600889	-0.092665
N	0.704520	-0.111873	-0.730062
N	0.365959	-1.219342	-1.024142

O	3.931788	0.599153	0.500833
C	5.154996	-0.066130	0.787841
H	5.836014	0.701525	1.153274
H	5.007346	-0.838704	1.546334
H	5.558795	-0.538760	-0.110687
C	-1.651963	0.110631	1.837516
C	-2.524385	0.927775	0.839364
C	-2.891378	-1.204995	0.198938
C	-1.906443	-1.359670	1.397079
H	-0.594520	0.384455	1.775491
H	-1.989462	0.282277	2.863591
H	-0.989678	-1.874232	1.103307
H	-2.383871	-1.933499	2.196185
C	-3.737229	-0.007112	0.668984
H	-4.444423	0.345708	-0.085439
H	-4.257394	-0.198311	1.612048
H	-2.743650	1.954016	1.147361
H	-3.420915	-2.119703	-0.070536
C	-1.874321	0.764464	-0.523724
C	-2.094863	-0.566166	-0.921653
C	-0.872926	1.538573	-1.062107
H	-0.538558	1.426207	-2.087342
C	-1.299863	-1.222933	-1.859249
H	-0.985244	-0.691264	-2.752628
H	-1.442455	-2.288079	-2.008331
O	-0.420739	2.678482	-0.513622
H	-0.730671	2.741800	0.400365

TS-[4+2]-6b-product

C	2.937576	-0.218883	0.081800
O	3.043697	-1.424251	0.099947
C	1.802451	0.590987	-0.313072
H	1.871316	1.662970	-0.279446
N	0.662505	0.068684	-0.771767
N	0.453647	-1.179097	-0.947954
O	3.947159	0.609618	0.477929
C	5.120731	-0.069239	0.901015
H	5.832876	0.706587	1.179802
H	4.908715	-0.717556	1.754968
H	5.524606	-0.686295	0.094544
C	-2.072373	0.463291	1.797401
C	-2.635040	1.086768	0.476845
C	-3.039630	-1.124916	0.211644
C	-2.334361	-1.057478	1.606113
H	-1.010395	0.685900	1.942426
H	-2.615954	0.854361	2.662019
H	-1.414701	-1.647404	1.619450
H	-2.997414	-1.444296	2.384640
C	-3.859603	0.179582	0.243038
H	-4.366093	0.388570	-0.701597
H	-4.573852	0.213634	1.071345
H	-2.811801	2.163438	0.511220
H	-3.576380	-2.054621	0.019488
C	-1.730439	0.569194	-0.619819
C	-1.958263	-0.739277	-0.773588
C	-0.456230	1.126268	-1.131058
H	-0.411791	1.140138	-2.224557
C	-0.891375	-1.553701	-1.420929
H	-0.940442	-1.442217	-2.516378
H	-0.995365	-2.619718	-1.209274
O	-0.142883	2.391325	-0.688774
H	-0.320827	2.440286	0.260240

TS-[4+2]-6c

C	2.967978	0.013693	-0.071323
O	3.078176	0.679884	-1.078201
C	1.777028	-0.111155	0.747978
H	1.745522	-0.716101	1.637886
N	0.703502	0.571262	0.393813
N	0.333399	1.285206	-0.485385
O	3.979048	-0.730768	0.441966
C	5.186436	-0.667565	-0.307209
H	5.896256	-1.309212	0.213128
H	5.026957	-1.022348	-1.328158
H	5.559972	0.358146	-0.352656
C	-1.790385	-1.748946	-0.515133
C	-2.593647	-1.192035	0.696226
C	-2.993296	0.327644	-0.926603
C	-2.072249	-0.709363	-1.636130
H	-0.726023	-1.841630	-0.283584
H	-2.165330	-2.738867	-0.789606
H	-1.161171	-0.246228	-2.020172
H	-2.606555	-1.164969	-2.474598
C	-3.823835	-0.594944	-0.013585
H	-4.486079	-0.048316	0.662723
H	-4.395140	-1.341052	-0.573488
H	-2.774203	-1.913219	1.494295
H	-3.536297	0.988801	-1.603355
C	-1.879837	0.078782	1.119643
C	-2.128541	1.025483	0.102978
C	-0.827934	0.208017	1.987621
H	-0.496094	1.186042	2.320099
C	-1.285025	2.115355	-0.102765
H	-0.925102	2.673401	0.756943
H	-1.406196	2.713109	-1.000225
H	-0.486775	-0.635577	2.581462

TS-[4+2]-6c-product

C	2.986606	0.014292	-0.081552
O	3.129024	0.946282	-0.840430
C	1.820352	-0.361167	0.688210
H	1.867554	-1.222207	1.332613
N	0.669280	0.325341	0.666240
N	0.452616	1.348712	-0.063692
O	3.984811	-0.881065	0.174505
C	5.191970	-0.617127	-0.525981
H	5.888201	-1.401462	-0.231287
H	5.027180	-0.638876	-1.606081
H	5.589067	0.365508	-0.259568
C	-2.230759	-1.644102	-0.850417
C	-2.693389	-1.198005	0.574096
C	-3.114942	0.627619	-0.693928
C	-2.509343	-0.385838	-1.719957
H	-1.178632	-1.941085	-0.860270
H	-2.823195	-2.498649	-1.189666
H	-1.605885	0.010919	-2.189617

H	-3.234141	-0.602713	-2.509551
C	-3.913837	-0.328953	0.212756
H	-4.351127	0.171805	1.079507
H	-4.683701	-0.885403	-0.330567
H	-2.851045	-2.014871	1.279983
H	-3.652253	1.463392	-1.143955
C	-1.719711	-0.111900	0.978289
C	-1.963108	0.966819	0.225828
C	-0.392830	-0.198225	1.631431
H	-0.317342	0.462566	2.501793
C	-0.872775	1.976616	0.085900
H	-0.858461	2.649102	0.958882
H	-1.002496	2.608725	-0.794796
H	-0.107077	-1.207014	1.924103

TS-[4+2]-6d

C	-3.057518	-0.574838	-0.058813
O	-3.181302	-1.726522	0.294703
C	-1.845030	0.226074	0.053038
H	-1.789837	1.240987	-0.306202
N	-0.782196	-0.333999	0.580890
N	-0.411073	-1.405584	0.958536
O	-4.055309	0.149640	-0.613883
C	-5.279046	-0.561812	-0.767213
H	-5.975772	0.137345	-1.226972
H	-5.137494	-1.437410	-1.404728
H	-5.654182	-0.895667	0.202920
C	1.911751	-0.438487	-1.795548
C	2.721815	0.431265	-0.789633
C	2.886568	-1.652565	0.078192
C	2.042426	-1.873983	-1.213823
H	0.877834	-0.093505	-1.870612
H	2.361466	-0.368984	-2.789363
H	1.077013	-2.333839	-0.993566
H	2.587018	-2.532053	-1.896894
C	3.846738	-0.542955	-0.390692
H	4.485938	-0.159907	0.409255
H	4.460829	-0.849579	-1.242427
H	2.996419	1.413341	-1.166709
H	3.325146	-2.560230	0.495375
C	1.896610	0.431775	0.481602
C	2.013683	-0.864165	1.030219
C	0.895693	1.289153	0.874425
H	0.504027	1.218097	1.885863
C	1.080855	-1.373579	1.944567
H	0.741144	-0.734761	2.755918
H	1.151658	-2.421313	2.218451
C	0.497438	2.490756	0.097488
O	0.847474	2.654894	-1.055905
C	-0.396608	3.477687	0.813943
H	-1.273392	2.964210	1.222552
H	0.142350	3.917432	1.659721
H	-0.706436	4.262862	0.125614

TS-[4+2]-6d-product

C	-2.957295	-0.632824	-0.066680
O	-3.096631	-1.769878	0.321959
C	-1.806524	0.239792	0.058938
H	-1.859396	1.223224	-0.372271
N	-0.654854	-0.147078	0.624113
N	-0.428029	-1.328439	1.041393
O	-3.946343	0.048482	-0.712507
C	-5.141802	-0.698010	-0.893673
H	-5.829787	-0.039116	-1.421853
H	-4.950316	-1.599908	-1.480027
H	-5.562476	-0.997072	0.069556
C	2.237198	-0.234859	-1.826030
C	2.717283	0.661175	-0.640713
C	3.113149	-1.438534	0.111699
C	2.494743	-1.676513	-1.305995
H	1.191106	-0.038064	-2.067999
H	2.834551	-0.024558	-2.717648
H	1.582635	-2.276138	-1.249228
H	3.208962	-2.207608	-1.941387
C	3.926847	-0.155315	-0.143508
H	4.374623	0.252529	0.765932
H	4.692242	-0.285229	-0.914723
H	2.882252	1.705006	-0.902662
H	3.637966	-2.298215	0.530535
C	1.742693	0.372465	0.483747
C	1.975800	-0.869192	0.928386
C	0.422255	0.952994	0.839816
H	0.355278	1.105429	1.925028
C	0.882442	-1.552530	1.677635
H	0.848015	-1.194448	2.720145
H	1.011677	-2.635238	1.718497
C	0.087134	2.262897	0.117454
O	0.380600	2.407009	-1.045058
C	-0.581032	3.333070	0.941505
H	-1.468725	2.922837	1.433105
H	0.103835	3.666353	1.728752
H	-0.850620	4.176224	0.307057

TS-[4+2]-6e

C	-3.128255	-0.540100	-0.099432
O	-3.215319	-1.742783	0.001341
C	-1.919912	0.249538	0.137128
H	-1.905733	1.325757	0.065270
N	-0.847915	-0.382189	0.529019
N	-0.418553	-1.486503	0.698896
O	-4.156762	0.261274	-0.449580
C	-5.376717	-0.429219	-0.703330
H	-6.101758	0.335657	-0.976461
H	-5.249495	-1.146370	-1.517232
H	-5.704573	-0.968779	0.187990
C	2.069820	-0.299763	-1.777089
C	2.798599	0.483025	-0.645631
C	2.892186	-1.662898	0.064876
C	2.158978	-1.778368	-1.305404
H	1.042658	0.051816	-1.901347
H	2.591566	-0.151439	-2.725973
H	1.181065	-2.252290	-1.204230
H	2.762482	-2.378493	-1.992500
C	3.887385	-0.527053	-0.236251
H	4.460476	-0.211842	0.639619
H	4.567604	-0.768578	-1.058242

H	3.104943	1.489018	-0.919571
H	3.295879	-2.602868	0.444350
C	1.877239	0.393260	0.556351
C	1.948018	-0.945238	1.005251
C	0.871403	1.242948	0.945439
H	0.382417	1.133143	1.906531
C	0.955945	-1.528023	1.811159
H	0.554757	-0.955024	2.643562
H	1.025232	-2.592542	2.011888
C	0.554129	2.468054	0.192788
O	1.070390	2.837137	-0.837706
O	-0.455065	3.155633	0.775252
H	-0.621103	3.926607	0.211352

TS-[4+2]-6e-product

C	3.374368	-0.414467	-0.093286
O	3.554074	-1.405480	0.577365
C	2.128842	0.219205	-0.468502
H	2.147379	1.106379	-1.078630
N	0.921337	-0.227844	-0.079794
N	0.748977	-1.256105	0.651843
O	4.403381	0.301925	-0.632781
C	5.690232	-0.220905	-0.334943
H	6.403744	0.440020	-0.825642
H	5.863268	-0.236067	0.743969
H	5.791986	-1.241111	-0.713067
C	-3.654783	0.881584	-0.110371
C	-2.796802	0.292306	-1.275857
C	-3.138540	-1.500562	0.059422
C	-3.866626	-0.344778	0.820834
H	-3.153473	1.707808	0.397870
H	-4.606757	1.252538	-0.500462
H	-3.442296	-0.188981	1.815311
H	-4.928539	-0.578201	0.936440
C	-3.436382	-1.106394	-1.401916
H	-2.927064	-1.744081	-2.127524
H	-4.507982	-1.063332	-1.620961
H	-2.760275	0.909249	-2.175398
H	-3.419196	-2.505634	0.377227
C	-1.469623	-0.100215	-0.660197
C	-1.668541	-1.150761	0.133926
C	-0.207105	0.670934	-0.567910
H	0.117130	1.096533	-1.517331
C	-0.602885	-1.629658	1.049512
H	-0.597276	-2.721694	1.129682
H	-0.785205	-1.244936	2.065182
C	-0.311152	1.775294	0.486252
O	-0.738869	1.600386	1.596722
O	0.131741	2.950528	0.023383
H	0.063732	3.590788	0.749700

TS-[4+2]-6f

C	3.074072	-0.337566	0.062930
O	3.176545	-1.539273	-0.036622
C	1.852171	0.431907	-0.175516
H	1.806742	1.505682	-0.068824
N	0.790105	-0.225388	-0.551827
N	0.369895	-1.336380	-0.695776
O	4.088470	0.479566	0.409295
C	5.320577	-0.189119	0.664983
H	6.031731	0.589522	0.935026
H	5.205533	-0.905187	1.481582
H	5.656910	-0.725777	-0.224869
C	-1.948774	0.051046	1.788688
C	-2.721254	0.781654	0.649665
C	-2.926181	-1.402169	0.099068
C	-2.117065	-1.451881	1.429331
H	-0.902110	0.364846	1.827554
H	-2.405021	0.284315	2.754026
H	-1.163018	-1.967261	1.306442
H	-2.697362	-1.979039	2.191850
C	-3.867033	-0.213039	0.379306
H	-4.482021	0.063617	-0.480632
H	-4.501321	-0.374786	1.255376
H	-2.982780	1.817544	0.867504
H	-3.384663	-2.349222	-0.188895
C	-1.890863	0.575557	-0.598098
C	-2.013890	-0.786030	-0.941962
C	-0.884436	1.373001	-1.087321
H	-0.437472	1.189357	-2.058052
C	-1.061603	-1.440640	-1.740108
H	-0.689886	-0.937251	-2.629431
H	-1.145437	-2.516328	-1.857550
C	-0.555130	2.619949	-0.474020
N	-0.244784	3.610568	0.042724

TS-[4+2]-6f-product

C	2.979287	-0.351243	0.080941
O	3.102621	-1.551136	-0.002932
C	1.819645	0.466784	-0.231437
H	1.879171	1.533302	-0.102817
N	0.673892	-0.050898	-0.680970
N	0.454600	-1.297444	-0.843661
O	3.979330	0.465566	0.507269
C	5.181117	-0.214086	0.847186
H	5.880253	0.556778	1.167824
H	5.005049	-0.930785	1.652867
H	5.576703	-0.755099	-0.015719
C	-2.159614	0.311939	1.780206
C	-2.690088	0.941743	0.452010
C	-3.066136	-1.272214	0.153439
C	-2.402971	-1.208661	1.569941
H	-1.108331	0.556650	1.953731
H	-2.734379	0.692300	2.628888
H	-1.480716	-1.793744	1.608061
H	-3.088608	-1.608523	2.321729
C	-3.897232	0.025897	0.168403
H	-4.376534	0.237110	-0.790079
H	-4.637691	0.045061	0.973297
H	-2.864844	2.017368	0.491506
H	-3.586536	-2.205455	-0.064445
C	-1.748046	0.438516	-0.618130
C	-1.957681	-0.871013	-0.793594
C	-0.436214	0.967162	-1.078036
H	-0.371687	0.973978	-2.172830
C	-0.857164	-1.673878	-1.399135

H	-0.845522	-1.546579	-2.494027
H	-0.964298	-2.742597	-1.206940
C	-0.180569	2.319822	-0.583779
N	-0.049012	3.401227	-0.200204

TS-[4+2]-7a

C	-2.957792	-0.714906	-0.212927
O	-3.197732	-1.892700	-0.049897
C	-1.698318	-0.053751	0.043411
H	-1.547224	1.000800	-0.112958
N	-0.706477	-0.789075	0.509856
N	-0.330435	-1.850652	0.829932
O	-3.881474	0.172016	-0.673762
C	-5.149227	-0.406956	-0.953581
H	-5.779333	0.406502	-1.312007
H	-5.060624	-1.185092	-1.715475
H	-5.578678	-0.854488	-0.054010
C	1.975177	0.306770	0.199136
C	2.233401	-1.047796	0.643949
C	3.147557	-1.836260	-0.139243
C	3.823280	-1.319710	-1.198512
C	3.637074	0.046360	-1.573711
C	2.736561	0.818635	-0.909622
H	3.301233	-2.868495	0.160870
H	4.524285	-1.936423	-1.751440
H	4.227211	0.469166	-2.379579
H	2.638433	1.863191	-1.178093
C	1.005623	1.065117	0.867749
C	1.536743	-1.659999	1.678828
H	0.741855	0.776608	1.880984
H	1.767137	-2.692167	1.916058
H	1.081911	-1.100716	2.486452
N	0.402515	2.203782	0.476399
C	0.305438	2.638937	-0.907881
H	1.053688	3.398990	-1.158996
H	0.418428	1.778958	-1.569723
H	-0.686665	3.072755	-1.064299
C	-0.335923	3.005216	1.438599
H	0.110605	4.000894	1.535476
H	-1.377909	3.116581	1.120828
H	-0.317480	2.520080	2.414697

TS-[4+2]-7a-product

C	-2.904961	-0.640899	-0.167878
O	-3.042976	-1.842149	-0.122290
C	-1.723161	0.158045	0.077678
H	-1.795442	1.223871	-0.002977
N	-0.540316	-0.360250	0.425255
N	-0.334875	-1.615064	0.554447
O	-3.936851	0.199917	-0.482576
C	-5.163436	-0.465317	-0.745412
H	-5.885287	0.316028	-0.981084
H	-5.059576	-1.155016	-1.586786
H	-5.491183	-1.036736	0.126668
C	1.883953	0.134244	0.150109
C	2.093801	-1.234770	0.300244
C	3.264377	-1.816505	-0.178865
C	4.237517	-1.022739	-0.777397
C	4.041813	0.352261	-0.894069
C	2.866540	0.934640	-0.429792
H	3.413215	-2.887441	-0.074971
H	5.152556	-1.473900	-1.147014
H	4.807841	0.973402	-1.346227
H	2.715547	2.006249	-0.500563
C	0.601859	0.687879	0.727221
C	1.001671	-1.986460	1.000053
H	0.651751	0.633860	1.822119
H	1.091342	-3.062131	0.836683
H	1.092685	-1.825031	2.089195
N	0.327711	2.018820	0.360487
C	0.177924	2.378914	-1.040399
H	0.728544	3.303705	-1.250076
H	0.572646	1.586489	-1.677574
H	-0.872901	2.540707	-1.315883
C	-0.356498	2.897844	1.286712
H	0.013396	3.919867	1.151964
H	-1.448199	2.913291	1.151057
H	-0.144348	2.593280	2.313854

TS-[4+2]-7b

C	2.908435	-0.220793	0.210466
O	3.192193	-1.399703	0.204427
C	1.619344	0.348148	-0.125659
H	1.395028	1.399964	-0.050828
N	0.650377	-0.498880	-0.422057
N	0.319800	-1.617984	-0.535831
O	3.794324	0.756136	0.530019
C	5.089044	0.276711	0.872259
H	5.683863	1.159129	1.104717
H	5.038726	-0.388968	1.737005
H	5.530931	-0.273845	0.038383
C	-1.933132	0.558851	-0.457738
C	-2.255538	-0.845963	-0.426565
C	-3.127364	-1.298886	0.621968
C	-3.691677	-0.428226	1.500034
C	-3.396029	0.971753	1.433280
C	-2.531872	1.448368	0.500661
H	-3.346118	-2.360966	0.676658
H	-4.372522	-0.791048	2.262966
H	-3.861434	1.648489	2.141960
H	-2.282662	2.502250	0.449565
C	-0.932326	1.005734	-1.300680
C	-1.597874	-1.758127	-1.242983
H	-0.601168	0.438222	-2.162679
H	-1.773326	-2.817020	-1.091033
H	-1.249790	-1.495475	-2.234320
O	-0.496619	2.272835	-1.214043
H	0.221991	2.417756	-1.840660

TS-[4+2]-7b-product

C	2.875023	-0.203059	0.160819
O	3.059226	-1.398230	0.134353
C	1.678766	0.541496	-0.177874
H	1.673679	1.610646	-0.071829
N	0.530112	-0.046322	-0.519273
N	0.334723	-1.312265	-0.553713

O	3.848902	0.680747	0.524003
C	5.083478	0.070188	0.872744
H	5.756189	0.884064	1.140462
H	4.954077	-0.611634	1.716765
H	5.487230	-0.498234	0.031193
C	-1.845411	0.476547	-0.240286
C	-2.078380	-0.896168	-0.242827
C	-3.200268	-1.400663	0.406302
C	-4.082899	-0.523312	1.032273
C	-3.839599	0.849683	1.026576
C	-2.711158	1.361005	0.390856
H	-3.380797	-2.471440	0.424089
H	-4.962578	-0.912551	1.534477
H	-4.529609	1.523218	1.523688
H	-2.499144	2.424138	0.381008
C	-0.608593	0.893681	-0.970869
C	-1.021081	-1.714363	-0.931660
H	-0.693300	0.642612	-2.038245
H	-1.104248	-2.771852	-0.675770
H	-1.153492	-1.642450	-2.026154
O	-0.331217	2.226663	-0.774818
H	0.283602	2.529941	-1.453403

TS-[4+2]-7c

C	2.919164	0.022511	-0.161307
O	3.075306	1.113670	-0.666313
C	1.689250	-0.478656	0.422373
H	1.595118	-1.454632	0.862533
N	0.650412	0.336576	0.397552
N	0.264453	1.384099	0.036013
O	3.903731	-0.903624	-0.066248
C	5.147955	-0.488536	-0.617756
H	5.832069	-1.323934	-0.475365
H	5.041446	-0.257519	-1.680138
H	5.519453	0.402072	-0.105602
C	-1.988113	-0.570787	0.755290
C	-2.283207	0.784299	0.346431
C	-3.209390	0.989182	-0.732898
C	-3.847903	-0.056744	-1.318462
C	-3.568333	-1.401654	-0.905792
C	-2.661198	-1.649093	0.071738
H	-3.404363	2.008347	-1.052635
H	-4.568348	0.116755	-2.110730
H	-4.081971	-2.223420	-1.393779
H	-2.433240	-2.666587	0.374733
C	-0.963035	-0.826853	1.637152
C	-1.522979	1.838410	0.836431
H	-0.601011	-0.094882	2.347360
H	-1.666064	2.828843	0.418335
H	-1.094242	1.819000	1.830617
H	-0.648465	-1.851605	1.811003

TS-[4+2]-7c-product

C	2.876903	0.031120	-0.125570
O	3.030209	1.196377	-0.412437
C	1.684902	-0.637719	0.352135
H	1.722543	-1.689929	0.575987
N	0.518110	-0.010730	0.549511
N	0.307246	1.228127	0.300674
O	3.884045	-0.885088	-0.213144
C	5.117167	-0.346948	-0.669749
H	5.818358	-1.180263	-0.692771
H	5.005892	0.086475	-1.666662
H	5.474077	0.433980	0.006225
C	-1.858046	-0.590668	0.404175
C	-2.116198	0.756025	0.160079
C	-3.277024	1.126558	-0.510620
C	-4.181748	0.146252	-0.911881
C	-3.918588	-1.200189	-0.665008
C	-2.746667	-1.575344	-0.013060
H	-3.472270	2.174637	-0.718376
H	-5.091958	0.431888	-1.428952
H	-4.622505	-1.958843	-0.990145
H	-2.528191	-2.623699	0.169810
C	-0.576596	-0.862595	1.127812
C	-1.039357	1.696516	0.628032
H	-0.645672	-0.563842	2.180658
H	-1.139595	2.680647	0.167509
H	-1.130010	1.844098	1.718617
H	-0.270683	-1.905295	1.073378

TS-[4+2]-7d

C	-2.984118	-0.651368	-0.215891
O	-3.168998	-1.795279	0.137267
C	-1.725824	0.075383	-0.115865
H	-1.587675	1.078604	-0.481983
N	-0.708666	-0.594264	0.379447
N	-0.319909	-1.638679	0.747606
O	-3.942920	0.133448	-0.753752
C	-5.209804	-0.502624	-0.891652
H	-5.869201	0.239905	-1.338076
H	-5.130381	-1.381649	-1.535016
H	-5.589860	-0.817780	0.082712
C	2.003303	0.314566	0.210151
C	2.210776	-1.035371	0.689781
C	3.120177	-1.892975	-0.012147
C	3.841522	-1.431200	-1.067518
C	3.661663	-0.087917	-1.523347
C	2.767275	0.748395	-0.930634
H	3.240799	-2.912231	0.342095
H	4.554398	-2.076377	-1.569665
H	4.245809	0.264926	-2.367240
H	2.612264	1.753202	-1.298464
C	0.991067	1.074654	0.785216
C	1.390411	-1.568988	1.686056
H	0.642331	0.817043	1.779195
H	1.494698	-2.621129	1.928246
H	0.991248	-0.961549	2.488835
C	0.479422	2.374912	0.295251
O	0.715731	2.818009	-0.814715
C	-0.426984	3.109142	1.260432
H	-1.276785	2.470515	1.525821
H	0.111110	3.338662	2.185663
H	-0.782554	4.029380	0.799112

TS-[4+2]-7d-product

C	-2.863790	-0.631705	-0.184253
O	-3.025243	-1.787441	0.133026
C	-1.683686	0.199158	-0.038352
H	-1.718927	1.210271	-0.401561
N	-0.522959	-0.263697	0.444323
N	-0.320819	-1.485072	0.768436
O	-3.850605	0.120169	-0.748688
C	-5.074080	-0.577336	-0.939362
H	-5.757304	0.135869	-1.398566
H	-4.928952	-1.442078	-1.591249
H	-5.472942	-0.929155	0.015287
C	1.859675	0.182318	0.058730
C	2.090206	-1.147418	0.416406
C	3.221000	-1.810046	-0.047815
C	4.133451	-1.129978	-0.849174
C	3.903501	0.198637	-1.199056
C	2.762319	0.862672	-0.755544
H	3.385674	-2.850089	0.218231
H	5.022220	-1.638501	-1.208244
H	4.612561	0.722005	-1.831622
H	2.577448	1.887597	-1.050590
C	0.601338	0.741766	0.670289
C	1.020518	-1.774085	1.267059
H	0.705918	0.721678	1.764245
H	1.110154	-2.861113	1.288758
H	1.123046	-1.425138	2.310701
C	0.208370	2.170892	0.269544
O	0.371766	2.571345	-0.857225
C	-0.376059	3.018882	1.370275
H	-1.196019	2.481456	1.856696
H	0.389702	3.210190	2.129839
H	-0.730054	3.963247	0.959386

TS-[4+2]-7e

C	-3.105214	-0.586381	-0.241119
O	-3.250351	-1.787108	-0.225093
C	-1.838950	0.119256	-0.031121
H	-1.753822	1.192955	-0.005023
N	-0.803951	-0.630378	0.224768
N	-0.323702	-1.699335	0.308753
O	-4.103527	0.293468	-0.452044
C	-5.377811	-0.307502	-0.670217
H	-6.071742	0.515739	-0.830415
H	-5.347683	-0.961407	-1.544325
H	-5.675681	-0.898566	0.198473
C	2.024071	0.266257	0.275181
C	2.117314	-1.124928	0.665634
C	3.077276	-1.972300	0.023438
C	3.944442	-1.477482	-0.898850
C	3.870958	-0.099919	-1.272071
C	2.944696	0.736132	-0.730354
H	3.110593	-3.018257	0.313489
H	4.689741	-2.119891	-1.355058
H	4.567607	0.284029	-2.010631
H	2.885578	1.772641	-1.031793
C	0.993928	1.045791	0.785639
C	1.157663	-1.703415	1.507735
H	0.473995	0.758733	1.689695
H	1.231389	-2.767638	1.705405
H	0.669352	-1.136304	2.291600
C	0.643890	2.386666	0.308123
O	1.164483	3.038137	-0.571648
O	-0.433672	2.862086	0.985607
H	-0.614810	3.740238	0.617243

TS-[4+2]-7e-product

C	-2.884256	-0.595055	-0.183589
O	-3.041558	-1.771491	0.047028
C	-1.698194	0.220454	-0.002359
H	-1.743595	1.259365	-0.273076
N	-0.538794	-0.273329	0.445140
N	-0.338814	-1.512096	0.702121
O	-3.879492	0.198604	-0.670308
C	-5.108829	-0.480787	-0.887163
H	-5.799960	0.266444	-1.274845
H	-4.980463	-1.292852	-1.606818
H	-5.487472	-0.904475	0.046204
C	1.851848	0.170188	0.086133
C	2.075770	-1.174399	0.383075
C	3.206072	-1.816861	-0.109682
C	4.121235	-1.102494	-0.877690
C	3.894870	0.240978	-1.168588
C	2.754432	0.885738	-0.696343
H	3.367797	-2.868553	0.107593
H	5.009436	-1.596140	-1.258192
H	4.605481	0.790590	-1.776530
H	2.569591	1.923417	-0.945895
C	0.594049	0.708567	0.715808
C	0.997000	-1.833129	1.196319
H	0.686096	0.680072	1.807703
H	1.079775	-2.920470	1.166779
H	1.094332	-1.534201	2.255544
C	0.239404	2.134105	0.326437
O	0.304871	2.591055	-0.783703
O	-0.152087	2.834507	1.398500
H	-0.372048	3.729546	1.094426

TS-[4+2]-7f

C	3.030894	-0.379057	0.199023
O	3.188108	-1.578949	0.191081
C	1.761896	0.309367	-0.039775
H	1.651412	1.382349	-0.025011
N	0.736693	-0.459813	-0.289896
N	0.281232	-1.541164	-0.345601
O	4.014794	0.511816	0.424478
C	5.291356	-0.072795	0.671293
H	5.971926	0.759831	0.839635
H	5.251757	-0.721450	1.548951
H	5.613077	-0.665683	-0.187607
C	-2.014756	0.477602	-0.367219
C	-2.193939	-0.934886	-0.601390
C	-3.143824	-1.651646	0.198193
C	-3.910078	-1.011367	1.120638
C	-3.740228	0.392103	1.343686
C	-2.819511	1.106868	0.644942
H	-3.252277	-2.718705	0.029358

H	-4.648450	-1.558359	1.696403
H	-4.353158	0.887488	2.089543
H	-2.681401	2.168034	0.826289
C	-0.982254	1.153863	-1.002710
C	-1.312474	-1.630962	-1.434566
H	-0.529675	0.790100	-1.915891
H	-1.416883	-2.708138	-1.507493
H	-0.856919	-1.165274	-2.300614
C	-0.603164	2.473178	-0.630365
N	-0.240229	3.528588	-0.311437

TS-[4+2]-7f-product

C	-2.884597	-0.357494	-0.167249
O	-3.022829	-1.557805	-0.134916
C	-1.703082	0.430502	0.142812
H	-1.753484	1.502522	0.070334
N	-0.546649	-0.123445	0.513907
N	-0.343436	-1.385755	0.615797
O	-3.885605	0.492709	-0.518582
C	-5.109242	-0.153050	-0.847419
H	-5.806155	0.641960	-1.108190
H	-4.971800	-0.834233	-1.690472
H	-5.483813	-0.727340	0.003283
C	1.854083	0.344781	0.187284
C	2.072595	-1.024993	0.308928
C	3.194623	-1.594553	-0.283291
C	4.094687	-0.784154	-0.970633
C	3.866485	0.586040	-1.085520
C	2.735889	1.161236	-0.511549
H	3.361006	-2.664951	-0.207985
H	4.975017	-1.224026	-1.427463
H	4.567066	1.209077	-1.630611
H	2.545392	2.225882	-0.606068
C	0.597631	0.816403	0.878064
C	0.997527	-1.774684	1.044259
H	0.697721	0.687785	1.963916
H	1.070718	-2.849469	0.872732
H	1.113472	-1.618477	2.131857
C	0.306808	2.226011	0.622121
N	0.148927	3.354310	0.434553

TS-[4+2]-7ba

C	-1.465792	-1.111047	0.522245
C	-1.729448	-1.359174	-0.876890
C	-2.157163	-2.683745	-1.239402
C	-2.338042	-3.664220	-0.315989
C	-2.062330	-3.412451	1.063165
C	-1.616770	-2.191912	1.460205
H	-2.342414	-2.878822	-2.291405
H	-2.684153	-4.645579	-0.623277
H	-2.211222	-4.200943	1.793193
H	-1.399435	-1.993102	2.502878
C	-0.920284	0.093614	0.978038
C	-1.347487	-0.480950	-1.890591
H	-1.433884	-0.828277	-2.914758
H	-1.338909	0.591547	-1.772545
C	3.302981	-0.243902	-0.239671
O	3.590654	-0.286414	-1.417471
C	1.965871	-0.245268	0.314758
H	1.755769	-0.260111	1.371851
N	0.963724	-0.348665	-0.541433
N	0.658514	-0.473908	-1.667047
O	4.233057	-0.177144	0.748550
C	5.575839	-0.179582	0.281751
H	6.203055	-0.127543	1.170991
H	5.788300	-1.090817	-0.282334
H	5.762380	0.678649	-0.368429
O	-0.346990	0.079621	2.201947
H	-0.208229	0.989877	2.496363
C	-1.199674	1.452867	0.448404
C	-2.518772	1.803978	0.133812
C	-0.192179	2.421587	0.384006
C	-2.819611	3.102044	-0.257021
H	-3.295372	1.047226	0.191705
C	-0.499896	3.720192	-0.011694
H	0.835941	2.138810	0.597341
C	-1.810567	4.062072	-0.331276
H	-3.843192	3.367897	-0.499100
H	0.289298	4.461282	-0.080089
H	-2.047416	5.074794	-0.640340

TS-[4+2]-7ba-product

C	-1.579337	-0.956229	0.386676
C	-1.704380	-1.320202	-0.951063
C	-2.737371	-2.168993	-1.336578
C	-3.646187	-2.628217	-0.386960
C	-3.512019	-2.259771	0.950486
C	-2.470075	-1.425601	1.346723
H	-2.827015	-2.470670	-2.376175
H	-4.455942	-3.284633	-0.688593
H	-4.215648	-2.630400	1.688414
H	-2.337718	-1.144155	2.385238
C	-0.441579	-0.023884	0.713032
C	-0.651446	-0.780604	-1.874887
H	-0.606732	-1.358766	-2.800125
H	-0.901763	0.256237	-2.155005
C	3.235290	-0.663455	-0.043830
O	3.485741	-0.703286	-1.227989
C	1.949390	-0.514645	0.605961
H	1.902537	-0.402102	1.672511
N	0.792777	-0.538609	-0.064014
N	0.692753	-0.836978	-1.305589
O	4.208333	-0.700396	0.910508
C	5.527439	-0.789915	0.390497
H	6.189708	-0.817134	1.254944
H	5.646475	-1.694413	-0.210774
H	5.756815	0.073451	-0.239227
O	-0.225107	-0.041365	2.082259
H	0.195777	0.791557	2.332228
C	-0.679616	1.412593	0.234198
C	-1.860056	2.033426	0.651481
C	0.259667	2.134046	-0.505262
C	-2.101969	3.364167	0.333117
H	-2.588782	1.462796	1.220484
C	0.006726	3.466028	-0.828414
H	1.172804	1.658852	-0.851588

C	-1.167248	4.083115	-0.409526
H	-3.021985	3.837907	0.659095
H	0.734981	4.019240	-1.411943
H	-1.357332	5.120563	-0.664393

A1

H	1.688182	-2.768128	0.615572
O	-0.573756	-2.516123	-1.157305
P	0.062300	-1.606443	-0.204218
O	-0.863172	-0.667276	0.718591
O	1.002637	-0.530311	-0.959539
O	0.956593	-2.230073	0.956868
C	-2.767185	2.466080	-1.261439
C	-3.484861	1.315877	-0.846067
C	-2.867551	0.266754	-0.210916
C	-1.482323	0.396856	0.064330
C	-0.735698	1.513767	-0.250776
C	-1.374944	2.566669	-0.983663
H	-4.549943	1.254213	-1.055641
C	2.643595	2.593850	1.244345
C	3.436414	1.491868	0.832913
C	2.897975	0.436792	0.140612
C	1.524646	0.516408	-0.211458
C	0.700280	1.562941	0.138181
C	1.254517	2.621378	0.931715
H	4.488991	1.470677	1.104259
C	3.671044	-0.797011	-0.182392
C	3.988203	-1.107002	-1.516106
C	4.036242	-1.672045	0.856947
C	4.657893	-2.297887	-1.791584
C	4.690971	-2.863673	0.533682
C	5.011800	-3.192839	-0.782583
H	4.901894	-2.536858	-2.824400
H	4.962855	-3.547896	1.334606
C	-3.613657	-0.958040	0.200184
C	-4.016743	-1.895372	-0.764046
C	-3.919868	-1.151390	1.556674
C	-4.739626	-3.012923	-0.346545
C	-4.645870	-2.280303	1.930079
C	-5.062642	-3.223541	0.992108
H	-5.052282	-3.742519	-1.090255
H	-4.891912	-2.426064	2.979748
C	-3.471803	-0.155875	2.596513
H	-2.381776	-0.169214	2.701001
H	-3.761680	0.863462	2.324024
H	-3.907891	-0.389050	3.570060
C	-3.652247	-1.730426	-2.218076
H	-4.015545	-0.783115	-2.625921
H	-2.564564	-1.754550	-2.336843
H	-4.077168	-2.542363	-2.811837
C	-5.815373	-4.457362	1.419805
H	-6.408255	-4.268699	2.318195
H	-6.487966	-4.804215	0.631540
H	-5.123545	-5.275389	1.646228
C	3.606544	-0.174911	-2.637018
H	2.529570	-0.219744	-2.825532
H	3.855326	0.861148	-2.390785
H	4.125812	-0.445472	-3.558543
C	3.722418	-1.360220	2.301440
H	3.859983	-2.248706	2.921812
H	4.382192	-0.578520	2.690390
H	2.694406	-1.009519	2.420452
C	5.746609	-4.467631	-1.107914
H	5.371536	-4.914690	-2.031930
H	6.815430	-4.274952	-1.246303
H	5.643022	-5.201147	-0.305208
C	-3.412127	3.511698	-1.974075
C	-0.665696	3.693860	-1.481200
C	0.466710	3.683016	1.454257
C	3.207057	3.649228	2.009405
C	-2.706586	4.597817	-2.418909
C	-1.314658	4.680306	-2.178197
C	1.038410	4.680324	2.201992
C	2.426797	4.674454	2.473571
H	-4.477376	3.424015	-2.167985
H	-3.207308	5.388976	-2.967025
H	-0.754398	5.529740	-2.554948
H	0.403163	3.761992	-1.311937
H	-0.600033	3.693405	1.261888
H	0.418389	5.479333	2.595052
H	2.865359	5.474006	3.061288
H	4.270622	3.617808	2.228594

A2

H	1.031673	-2.348130	0.977935
O	-0.653357	-1.760958	-0.973934
P	-0.006135	-0.803437	-0.079536
O	-0.927345	0.199214	0.785777
O	0.954123	0.233276	-0.862034
O	0.881453	-1.400942	1.099411
C	-2.688375	3.322877	-1.340335
C	-3.446464	2.194996	-0.940768
C	-2.883073	1.149091	-0.249593
C	-1.508220	1.256648	0.092524
C	-0.726863	2.345519	-0.225769
C	-1.308043	3.399697	-1.003469
H	-4.502355	2.158306	-1.195773
C	2.636162	3.338152	1.352131
C	3.413740	2.226552	0.944275
C	2.871555	1.188650	0.225521
C	1.501400	1.284993	-0.137982
C	0.700384	2.354353	0.195929
C	1.258578	3.401427	1.000590
H	4.465802	2.196310	1.215780
C	3.682026	-0.003177	-0.126801
C	4.472985	-1.639966	-1.719746
C	5.310408	-1.672546	0.519683
C	-3.680177	-0.052121	0.101939
C	-5.325830	-1.710524	-0.526209
C	-4.408133	-1.731253	1.680141
C	-3.281197	4.367956	-2.097383
C	-0.553516	4.502022	-1.487548
C	0.483456	4.483184	1.498647
C	3.206083	4.376800	2.135006
C	-2.533235	5.430639	-2.529060
C	-1.151746	5.488474	-2.229026

C	1.059711	5.463698	2.265119
C	2.438634	5.420499	2.578563
H	-4.338521	4.299259	-2.336243
H	-2.992061	6.222051	-3.111986
H	-0.558210	6.319501	-2.595398
H	0.508065	4.552208	-1.273318
H	-0.576460	4.522833	1.274855
H	0.450176	6.278828	2.640836
H	2.879847	6.207360	3.180919
H	4.261780	4.318437	2.383778
C	-6.198805	-2.327944	-1.583575
F	-7.255283	-2.952704	-1.045307
F	-5.530217	-3.233276	-2.308820
F	-6.662526	-1.403448	-2.437507
C	-4.356606	-2.288695	3.075620
F	-4.842870	-3.534997	3.133079
F	-5.073921	-1.541250	3.927910
F	-3.101191	-2.316510	3.544075
C	4.418266	-2.244352	-3.096847
F	4.090846	-1.335124	-4.023142
F	3.508537	-3.225602	-3.162015
F	5.598422	-2.777121	-3.443487
C	6.145988	-2.308453	1.595907
F	7.195770	-2.963693	1.085417
F	5.432672	-3.193554	2.307938
F	6.611741	-1.395724	2.460022
C	3.666570	-0.550204	-1.415206
H	3.036131	-0.117090	-2.183511
C	4.508725	-0.581021	0.839036
H	4.519646	-0.182380	1.848708
C	5.303472	-2.210952	-0.760299
H	5.940224	-3.052104	-1.010474
C	-3.617917	-0.629215	1.373280
H	-2.953045	-0.219844	2.126011
C	-4.540872	-0.609543	-0.847446
H	-4.585646	-0.191744	-1.848117
C	-5.269206	-2.282496	0.739158
H	-5.881019	-3.142523	0.985751

A3

P	-0.002556	-1.340724	-0.000743
O	0.549740	-2.353574	0.896694
O	-0.992577	-0.324382	0.778289
O	0.994015	-0.327960	-0.760111
C	-1.500102	0.744139	0.056038
C	-0.684978	1.821447	-0.215369
C	1.517289	0.717361	-0.011082
C	0.718591	1.803683	0.277642
C	-1.213480	2.886156	-1.017152
C	-2.328738	4.939249	-2.599371
C	-0.418842	3.976984	-1.463249
C	-2.577612	2.833366	-1.421138
C	-3.113802	3.888267	-2.206011
C	-0.963108	4.974094	-2.231535
H	0.631488	4.009358	-1.196141
H	-4.159436	3.836837	-2.495898
H	-0.338440	5.795684	-2.566420
H	-2.745742	5.738693	-3.202679
C	1.263519	2.845385	1.098005
C	2.410993	4.852508	2.715623
C	0.485898	3.940308	1.564218
C	2.627001	2.764690	1.499001
C	3.179498	3.796894	2.302692
C	1.045744	4.915121	2.349564
H	-0.564183	3.993629	1.299351
H	4.224309	3.723929	2.590761
H	0.433956	5.740071	2.699700
H	2.840544	5.634325	3.333069
C	-3.375730	1.717562	-1.059846
H	-4.415558	1.686994	-1.375134
C	-2.858364	0.663751	-0.349086
C	3.407924	1.645049	1.114128
H	4.447941	1.592839	1.425385
C	2.875484	0.611859	0.384240
O	-0.802978	-1.833137	-1.286481
H	-1.313514	-2.638357	-1.124233
C	-3.680987	-0.530697	-0.001757
C	-4.092439	-0.728119	1.331168
C	-4.055645	-1.442778	-1.008268
C	-3.732153	0.170365	2.386858
C	-4.910777	-1.860728	1.659043
C	-4.880604	-2.569872	-0.667684
C	-3.623536	-1.314105	-2.371107
C	-4.146597	-0.048249	3.666884
H	-3.119899	1.035203	2.154624
C	-5.325927	-2.052591	3.014632
C	-5.288845	-2.749465	0.652960
C	-5.260421	-3.492732	-1.694328
H	-2.967930	-0.491970	-2.634914
C	-3.999101	-2.222633	-3.316003
C	-4.955641	-1.177351	3.989733
H	-3.859049	0.642372	4.452796
H	-5.943450	-2.916115	3.245150
H	-5.912458	-3.604189	0.904993
C	-4.838300	-3.326227	-2.977986
H	-5.891326	-4.333395	-1.419492
H	-3.652545	-2.110699	-4.338147
H	-5.273417	-1.332313	5.015501
H	-5.129264	-4.033459	-3.747674
C	3.685299	-0.582788	0.010369
C	4.001423	-1.545506	0.986436
C	4.144029	-0.722560	-1.313141
C	3.513225	-1.471608	2.332067
C	4.830717	-2.662746	0.628781
C	4.960989	-1.849878	-1.660785
C	3.834682	0.227734	-2.339217
C	3.849042	-2.418381	3.252335
H	2.851658	-0.657126	2.605129
C	5.165051	-3.630115	1.628866
C	5.290680	-2.786315	-0.680980
C	5.425886	-1.983722	-3.007034
H	3.223491	1.089059	-2.089969
C	4.295076	0.063037	-3.611905
C	4.695443	-3.511540	2.901031
H	3.459367	-2.350618	4.262643
H	5.799665	-4.464540	1.343585

H	5.916900	-3.635201	-0.946407
C	5.103787	-1.060312	-3.954962
H	6.042766	-2.843490	-3.253549
H	4.045653	0.792595	-4.375566
H	4.951765	-4.252394	3.651350
H	5.460192	-1.172385	-4.973725

A4

H	1.725016	-2.754656	0.614332
O	-0.521817	-2.588102	-1.046038
P	0.101133	-1.588626	-0.179993
O	-0.819991	-0.658119	0.758362
O	0.925993	-0.490217	-1.032156
O	1.097319	-2.101005	0.954345
C	-2.842183	2.459487	-1.134745
C	-3.530616	1.304824	-0.689172
C	-2.883630	0.261605	-0.069967
C	-1.484937	0.400430	0.145454
C	-0.765583	1.523518	-0.209112
C	-1.441731	2.572619	-0.912908
H	-4.603895	1.240718	-0.846852
C	2.671513	2.596442	1.146191
C	3.446027	1.502778	0.684512
C	2.886275	0.462247	-0.016500
C	1.498836	0.549885	-0.313553
C	0.689717	1.583227	0.100805
C	1.272174	2.631151	0.886959
H	4.508817	1.480697	0.911270
C	3.672130	-0.746808	-0.372999
C	4.329025	-2.482788	-1.941449
C	5.235017	-2.478146	0.320993
C	-3.623116	-0.958764	0.340761
C	-5.284418	-2.656527	-0.170844
C	-4.194179	-2.627689	2.007347
C	-3.525305	3.500127	-1.818703
C	-0.762887	3.706643	-1.435935
C	0.505845	3.684464	1.455126
C	3.265282	3.639020	1.905968
C	-2.847933	4.593024	-2.289893
C	-1.448339	4.688117	-2.104802
C	1.106934	4.669054	2.197070
C	2.504470	4.657082	2.416158
H	-4.596833	3.403440	-1.968937
H	-3.377395	5.380410	-2.816031
H	-0.911498	5.543421	-2.501805
H	0.311209	3.784386	-1.309355
H	-0.567318	3.699333	1.302586
H	0.503572	5.462663	2.625419
H	2.966299	5.446692	2.999510
H	4.336472	3.603751	2.083435
C	-6.237638	-3.291566	-1.150939
C	-4.014347	-3.235006	3.375451
C	4.243129	-3.092453	-3.317533
C	6.132911	-3.091872	1.365033
C	3.596669	-1.332304	-1.639001
H	2.955302	-0.891844	-2.396118
C	4.493391	-1.331980	0.599423
H	4.524998	-0.898348	1.595792
C	5.137184	-3.043587	-0.953336
H	5.700974	-3.946842	-1.177703
C	-3.456478	-1.516077	1.614612
H	-2.749625	-1.068535	2.306549
C	-4.536462	-1.536279	-0.540383
H	-4.648911	-1.120905	-1.538952
C	-5.105646	-3.184454	1.104457
H	-5.685122	-4.055327	1.405380
H	-6.931175	-3.968387	-0.646946
H	-5.691433	-3.870194	-1.902606
H	-6.822660	-2.535376	-1.681340
H	-3.534427	-4.216134	3.305118
H	-4.977333	-3.376526	3.874366
H	-3.390637	-2.602332	4.010319
H	6.110126	-4.183435	1.314913
H	7.171336	-2.778623	1.216198
H	5.835958	-2.788639	2.371471
H	3.202525	-3.194543	-3.636464
H	4.751783	-2.462420	-4.053824
H	4.708237	-4.080162	-3.343222

B1

H	1.461269	-2.098062	0.650605
P	0.003730	-0.774198	-0.230769
O	0.737388	-1.529251	0.960443
O	-0.611171	-1.565735	-1.297441
H	-1.252443	4.513999	-2.756139
H	-1.552397	5.184553	-1.154695
H	-3.832873	3.311992	-2.386948
C	-1.189940	4.296408	-1.686600
C	-3.253974	2.683679	-1.716660
H	0.865211	4.778524	-1.003227
C	0.233810	3.916676	-1.237293
C	-1.986876	3.070191	-1.302545
H	0.726986	3.334591	-2.022889
C	-3.772661	1.471363	-1.267315
H	-4.769942	1.161918	-1.565144
H	-0.883705	4.720931	1.052249
H	1.528500	5.162014	1.244420
C	-1.245900	2.265419	-0.431592
C	0.015100	2.995074	-0.004585
C	-0.236916	3.864450	1.261455
C	1.170739	4.254969	1.746835
C	-3.028646	0.607511	-0.456461
C	-1.752407	1.027783	-0.063808
C	1.288715	2.281347	0.409300
C	1.991779	3.053123	1.340119
H	-0.728731	3.242380	2.016872
O	1.086932	0.255522	-0.855437
H	1.213190	4.443693	2.822783
C	1.819866	1.067216	0.002397
C	-3.874276	-1.705311	-0.958553
C	-3.588155	-0.702757	-0.014818
C	3.244873	2.659108	1.788889
O	-0.943830	0.159695	0.677205
C	3.910869	-0.972367	-1.294641
C	3.072729	0.628818	0.454186
H	3.793497	3.266116	2.502661

C	3.780613	1.458433	1.329298
C	-4.427330	-2.905272	-0.514478
H	4.613259	-2.439722	-2.688198
C	-3.861975	-0.912782	1.347383
H	-4.641358	-3.684418	-1.242992
C	4.374393	-2.239417	-1.645980
C	3.605025	-0.705839	0.053229
H	4.758441	1.132348	1.671127
C	-4.705216	-3.137053	0.831254
C	-4.420233	-2.126765	1.746286
C	4.534200	-3.254410	-0.704139
C	3.790452	-1.706064	1.028718
H	-4.639915	-2.284119	2.800163
C	4.240311	-2.966929	0.627528
H	4.369395	-3.741599	1.380310
C	4.992448	-4.627669	-1.121829
H	5.772466	-4.567177	-1.885016
H	5.386788	-5.189846	-0.272482
H	4.162579	-5.201989	-1.546073
C	3.499460	-1.458310	2.491414
H	3.375660	-2.406657	3.019473
H	4.320631	-0.918455	2.973197
H	2.592723	-0.864184	2.625199
C	3.755093	0.086880	-2.355846
H	2.701594	0.214860	-2.621532
H	4.127421	1.053807	-2.006764
H	4.304291	-0.190821	-3.257805
C	-5.272624	-4.457734	1.284733
H	-5.808102	-4.355154	2.231687
H	-5.963118	-4.867601	0.543174
H	-4.475330	-5.193639	1.432868
C	-3.581572	-1.515729	-2.426188
H	-3.668942	-2.468255	-2.953318
H	-4.278927	-0.812044	-2.891773
H	-2.566899	-1.137699	-2.567122
C	-3.576128	0.151452	2.377739
H	-2.499796	0.241905	2.555704
H	-3.938908	1.130562	2.051412
H	-4.056908	-0.094595	3.327008

B2

H	0.939770	-1.413031	0.935903
P	-0.061793	0.172240	-0.095214
O	0.730454	-0.486661	1.118122
O	-0.703446	-0.727930	-1.053107
H	-1.284427	5.410946	-2.838254
H	-1.603047	6.107653	-1.250883
H	-3.826185	4.154012	-2.527634
C	-1.229247	5.213725	-1.764696
C	-3.261175	3.562018	-1.814457
H	0.819894	5.719925	-1.082174
C	0.192120	4.850364	-1.295377
C	-2.020864	3.990916	-1.362732
H	0.690162	4.248757	-2.062608
C	-3.766574	2.348219	-1.356408
H	-4.739199	2.003636	-1.694160
H	-0.892676	5.728252	0.983820
H	1.528559	6.128247	1.152609
C	-1.294617	3.229026	-0.441948
C	-0.030982	3.963451	-0.037041
C	-0.261193	4.864715	1.209711
C	1.156393	5.240399	1.677999
C	-3.039041	1.536875	-0.479326
C	-1.793336	2.002347	-0.036044
C	1.235740	3.238421	0.379625
C	1.954186	4.016131	1.294320
H	-0.758806	4.270520	1.982994
O	0.980454	1.175469	-0.820658
H	1.208792	5.452617	2.748865
C	1.745867	2.010577	-0.011200
C	-4.126677	-0.639379	-1.026482
C	-3.559824	0.208948	-0.071434
C	3.197927	3.606427	1.753738
O	-0.993810	1.176414	0.758560
C	3.479540	-0.224622	-1.262487
C	2.996986	1.565975	0.441341
H	3.756378	4.214325	2.458578
C	3.715590	2.392595	1.311254
C	-4.644306	-1.872401	-0.651883
C	-3.513798	-0.211954	1.259008
C	4.005048	-1.468862	-1.591254
C	3.533628	0.236864	0.057895
H	4.692648	2.063671	1.651981
C	-4.601581	-2.293132	0.673135
C	-4.028859	-1.453174	1.619245
C	4.595342	-2.278252	-0.626055
C	4.118943	-0.579948	1.029197
C	4.646438	-1.820520	0.684724
C	-5.207155	-2.793444	-1.698598
F	-6.196383	-3.551505	-1.202714
F	-4.274980	-3.627681	-2.176366
F	-5.700764	-2.111555	-2.742068
C	-3.919956	-1.891698	3.052632
F	-4.165672	-0.878316	3.895840
F	-2.687695	-2.341303	3.334236
F	-4.778245	-2.879007	3.340208
H	-4.146927	-0.341319	-2.069536
H	-5.015688	-3.252141	0.962786
H	-3.083944	0.432512	2.018610
H	3.030489	0.389756	-2.034775
H	4.139340	-0.256548	2.065312
H	5.004667	-3.246577	-0.890977
C	3.888346	-1.974432	-3.003994
F	2.755022	-2.664489	-3.182500
F	4.903174	-2.793455	-3.314665
F	3.887393	-0.969512	-3.888921
C	5.322668	-2.648965	1.742054
F	6.603976	-2.288051	1.901014
F	5.312413	-3.951636	1.432435
F	4.724474	-2.505757	2.933239

B3

H	1.256358	-1.857564	0.988603
P	-0.019320	-0.490033	-0.103528
O	0.640814	-1.137334	1.189630
O	-0.566666	-1.363871	-1.140854

H	-1.019689	4.755407	-2.894302
H	-1.453588	5.452761	-1.335198
H	-3.610188	3.537286	-2.748256
C	-1.048538	4.555977	-1.819848
C	-3.097924	2.933018	-2.005701
H	0.944301	5.048150	-0.976956
C	0.330815	4.183049	-1.244192
C	-1.877681	3.337903	-1.481868
H	0.884305	3.583110	-1.974501
C	-3.655745	1.732149	-1.572839
H	-4.613115	1.401420	-1.964064
H	-0.939542	5.041004	0.948508
H	1.456685	5.455715	1.312655
C	-1.220447	2.558865	-0.525350
C	0.008211	3.286988	-0.014612
C	-0.322194	4.178992	1.216172
C	1.052766	4.558217	1.796879
C	-2.993480	0.900442	-0.662407
C	-1.758387	1.332655	-0.165375
C	1.239925	2.564879	0.497994
C	1.888125	3.343824	1.461848
H	-0.875097	3.574961	1.943534
O	1.093100	0.510113	-0.730809
H	1.020350	4.758126	2.871137
C	1.784731	1.341647	0.139069
C	3.107009	2.946292	1.994159
O	-1.027978	0.496798	0.678272
C	3.016915	0.915242	0.653074
H	3.611585	3.554483	2.738665
C	3.671994	1.746164	1.568104
H	4.627625	1.419113	1.967166
C	-3.606553	-0.389579	-0.234993
C	-4.032594	-0.549579	1.099902
C	-3.813948	-1.415346	-1.178422
C	-3.856949	0.463644	2.098171
C	-4.692464	-1.763915	1.489454
C	-4.499509	-2.612784	-0.781189
C	-3.344928	-1.328084	-2.530124
C	-4.281070	0.273950	3.379807
H	-3.381400	1.397985	1.820391
C	-5.120918	-1.923922	2.845235
C	-4.919328	-2.758791	0.539536
C	-4.735183	-3.638302	-1.751371
H	-2.761232	-0.463835	-2.824364
C	-3.584540	-2.329361	-3.422535
C	-4.920028	-0.940840	3.765472
H	-4.134858	1.056039	4.117921
H	-5.613229	-2.852734	3.120161
H	-5.433760	-3.670057	0.836695
C	-4.301921	-3.499418	-3.034160
H	-5.265433	-4.532067	-1.434283
H	-3.209373	-2.247893	-4.437426
H	-5.248268	-1.072535	4.791362
H	-4.483824	-4.283089	-3.762567
C	3.618706	-0.386368	0.242307
C	4.042126	-0.574849	-1.090313
C	3.799925	-1.411331	1.196750
C	3.898512	0.435951	-2.095704
C	4.660500	-1.814220	-1.469755
C	4.430950	-2.642485	0.805171
C	3.344732	-1.296005	2.554413
C	4.319289	0.221778	-3.374137
H	3.450167	1.385285	-1.825018
C	5.085664	-1.999760	-2.823415
C	4.844680	-2.813069	-0.514923
C	4.614561	-3.675820	1.778649
H	2.823033	-0.394239	2.854466
C	3.528974	-2.310489	3.447228
C	4.919007	-1.016292	-3.749458
H	4.198693	1.001354	-4.119199
H	5.545435	-2.946832	-3.091208
H	5.318782	-3.747298	-0.806946
C	4.183727	-3.517144	3.060392
H	5.102255	-4.594164	1.463988
H	3.166426	-2.203757	4.464334
H	5.243093	-1.166013	-4.774019
H	4.324056	-4.308515	3.789163

B4

H	1.558789	-1.958674	0.620375
P	0.002449	-0.699131	-0.190388
O	0.845750	-1.397501	0.963269
O	-0.680723	-1.534522	-1.178102
H	-1.410413	4.595633	-2.667116
H	-1.619372	5.253943	-1.045669
H	-3.931298	3.343350	-2.203995
C	-1.283321	4.371885	-1.604597
C	-3.319734	2.728035	-1.550917
H	0.807763	4.862581	-1.048261
C	0.165851	3.998406	-1.242014
C	-2.046675	3.138075	-1.180920
H	0.610978	3.416781	-2.055865
C	-3.800786	1.507999	-1.083893
H	-4.800124	1.178697	-1.351126
H	-0.782039	4.809490	1.120493
H	1.642717	5.226454	1.149712
C	-1.259479	2.346237	-0.338828
C	0.027392	3.077660	0.003098
C	-0.130814	3.946408	1.284388
C	1.310007	4.323092	1.675599
C	-3.018957	0.664490	-0.286240
C	-1.736322	1.107528	0.065583
C	1.323669	2.356950	0.323493
C	2.090000	3.113297	1.215697
H	-0.575330	3.327643	2.070662
O	1.003500	0.343771	-0.927483
H	1.425131	4.511540	2.746260
C	1.812775	1.142429	-0.129858
C	-4.186464	-1.480460	-0.777805
C	-3.535816	-0.659916	0.141807
C	3.356834	2.692243	1.595652
O	-0.881425	0.252620	0.766365
C	3.409486	-1.147146	-1.451888
C	3.080032	0.676837	0.254386
H	3.953972	3.283309	2.283314
C	3.844165	1.484145	1.103855

C	-4.715696	-2.713995	-0.393296
C	-3.410584	-1.087191	1.469102
C	3.818089	-2.438029	-1.798903
C	3.559531	-0.671158	-0.146957
H	4.831636	1.138389	1.394400
C	-4.586134	-3.110292	0.935048
C	-3.932145	-2.310565	1.877146
C	4.386967	-3.248648	-0.818423
C	4.134386	-1.511272	0.818582
C	4.557390	-2.798995	0.494681
C	-5.383949	-3.603664	-1.410431
C	-3.788046	-2.778844	3.303056
H	-4.255155	-1.165856	-1.816243
H	-4.998633	-4.068058	1.247118
H	-2.905073	-0.450204	2.189163
H	2.955249	-0.509653	-2.204140
H	4.221498	-1.158212	1.843127
H	4.698886	-4.258071	-1.078112
C	3.620894	-2.934928	-3.208015
C	5.194798	-3.688612	1.531289
H	-3.453399	-1.968169	3.953792
H	-4.736323	-3.160595	3.691811
H	-5.930284	-4.417047	-0.927587
H	-6.087788	-3.039411	-2.028519
H	-4.642495	-4.048349	-2.081580
H	-3.054691	-3.588399	3.374385
H	2.557531	-2.956658	-3.463800
H	4.117634	-2.277293	-3.927048
H	4.022922	-3.942273	-3.333793
H	4.863180	-4.724221	1.421589
H	6.284863	-3.680620	1.430315
H	4.952058	-3.356043	2.542881

TS-[4+2]-A1-R-1

H	-0.122324	2.535997	-1.027990
O	-0.531983	-0.031843	0.753699
P	0.576757	0.287200	-0.206752
O	1.028441	-1.032573	-1.034960
O	1.894997	0.590987	0.692005
O	0.384831	1.356358	-1.260585
C	2.773851	-4.072347	1.214195
C	1.425899	-4.163123	0.787353
C	0.817540	-3.161350	0.069674
C	1.614178	-2.040298	-0.283975
C	2.938372	-1.899413	0.077865
C	3.539420	-2.918642	0.885007
H	0.848868	-5.044968	1.055295
C	5.537966	0.566381	-1.324668
C	4.946770	1.781450	-0.895342
C	3.738340	1.808784	-0.243470
C	3.112347	0.564445	0.029604
C	3.661705	-0.655989	-0.306584
C	4.887149	-0.668648	-1.047601
H	5.458636	2.718030	-1.103170
C	3.116296	3.097416	0.181070
C	3.081847	3.434952	1.546203
C	2.609043	3.982770	-0.781616
C	2.561502	4.670554	1.923069
C	2.096714	5.212026	-0.360823
C	2.075716	5.578949	0.981164
H	2.544656	4.935457	2.978431
H	1.697292	5.895205	-1.107873
C	-0.623100	-3.274491	-0.307343
C	-1.607799	-3.277148	0.699525
C	-0.986651	-3.463218	-1.650517
C	-2.933129	-3.521900	0.342779
C	-2.330647	-3.672365	-1.965142
C	-3.317064	-3.720076	-0.982759
H	-3.687955	-3.539720	1.126089
H	-2.609440	-3.819821	-3.006846
C	0.051959	-3.465028	-2.743102
H	0.455444	-2.460115	-2.897867
H	0.891232	-4.118957	-2.487538
H	-0.378221	-3.811545	-3.685110
C	-1.271827	-2.970948	2.139790
H	-0.731273	-3.791006	2.622715
H	-0.645941	-2.075572	2.200995
H	-2.188845	-2.785704	2.707596
C	-4.760237	-3.980197	-1.332635
H	-5.420623	-3.261203	-0.836944
H	-4.929429	-3.893055	-2.408503
H	-5.065723	-4.984061	-1.019924
C	3.607629	2.482044	2.589092
H	2.969792	1.595490	2.659882
H	4.616411	2.140087	2.338800
H	3.640038	2.960383	3.570248
C	2.586361	3.621973	-2.246489
H	1.963546	4.327777	-2.800746
H	3.589768	3.641979	-2.683448
H	2.181883	2.616706	-2.391621
C	1.563636	6.931203	1.411544
H	0.965751	7.398611	0.623961
H	0.948484	6.857764	2.313549
H	2.392501	7.609181	1.639578
C	3.362587	-5.100263	1.997954
C	4.857980	-2.812479	1.406956
C	5.464722	-1.865868	-1.551931
C	6.760491	0.562196	-2.047473
C	4.645182	-4.981752	2.462540
C	5.393906	-3.816645	2.171534
C	6.639885	-1.835543	-2.257670
C	7.304461	-0.610017	-2.500864
H	2.766758	-5.978776	2.229410
H	5.085267	-5.770212	3.064114
H	6.400802	-3.714501	2.563049
H	5.437943	-1.920113	1.200514
H	4.957580	-2.808731	-1.379115
H	7.061967	-2.759515	-2.639256
H	8.236327	-0.602455	-3.056544
H	7.249394	1.512808	-2.241554
N	-3.845666	2.278507	-0.276221
C	-2.577848	2.332472	-0.716089
N	-4.800962	2.763896	0.157607
H	-2.157411	1.448526	-1.169185
C	-1.796891	3.470105	-0.508355
O	-0.552842	3.528884	-0.798287

O	-2.361879	4.534343	0.032684
C	-1.484771	5.620817	0.356170
H	-2.110333	6.354433	0.860241
H	-0.677351	5.274094	1.004147
H	-1.050982	6.040571	-0.553908
C	-4.855735	-0.214060	-0.956069
C	-6.091700	0.474560	-0.650205
C	-7.064955	0.545891	-1.711386
C	-6.851939	-0.002021	-2.937052
C	-5.616482	-0.653162	-3.233574
C	-4.647790	-0.729473	-2.281963
H	-7.997695	1.059083	-1.496794
H	-7.622193	0.060228	-3.699425
H	-5.456193	-1.088844	-4.214020
H	-3.705698	-1.229845	-2.480744
C	-3.770698	-0.322590	-0.053815
C	-6.297731	1.263552	0.478252
H	-7.207351	1.853459	0.523608
H	-5.806350	1.094813	1.423503
O	-2.591083	-0.557229	-0.557274
H	-1.798012	-0.490864	0.098560
C	-3.906828	-0.371234	1.425644
C	-4.877267	-1.219529	1.975677
C	-3.040671	0.329551	2.267570
C	-4.974116	-1.369469	3.352083
H	-5.551636	-1.753028	1.311718
C	-3.152866	0.186460	3.648531
H	-2.277888	0.973949	1.844182
C	-4.111330	-0.662982	4.191517
H	-5.721087	-2.035058	3.771794
H	-2.481148	0.736806	4.298480
H	-4.188356	-0.777697	5.267919

TS-[4+2]-A1-R-2

P	-0.576634	0.258936	-1.190311
O	0.257212	1.402833	-0.748323
O	-0.757185	-0.732538	0.089240
O	-2.107186	0.644248	-1.524412
C	-1.731208	-1.717316	0.018405
C	-3.055865	-1.354447	0.145864
C	-2.882391	1.041848	-0.442280
C	-3.390409	0.073499	0.396932
C	-4.054378	-2.371662	0.004848
C	-5.959074	-4.432190	-0.277205
C	-5.445353	-2.080189	-0.020300
C	-3.641665	-3.724551	-0.150710
C	-4.624789	-4.741433	-0.277615
C	-6.369998	-3.083404	-0.157755
H	-5.769216	-1.048285	0.060236
H	-4.293359	-5.770388	-0.385710
H	-7.427300	-2.840601	-0.181766
H	-6.702660	-5.215543	-0.380252
C	-4.151070	0.494799	1.537160
C	-5.642921	1.409510	3.752145
C	-4.610952	-0.410415	2.532837
C	-4.423669	1.881660	1.707600
C	-5.189384	2.309271	2.824552
C	-5.336739	0.035845	3.607609
H	-4.375722	-1.464479	2.438567
H	-5.397865	3.370058	2.931788
H	-5.675685	-0.671346	4.357654
H	-6.224094	1.746644	4.604073
C	-2.258542	-4.034665	-0.191923
H	-1.955035	-5.074379	-0.287944
C	-1.293609	-3.059235	-0.131671
C	-3.894400	2.819896	0.785349
H	-4.094869	3.877758	0.936465
C	-3.106655	2.432640	-0.270000
O	-0.177060	-0.567994	-2.418567
H	0.849105	-0.861667	-2.673052
C	0.158127	-3.398921	-0.190871
C	0.950886	-3.273229	0.963714
C	0.711622	-3.907141	-1.375885
C	2.291788	-3.648648	0.913676
C	2.044918	-4.319005	-1.367191
C	2.856692	-4.185550	-0.243090
C	-2.472538	3.423844	-1.185299
C	-1.402132	4.204607	-0.724144
C	-2.947266	3.567121	-2.499365
C	-0.827398	5.133047	-1.593242
C	-2.350197	4.510162	-3.331678
C	-1.289723	5.304502	-2.895144
N	3.805682	-0.656218	-0.051303
C	2.883783	-0.554473	-1.008897
N	4.678465	-1.256283	0.434380
H	2.217651	0.291124	-0.988699
C	2.917065	-1.372401	-2.164068
O	2.025806	-1.355441	-3.044477
O	4.000071	-2.131953	-2.316546
C	4.102865	-2.857327	-3.540352
H	4.856373	-3.624764	-3.366317
H	3.145303	-3.303216	-3.808359
H	4.422498	-2.186236	-4.341188
C	4.735590	1.819745	0.903619
C	5.646583	0.933200	1.590274
C	7.053340	1.173546	1.409204
C	7.520063	2.156876	0.593938
C	6.611712	2.977256	-0.139936
C	5.270271	2.793650	-0.006344
H	7.744739	0.526016	1.940045
H	8.588962	2.313057	0.488164
H	6.993801	3.753490	-0.793995
H	4.568683	3.416577	-0.548233
C	3.333355	1.713533	0.999204
C	5.250825	-0.273005	2.167357
H	6.022221	-0.926365	2.561318
H	4.254851	-0.441111	2.551589
O	2.637898	2.251822	0.011839
H	1.667110	2.077084	0.030275
C	2.588996	1.341636	2.228876
C	3.070017	1.794796	3.466230
C	1.347197	0.704659	2.163826
C	2.316532	1.611719	4.616835
H	4.030318	2.298395	3.511218
C	0.587686	0.542595	3.319900
H	0.968107	0.335196	1.217607

C	1.068511	0.992421	4.545067
H	2.693190	1.971073	5.568762
H	-0.387912	0.071788	3.253131
H	0.471135	0.868220	5.442388
H	2.906221	-3.539009	1.804911
H	2.463772	-4.753483	-2.272208
H	-2.718583	4.624323	-4.349083
H	0.010815	5.731528	-1.243164
C	-4.079904	2.710416	-3.004529
H	-3.761859	1.667187	-3.099593
H	-4.931544	2.732608	-2.317897
H	-4.418783	3.053174	-3.984358
C	-0.674561	6.332226	-3.810167
H	-0.572439	5.944457	-4.827119
H	-1.297215	7.231531	-3.863249
H	0.314873	6.633241	-3.458560
C	-0.858209	4.047915	0.674997
H	0.125901	4.516779	0.754499
H	-1.512854	4.516745	1.417302
H	-0.758140	2.992606	0.941907
C	4.309775	-4.577070	-0.286604
H	4.492340	-5.326904	-1.061536
H	4.928496	-3.700208	-0.504441
H	4.639047	-4.987337	0.671555
C	-0.097200	-3.999446	-2.646364
H	0.554766	-4.210681	-3.497124
H	-0.852789	-4.789456	-2.594266
H	-0.618076	-3.057818	-2.840941
C	0.347350	-2.799198	2.259835
H	-0.162875	-1.842932	2.131588
H	-0.392923	-3.517938	2.627767
H	1.115473	-2.671962	3.025982

TS-[4+2]-A1-S-1

P	0.564041	0.264623	-0.158542
O	-0.576424	0.066645	0.795224
O	1.884654	0.572080	0.734951
O	0.980111	-1.114670	-0.904735
C	3.099638	0.524190	0.066504
C	3.641260	-0.704454	-0.251610
C	1.598344	-2.096310	-0.149593
C	2.931172	-1.940836	0.172617
C	4.855432	-0.737438	-1.012307
C	7.250525	-0.717635	-2.504638
C	5.415304	-1.945562	-1.510879
C	5.511505	0.487539	-1.317367
C	6.722917	0.464611	-2.058257
C	6.579131	-1.933942	-2.235801
H	4.903697	-2.882216	-1.319748
H	7.215799	1.408871	-2.272232
H	6.986630	-2.866282	-2.612869
H	8.173692	-0.725135	-3.074663
C	3.565748	-2.949837	0.967927
C	4.744284	-5.000827	2.509329
C	4.892210	-2.820904	1.464451
C	2.830472	-4.120188	1.305878
C	3.455198	-5.141820	2.069884
C	5.463098	-3.818614	2.211894
H	5.450225	-1.915875	1.253146
H	2.881240	-6.033105	2.307763
H	6.474917	-3.697983	2.585001
H	5.212134	-5.784043	3.096616
C	4.935282	1.712111	-0.896501
H	5.451997	2.641928	-1.121779
C	3.734140	1.758377	-0.232599
C	1.474502	-4.230686	0.911523
H	0.919004	-5.123950	1.187063
C	0.830347	-3.230483	0.223937
O	0.435834	1.260782	-1.292776
H	-0.008762	2.462676	-1.263585
C	3.135669	3.062004	0.175932
C	3.107539	3.419156	1.537680
C	2.660906	3.948649	-0.800004
C	2.621390	4.672581	1.895759
C	2.186313	5.199804	-0.397004
C	2.163856	5.582263	0.939843
C	-0.625455	-3.338667	-0.084290
C	-1.551621	-3.333362	0.973225
C	-1.062416	-3.513548	-1.408511
C	-2.903572	-3.536516	0.688648
C	-2.420826	-3.706751	-1.648475
C	-3.354220	-3.741711	-0.613576
N	-3.657534	2.488943	-0.201698
C	-2.442063	2.381349	-0.750562
N	-4.542885	3.089306	0.227859
H	-2.057540	1.402905	-0.984181
C	-1.649680	3.525758	-0.887910
O	-0.428470	3.500341	-1.253723
O	-2.201428	4.692338	-0.607126
C	-1.332441	5.830782	-0.617245
H	-1.948415	6.664114	-0.286060
H	-0.491223	5.666763	0.058577
H	-0.953073	6.007516	-1.625808
C	-4.169650	0.119272	1.313659
C	-5.305589	0.937153	1.702221
C	-5.480936	1.174637	3.114817
C	-4.608321	0.711587	4.047085
C	-3.454947	-0.030065	3.649788
C	-3.241038	-0.290604	2.332754
H	-6.343936	1.761285	3.415523
H	-4.782858	0.911285	5.099765
H	-2.758638	-0.397937	4.395615
H	-2.377608	-0.873823	2.038861
C	-3.878093	-0.289420	-0.009954
C	-6.075780	1.683109	0.821618
H	-6.843603	2.331948	1.228953
H	-6.156300	1.460113	-0.231834
O	-2.669256	-0.612381	-0.386477
H	-1.875416	-0.338543	0.217515
C	-4.874216	-0.589338	-1.068585
C	-6.174588	-1.003140	-0.752525
C	-4.462474	-0.585680	-2.405294
C	-7.058243	-1.365135	-1.758974
H	-6.484110	-1.040080	0.287024
C	-5.350827	-0.949380	-3.412923
H	-3.442020	-0.304403	-2.641346

C	-6.650332	-1.333692	-3.093216
H	-8.062209	-1.687571	-1.503692
H	-5.025834	-0.934755	-4.447948
H	-7.342360	-1.618487	-3.879271
H	2.606816	4.951787	2.947385
H	1.819983	5.888060	-1.156516
H	-2.759761	-3.851506	-2.672596
H	-3.620387	-3.530654	1.508041
C	1.659462	6.940988	1.358189
H	1.331662	7.525507	0.494269
H	0.816518	6.855610	2.051848
H	2.441506	7.510530	1.869333
C	2.637294	3.575564	-2.262104
H	1.982163	4.254039	-2.813316
H	3.634956	3.629753	-2.709767
H	2.269316	2.555206	-2.398342
C	3.606504	2.467692	2.594776
H	2.939689	1.604552	2.683524
H	4.602574	2.088651	2.346859
H	3.658275	2.961884	3.567111
C	-0.082806	-3.524141	-2.554093
H	0.310044	-2.520298	-2.739420
H	0.770621	-4.173796	-2.337327
H	-0.561701	-3.881032	-3.468393
C	-1.112307	-3.097002	2.399918
H	-1.982527	-2.961771	3.047460
H	-0.527996	-3.933013	2.794576
H	-0.484527	-2.201567	2.467741
C	-4.801700	-4.036624	-0.907841
H	-4.949590	-5.109041	-1.075666
H	-5.446148	-3.736388	-0.078038
H	-5.136563	-3.509087	-1.806188

TS-[4+2]-A1-S-2

P	-0.647048	0.266512	-1.093631
O	0.304225	1.301996	-0.603983
O	-0.861983	-0.779113	0.126221
O	-2.144811	0.791015	-1.355637
C	-1.860789	-1.727835	-0.039724
C	-3.177573	-1.340509	0.092854
C	-2.891244	1.097942	-0.222224
C	-3.469016	0.066714	0.487546
C	-4.192081	-2.315849	-0.173498
C	-6.132083	-4.288380	-0.715778
C	-5.575194	-1.990822	-0.196576
C	-3.802583	-3.654290	-0.465008
C	-4.804787	-4.627152	-0.721145
C	-6.517751	-2.951250	-0.460448
H	-5.877401	-0.965732	-0.010671
H	-4.493482	-5.646397	-0.932038
H	-7.568938	-2.682835	-0.479821
H	-6.889088	-5.038796	-0.918191
C	-4.227396	0.397644	1.659274
C	-5.714341	1.137433	3.942864
C	-4.774446	-0.587343	2.526779
C	-4.405737	1.769321	1.999155
C	-5.171122	2.109578	3.145916
C	-5.499195	-0.226033	3.633528
H	-4.606568	-1.635885	2.309769
H	-5.305985	3.161229	3.382680
H	-5.905983	-0.994323	4.282932
H	-6.294892	1.407691	4.818699
C	-2.425249	-3.995068	-0.512601
H	-2.144773	-5.025210	-0.717685
C	-1.443576	-3.054660	-0.323853
C	-3.774356	2.775500	1.223894
H	-3.882470	3.815615	1.521344
C	-2.996132	2.466969	0.136610
O	-0.341368	-0.502349	-2.385534
H	0.663572	-0.797409	-2.685713
C	0.013634	-3.370122	-0.386967
C	0.783421	-3.311254	0.788320
C	0.616264	-3.703284	-1.612244
C	2.151570	-3.571477	0.717546
C	1.987132	-3.960304	-1.636838
C	2.774571	-3.877879	-0.489866
C	-2.224905	3.502820	-0.611220
C	-1.061041	4.041798	-0.043349
C	-2.650348	3.909173	-1.887037
C	-0.345983	5.000724	-0.763661
C	-1.912350	4.872165	-2.569406
C	-0.756745	5.431372	-2.021315
N	4.021498	-0.429477	-0.502464
C	2.873218	-0.726214	-1.113536
N	5.177124	-0.322215	-0.530964
H	1.970232	-0.754037	-0.523184
C	2.869131	-1.061725	-2.487553
O	1.837976	-1.197000	-3.183893
O	4.069724	-1.224228	-3.045800
C	4.072189	-1.513166	-4.444062
H	5.121186	-1.585479	-4.723906
H	3.576593	-0.715467	-5.000015
H	3.554997	-2.454914	-4.638247
C	3.711100	-0.122180	2.280764
C	5.155319	-0.143185	2.187263
C	5.838680	-1.158925	2.950066
C	5.180738	-2.039246	3.748870
C	3.754774	-2.003638	3.839727
C	3.053520	-1.097387	3.108139
H	6.921439	-1.192949	2.873588
H	5.737509	-2.772743	4.323437
H	3.236573	-2.697403	4.494050
H	1.972141	-1.059378	3.163541
C	2.889214	0.733005	1.520306
C	5.889266	0.575357	1.251673
H	6.952885	0.375306	1.176752
H	5.560244	1.513222	0.831674
O	1.625831	0.382058	1.382773
H	1.112472	0.934060	0.713076
C	3.246833	2.113763	1.093358
C	3.797030	2.972197	2.055094
C	2.925452	2.608952	-0.173781
C	4.023887	4.308099	1.750640
H	4.040907	2.580441	3.037965
C	3.164797	3.947128	-0.474827
H	2.482109	1.954933	-0.915915

C	3.708235	4.797970	0.483455
H	4.441997	4.968640	2.502927
H	2.911945	4.323146	-1.460926
H	3.885414	5.842234	0.245970
H	2.459014	-4.188229	-2.591662
H	2.748769	-3.501143	1.623498
C	-0.177025	-3.750268	-2.894941
H	0.496827	-3.744791	-3.754412
H	-0.795830	-4.651826	-2.952768
H	-0.842026	-2.886827	-2.977662
C	0.157266	-2.948837	2.111075
H	-0.026939	-1.869544	2.162288
H	-0.800431	-3.456773	2.255701
H	0.820707	-3.222569	2.935270
C	4.270752	-4.035907	-0.574852
H	4.550822	-5.009003	-0.989859
H	4.694902	-3.263455	-1.226928
H	4.735189	-3.932497	0.408843
H	-2.242458	5.188787	-3.556725
H	0.563753	5.408910	-0.327844
C	-3.878896	3.299300	-2.511825
H	-3.709113	2.242170	-2.741205
H	-4.737138	3.353400	-1.835351
H	-4.138964	3.811496	-3.440502
C	0.018245	6.481931	-2.775236
H	0.140309	6.205551	-3.826156
H	-0.499285	7.446486	-2.749196
H	1.011235	6.626846	-2.342161
C	-0.554695	3.603219	1.308928
H	0.513196	3.824292	1.400928
H	-1.079374	4.120816	2.119610
H	-0.694798	2.530149	1.457828

TS-[4+2]-A2-R-1

P	-0.726029	0.455835	-0.131398
O	0.439530	0.290852	0.797192
O	-2.001306	0.769909	0.833970
O	-0.636140	1.856130	-0.961721
C	-3.118656	1.329273	0.249099
C	-3.106580	2.679153	-0.033133
C	-0.663547	2.998024	-0.179636
C	-1.877028	3.455398	0.290687
C	-4.251177	3.257284	-0.669145
C	-6.557816	4.321348	-1.895088
C	-4.286349	4.609211	-1.105220
C	-5.392316	2.439623	-0.903288
C	-6.544954	3.007812	-1.508428
C	-5.408993	5.124552	-1.700711
H	-3.408206	5.230464	-0.968126
H	-7.411798	2.373242	-1.669731
H	-5.415411	6.157730	-2.031996
H	-7.439996	4.745930	-2.362320
C	-1.891039	4.598466	1.155420
C	-1.827547	6.855090	2.851014
C	-3.075335	5.077331	1.778951
C	-0.663170	5.257722	1.445424
C	-0.664661	6.399610	2.289475
C	-3.042458	6.174971	2.600551
H	-4.011334	4.558536	1.606586
H	0.280387	6.896736	2.488921
H	-3.957447	6.521797	3.069430
H	-1.819314	7.725481	3.498480
C	-5.351179	1.064714	-0.566301
H	-6.234202	0.459767	-0.754813
C	-4.228513	0.481757	-0.026045
C	0.548804	4.744843	0.920704
H	1.480033	5.252226	1.159830
C	0.575346	3.620064	0.133047
O	-1.065780	-0.595441	-1.152783
H	-1.228695	-1.943989	-1.050850
C	-4.158118	-0.983468	0.203301
C	-3.477067	-1.542589	1.289618
C	-4.778253	-1.849326	-0.707720
C	-3.423945	-2.923353	1.450010
C	-4.753105	-3.221992	-0.507948
C	-4.083869	-3.775480	0.577791
H	-4.068514	-4.849572	0.727534
C	1.863219	3.055918	-0.343954
C	2.905281	2.847756	0.566692
C	2.072638	2.747613	-1.689146
C	4.133450	2.369345	0.128084
C	3.313395	2.280797	-2.113932
C	4.355250	2.093282	-1.216921
H	5.309343	1.701918	-1.551985
H	-5.267818	-1.448616	-1.588491
H	-2.976362	-0.906046	2.008180
H	1.267161	2.874892	-2.405684
H	2.739891	3.030918	1.623474
C	3.487827	1.940936	-3.567551
F	2.651228	0.959547	-3.936917
F	4.733872	1.523345	-3.840975
F	3.229404	2.991584	-4.357595
C	5.256860	2.154879	1.101204
F	6.097066	3.200066	1.130977
F	5.990297	1.078774	0.764037
F	4.813194	1.967486	2.350192
C	-5.378183	-4.158927	-1.500868
F	-6.140152	-5.078897	-0.891616
F	-4.437507	-4.834154	-2.186428
F	-6.141654	-3.520484	-2.393638
C	-2.529775	-3.484229	2.516117
F	-2.828973	-4.760077	2.806696
F	-2.577970	-2.780801	3.650661
F	-1.242058	-3.475025	2.106638
N	2.145154	-3.511181	-0.330283
C	1.028491	-2.886537	-0.753758
N	2.701379	-4.457450	0.023968
H	1.091462	-1.844142	-1.022109
C	-0.183839	-3.572940	-0.743911
O	-1.317992	-3.012246	-0.969157
O	-0.153128	-4.864659	-0.490326
C	-1.387176	-5.579982	-0.373404
H	-1.141522	-6.617429	-0.592401
H	-1.751165	-5.492800	0.652066
H	-2.129452	-5.200761	-1.075865
C	4.306926	-1.828519	-0.638542

C	5.027770	-3.046000	-0.328890
C	5.986398	-3.497100	-1.310339
C	6.193572	-2.844849	-2.483251
C	5.417195	-1.690647	-2.813777
C	4.495493	-1.225608	-1.931698
H	6.549548	-4.395787	-1.076774
H	6.936525	-3.211507	-3.184497
H	5.557849	-1.188871	-3.764989
H	3.874550	-0.375968	-2.179857
C	3.337811	-1.242204	0.202776
C	4.696276	-3.914960	0.701908
H	5.208158	-4.870929	0.745122
H	4.196267	-3.611092	1.608190
O	2.530804	-0.359692	-0.330376
H	1.741028	-0.040892	0.264286
C	3.264878	-1.419024	1.678892
C	4.416282	-1.186492	2.440047
C	2.064771	-1.749086	2.315587
C	4.367587	-1.300559	3.823697
H	5.340835	-0.919004	1.939639
C	2.028727	-1.881318	3.699764
H	1.164048	-1.907188	1.732697
C	3.176889	-1.658075	4.454552
H	5.260406	-1.111286	4.410261
H	1.096670	-2.156355	4.182589
H	3.144204	-1.756645	5.534843

TS-[4+2]-A2-R-2

P	-0.591286	0.662920	0.507658
O	-0.612253	-0.694760	-0.118654
O	-0.198625	1.740929	-0.655489
O	-2.091910	1.166060	0.884404
C	-0.384221	3.064059	-0.298017
C	-1.652480	3.601123	-0.343046
C	-2.935687	1.506014	-0.156453
C	-2.771466	2.723917	-0.783056
C	-1.840215	4.946512	0.113016
C	-2.129563	7.596178	1.040041
C	-3.123104	5.551285	0.205984
C	-0.706967	5.696541	0.538672
C	-0.882727	7.032008	0.987245
C	-3.261266	6.839686	0.655064
H	-3.998808	4.977097	-0.075293
H	-0.006026	7.593242	1.297878
H	-4.249802	7.281932	0.722255
H	-2.254921	8.615883	1.388393
C	-3.626631	3.051084	-1.884713
C	-5.360034	3.623065	-4.036842
C	-3.460857	4.229748	-2.661450
C	-4.662095	2.143954	-2.245962
C	-5.528329	2.465926	-3.324229
C	-4.305308	4.506386	-3.706077
H	-2.649913	4.909156	-2.424036
H	-6.320489	1.767430	-3.578401
H	-4.159697	5.409408	-4.289733
H	-6.022856	3.859086	-4.862546
C	0.576280	5.091784	0.540914
H	1.431923	5.670748	0.878851
C	0.751126	3.791242	0.142885
C	-4.792105	0.917355	-1.549843
H	-5.584736	0.232388	-1.840148
C	-3.938712	0.571095	-0.530003
O	0.233357	0.938383	1.735973
H	1.260120	0.432931	2.363469
C	2.079387	3.124280	0.191859
C	2.727931	2.743297	-0.981750
C	2.686845	2.864460	1.423975
C	3.982163	2.140208	-0.921869
C	3.925998	2.238995	1.467944
C	4.588692	1.877375	0.298579
C	-4.031580	-0.755126	0.127333
C	-4.182446	-1.898771	-0.656907
C	-3.986413	-0.894768	1.519459
C	-4.300683	-3.152111	-0.062248
C	-4.101974	-2.151160	2.098596
C	-4.264142	-3.292297	1.317956
N	2.930877	-2.669357	0.857457
C	2.456717	-1.452742	1.179095
N	3.523113	-3.624136	1.097912
H	1.831466	-0.937832	0.468738
C	2.650287	-0.992706	2.484537
O	2.094448	0.055253	2.963451
O	3.437341	-1.694993	3.273213
C	3.506741	-1.292320	4.648622
H	4.221856	-1.972662	5.105139
H	2.525599	-1.392875	5.115453
H	3.846717	-0.260492	4.721777
C	2.873260	-2.761742	-2.565236
C	2.996065	-3.808659	-3.485927
C	4.052110	-3.819203	-4.386135
C	4.991979	-2.788436	-4.371537
C	4.865957	-1.739426	-3.465786
C	3.800872	-1.719000	-2.570081
H	4.140826	-4.627720	-5.104133
H	5.818848	-2.800008	-5.074389
H	5.586881	-0.930757	-3.459650
H	3.681761	-0.901001	-1.866014
C	1.696428	-2.699009	-1.663760
O	1.149992	-1.508212	-1.687478
H	0.388801	-1.298903	-1.034487
C	1.136053	-3.807476	-1.000037
C	1.907277	-4.986638	-0.626853
C	-0.267001	-3.765217	-0.665945
C	1.173564	-6.079603	-0.031506
C	-0.893927	-4.825833	-0.095248
H	-0.847045	-2.887991	-0.931353
C	-0.156765	-6.009625	0.221599
H	1.735868	-6.972067	0.226554
H	-1.958506	-4.792065	0.101119
H	-0.670529	-6.855186	0.668022
H	2.168822	3.117575	2.342970
H	2.254946	2.917697	-1.943244
H	5.557523	1.391197	0.340169
H	-3.865924	-0.020542	2.148937
H	-4.183382	-1.814092	-1.739618
H	-4.357280	-4.268932	1.778908

C	-3.999939	-2.289686	3.592519
F	-2.730124	-2.458851	3.985615
F	-4.693018	-3.349377	4.035696
F	-4.467528	-1.204187	4.223038
C	-4.498380	-4.348770	-0.948892
F	-5.732908	-4.379513	-1.471079
F	-4.318574	-5.499382	-0.281738
F	-3.639572	-4.339230	-1.978197
C	4.603661	1.942630	2.774431
F	5.728110	2.659546	2.917297
F	4.970113	0.646469	2.841941
F	3.827271	2.196252	3.832085
C	4.713415	1.840995	-2.199199
F	5.672693	0.915729	-2.010483
F	5.313307	2.933116	-2.691274
F	3.892171	1.380483	-3.150383
C	3.288812	-5.046920	-0.583393
H	3.752521	-5.945198	-0.190088
H	3.939927	-4.373966	-1.120117
H	2.260977	-4.607338	-3.483797

TS-[4+2]-A2-S-1

P	0.764022	0.383393	-0.022751
O	-0.300041	-0.030750	-0.993552
O	2.039122	0.840268	-0.925092
O	0.400715	1.780308	0.734820
C	2.998582	1.597800	-0.279504
C	2.764366	2.941895	-0.087072
C	0.300782	2.901724	-0.068377
C	1.455442	3.505230	-0.520925
C	3.742969	3.713260	0.620757
C	5.724007	5.157996	2.019136
C	3.549362	5.080985	0.955212
C	4.942990	3.077005	1.048255
C	5.927680	3.833553	1.737057
C	4.514290	5.781513	1.632842
H	2.622187	5.567927	0.675261
H	6.841954	3.334422	2.045346
H	4.345551	6.824135	1.881386
H	6.479529	5.727459	2.549929
C	1.340943	4.611342	-1.423153
C	1.031469	6.779853	-3.199584
C	2.470601	5.220427	-2.033016
C	0.045411	5.097329	-1.757103
C	-0.077719	6.199292	-2.644201
C	2.318007	6.275016	-2.896338
H	3.460148	4.834207	-1.814200
H	-1.072843	6.565505	-2.880120
H	3.192108	6.723920	-3.356519
H	0.927601	7.618009	-3.880435
C	5.122755	1.690294	0.818614
H	6.036991	1.215502	1.165899
C	4.167283	0.935893	0.182480
C	-1.101927	4.466961	-1.213731
H	-2.083733	4.864448	-1.458429
C	-1.001663	3.373498	-0.388173
O	1.193930	-0.541764	1.088038
H	1.456582	-1.836920	0.993544
C	4.324900	-0.531766	0.028392
C	4.123073	-1.167884	-1.201346
C	4.699268	-1.300634	1.132597
C	4.335649	-2.535916	-1.319706
C	4.896821	-2.671051	1.000606
C	4.734659	-3.298087	-0.226717
H	4.908949	-4.364252	-0.328986
C	-2.210468	2.705894	0.157037
C	-3.288210	2.412030	-0.678722
C	-2.319051	2.404540	1.519311
C	-4.442990	1.830278	-0.161951
C	-3.483991	1.839334	2.022827
C	-4.557535	1.538904	1.190390
H	-5.455969	1.075874	1.586093
N	-1.718811	-3.721409	0.084460
C	-0.697261	-2.983000	0.548125
N	-2.184509	-4.720130	-0.250682
H	-0.850804	-1.930377	0.712740
C	0.567553	-3.566586	0.653936
O	1.636304	-2.911214	0.919049
O	0.664500	-4.863641	0.444316
C	1.984044	-5.423118	0.387709
H	1.834023	-6.499868	0.352189
H	2.487720	-5.077253	-0.517097
H	2.559978	-5.135466	1.267774
C	-3.288321	-2.083649	-1.606076
C	-3.863617	-3.382175	-1.906376
C	-3.823139	-3.806587	-3.284885
C	-3.238228	-3.060525	-4.256861
C	-2.627070	-1.807645	-3.941080
C	-2.640072	-1.350605	-2.661702
H	-4.269326	-4.767446	-3.523382
H	-3.230798	-3.415844	-5.282527
H	-2.173331	-1.214103	-4.726762
H	-2.204378	-0.383887	-2.434264
C	-3.312154	-1.498887	-0.324974
C	-4.216636	-4.318094	-0.946615
H	-4.551035	-5.295903	-1.276099
H	-4.433419	-4.063592	0.080427
O	-2.482530	-0.554198	0.041800
H	-1.623928	-0.396119	-0.514310
C	-4.368345	-1.691946	0.697986
C	-5.715149	-1.742186	0.322737
C	-4.023554	-1.629338	2.050770
C	-6.704354	-1.737514	1.298745
H	-5.974830	-1.756236	-0.730717
C	-5.016172	-1.638176	3.024362
H	-2.978207	-1.543029	2.328487
C	-6.357217	-1.688775	2.649137
H	-7.748667	-1.755283	1.005175
H	-4.741459	-1.574956	4.071739
H	-7.133060	-1.678491	3.407861
H	4.818956	-0.827663	2.101908
H	3.804339	-0.593486	-2.063842
H	-1.495162	2.628125	2.189197
H	-3.219189	2.622055	-1.742498
C	5.206345	-3.502641	2.211630
F	5.839896	-2.797041	3.155732

F	5.972801	-4.558868	1.903379
F	4.083445	-3.988532	2.770714
C	4.197745	-3.208063	-2.656399
F	3.672525	-4.442125	-2.528344
F	5.386618	-3.360160	-3.256830
F	3.413691	-2.518304	-3.488936
C	-3.555558	1.546629	3.495588
F	-2.811064	0.479362	3.833724
F	-4.808451	1.299415	3.901051
F	-3.091933	2.576960	4.218491
C	-5.535413	1.454247	-1.119399
F	-6.674498	1.130663	-0.494896
F	-5.176887	0.395043	-1.869415
F	-5.807995	2.451270	-1.974502

TS-[4+2]-A2-S-2

P	-0.624775	0.625112	0.471646
O	-0.696905	-0.748543	-0.112393
O	-0.165592	1.629887	-0.732729
O	-2.103547	1.214678	0.802151
C	-0.397356	2.975213	-0.516185
C	-1.669043	3.475831	-0.698417
C	-2.922548	1.397080	-0.298748
C	-2.750739	2.523392	-1.075339
C	-1.903357	4.860372	-0.415117
C	-2.285182	7.594848	0.169699
C	-3.196546	5.446803	-0.478282
C	-0.810191	5.676803	-0.005804
C	-1.031575	7.052220	0.268232
C	-3.379537	6.776400	-0.196360
H	-4.044810	4.826763	-0.746045
H	-0.184771	7.662726	0.568686
H	-4.375357	7.204252	-0.247559
H	-2.445454	8.645969	0.384893
C	-3.558305	2.673643	-2.248341
C	-5.184971	2.894209	-4.542280
C	-3.384344	3.745395	-3.165072
C	-4.545584	1.688653	-2.536484
C	-5.358592	1.835044	-3.691583
C	-4.177451	3.851908	-4.278751
H	-2.607706	4.478694	-2.977860
H	-6.114972	1.081308	-3.891180
H	-4.027156	4.675536	-4.968950
H	-5.807706	2.995110	-5.424822
C	0.473950	5.099358	0.165803
H	1.293228	5.726850	0.507380
C	0.693173	3.765539	-0.068150
C	-4.681046	0.560001	-1.689255
H	-5.434256	-0.187004	-1.927044
C	-3.878420	0.386188	-0.588307
O	0.192429	0.912120	1.705583
H	1.243414	0.405019	2.235308
C	2.000632	3.115238	0.208407
C	2.723078	2.477604	-0.806456
C	2.490435	3.089602	1.513066
C	3.928079	1.855805	-0.511244
C	3.687042	2.436027	1.796924
C	4.419499	1.824935	0.790754
C	-3.962550	-0.831226	0.256424
C	-3.971431	-2.093671	-0.339601
C	-4.027381	-0.741463	1.650485
C	-4.055466	-3.239506	0.445513
C	-4.109121	-1.893888	2.421763
C	-4.126283	-3.152279	1.830102
N	3.346870	-2.266053	0.359533
C	2.709902	-1.175316	0.824738
N	4.053392	-3.161785	0.468208
H	2.107896	-0.600711	0.137294
C	2.801146	-0.893567	2.193412
O	2.117404	0.000030	2.793870
O	3.639576	-1.619282	2.908692
C	3.588428	-1.454949	4.334213
H	4.358857	-2.117976	4.720954
H	2.605144	-1.747056	4.706693
H	3.792206	-0.420003	4.602585
C	2.923408	-2.545311	-2.508117
C	3.910221	-3.595722	-2.308051
C	5.119160	-3.502653	-3.098527
C	5.332938	-2.505299	-3.991490
C	4.361053	-1.469640	-4.168936
C	3.221903	-1.481338	-3.432881
H	5.863511	-4.280482	-2.956219
H	6.247973	-2.487246	-4.575239
H	4.540649	-0.675318	-4.885024
H	2.481208	-0.699457	-3.550453
C	1.711561	-2.452428	-1.803361
C	3.868563	-4.546363	-1.307570
H	4.724904	-5.200006	-1.180071
H	2.966921	-4.839556	-0.792708
O	1.137558	-1.266087	-1.755741
H	0.294039	-1.200658	-1.193734
C	0.928837	-3.609753	-1.298782
C	0.774516	-4.720081	-2.140872
C	0.247574	-3.569914	-0.078473
C	-0.042658	-5.775619	-1.763129
H	1.301302	-4.741033	-3.089906
C	-0.571473	-4.632387	0.293975
H	0.342143	-2.704738	0.568105
C	-0.719080	-5.732918	-0.544464
H	-0.164614	-6.626509	-2.424994
H	-1.107583	-4.592087	1.236708
H	-1.376779	-6.546187	-0.257668
H	1.905523	3.527373	2.315389
H	2.336547	2.460749	-1.819621
H	5.345076	1.305037	1.016541
H	-4.014063	0.229476	2.132785
H	-3.879929	-2.182676	-1.417292
H	-4.192372	-4.047485	2.438670
C	-4.122254	-1.787219	3.921249
F	-2.881950	-1.837526	4.428629
F	-4.813388	-2.792852	4.478802
F	-4.671615	-0.637420	4.332229
C	-4.129795	-4.589676	-0.208797
F	-5.399600	-4.950797	-0.449541
F	-3.599123	-5.546524	0.574962
F	-3.484584	-4.617833	-1.380091

C	4.198279	2.377635	3.207158
F	5.038041	3.386905	3.479047
F	4.883229	1.236461	3.422250
F	3.210764	2.429968	4.106114
C	4.723157	1.146016	-1.569285
F	4.785322	-0.171124	-1.320542
F	5.989266	1.589611	-1.604599
F	4.201846	1.316645	-2.790192

TS-[4+2]-A3-R-1

P	0.550848	0.048248	-0.218191
O	-0.611324	-0.054915	0.702847
O	1.850279	0.400155	0.689006
O	0.976364	-1.360380	-0.897045
C	3.098599	0.192986	0.130947
C	3.577123	-1.095317	0.013105
C	1.440028	-2.329230	-0.022684
C	2.724846	-2.226539	0.467633
C	4.850985	-1.296533	-0.611485
C	7.367083	-1.604506	-1.852988
C	5.373445	-2.588739	-0.892481
C	5.611718	-0.160116	-1.006046
C	6.879850	-0.346599	-1.617496
C	6.596596	-2.735948	-1.494652
H	4.788083	-3.463672	-0.632920
H	7.450088	0.532868	-1.902877
H	6.975432	-3.730872	-1.704688
H	8.335136	-1.737884	-2.324291
C	3.166021	-3.191205	1.430777
C	3.954422	-5.125384	3.327222
C	4.421641	-3.096468	2.090502
C	2.299854	-4.266764	1.774690
C	2.729503	-5.231597	2.723890
C	4.802981	-4.037870	3.011898
H	5.075487	-2.261696	1.863131
H	2.059581	-6.051443	2.967021
H	5.763076	-3.945235	3.509015
H	4.272652	-5.864959	4.054444
C	5.084057	1.140104	-0.805141
H	5.672763	2.002107	-1.108218
C	3.839134	1.337669	-0.260643
C	1.016424	-4.352066	1.177614
H	0.368000	-5.185698	1.434618
C	0.565109	-3.399294	0.298241
O	0.502569	0.978128	-1.433442
H	0.127262	2.030237	-1.400837
C	3.296942	2.714492	-0.077034
C	3.248183	3.278166	1.213265
C	2.903722	3.463816	-1.201031
C	3.615524	2.544016	2.386704
C	2.832464	4.642393	1.372659
C	2.515600	4.836375	-1.032049
C	2.851989	2.904700	-2.520516
C	3.559237	3.118870	3.621792
H	3.938638	1.513733	2.281413
C	2.792105	5.209190	2.685245
C	2.495749	5.393150	0.245319
C	2.154937	5.603234	-2.185054
H	3.092717	1.855804	-2.652604
C	2.471831	3.661807	-3.587683
C	3.140628	4.472962	3.777020
H	3.836200	2.543166	4.498905
H	2.475965	6.243610	2.788553
H	2.210067	6.436407	0.367507
C	2.132269	5.037709	-3.423270
H	1.892422	6.649203	-2.044182
H	2.422026	3.215715	-4.575425
H	3.105243	4.912262	4.768656
H	1.850907	5.626737	-4.290508
C	-0.784214	-3.509142	-0.327262
C	-1.937622	-3.270805	0.440498
C	-0.889551	-3.911428	-1.674376
C	-1.879456	-2.773881	1.786413
C	-3.231792	-3.489946	-0.144624
C	-2.187534	-4.106193	-2.253651
C	0.257705	-4.149284	-2.497365
C	-3.019472	-2.547451	2.498549
H	-0.910782	-2.542762	2.215389
C	-4.402956	-3.265425	0.648285
C	-3.325904	-3.904393	-1.471090
C	-2.286509	-4.517990	-3.619355
H	1.246816	-4.013391	-2.072938
C	0.121841	-4.537961	-3.797373
C	-4.301406	-2.819906	1.930525
H	-2.961385	-2.137307	3.502609
H	-5.373666	-3.448388	0.194921
H	-4.309127	-4.069066	-1.907963
C	-1.169446	-4.725642	-4.370890
H	-3.277168	-4.660402	-4.042187
H	1.004380	-4.706985	-4.405629
H	-5.192706	-2.651041	2.526256
H	-1.255362	-5.035723	-5.407179
N	-3.668490	2.613997	-0.484077
C	-2.423653	2.352529	-0.893797
N	-4.509337	3.376438	-0.244379
H	-2.125494	1.323974	-1.014263
C	-1.513377	3.410019	-1.112218
O	-0.301451	3.249597	-1.402820
O	-2.004763	4.637726	-0.976006
C	-1.076427	5.706597	-1.162871
H	-1.648790	6.618158	-1.000719
H	-0.255373	5.625827	-0.446669
H	-0.662674	5.677935	-2.172538
C	-5.237732	0.288510	-0.413163
C	-6.274145	1.287869	-0.267517
C	-7.340252	1.260139	-1.238191
C	-7.392797	0.343214	-2.239209
C	-6.350140	-0.621681	-2.388195
C	-5.302209	-0.625703	-1.522315
H	-8.121864	2.007574	-1.139021
H	-8.225288	0.346792	-2.935801
H	-6.397245	-1.348290	-3.192456
H	-4.498663	-1.346868	-1.624872
C	-4.086301	0.223395	0.399473
C	-6.190647	2.390570	0.576538
H	-6.956451	3.154197	0.489038

H	-5.638027	2.392672	1.502627
O	-3.052044	-0.418390	-0.103678
H	-2.218228	-0.402511	0.441015
C	-4.015631	0.603702	1.832925
C	-5.085920	0.263575	2.671883
C	-2.857663	1.160027	2.381333
C	-4.998444	0.479572	4.039420
H	-5.980566	-0.170638	2.235324
C	-2.779026	1.383048	3.754073
H	-2.018793	1.411120	1.740577
C	-3.841739	1.040903	4.583641
H	-5.828308	0.207355	4.683375
H	-1.878359	1.819945	4.171841
H	-3.772654	1.209471	5.653564

TS-[4+2]-A3-R-2

P	-0.709369	-0.046726	1.068631
O	0.163332	-1.209559	0.800507
O	-0.851441	0.816372	-0.309948
O	-2.255694	-0.426924	1.346121
C	-1.769378	1.853462	-0.294358
C	-3.114997	1.563766	-0.392554
C	-3.013006	-0.819798	0.252947
C	-3.518454	0.146198	-0.593014
C	-4.050577	2.643130	-0.283987
C	-5.829599	4.820645	-0.066138
C	-5.455167	2.434014	-0.228632
C	-3.558833	3.975478	-0.189501
C	-4.480034	5.052141	-0.094504
C	-6.318714	3.493962	-0.122560
H	-5.837897	1.419662	-0.261781
H	-4.088547	6.063638	-0.033796
H	-7.387712	3.314069	-0.074863
H	-6.525642	5.649168	0.012071
C	-4.307937	-0.273669	-1.714978
C	-5.870956	-1.186732	-3.884407
C	-4.772433	0.626885	-2.713350
C	-4.607064	-1.657243	-1.867526
C	-5.408373	-2.084290	-2.959539
C	-5.533586	0.181912	-3.763832
H	-4.514031	1.676953	-2.642036
H	-5.634592	-3.142874	-3.050553
H	-5.875796	0.886884	-4.514480
H	-6.479988	-1.522115	-4.717279
C	-2.159881	4.208085	-0.168145
H	-1.795127	5.229865	-0.100379
C	-1.257048	3.173832	-0.194008
C	-4.042801	-2.598437	-0.970054
H	-4.219404	-3.657950	-1.136046
C	-3.221885	-2.210726	0.058921
O	-0.375217	0.918371	2.216409
H	0.643844	1.088197	2.561230
C	0.212045	3.403842	-0.118342
C	1.026347	3.104205	-1.229039
C	0.774993	3.946364	1.052743
C	0.490415	2.639007	-2.472473
C	2.445476	3.295913	-1.138941
C	2.183688	4.224967	1.090675
C	0.000881	4.231220	2.226050
C	1.307595	2.341751	-3.522977
H	-0.585547	2.534385	-2.573784
C	3.271925	2.930606	-2.248956
C	2.990958	3.858926	0.014437
C	2.734978	4.860573	2.247108
H	-1.046204	3.951961	2.242041
C	0.568353	4.823957	3.314039
C	2.723075	2.461558	-3.405210
H	0.881473	1.991884	-4.458054
H	4.347377	3.045382	-2.143945
H	4.066032	4.011828	0.075976
C	1.951661	5.170711	3.317455
H	3.798747	5.084319	2.247823
H	-0.034385	5.028583	4.192738
H	3.355763	2.191521	-4.244927
H	2.380151	5.658673	4.187649
C	-2.469509	-3.212344	0.867325
C	-1.326460	-3.808588	0.300748
C	-2.884497	-3.545929	2.167054
C	-0.828715	-3.451439	-0.996572
C	-0.588778	-4.776853	1.061311
C	-2.146547	-4.524045	2.914198
C	-4.028267	-2.942585	2.781473
C	0.301612	-4.023321	-1.501696
H	-1.347550	-2.688852	-1.568272
C	0.588898	-5.359769	0.491922
C	-1.020976	-5.117669	2.342744
C	-2.584148	-4.862426	4.233606
H	-4.588135	-2.199094	2.223103
C	-4.409768	-3.289034	4.043382
C	1.022524	-4.998454	-0.747751
H	0.667323	-3.721299	-2.479790
H	1.134765	-6.091196	1.081481
H	-0.460590	-5.854018	2.914550
C	-3.678734	-4.266015	4.782631
H	-2.017892	-5.605634	4.788092
H	-5.276757	-2.818549	4.495639
H	1.924566	-5.436230	-1.163943
H	-4.000138	-4.528064	5.785379
N	3.833810	0.551717	0.206254
C	2.813350	0.583753	1.062602
N	4.808640	1.046664	-0.204577
H	2.057275	-0.177206	0.974485
C	2.835511	1.362176	2.247260
O	1.867208	1.429380	3.036437
O	3.986560	1.975300	2.529843
C	4.130228	2.452358	3.869276
H	5.003928	3.102846	3.859180
H	3.242888	2.998727	4.183399
H	4.300957	1.606015	4.539927
C	4.698544	-2.031106	-0.560428
C	5.683454	-1.225441	-1.239063
C	7.064056	-1.542102	-0.997486
C	7.439337	-2.525061	-0.133914
C	6.457737	-3.265980	0.587839
C	5.134882	-3.005592	0.397196
H	7.813414	-0.954980	-1.519996

H	8.492257	-2.740969	0.017838
H	6.767778	-4.043993	1.277009
H	4.374368	-3.568760	0.925853
C	3.309703	-1.844324	-0.719716
C	5.373272	-0.017679	-1.869072
H	6.193912	0.570588	-2.268264
H	4.400748	0.189295	-2.295974
O	2.545441	-2.276561	0.265432
H	1.580775	-2.139532	0.130056
C	2.631937	-1.524091	-2.000782
C	3.093264	-2.148077	-3.169587
C	1.438473	-0.800655	-2.028978
C	2.350046	-2.068397	-4.339744
H	4.020820	-2.711201	-3.141249
C	0.687182	-0.744126	-3.199064
H	1.083677	-0.288291	-1.142716
C	1.134892	-1.380552	-4.352368
H	2.705616	-2.563343	-5.237564
H	-0.248426	-0.193969	-3.194360
H	0.542771	-1.342209	-5.261278

TS-[4+2]-A3-S-1

P	0.618152	0.115038	-0.110902
O	-0.525110	0.214087	0.855868
O	1.974201	0.074863	0.784233
O	0.669037	-1.334553	-0.846289
C	3.124372	-0.302536	0.115256
C	3.335027	-1.638364	-0.158438
C	0.997133	-2.436405	-0.081316
C	2.316549	-2.632946	0.274725
C	4.500309	-2.005310	-0.908370
C	6.819760	-2.643141	-2.386253
C	4.739675	-3.333654	-1.355587
C	5.439845	-0.995805	-1.260342
C	6.604271	-1.349435	-1.992464
C	5.867440	-3.641464	-2.072479
H	4.012365	-4.105689	-1.131278
H	7.315056	-0.566726	-2.242100
H	6.028378	-4.660601	-2.408598
H	7.709973	-2.903778	-2.949014
C	2.644727	-3.761002	1.094687
C	3.206997	-6.018297	2.693680
C	3.946228	-3.973723	1.626321
C	1.621358	-4.693839	1.421962
C	1.937463	-5.827454	2.217291
C	4.217452	-5.071377	2.402260
H	4.726527	-3.250263	1.417935
H	1.145111	-6.534043	2.447729
H	5.216194	-5.212747	2.802359
H	3.438798	-6.884697	3.304203
C	5.187220	0.352217	-0.902188
H	5.908042	1.116671	-1.180934
C	4.040671	0.720591	-0.242608
C	0.296030	-4.462534	0.977607
H	-0.479620	-5.177411	1.240602
C	-0.044561	-3.341751	0.259048
O	0.747335	1.103962	-1.244866
H	0.568167	2.401762	-1.255603
C	3.773290	2.150373	0.084024
C	3.844868	2.590637	1.420849
C	3.513870	3.063278	-0.955933
C	4.092130	1.696290	2.511553
C	3.683484	3.985896	1.715655
C	3.385854	4.461535	-0.651631
C	3.344594	2.652158	-2.319847
C	4.157002	2.153112	3.794356
H	4.224658	0.639851	2.304564
C	3.761728	4.424627	3.074750
C	3.474899	4.888706	0.671889
C	3.167702	5.388228	-1.720470
H	3.375859	1.593880	-2.552379
C	3.107567	3.564858	-3.303672
C	3.987961	3.538739	4.084202
H	4.338688	1.457424	4.606959
H	3.636331	5.484069	3.280652
H	3.383946	5.949766	0.897123
C	3.034985	4.958125	-3.005436
H	3.107293	6.446646	-1.477037
H	2.967267	3.231259	-4.326547
H	4.043503	3.881482	5.112273
H	2.867495	5.669782	-3.808007
C	-1.461213	-3.086664	-0.128184
C	-2.429401	-2.887524	0.878984
C	-1.839700	-3.099328	-1.485659
C	-2.096918	-2.804467	2.272140
C	-3.809662	-2.728246	0.510569
C	-3.219998	-2.926366	-1.837757
C	-0.899338	-3.307362	-2.546474
C	-3.060349	-2.598823	3.216573
H	-1.057031	-2.881077	2.568373
C	-4.786538	-2.508653	1.532841
C	-4.172553	-2.756845	-0.834776
C	-3.597425	-2.937950	-3.217884
H	0.145701	-3.461083	-2.301102
C	-1.297573	-3.312225	-3.850144
C	-4.428673	-2.449111	2.846294
H	-2.781566	-2.525200	4.263125
H	-5.822713	-2.385544	1.227990
H	-5.216837	-2.617355	-1.110900
C	-2.667644	-3.119384	-4.196321
H	-4.647554	-2.796840	-3.458990
H	-0.565943	-3.465614	-4.636729
H	-5.175362	-2.271129	3.613141
H	-2.962324	-3.126996	-5.240850
N	-3.028378	3.228101	-0.309062
C	-1.839398	2.834651	-0.785687
N	-3.781753	4.035704	0.023353
H	-1.656515	1.783239	-0.927587
C	-0.824867	3.780512	-0.959471
O	0.378947	3.486826	-1.268348
O	-1.131939	5.051073	-0.775001
C	-0.054036	5.989986	-0.864906
H	-0.500658	6.957859	-0.647215
H	0.723093	5.741927	-0.138428
H	0.380390	5.972077	-1.865598
C	-3.997628	1.198391	1.405485

C	-4.957433	2.250491	1.685441
C	-5.075834	2.671464	3.059455
C	-4.295318	2.157043	4.045712
C	-3.305388	1.172832	3.746576
C	-3.151956	0.731889	2.469192
H	-5.809828	3.439797	3.283850
H	-4.418737	2.500269	5.068371
H	-2.688981	0.762632	4.539060
H	-2.423471	-0.042207	2.257227
C	-3.827570	0.603514	0.134367
C	-5.572050	3.022975	0.709867
H	-6.208717	3.842984	1.024409
H	-5.686412	2.701059	-0.314901
O	-2.731861	-0.006022	-0.224004
H	-1.865498	0.119150	0.345624
C	-4.904423	0.403538	-0.868007
C	-6.215910	0.132536	-0.457681
C	-4.570854	0.314114	-2.221118
C	-7.181835	-0.207553	-1.394877
H	-6.461831	0.181912	0.598646
C	-5.546197	-0.009076	-3.160103
H	-3.541859	0.477620	-2.524803
C	-6.849601	-0.274765	-2.749578
H	-8.194015	-0.427120	-1.071335
H	-5.280337	-0.071781	-4.210403
H	-7.606950	-0.538880	-3.480831

TS-[4+2]-A3-S-2

P	0.778820	-0.026655	-0.988363
O	-0.113214	-1.193885	-0.788938
O	0.669405	0.933197	0.316765
O	2.350361	-0.383280	-1.018746
C	1.620408	1.932351	0.456940
C	2.893975	1.583572	0.861699
C	2.880456	-0.798005	0.197314
C	3.191104	0.153438	1.145972
C	3.888602	2.609319	0.955210
C	5.781090	4.694075	1.132090
C	5.256717	2.331334	1.223663
C	3.502692	3.961019	0.737699
C	4.475006	4.990892	0.847703
C	6.174788	3.346123	1.309313
H	5.571157	1.301481	1.351789
H	4.159918	6.018314	0.689112
H	7.215674	3.113554	1.509099
H	6.518614	5.486029	1.209069
C	3.708509	-0.288168	2.408371
C	4.736714	-1.241601	4.858991
C	3.943776	0.596975	3.496234
C	3.959974	-1.675851	2.602218
C	4.491054	-2.123761	3.840990
C	4.445223	0.131975	4.684789
H	3.714308	1.650042	3.381045
H	4.686655	-3.185014	3.965443
H	4.614215	0.824031	5.503290
H	5.139086	-1.592782	5.803368
C	2.164028	4.257077	0.382702
H	1.883137	5.292993	0.210975
C	1.219589	3.272989	0.205057
C	3.629020	-2.598401	1.578061
H	3.785922	-3.659758	1.752144
C	3.064426	-2.191082	0.394930
O	0.599550	0.853302	-2.241660
H	-0.398906	1.195756	-2.377152
C	-0.155219	3.623216	-0.252830
C	-1.272458	3.341929	0.558370
C	-0.321845	4.293151	-1.485533
C	-1.161718	2.670480	1.818168
C	-2.584341	3.737134	0.125860
C	-1.627338	4.756472	-1.864327
C	0.753325	4.503975	-2.410189
C	-2.270418	2.330669	2.532686
H	-0.178054	2.422955	2.200885
C	-3.725064	3.351482	0.901085
C	-2.725303	4.462884	-1.055752
C	-1.784194	5.481280	-3.088053
H	1.730648	4.096565	-2.179087
C	0.556529	5.173422	-3.582062
C	-3.578181	2.643353	2.055229
H	-2.165206	1.812114	3.478308
H	-4.711212	3.608942	0.524329
H	-3.717795	4.784266	-1.366102
C	-0.727375	5.690160	-3.921512
H	-2.774965	5.851944	-3.339602
H	1.383904	5.306769	-4.271316
H	-4.444695	2.313281	2.621522
H	-0.858867	6.235271	-4.850573
C	2.593809	-3.177550	-0.618384
C	1.426066	-3.919611	-0.358472
C	3.315178	-3.367710	-1.810571
C	0.623053	-3.715535	0.812559
C	0.987199	-4.897828	-1.313573
C	2.866255	-4.346701	-2.758770
C	4.497615	-2.620589	-2.117293
C	-0.512291	-4.440799	1.022482
H	0.917605	-2.951231	1.524276
C	-0.202625	-5.647924	-1.045467
C	1.719235	-5.091660	-2.484307
C	3.611052	-4.537160	-3.965337
H	4.847019	-1.879256	-1.406011
C	5.177195	-2.829043	-3.280380
C	-0.928687	-5.432935	0.085846
H	-1.116475	-4.255627	1.906008
H	-0.518781	-6.386969	-1.777013
H	1.384407	-5.835804	-3.203705
C	4.729281	-3.802861	-4.221277
H	3.259787	-5.282422	-4.673649
H	6.068505	-2.249542	-3.497655
H	-1.839906	-5.992457	0.270464
H	5.285360	-3.953480	-5.140807
N	-3.968598	0.257854	-0.263412
C	-2.788697	0.644779	-0.743186
N	-5.129655	0.295738	-0.321963
H	-1.899618	0.358660	-0.206060
C	-2.731296	1.390866	-1.950668
O	-1.692143	1.669380	-2.579723

O	-3.918455	1.778504	-2.426803
C	-3.892127	2.426148	-3.698021
H	-4.924542	2.704396	-3.903348
H	-3.520562	1.742848	-4.464879
H	-3.246600	3.305646	-3.667113
C	-3.848761	-1.165680	2.211881
C	-5.279325	-0.988905	2.072487
C	-5.969850	-0.371014	3.177395
C	-5.337607	-0.004466	4.323244
C	-3.927026	-0.186813	4.453029
C	-3.214663	-0.713847	3.421176
H	-7.040569	-0.222754	3.072148
H	-5.902731	0.427532	5.143125
H	-3.427653	0.094552	5.374444
H	-2.141794	-0.845273	3.502615
C	-3.006039	-1.658447	1.192355
C	-5.984801	-1.166929	0.886660
H	-7.026679	-0.865200	0.868462
H	-5.695392	-1.873975	0.125307
O	-1.727037	-1.332600	1.286369
H	-1.160810	-1.616663	0.525414
C	-3.371541	-2.701718	0.200282
C	-4.176607	-3.771398	0.617478
C	-2.836991	-2.704885	-1.092403
C	-4.480925	-4.803110	-0.260230
H	-4.573206	-3.773142	1.628563
C	-3.149342	-3.741166	-1.967796
H	-2.183290	-1.901293	-1.415616
C	-3.973980	-4.784591	-1.560001
H	-5.109367	-5.623844	0.070170
H	-2.735115	-3.732569	-2.970364
H	-4.213257	-5.589919	-2.247317

TS-[4+2]-A4-R-1

P	0.704098	0.260989	-0.127639
O	-0.426824	-0.099268	0.771049
O	1.989231	0.601242	0.795257
O	1.242966	-0.978996	-1.017332
C	3.207426	0.688440	0.134867
C	3.840253	-0.474804	-0.245087
C	1.889663	-1.984214	-0.309181
C	3.194274	-1.774870	0.084697
C	5.053576	-0.375510	-0.999423
C	7.430091	-0.093893	-2.491555
C	5.723819	-1.513410	-1.524681
C	5.588566	0.914618	-1.274868
C	6.793732	1.022759	-2.018083
C	6.880100	-1.374701	-2.248936
H	5.304177	-2.498513	-1.352518
H	7.194947	2.013810	-2.210729
H	7.375303	-2.255100	-2.645316
H	8.348197	-0.000208	-3.062090
C	3.841894	-2.778211	0.875170
C	5.038948	-4.801664	2.433860
C	5.146906	-2.608793	1.412671
C	3.135905	-3.976759	1.174915
C	3.770210	-4.982870	1.951082
C	5.727861	-3.594528	2.168600
H	5.679611	-1.683315	1.224636
H	3.221435	-5.896668	2.160970
H	6.723823	-3.445360	2.572672
H	5.513932	-5.574438	3.029179
C	4.902470	2.070846	-0.824403
H	5.323012	3.050396	-1.036697
C	3.718447	1.984918	-0.134216
C	1.805095	-4.139188	0.716770
H	1.278438	-5.061280	0.948471
C	1.159926	-3.165128	-0.007325
O	0.522654	1.355348	-1.189607
H	0.013351	2.308492	-0.993680
C	2.977382	3.195746	0.300769
C	2.629969	3.375830	1.645671
C	2.634086	4.169971	-0.632000
C	1.981466	4.532027	2.063265
C	1.953554	5.326614	-0.241182
C	1.638453	4.752754	3.514567
C	1.657480	5.501511	1.106807
C	1.504312	6.320231	-1.279285
H	0.589180	5.039208	3.631564
H	1.147701	6.409807	1.426071
H	1.087512	7.219647	-0.818467
C	-0.247768	-3.353947	-0.444076
C	-1.209977	-3.756887	0.486410
C	-0.613540	-3.202065	-1.783674
C	-2.519850	-4.030402	0.092448
C	-1.912768	-3.484707	-2.203596
C	-3.541596	-4.487650	1.102470
C	-2.852010	-3.896142	-1.256167
C	-2.286043	-3.349757	-3.659190
H	-3.407057	-5.547934	1.341325
H	-3.871979	-4.101917	-1.576020
H	-3.356518	-3.513739	-3.808805
N	-3.821896	2.012201	-0.236266
C	-2.548193	2.114655	-0.620446
N	-4.811797	2.507941	0.123629
H	-2.051871	1.226882	-0.975437
C	-1.849874	3.339776	-0.544994
O	-0.628575	3.460744	-0.811137
O	-2.560231	4.394970	-0.153022
C	-1.856019	5.633108	-0.066573
H	-2.536856	6.321927	0.430437
H	-0.932450	5.510363	0.502395
H	-1.612896	5.999264	-1.066987
C	-4.816798	-0.467597	-0.901620
C	-6.055074	0.222496	-0.621681
C	-7.028825	0.256906	-1.681644
C	-6.812528	-0.325161	-2.891773
C	-5.567771	-0.964884	-3.170544
C	-4.600673	-1.006555	-2.215083
H	-7.964662	0.770416	-1.481819
H	-7.582936	-0.291753	-3.655651
H	-5.394187	-1.412984	-4.143569
H	-3.645226	-1.479067	-2.406243
C	-3.736416	-0.532318	0.006540
C	-6.251847	1.057870	0.479096
H	-7.160152	1.651257	0.501729

H	-5.784004	0.897703	1.437849
O	-2.550943	-0.804906	-0.489092
H	-1.785367	-0.723112	0.157205
C	-3.875273	-0.549869	1.485522
C	-4.848635	-1.383423	2.051244
C	-3.014096	0.175162	2.313065
C	-4.963950	-1.483877	3.431328
H	-5.514398	-1.939591	1.398027
C	-3.144141	0.079077	3.695751
H	-2.249571	0.808725	1.875249
C	-4.113457	-0.747571	4.255877
H	-5.716218	-2.135195	3.864043
H	-2.480394	0.651174	4.335044
H	-4.206673	-0.821485	5.334598
H	2.329084	6.621369	-1.931386
H	0.731672	5.866574	-1.908928
H	2.865297	4.006045	-1.681793
H	2.880326	2.603826	2.367941
H	1.811216	3.849305	4.102890
H	2.246168	5.555885	3.943439
H	0.129532	-2.875123	-2.506239
H	-0.930559	-3.843149	1.533824
H	-2.035996	-2.353833	-4.038443
H	-1.745027	-4.077169	-4.272061
H	-3.455642	-3.922834	2.034774
H	-4.557592	-4.360956	0.719606

TS-[4+2]-A4-R-2

P	0.648580	-0.159992	-1.106416
O	-0.501372	-1.023860	-0.718071
O	1.128271	0.660729	0.210486
O	1.960541	-1.007542	-1.489016
C	2.386770	1.249991	0.158011
C	3.501967	0.442216	0.261820
C	2.516568	-1.714236	-0.425571
C	3.318133	-1.022933	0.456177
C	4.797036	1.037512	0.125043
C	7.308723	2.292088	-0.147351
C	5.994584	0.272082	0.091753
C	4.891186	2.448626	-0.023325
C	6.170762	3.053613	-0.143343
C	7.214532	0.883971	-0.040428
H	5.933153	-0.808134	0.162951
H	6.224704	4.133995	-0.243591
H	8.117092	0.282359	-0.069374
H	8.281791	2.761885	-0.245170
C	3.870698	-1.725919	1.575707
C	4.933918	-3.196939	3.735402
C	4.624903	-1.083290	2.594810
C	3.623109	-3.122099	1.695170
C	4.185151	-3.838574	2.785293
C	5.142572	-1.800545	3.642761
H	4.782896	-0.012210	2.540464
H	3.996525	-4.906188	2.854325
H	5.713109	-1.291129	4.412423
H	5.355417	-3.751666	4.567133
C	3.708828	3.225138	-0.076233
H	3.795779	4.303344	-0.180176
C	2.456401	2.659527	-0.013004
C	2.781133	-3.768011	0.757057
H	2.577054	-4.828243	0.880810
C	2.191251	-3.090692	-0.284256
O	0.499235	0.817506	-2.276512
H	-0.252966	1.614734	-2.214949
C	1.246884	3.513033	-0.149410
C	0.170227	3.427848	0.742578
C	1.220447	4.480639	-1.155289
C	-0.897912	4.319502	0.654998
C	0.150956	5.367642	-1.277683
C	-0.892297	5.281891	-0.359302
C	1.187232	-3.752043	-1.155684
C	0.199088	-4.536621	-0.559318
C	1.197206	-3.609211	-2.547814
C	-0.772539	-5.183054	-1.327206
C	0.236640	-4.237861	-3.334374
C	-0.738689	-5.022969	-2.710601
N	-3.727585	1.236766	-0.256774
C	-2.471611	1.545907	-0.584794
N	-4.868520	1.422956	-0.385095
H	-1.679219	0.945733	-0.173813
C	-2.217029	2.496357	-1.604951
O	-1.137604	2.603583	-2.228698
O	-3.239102	3.297025	-1.906054
C	-3.035922	4.179688	-3.008643
H	-3.982283	4.700431	-3.142416
H	-2.774409	3.616793	-3.906567
H	-2.233522	4.885116	-2.782078
C	-3.627438	-0.161709	2.647136
C	-4.576503	-0.826228	3.429045
C	-5.010214	-0.258593	4.620235
C	-4.505075	0.974660	5.032385
C	-3.549910	1.631681	4.260424
C	-3.098714	1.055961	3.077818
H	-5.742609	-0.777172	5.229969
H	-4.853049	1.419522	5.959066
H	-3.153269	2.589427	4.582226
H	-2.345557	1.542531	2.465254
C	-3.094889	-0.777548	1.406886
O	-1.785816	-0.748630	1.396369
H	-1.321122	-0.964294	0.509892
C	-3.863206	-1.470091	0.445612
C	-5.260078	-1.177816	0.183418
C	-3.199123	-2.463740	-0.358028
C	-5.903204	-1.960545	-0.840541
C	-3.863296	-3.169592	-1.311996
H	-2.150912	-2.681685	-0.176701
C	-5.246475	-2.913962	-1.552716
H	-6.950468	-1.753417	-1.039959
H	-3.336762	-3.926228	-1.885053
H	-5.773514	-3.482400	-2.312698
H	2.041141	4.527667	-1.866953
H	0.183717	2.676870	1.528502
H	-1.725228	5.979847	-0.429732
H	1.962633	-3.000221	-3.018626
H	0.172165	-4.625582	0.524408
H	-1.488745	-5.521945	-3.322158

C	0.227249	-4.058865	-4.831012
C	-1.831734	-6.022257	-0.657388
C	0.126608	6.373639	-2.399722
C	-2.053336	4.251194	1.620047
H	0.002112	5.869360	-3.364102
H	1.060987	6.939955	-2.447261
H	-0.695156	7.084065	-2.279405
H	-2.449688	5.247880	1.830279
H	-2.869242	3.647708	1.205328
H	-1.747776	3.800225	2.568066
H	1.200219	-3.722426	-5.195285
H	-0.026892	-4.992150	-5.340411
H	-0.514467	-3.309239	-5.124787
H	-1.381316	-6.814229	-0.051806
H	-2.488722	-6.491627	-1.393737
H	-2.453667	-5.411181	0.004821
C	-5.932921	-0.051096	0.651162
H	-5.676921	0.465113	1.563006
H	-6.939543	0.121528	0.285382
H	-4.974531	-1.777614	3.089186

TS-[4+2]-A4-S-1

P	0.706613	0.303292	-0.140294
O	-0.443946	0.061059	0.793936
O	2.008989	0.531014	0.797727
O	1.121255	-1.034004	-0.961876
C	3.240067	0.415737	0.172567
C	3.727909	-0.846225	-0.091162
C	1.596702	-2.086459	-0.193284
C	2.893893	-2.025957	0.272162
C	4.975104	-0.966116	-0.785556
C	7.439451	-1.111108	-2.152267
C	5.511358	-2.218003	-1.192783
C	5.690462	0.217875	-1.121121
C	6.935060	0.111528	-1.796866
C	6.710223	-2.286622	-1.855284
H	4.956000	-3.124511	-0.979776
H	7.473440	1.024650	-2.035021
H	7.100973	-3.251835	-2.160540
H	8.389207	-1.181826	-2.672085
C	3.361477	-3.067886	1.136072
C	4.201628	-5.156491	2.834975
C	4.640823	-3.035010	1.754357
C	2.497093	-4.160992	1.423452
C	2.954026	-5.204331	2.271778
C	5.048090	-4.051818	2.579608
H	5.292621	-2.187588	1.572269
H	2.286393	-6.037817	2.471613
H	6.026829	-4.006728	3.046020
H	4.539792	-5.956350	3.485461
C	5.138157	1.484533	-0.807257
H	5.692169	2.380154	-1.076400
C	3.919487	1.611283	-0.184963
C	1.190056	-4.183993	0.876295
H	0.546141	-5.032927	1.091164
C	0.712768	-3.165842	0.085816
O	0.595503	1.380572	-1.198473
H	0.194502	2.573533	-0.965702
C	3.320567	2.946945	0.066360
C	2.813557	3.294823	1.320504
C	3.292199	3.888185	-0.966776
C	2.317573	4.576597	1.558365
C	2.785978	5.169184	-0.757845
C	2.324149	5.503075	0.515466
H	1.951949	6.510566	0.696759
C	-0.673669	-3.196143	-0.448124
C	-1.740856	-3.505865	0.399991
C	-0.926690	-2.965485	-1.803226
C	-3.047069	-3.584175	-0.086657
C	-2.219333	-3.058163	-2.315312
C	-3.266448	-3.370492	-1.447573
H	-4.282142	-3.419762	-1.838283
N	-3.475244	2.502577	0.088119
C	-2.258876	2.464528	-0.471524
N	-4.358164	3.044845	0.594909
H	-1.885565	1.524085	-0.839408
C	-1.437399	3.596416	-0.415316
O	-0.208104	3.603168	-0.752766
O	-1.976837	4.717251	0.032949
C	-1.090810	5.822491	0.234675
H	-1.728119	6.646376	0.548860
H	-0.358403	5.577856	1.006390
H	-0.562946	6.066047	-0.689148
C	-3.970829	-0.016204	1.377552
C	-5.111290	0.747854	1.844903
C	-5.286264	0.840839	3.273090
C	-4.411134	0.282286	4.149991
C	-3.260369	-0.419404	3.679115
C	-3.041052	-0.539403	2.341476
H	-6.148902	1.392610	3.634785
H	-4.583886	0.371206	5.218112
H	-2.572200	-0.869088	4.386038
H	-2.181191	-1.096133	1.983338
C	-3.697351	-0.268250	0.012204
C	-5.885783	1.565735	1.033337
H	-6.668792	2.159041	1.493053
H	-5.953170	1.439567	-0.037468
O	-2.498528	-0.523406	-0.424382
H	-1.685850	-0.295211	0.197995
C	-4.720400	-0.489656	-1.039624
C	-5.932782	-1.118465	-0.731439
C	-4.393925	-0.233396	-2.373223
C	-6.808479	-1.476103	-1.747731
H	-6.171485	-1.334473	0.305558
C	-5.280325	-0.579532	-3.388244
H	-3.435871	0.222283	-2.602875
C	-6.484932	-1.205610	-3.078332
H	-7.741231	-1.974535	-1.505121
H	-5.022856	-0.373610	-4.422253
H	-7.170734	-1.487070	-3.870963
H	3.651166	3.602885	-1.952536
H	2.820604	2.562038	2.122263
H	-0.101465	-2.716984	-2.464867
H	-1.549388	-3.665034	1.459484
C	2.694836	6.153704	-1.894854
C	1.775268	4.940146	2.917953

C	-2.475349	-2.803859	-3.778888
C	-4.196675	-3.849664	0.852398
H	1.556869	6.008999	2.986133
H	2.487585	4.689616	3.708825
H	0.851840	4.390391	3.129000
H	1.782700	5.979569	-2.476154
H	3.541756	6.054993	-2.578369
H	2.667672	7.183238	-1.529207
H	-3.523658	-2.978962	-4.031888
H	-1.854888	-3.449662	-4.407340
H	-2.235816	-1.767341	-4.039045
H	-5.131980	-3.976500	0.301514
H	-4.025597	-4.750310	1.449528
H	-4.325332	-3.014267	1.551181

TS-[4+2]-A4-S-2

P	0.691202	0.201883	1.147214
O	-0.205690	1.315326	0.732504
O	0.843703	-0.793921	-0.125268
O	2.210804	0.652512	1.422708
C	1.902983	-1.690828	-0.121867
C	3.176545	-1.212385	-0.356770
C	2.865919	1.148635	0.299275
C	3.369024	0.243590	-0.609278
C	4.275964	-2.127427	-0.288598
C	6.381627	-3.999406	-0.148269
C	5.630856	-1.710570	-0.395777
C	4.007370	-3.506642	-0.067484
C	5.087647	-4.427543	-0.016294
C	6.652955	-2.622205	-0.328068
H	5.850750	-0.656512	-0.523595
H	4.863685	-5.478853	0.141218
H	7.680926	-2.283887	-0.407211
H	7.200825	-4.709346	-0.102748
C	3.986394	0.746808	-1.800732
C	5.189559	1.823607	-4.113975
C	4.443344	-0.099912	-2.846877
C	4.109779	2.155260	-1.966220
C	4.733634	2.666266	-3.135414
C	5.029490	0.425280	-3.970011
H	4.316770	-1.172465	-2.751734
H	4.830805	3.743170	-3.240497
H	5.368992	-0.237704	-4.759071
H	5.660835	2.224063	-5.005465
C	2.672207	-3.937155	0.124565
H	2.481951	-4.995090	0.284259
C	1.612371	-3.060239	0.126213
C	3.575484	3.028439	-0.985990
H	3.661104	4.101566	-1.135697
C	2.932718	2.558334	0.133968
O	0.358080	-0.622159	2.399410
H	-0.581453	-1.148919	2.474817
C	0.236025	-3.547455	0.407840
C	-0.860666	-3.183904	-0.384617
C	0.044574	-4.441027	1.463781
C	-2.121783	-3.729027	-0.149108
C	-1.211673	-4.987079	1.729361
C	-2.278872	-4.630076	0.909011
C	2.270575	3.479027	1.092558
C	1.424910	4.473519	0.602501
C	2.464908	3.364524	2.473382
C	0.768720	5.351382	1.467839
C	1.832846	4.236082	3.355217
C	0.985976	5.220904	2.837057
N	-3.946215	-0.472321	0.269273
C	-2.797532	-0.760541	0.871553
N	-5.104740	-0.548510	0.204387
H	-1.884072	-0.434524	0.404898
C	-2.761752	-1.596412	2.018203
O	-1.732887	-1.842816	2.679053
O	-3.930329	-2.131725	2.371656
C	-3.907987	-2.946488	3.543534
H	-4.933122	-3.284963	3.681981
H	-3.573206	-2.365893	4.405223
H	-3.234210	-3.793686	3.398966
C	-3.551326	0.312892	-2.430373
C	-4.990001	0.157728	-2.399346
C	-5.563273	-0.761663	-3.350943
C	-4.810911	-1.445115	-4.252460
C	-3.391098	-1.289076	-4.271582
C	-2.789782	-0.461982	-3.375910
H	-6.641092	-0.892523	-3.327025
H	-5.287529	-2.114858	-4.961249
H	-2.797585	-1.827958	-5.002208
H	-1.713501	-0.335504	-3.377163
C	-2.819229	1.088697	-1.507619
C	-5.809667	0.631055	-1.380079
H	-6.855872	0.345108	-1.395841
H	-5.572160	1.496595	-0.780749
O	-1.541005	0.788107	-1.383337
H	-1.045641	1.245918	-0.640046
C	-3.283881	2.349301	-0.871506
C	-3.986201	3.273819	-1.656731
C	-2.923569	2.686281	0.436949
C	-4.337864	4.510502	-1.133866
H	-4.253934	3.008900	-2.675155
C	-3.283661	3.926762	0.956482
H	-2.362949	1.985649	1.046559
C	-3.988683	4.838761	0.176253
H	-4.877605	5.222240	-1.749655
H	-3.001018	4.180129	1.973070
H	-4.262217	5.806485	0.584830
H	0.886217	-4.693915	2.104095
H	-0.731005	-2.468651	-1.192887
H	-3.265305	-5.050167	1.101378
H	3.114979	2.584864	2.859352
H	1.245451	4.538274	-0.468075
H	0.478830	5.897297	3.522716
C	2.070643	4.137352	4.840716
C	-0.177306	6.390088	0.920546
C	-1.402035	-5.914412	2.902736
C	-3.307727	-3.355578	-1.001237
H	-1.269588	-5.374988	3.846762
H	-0.671936	-6.728645	2.888725
H	-2.401779	-6.356070	2.901451
H	-3.574482	-4.170877	-1.682225

H	-4.182024	-3.145694	-0.376490
H	-3.101475	-2.468516	-1.605666
H	2.427520	3.143089	5.117710
H	2.822001	4.864677	5.165670
H	1.154277	4.339891	5.401139
H	0.295797	6.976805	0.127856
H	-0.503969	7.078891	1.703145
H	-1.067136	5.917107	0.491733

TS-[4+2]-B2-R

P	-0.687682	1.299459	-0.168978
O	0.366400	0.757478	0.749631
O	-1.890599	1.763597	0.834628
O	-0.223966	2.714345	-0.835682
C	-3.027484	2.297273	0.256915
C	-3.056448	3.662921	0.011667
C	0.270410	3.655960	0.055577
C	-0.613184	4.534792	0.666048
C	-4.134675	4.223338	-0.676182
C	-5.232303	3.443550	-1.011484
C	-0.144784	5.405953	1.655457
C	1.201309	5.447708	1.987176
C	-5.221811	2.091519	-0.689422
H	-6.099629	1.496383	-0.915186
C	-4.113409	1.472639	-0.091112
C	2.080849	4.589434	1.335617
H	3.139800	4.617680	1.573763
C	1.636100	3.668855	0.380070
O	-1.230279	0.498760	-1.318137
H	-1.732880	-0.743531	-1.588629
C	-4.122055	0.000940	0.131602
C	-3.359959	-0.625564	1.134590
C	-4.940168	-0.813226	-0.657751
C	-3.425899	-1.999808	1.316869
C	-5.032832	-2.183401	-0.429523
C	-4.273388	-2.798135	0.552527
H	-4.336917	-3.867230	0.724715
C	2.611287	2.735083	-0.235936
C	3.576248	2.117373	0.567008
C	2.624777	2.489642	-1.613111
C	4.549041	1.305527	-0.002000
C	3.610176	1.680520	-2.167436
C	4.588571	1.093472	-1.374001
H	5.344474	0.448468	-1.812433
N	0.583336	-3.361675	-0.145168
C	-0.148099	-2.366390	-0.681089
N	0.715554	-4.456995	0.186933
H	0.289744	-1.385430	-0.750304
C	-1.386310	-2.636304	-1.251424
O	-2.115331	-1.722708	-1.786768
O	-1.815849	-3.883183	-1.259151
C	-2.900250	-4.240507	-2.126815
H	-2.478252	-4.693099	-3.026386
H	-3.502378	-4.970980	-1.589427
H	-3.497913	-3.370505	-2.389001
C	3.250714	-2.683754	-0.345719
C	3.414835	-4.068935	0.044412
C	4.167812	-4.909243	-0.857116
C	4.662823	-4.452954	-2.036450
C	4.418585	-3.105884	-2.449828
C	3.720697	-2.268099	-1.640190
H	4.322326	-5.942557	-0.560874
H	5.231549	-5.117264	-2.679551
H	4.789568	-2.752961	-3.406391
H	3.516239	-1.250688	-1.946812
C	2.563053	-1.723915	0.422928
C	2.705859	-4.683905	1.066887
H	2.801481	-5.759021	1.178994
H	2.290210	-4.158582	1.913188
O	2.184139	-0.624185	-0.181489
H	1.528807	-0.012921	0.337647
C	2.406284	-1.783239	1.900842
C	3.556606	-1.964333	2.678457
C	1.163645	-1.620309	2.518730
C	3.458707	-1.996934	4.063426
H	4.516937	-2.079261	2.187461
C	1.071560	-1.675008	3.906406
H	0.273772	-1.460741	1.918715
C	2.214906	-1.862613	4.677939
H	4.352924	-2.130883	4.663076
H	0.101488	-1.574243	4.379032
H	2.137733	-1.901209	5.759833
H	-6.089576	3.876077	-1.517774
H	1.564160	6.127692	2.751621
C	-2.097503	4.759846	0.438787
C	-3.877983	5.685462	-0.957151
C	-2.369710	5.814666	-0.669942
C	-2.506985	5.338919	1.824602
C	-1.292917	6.172913	2.267153
H	-2.065998	6.820781	-0.367878
H	-1.798020	5.537707	-1.561575
H	-4.469731	6.322697	-0.288926
H	-4.140867	5.961869	-1.981673
H	-3.439284	5.908335	1.776025
H	-2.651902	4.504616	2.518665
H	-1.340514	7.192370	1.864980
H	-1.206371	6.257287	3.353538
H	-5.507191	-0.387676	-1.478543
H	-2.717647	-0.041247	1.779650
H	1.869264	2.934244	-2.250784
H	3.545114	2.246771	1.643679
C	-5.997259	-2.975131	-1.265636
F	-5.879052	-4.296077	-1.061057
F	-5.804017	-2.754533	-2.578250
F	-7.267185	-2.641070	-1.003786
C	-2.565871	-2.672677	2.349550
F	-1.577086	-3.381815	1.779874
F	-3.274100	-3.530797	3.095806
F	-1.992336	-1.788353	3.180310
C	3.663231	1.440525	-3.649650
F	3.831203	0.132990	-3.923420
F	4.697388	2.082363	-4.214166
F	2.551678	1.844948	-4.270680
C	5.566318	0.604379	0.850515
F	6.800417	1.091698	0.656813
F	5.619818	-0.706899	0.549110

F	5.294121	0.704804	2.157101

TS-[4+2]-B1-S

P	-1.222641	-0.115976	-0.669009
O	-0.462709	1.050484	-0.131544
O	-1.121213	-1.289062	0.444539
O	-2.802190	0.159846	-0.817415
C	-1.690146	-2.518499	0.117894
C	-3.049948	-2.708433	0.317591
C	-3.452183	0.590233	0.339687
C	-3.976591	-0.363558	1.199814
C	-3.652256	-3.877585	-0.156606
C	-2.886717	-4.886109	-0.724972
C	-4.550474	0.047456	2.406508
C	-4.664976	1.396154	2.712957
C	-1.509298	-4.709769	-0.830934
H	-0.891147	-5.498574	-1.248959
C	-0.884588	-3.520477	-0.438119
C	-4.169441	2.336227	1.813806
H	-4.249781	3.396391	2.034947
C	-3.531471	1.958834	0.626353
O	-0.867841	-0.693581	-2.043443
H	0.119964	-0.626463	-2.510779
C	0.589316	-3.353293	-0.599620
C	1.406232	-3.187728	0.534967
C	1.171884	-3.433975	-1.879381
C	2.788497	-3.083186	0.369166
C	2.557972	-3.339550	-1.996359
C	3.381648	-3.145526	-0.888541
C	-2.954199	2.999745	-0.272591
C	-1.901164	3.809373	0.187240
C	-3.497268	3.204457	-1.553104
C	-1.418457	4.820193	-0.643770
C	-2.976072	4.218794	-2.355052
C	-1.936118	5.037389	-1.918218
C	-4.073925	-1.871370	1.062345
H	-3.351411	-5.799276	-1.084645
H	-5.118211	1.715791	3.646550
C	-5.376374	-2.316009	0.340847
H	-5.464157	-1.753897	-0.594833
H	-6.269408	-2.121264	0.941544
C	-5.150848	-3.808924	0.033747
H	-5.696957	-4.146586	-0.851206
H	-5.470675	-4.441474	0.870828
C	-4.138061	-2.282134	2.562597
H	-3.117241	-2.300548	2.959274
H	-4.574841	-3.275099	2.700826
C	-4.935840	-1.153396	3.238580
H	-6.015501	-1.339389	3.182178
H	-4.684402	-1.027918	4.295102
N	3.581655	0.265501	-0.685435
C	2.426155	-0.140298	-1.209696
N	4.697412	0.559155	-0.802865
H	1.606627	-0.351519	-0.542176
C	2.322979	-0.368688	-2.599507
O	1.253010	-0.617683	-3.200862
O	3.463081	-0.287134	-3.286314
C	3.356770	-0.490510	-4.695089
H	4.365348	-0.365341	-5.083870
H	2.677035	0.239544	-5.137655
H	2.984351	-1.495420	-4.906175
C	3.538088	0.321588	2.177496
C	4.942147	0.569390	1.920805
C	5.880949	-0.343137	2.528949
C	5.494125	-1.357690	3.345367
C	4.107602	-1.574741	3.615913
C	3.174106	-0.781942	3.026093
H	6.934493	-0.180301	2.321429
H	6.238773	-2.003238	3.800300
H	3.804539	-2.368779	4.290693
H	2.119209	-0.937974	3.216689
C	2.479377	1.024995	1.564277
C	5.429683	1.460603	0.974156
H	6.496289	1.459471	0.776581
H	4.897687	2.345092	0.660041
O	1.308812	0.423726	1.542665
H	0.592492	0.857032	0.967488
C	2.519753	2.460819	1.172376
C	3.068509	3.374345	2.082907
C	1.944067	2.929700	-0.012657
C	3.063938	4.733836	1.800283
H	3.504794	3.004399	3.005884
C	1.968876	4.291273	-0.302741
H	1.482560	2.236908	-0.707136
C	2.523253	5.194337	0.599634
H	3.485372	5.434104	2.513830
H	1.537095	4.642364	-1.234341
H	2.531630	6.255689	0.372018
H	3.003628	-3.376080	-2.990104
H	3.413495	-2.928936	1.245882
H	-3.401081	4.378416	-3.343968
H	-0.611392	5.451971	-0.279023
C	0.335371	-3.587463	-3.127095
H	0.890328	-3.224497	-3.995050
H	0.069283	-4.634015	-3.309367
H	-0.592771	-3.015975	-3.053406
C	4.864694	-2.941422	-1.062078
H	5.357891	-3.853980	-1.412450
H	5.054707	-2.155028	-1.800279
H	5.331405	-2.636624	-0.121745
C	0.820901	-3.128206	1.923514
H	0.387028	-2.140731	2.113938
H	0.029131	-3.871257	2.055263
H	1.597420	-3.312662	2.669706
C	-4.639348	2.359969	-2.060317
H	-4.299424	1.347768	-2.299720
H	-5.430043	2.271270	-1.309474
H	-5.070140	2.797801	-2.963345
C	-1.370756	6.110550	-2.813419
H	-0.684264	5.682600	-3.551995
H	-2.161741	6.625488	-3.365220
H	-0.816968	6.855695	-2.236754
C	-1.271331	3.608262	1.544356
H	-0.292077	4.094095	1.582218
H	-1.886638	4.031310	2.345364
H	-1.138019	2.544523	1.755182

TS-[4+2]-B2-R

H	-0.934045	-0.651980	-2.553107
P	-1.016392	1.052343	-0.216873
O	-1.102773	0.161339	-1.415844
O	-0.014580	0.792939	0.870272
H	-4.109740	5.660875	2.519258
H	-4.043258	6.452366	0.944587
H	-1.379069	6.354848	2.789557
C	-3.825527	5.516289	1.473750
C	-1.269136	5.595907	2.021205
H	-5.539109	4.562948	0.437162
C	-4.541872	4.323706	0.817186
C	-2.371958	5.138300	1.313129
H	-4.640194	3.512322	1.545663
C	-0.018043	5.051888	1.744905
H	0.858648	5.398656	2.284035
H	-4.002929	5.737107	-1.399635
H	-5.995156	4.385886	-1.883852
C	-2.235431	4.154434	0.329441
C	-3.578063	3.856562	-0.313610
C	-3.838141	4.675953	-1.607583
C	-5.049358	3.981377	-2.264438
C	0.144468	4.049595	0.783090
C	-0.985020	3.604041	0.083770
C	-3.945834	2.466414	-0.792540
C	-4.870487	2.540459	-1.838844
H	-2.963137	4.585398	-2.259294
O	-2.465730	1.127150	0.537163
H	-5.064454	4.095279	-3.351549
C	-3.537595	1.225318	-0.334982
C	-5.438883	1.388197	-2.365846
O	-0.870555	2.564186	-0.823254
C	-4.121019	0.049751	-0.825265
H	-6.151119	1.445669	-3.183172
C	-5.077653	0.148458	-1.836862
H	-5.527465	-0.762104	-2.221789
C	1.492511	3.480584	0.530366
C	2.043550	3.481170	-0.753095
C	2.246379	2.971613	1.590625
C	3.345932	3.035369	-0.953158
C	3.538104	2.508420	1.370937
C	4.110711	2.562010	0.106452
H	5.124828	2.210367	-0.053716
C	-3.702926	-1.257206	-0.255439
C	-3.858793	-1.493651	1.110682
C	-3.138905	-2.256052	-1.054092
C	-3.488689	-2.716603	1.662329
C	-2.751569	-3.464607	-0.485282
C	-2.931562	-3.712870	0.872646
H	-2.635614	-4.662532	1.305109
N	1.739837	-2.961060	-1.347519
C	0.891282	-2.021160	-1.798051
N	2.179150	-4.028753	-1.349792
H	0.880372	-1.063627	-1.305904
C	0.076540	-2.248728	-2.896547
O	-0.809521	-1.388749	-3.286545
O	0.215559	-3.353748	-3.594837
C	-0.545249	-3.476485	-4.803000
H	-0.373106	-4.494769	-5.143599
H	-1.603335	-3.308887	-4.610236
H	-0.183419	-2.757836	-5.540693
C	3.841919	-1.693532	-0.094781
C	4.338677	-3.052401	-0.068026
C	5.615647	-3.287184	-0.696575
C	6.297586	-2.310067	-1.350102
C	5.743248	-0.998707	-1.466226
C	4.553316	-0.717376	-0.873182
H	6.016508	-4.295252	-0.646907
H	7.257684	-2.530610	-1.806119
H	6.268260	-0.229744	-2.022977
H	4.113228	0.266174	-0.961813
C	2.649637	-1.259589	0.528856
C	3.571115	-4.160597	0.275199
H	4.009572	-5.144544	0.144686
H	2.712774	-4.112986	0.928730
O	2.147990	-0.118282	0.142433
H	1.258451	0.217717	0.586077
C	2.013102	-1.925372	1.693679
C	2.811584	-2.251064	2.796352
C	0.636568	-2.166436	1.730345
C	2.239381	-2.829375	3.921143
H	3.876370	-2.045423	2.757986
C	0.074128	-2.759261	2.856755
H	0.011667	-1.906555	0.878973
C	0.870355	-3.090292	3.949003
H	2.859913	-3.074283	4.776679
H	-0.989645	-2.959233	2.887121
H	0.420515	-3.546217	4.825043
H	1.457229	3.840155	-1.592298
H	1.808710	2.915817	2.581951
H	-4.270445	-0.715896	1.746554
H	-2.976282	-2.070463	-2.111112
C	-2.070782	-4.517888	-1.309924
F	-2.506239	-5.746389	-1.003075
F	-0.743060	-4.516463	-1.115194
F	-2.277549	-4.332414	-2.625463
C	-3.747165	-2.957178	3.123276
F	-3.069428	-4.024634	3.578319
F	-5.045966	-3.177962	3.366557
F	-3.381398	-1.903898	3.864702
C	3.968890	3.110015	-2.317790
F	4.792829	2.068298	-2.536191
F	4.706711	4.220443	-2.466477
F	3.050580	3.111027	-3.290204
C	4.300041	1.841786	2.478458
F	3.884001	2.236956	3.687808
F	5.614770	2.088735	2.396622
F	4.153258	0.504375	2.426787

TS-[4+2]-B2-S

H	-1.362071	-1.051773	-2.013381
P	-1.213954	0.995503	-0.095912
O	-1.504266	0.084881	-1.246847
O	-0.145840	0.669269	0.909274
H	-3.396745	5.958607	2.858206
H	-3.526212	6.696164	1.261779

H	-0.622947	6.452845	2.632999
C	-3.301963	5.759796	1.787541
C	-0.696555	5.649279	1.906825
H	-5.233245	4.930584	1.081111
C	-4.210148	4.616757	1.306158
C	-1.930518	5.250363	1.413594
H	-4.253413	3.835970	2.072478
C	0.447509	4.992070	1.467523
H	1.423380	5.298605	1.831977
H	-3.870334	5.949140	-0.996861
H	-6.049565	4.821608	-1.120210
C	-2.032145	4.217062	0.475804
C	-3.483807	4.040099	0.055996
C	-3.857881	4.874743	-1.201064
C	-5.226969	4.314601	-1.639022
C	0.378136	3.927248	0.562058
C	-0.881885	3.546150	0.076594
C	-4.066395	2.695678	-0.330851
C	-5.133171	2.864983	-1.217935
H	-3.114136	4.682516	-1.981094
O	-2.551303	1.240837	0.804085
H	-5.406163	4.424565	-2.711765
C	-3.714897	1.420573	0.075082
C	-5.893141	1.776007	-1.624585
O	-0.987456	2.460930	-0.778897
C	-4.459617	0.301181	-0.323434
H	-6.724573	1.905481	-2.310534
C	-5.561235	0.504381	-1.159406
H	-6.148071	-0.356171	-1.467399
C	1.629434	3.234651	0.161437
C	1.940544	2.985816	-1.179016
C	2.565407	2.885231	1.136472
C	3.171755	2.436760	-1.523573
C	3.784231	2.320184	0.778065
C	4.109524	2.098358	-0.553305
H	5.060501	1.653023	-0.828130
C	-4.010129	-1.057879	0.064270
C	-3.598331	-1.340756	1.369505
C	-3.921205	-2.064431	-0.900969
C	-3.091872	-2.595412	1.692359
C	-3.418159	-3.313937	-0.563297
C	-2.991152	-3.592943	0.731413
H	-2.572210	-4.562115	0.981747
N	1.485177	-3.108977	-0.618639
C	0.454338	-2.333941	-1.003361
N	2.130670	-4.062315	-0.686460
H	0.189973	-1.491603	-0.384911
C	-0.221502	-2.611869	-2.185755
O	-1.213785	-1.909695	-2.614116
O	0.182475	-3.624880	-2.921473
C	-0.501469	-3.851333	-4.160798
H	-0.027834	-4.733038	-4.586276
H	-1.560606	-4.029569	-3.979989
H	-0.377012	-2.990448	-4.819648
C	2.422369	-1.961032	1.673354
C	2.916513	-3.317504	1.822906
C	2.376419	-4.074164	2.924765
C	1.468105	-3.559878	3.795059
C	1.006353	-2.217547	3.649406
C	1.464769	-1.455423	2.621545
H	2.720830	-5.097994	3.037497
H	1.089316	-4.170579	4.608571
H	0.292584	-1.810243	4.355818
H	1.126449	-0.429774	2.527335
C	2.767068	-1.115625	0.591648
C	3.638405	-4.014179	0.859944
H	3.817104	-5.070854	1.029707
H	4.279287	-3.545472	0.130853
O	2.076193	-0.075877	0.234389
H	1.129191	0.150017	0.621189
C	4.010361	-1.195417	-0.216302
C	3.923725	-1.025359	-1.599910
C	5.259027	-1.261355	0.406309
C	5.081793	-0.945999	-2.364546
H	2.944923	-0.930321	-2.059146
C	6.415431	-1.162113	-0.359967
H	5.313209	-1.367886	1.485035
C	6.328353	-1.009733	-1.743439
H	5.009551	-0.805447	-3.437630
H	7.385653	-1.192035	0.124558
H	7.233679	-0.931239	-2.336756
H	1.228163	3.247697	-1.954883
H	2.331159	3.040486	2.185636
H	-3.641282	-0.568878	2.129398
H	-4.193901	-1.853054	-1.929451
C	-3.282241	-4.391621	-1.597057
F	-4.000961	-5.477471	-1.282612
F	-2.003016	-4.799739	-1.707955
F	-3.673585	-3.988342	-2.815120
C	-2.690035	-2.888736	3.111360
F	-1.709914	-3.800822	3.171968
F	-3.721260	-3.374191	3.821120
F	-2.264281	-1.787379	3.745203
C	3.468954	2.198817	-2.977116
F	4.777840	2.018997	-3.202064
F	3.066105	3.229543	-3.735062
F	2.835532	1.109850	-3.451051
C	4.694131	1.857357	1.876686
F	4.802082	2.771350	2.852551
F	5.929206	1.581271	1.440511
F	4.215387	0.737403	2.454889

TS-[4+2]-B3-R

H	-0.133763	-0.642942	2.722100
P	1.157419	0.223295	0.501792
O	0.843791	-0.495327	1.784086
O	0.088430	0.795624	-0.370266
H	5.877070	1.389583	-3.346980
H	6.729634	1.899983	-1.889977
H	4.471268	3.840929	-3.174819
C	5.806482	1.434215	-2.256955
C	4.021765	3.344448	-2.320182
H	6.501794	-0.517019	-1.463347
C	5.582693	0.056558	-1.612584
C	4.593492	2.199133	-1.783630
H	4.910081	-0.535073	-2.243118

C	2.843463	3.832890	-1.763247
H	2.369242	4.717399	-2.178093
H	6.692662	1.338979	0.473922
H	7.255017	-1.038172	0.684641
C	4.014872	1.558215	-0.684842
C	4.852553	0.360433	-0.269188
C	5.897150	0.680210	0.834233
C	6.404471	-0.704220	1.291202
C	2.214297	3.192390	-0.688674
C	2.828147	2.049544	-0.155109
C	4.249166	-0.914332	0.291933
C	5.196907	-1.588841	1.066522
H	5.385427	1.180344	1.662999
O	1.995230	-0.757008	-0.502020
H	6.732512	-0.710462	2.334188
C	3.004924	-1.491851	0.089973
C	4.945836	-2.874671	1.528189
O	2.245632	1.364870	0.899438
C	2.734766	-2.800315	0.509645
H	5.683019	-3.403492	2.124811
C	3.731243	-3.484547	1.212835
H	3.527764	-4.499203	1.542683
C	0.923826	3.739899	-0.173195
C	0.869991	4.344286	1.097935
C	-0.224813	3.703905	-0.991579
C	2.003604	4.398999	1.972895
C	-0.354874	4.947084	1.545241
C	-1.438929	4.323334	-0.540253
C	-0.255882	3.007011	-2.245554
C	1.920532	4.991204	3.197744
H	2.938340	3.957819	1.644667
C	-0.398694	5.559617	2.837727
C	-1.473355	4.934551	0.712364
C	-2.601684	4.275804	-1.375880
H	0.633112	2.476407	-2.566377
C	-1.395215	2.947017	-2.992146
C	0.700003	5.580507	3.641775
H	2.790938	5.017641	3.845363
H	-1.334118	6.008409	3.160604
H	-2.395049	5.402937	1.051663
C	-2.586169	3.605392	-2.561065
H	-3.505423	4.769366	-1.027491
H	-1.405895	2.376993	-3.916253
H	0.655027	6.046736	4.620714
H	-3.479310	3.557915	-3.176717
C	1.423045	-3.434938	0.185525
C	1.121160	-3.762720	-1.154831
C	0.512791	-3.755898	1.211010
C	2.035538	-3.522660	-2.232702
C	-0.124131	-4.407278	-1.467704
C	-0.739525	-4.381369	0.882685
C	0.792955	-3.497553	2.592379
C	1.748558	-3.920888	-3.506365
H	2.980222	-3.035232	-2.017201
C	-0.391636	-4.799682	-2.818021
C	-1.035805	-4.675647	-0.446562
C	-1.647034	-4.724780	1.934831
H	1.707774	-2.975919	2.848961
C	-0.077114	-3.884045	3.568002
C	0.518320	-4.576784	-3.807236
H	2.464569	-3.740515	-4.301690
H	-1.338338	-5.288184	-3.031052
H	-1.980513	-5.157437	-0.688152
C	-1.318817	-4.505408	3.238347
H	-2.596300	-5.180432	1.667607
H	0.168591	-3.694556	4.608686
H	0.310566	-4.888711	-4.825705
H	-2.005802	-4.790474	4.029766
N	-3.371124	-1.422705	0.924964
C	-2.206249	-1.070651	1.494162
N	-4.350869	-2.031874	0.880304
H	-1.533575	-0.445783	0.934377
C	-1.972888	-1.275184	2.849638
O	-0.899503	-0.883051	3.435195
O	-2.921079	-1.827218	3.583309
C	-2.684388	-1.911252	4.990748
H	-3.555559	-2.420611	5.397501
H	-1.774235	-2.478153	5.190630
H	-2.589418	-0.911217	5.417546
C	-4.534664	0.812949	-0.446253
C	-5.575398	-0.169001	-0.651676
C	-6.904124	0.202364	-0.235934
C	-7.167768	1.386133	0.379698
C	-6.115187	2.308603	0.658280
C	-4.842103	2.014210	0.275830
H	-7.702329	-0.511995	-0.414812
H	-8.184421	1.628135	0.674215
H	-6.335270	3.244524	1.160391
H	-4.026366	2.703650	0.464900
C	-3.186212	0.631416	-0.837830
C	-5.336304	-1.500879	-0.977208
H	-6.182644	-2.178340	-1.021819
H	-4.436219	-1.831795	-1.475615
O	-2.292368	1.329688	-0.202515
H	-1.296086	1.150378	-0.418440
C	-2.759438	-0.127253	-2.043579
C	-3.469134	0.079175	-3.234601
C	-1.611938	-0.924701	-2.054504
C	-3.027798	-0.496705	-4.418749
H	-4.358679	0.701605	-3.218994
C	-1.166885	-1.488821	-3.245298
H	-1.048761	-1.102499	-1.145983
C	-1.871226	-1.276942	-4.426484
H	-3.579195	-0.327537	-5.338040
H	-0.260538	-2.083869	-3.240715
H	-1.518235	-1.718190	-5.353488

TS-[4+2]-B3-S

P	-1.177708	0.332723	-0.224440
O	0.033998	0.586423	0.627144
O	-2.273439	-0.222727	0.839456
O	-1.851678	1.722689	-0.733800
C	-3.493867	-0.609734	0.320136
C	-4.499782	0.334721	0.193722
C	-2.125865	2.677797	0.230903
C	-3.350322	2.649197	0.889190

C	-5.692805	-0.015735	-0.443756
C	-5.919201	-1.326404	-0.843267
C	-3.589454	3.561225	1.922414
C	-2.656974	4.538332	2.241870
C	-4.921851	-2.279367	-0.641107
H	-5.081649	-3.307452	-0.952441
C	-3.679444	-1.936587	-0.094670
C	-1.458340	4.581942	1.536332
H	-0.710444	5.332232	1.775166
C	-1.158552	3.645594	0.539816
O	-1.116630	-0.534233	-1.443725
H	-0.337804	-1.304509	-2.255676
C	-2.564219	-2.922070	-0.003181
C	-1.987407	-3.232648	1.246707
C	-2.079257	-3.538264	-1.178096
C	-2.479461	-2.692675	2.479971
C	-0.876781	-4.141204	1.313209
C	-1.001213	-4.483677	-1.089141
C	-2.605179	-3.252342	-2.481841
C	-1.903224	-3.014380	3.672371
H	-3.334350	-2.026214	2.455101
C	-0.285590	-4.436644	2.582665
C	-0.409451	-4.742830	0.146529
C	-0.558173	-5.156261	-2.272555
H	-3.352457	-2.474940	-2.584881
C	-2.170225	-3.927294	-3.583759
C	-0.782283	-3.894316	3.727964
H	-2.300396	-2.598379	4.592883
H	0.570789	-5.104830	2.607184
H	0.423843	-5.439831	0.202644
C	-1.148004	-4.914575	-3.477171
H	0.246246	-5.881130	-2.178871
H	-2.592070	-3.699065	-4.557259
H	-0.330972	-4.128809	4.687396
H	-0.831302	-5.458891	-4.362243
C	0.170793	3.693421	-0.136483
C	1.342238	3.498368	0.624316
C	0.261554	3.991261	-1.511870
C	1.309572	3.097393	2.001252
C	2.628567	3.645797	0.001828
C	1.553764	4.103809	-2.129441
C	-0.893028	4.208377	-2.331982
C	2.461041	2.904157	2.707242
H	0.348095	2.914585	2.467722
C	3.811970	3.451633	0.782262
C	2.704089	3.938689	-1.357937
C	1.635908	4.400419	-3.526832
H	-1.875993	4.145236	-1.878719
C	-0.772557	4.491422	-3.659970
C	3.734516	3.098563	2.095281
H	2.410973	2.582532	3.742955
H	4.776700	3.558857	0.290835
H	3.681420	4.032388	-1.827222
C	0.511621	4.585412	-4.272392
H	2.622092	4.478199	-3.976574
H	-1.661999	4.648984	-4.261360
H	4.639660	2.939421	2.673324
H	0.585611	4.810496	-5.331455
N	2.828654	-2.403409	-0.459767
C	1.662041	-1.993606	-0.986460
N	3.755040	-3.096158	-0.443800
H	1.053271	-1.323975	-0.401515
C	1.308105	-2.356687	-2.281372
O	0.259449	-1.926359	-2.882295
O	2.125283	-3.148798	-2.953999
C	1.860596	-3.317157	-4.350069
H	2.610794	-4.023871	-4.698957
H	0.854438	-3.707362	-4.500447
H	1.964382	-2.361752	-4.868745
C	4.673114	0.360440	0.144371
C	4.730641	0.739394	-1.198374
C	5.913523	1.246659	-1.727427
C	7.030392	1.404310	-0.910625
C	6.968922	1.044292	0.436579
C	5.796033	0.519901	0.962915
H	5.960006	1.529617	-2.774019
H	7.949193	1.811741	-1.320297
H	7.835084	1.179442	1.075799
H	5.733472	0.240064	2.010385
C	3.360130	-0.016748	0.727447
O	2.415896	0.693155	0.213715
H	1.389498	0.573715	0.454936
C	3.169132	-0.936314	1.799881
C	4.040154	-2.064546	2.061239
C	2.012143	-0.734749	2.627041
C	3.672235	-2.909251	3.166813
C	1.726415	-1.563308	3.668535
H	1.377822	0.122985	2.434477
C	2.575571	-2.674621	3.938161
H	4.309063	-3.765525	3.369967
H	0.855429	-1.380006	4.288039
H	2.345047	-3.338321	4.766615
H	-6.852462	-1.607100	-1.322171
H	-2.849280	5.247762	3.041089
C	-4.573934	1.767854	0.686156
C	-6.563615	1.208188	-0.622052
C	-5.573957	2.358777	-0.347200
C	-5.199040	1.833008	2.110207
C	-4.911268	3.264857	2.591301
H	-6.054295	3.272265	0.014845
H	-5.024306	2.600426	-1.263017
H	-7.391062	1.213033	0.097895
H	-7.006193	1.259514	-1.620505
H	-6.261182	1.572601	2.108711
H	-4.672700	1.117340	2.750856
H	-5.687648	3.962573	2.253770
H	-4.855158	3.346354	3.680101
C	5.007358	-2.540558	1.176400
H	5.532201	-1.912231	0.474436
H	5.501114	-3.474926	1.422694
H	3.837352	0.647728	-1.807837

TS-[4+2]-B4-R

P	1.197663	-0.234817	-0.435362
O	0.083307	-0.846515	0.358552
O	2.193103	0.361394	0.706413

O	2.110995	-1.363457	-1.161222
C	3.380616	0.945763	0.300442
C	4.489954	0.125987	0.129892
C	2.441185	-2.451030	-0.360550
C	3.586231	-2.381424	0.418265
C	5.680495	0.665969	-0.362568
C	5.794227	2.031327	-0.577842
C	3.857278	-3.401492	1.335983
C	3.033280	-4.514301	1.419525
C	4.692904	2.844574	-0.339447
H	4.793253	3.915936	-0.472071
C	3.449201	2.329831	0.059506
C	1.913378	-4.587902	0.595881
H	1.259405	-5.453196	0.644955
C	1.578620	-3.555775	-0.287889
O	0.932050	0.777946	-1.517432
H	0.252530	1.868319	-1.708904
C	2.286577	3.254475	0.187634
C	1.232964	3.048822	1.095601
C	2.257231	4.409543	-0.600462
C	0.196051	3.972001	1.217299
C	1.255446	5.370292	-0.463027
C	0.227200	5.136483	0.444425
H	-0.575606	5.865299	0.548743
C	0.315354	-3.622578	-1.065953
C	-0.857418	-4.036391	-0.433706
C	0.271827	-3.284305	-2.424141
C	-2.064858	-4.115756	-1.130313
C	-0.915740	-3.373070	-3.144747
C	-2.075045	-3.793349	-2.484949
H	-3.009894	-3.855814	-3.040363
N	-3.148969	1.844331	0.030953
C	-1.970880	1.721616	-0.598701
N	-4.038570	2.460611	0.425958
H	-1.506270	0.751817	-0.655502
C	-1.439525	2.818873	-1.286454
O	-0.329620	2.786859	-1.909433
O	-2.158710	3.927402	-1.312514
C	-1.744521	4.956494	-2.217771
H	-2.029232	4.678511	-3.235169
H	-2.281666	5.850816	-1.906688
H	-0.668374	5.105701	-2.160565
C	-4.500601	-0.651313	0.029341
C	-5.553095	0.175967	0.587501
C	-6.818038	0.169205	-0.112095
C	-7.013724	-0.531623	-1.257673
C	-5.944522	-1.283991	-1.838522
C	-4.732350	-1.317445	-1.226116
H	-7.622834	0.762827	0.311438
H	-7.983585	-0.513739	-1.745181
H	-6.107716	-1.831056	-2.760984
H	-3.909150	-1.884796	-1.647949
C	-3.211499	-0.783384	0.587632
C	-5.370094	1.122639	1.582432
H	-6.204071	1.768616	1.836039
H	-4.555817	1.102229	2.290834
O	-2.267810	-1.230365	-0.195886
H	-1.283362	-1.185013	0.140273
C	-2.910104	-0.643887	2.039082
C	-3.738748	-1.303897	2.955261
C	-1.794429	0.060168	2.498696
C	-3.463220	-1.244895	4.314863
H	-4.603420	-1.849795	2.589802
C	-1.530361	0.125438	3.864052
H	-1.132122	0.547407	1.790899
C	-2.361460	-0.523061	4.772451
H	-4.107258	-1.761927	5.018453
H	-0.664565	0.678305	4.214887
H	-2.148409	-0.473279	5.835373
H	6.726182	2.463536	-0.929563
H	3.245666	-5.309698	2.127653
C	4.695547	-1.345761	0.452848
C	6.699639	-0.423463	-0.600237
C	5.832425	-1.693929	-0.549017
C	5.207980	-1.537818	1.909265
C	5.067070	-3.048400	2.169696
H	6.383437	-2.591381	-0.254138
H	5.384154	-1.875569	-1.531249
H	7.462387	-0.427617	0.188145
H	7.222078	-0.302264	-1.553100
H	6.225673	-1.160375	2.043671
H	4.546273	-0.984385	2.583593
H	5.954752	-3.595891	1.829426
H	4.927469	-3.286380	3.227673
H	3.025078	4.566224	-1.352197
H	1.228088	2.164752	1.723727
H	1.178337	-2.949230	-2.919183
H	-0.838593	-4.251525	0.632356
C	1.301078	6.633356	-1.287258
C	-0.955584	3.741125	2.162462
C	-0.950880	-3.044867	-4.615748
C	-3.333694	-4.474203	-0.401509
H	2.115552	7.285296	-0.956530
H	1.472837	6.411493	-2.345278
H	0.369257	7.198476	-1.201510
H	-1.911300	3.795850	1.628885
H	-0.979380	4.502438	2.948591
H	-0.892935	2.762297	2.642109
H	-0.112047	-2.404164	-4.895918
H	-1.877809	-2.530406	-4.882508
H	-0.893884	-3.955351	-5.221608
H	-4.163828	-4.629811	-1.094841
H	-3.619595	-3.664569	0.280855
H	-3.208576	-5.381179	0.196814

TS-[4+2]-B4-S

H	0.624546	1.950221	-1.590033
P	1.223944	-0.287796	-0.278322
O	1.091187	0.722464	-1.383484
O	0.067300	-0.585878	0.639140
H	5.018953	-3.882685	2.913190
H	5.705183	-4.347175	1.356915
H	2.872420	-5.598511	2.237757
C	4.991854	-3.668765	1.841343
C	2.654218	-4.792536	1.543498
H	6.375871	-1.979012	1.457183

C	5.306463	-2.200381	1.514173
C	3.609222	-3.828655	1.256152
H	4.864052	-1.551225	2.276881
C	1.401910	-4.700090	0.945721
H	0.644485	-5.448774	1.155954
H	5.921479	-3.402500	-0.807421
H	7.377730	-1.441016	-0.567732
C	3.335278	-2.794148	0.354749
C	4.578145	-1.935169	0.163602
C	5.468691	-2.427947	-1.010915
C	6.499512	-1.298229	-1.209104
C	1.069774	-3.648607	0.082387
C	2.067519	-2.703055	-0.207068
C	4.547560	-0.444541	-0.132146
C	5.716376	-0.072626	-0.797165
H	4.843888	-2.520955	-1.905104
O	2.418912	0.080463	0.754389
H	6.861505	-1.230832	-2.238701
C	3.611565	0.520802	0.208413
C	5.998124	1.270941	-1.000731
O	1.777005	-1.617154	-1.024512
C	3.838701	1.891301	-0.017102
H	6.920432	1.578965	-1.484089
C	5.079226	2.228409	-0.583300
H	5.327048	3.275064	-0.716171
C	-0.316293	-3.556160	-0.450302
C	-0.577296	-3.268340	-1.794669
C	-1.393416	-3.802789	0.406270
C	-1.883051	-3.255203	-2.283354
C	-2.709483	-3.775066	-0.056822
C	-2.937933	-3.516804	-1.406549
H	-3.961985	-3.473948	-1.775898
C	2.827184	2.953726	0.269043
C	1.769608	2.786806	1.180198
C	2.913759	4.180149	-0.402608
C	0.816949	3.784156	1.385510
C	2.016522	5.219465	-0.160700
C	0.957363	5.003351	0.718984
H	0.223296	5.791108	0.882167
N	-2.760630	2.348779	0.075731
C	-1.580835	2.103505	-0.504109
N	-3.637968	3.017156	0.410600
H	-1.156358	1.120518	-0.420668
C	-0.923243	3.105603	-1.221621
O	0.199737	2.929171	-1.803480
O	-1.514445	4.280948	-1.328024
C	-0.898917	5.239793	-2.194904
H	-1.433343	6.171331	-2.018984
H	0.158444	5.341308	-1.955493
H	-1.012709	4.924710	-3.234432
C	-3.308798	0.073780	1.668039
C	-4.284585	1.019501	2.178143
C	-4.181484	1.354770	3.577915
C	-3.228567	0.826890	4.390042
C	-2.269778	-0.097439	3.875633
C	-2.304374	-0.442145	2.560003
H	-4.904042	2.063548	3.971886
H	-3.197294	1.103976	5.439283
H	-1.528760	-0.535732	4.534696
H	-1.591674	-1.164716	2.177149
C	-3.254338	-0.368477	0.320311
C	-5.135763	1.782599	1.391033
H	-5.754785	2.528620	1.877502
H	-5.434010	1.501440	0.392556
O	-2.179173	-0.832871	-0.228254
H	-1.228437	-0.742200	0.242313
C	-4.419533	-0.526977	-0.586940
C	-4.235984	-0.355176	-1.961589
C	-5.639373	-1.010211	-0.102905
C	-5.276285	-0.631991	-2.842586
H	-3.269918	-0.016122	-2.323228
C	-6.668288	-1.308222	-0.987900
H	-5.768050	-1.154197	0.965918
C	-6.490159	-1.114428	-2.357725
H	-5.135593	-0.483365	-3.908487
H	-7.609094	-1.695354	-0.610837
H	-7.297015	-1.343638	-3.046415
H	0.251283	-3.060760	-2.465741
H	-1.201435	-3.984479	1.461767
H	1.668203	1.864263	1.736277
H	3.681549	4.334589	-1.154078
C	2.200363	6.550876	-0.847720
C	-0.347941	3.545002	2.314802
C	-2.153336	-2.970605	-3.738987
C	-3.855290	-3.941017	0.908567
H	1.304558	7.171498	-0.760489
H	2.429847	6.424268	-1.910347
H	3.030586	7.106716	-0.400575
H	-1.251597	4.036748	1.940398
H	-0.146042	3.943583	3.314648
H	-0.559853	2.476355	2.413018
H	-2.089519	-3.884780	-4.338751
H	-1.427341	-2.260001	-4.142239
H	-3.155812	-2.555093	-3.873902
H	-4.811006	-4.001678	0.382283
H	-3.903469	-3.085250	1.593786
H	-3.738624	-4.840335	1.520548

TS-(3+2)-B2-1R2S5R

H	-0.182723	-0.144186	1.711218
P	-1.334108	-1.003920	0.115866
O	-1.149915	-0.331768	1.519261
O	-0.206235	-0.944351	-0.825156
H	-5.065243	-3.803534	-3.730600
H	-5.595414	-4.819210	-2.391273
H	-2.703534	-5.429855	-3.708447
C	-4.982342	-3.947498	-2.650363
C	-2.525259	-4.858965	-2.802576
H	-6.486879	-2.642240	-1.672535
C	-5.409137	-2.702827	-1.846840
C	-3.551946	-4.142047	-2.202450
H	-5.097686	-1.798045	-2.378835
C	-1.249046	-4.815537	-2.243955
H	-0.436413	-5.368251	-2.706025
H	-5.725650	-4.639882	-0.027581
H	-7.334297	-2.867561	0.524331

C	-3.316653	-3.411705	-1.034640
C	-4.601277	-2.799553	-0.519235
C	-5.329887	-3.750765	0.470854
C	-6.412458	-2.870782	1.118304
C	-0.973986	-4.046401	-1.108846
C	-2.036840	-3.349232	-0.517521
C	-4.649448	-1.495477	0.265677
C	-5.765433	-1.505147	1.111746
H	-4.613174	-4.076020	1.231961
O	-2.672546	-0.355516	-0.520573
H	-6.679663	-3.197466	2.126643
C	-3.853181	-0.356174	0.217731
C	1.454467	-3.621344	-1.481236
C	0.407903	-3.887833	-0.595132
C	-6.141894	-0.371814	1.817379
O	-1.801964	-2.492716	0.553351
C	-3.931350	3.050050	-0.164566
C	-4.232688	0.813146	0.892169
H	-7.010404	-0.387386	2.468412
C	-5.389244	0.790450	1.675118
C	2.739328	-3.389768	-1.006227
C	0.684539	-3.923373	0.772414
C	-3.264944	4.266461	-0.298339
C	-3.475972	2.092120	0.741899
H	-5.678314	1.697977	2.196089
C	3.017064	-3.413330	0.357074
C	1.974661	-3.681216	1.235308
C	-2.126960	4.541201	0.447131
C	-2.346961	2.377536	1.513018
C	-1.672264	3.580425	1.343132
C	3.802855	-3.003815	-1.995713
F	5.025022	-3.015760	-1.452749
F	3.585315	-1.765240	-2.472625
F	3.813075	-3.828087	-3.052774
C	2.200368	-3.697506	2.719015
F	1.343129	-2.862853	3.338781
F	3.439912	-3.314959	3.053314
F	1.996269	-4.912785	3.243459
H	1.252279	-3.543939	-2.545322
H	4.015505	-3.206126	0.724710
H	-0.113888	-4.113805	1.482277
H	-4.811901	2.847376	-0.766729
H	-1.985138	1.642362	2.219643
H	-1.583019	5.468367	0.305135
C	-3.743232	5.246975	-1.331032
F	-3.313615	4.911498	-2.561040
F	-3.304800	6.486954	-1.084720
F	-5.081347	5.286922	-1.389210
C	-0.408679	3.834914	2.113625
F	-0.634046	4.441263	3.285189
F	0.447849	4.598237	1.424839
F	0.236115	2.678139	2.393567
C	4.502197	2.108218	-0.442178
C	4.723048	1.905178	-1.892772
C	6.090320	2.147808	-2.349039
C	7.065241	2.603650	-1.535382
C	6.801716	2.889113	-0.144081
C	5.575829	2.647226	0.370371
H	6.296534	1.951768	-3.397697
H	8.062394	2.773295	-1.930487
H	7.587312	3.305064	0.477196
H	5.352932	2.864912	1.408170
C	3.185453	2.051218	0.116551
C	3.812756	1.413110	-2.766434
H	2.783517	1.198314	-2.509836
C	2.443166	-0.183899	1.560531
O	1.332723	0.072157	2.007017
C	2.823755	-0.022019	0.140382
H	2.092450	-0.350982	-0.598639
N	4.102822	-0.487981	-0.083011
N	5.160950	-0.082014	-0.233917
O	3.462253	-0.495005	2.342735
C	3.244983	-0.340031	3.751673
H	4.171516	-0.662672	4.220581
H	3.044764	0.711526	3.964890
H	2.409791	-0.957939	4.076496
O	3.123375	2.349720	1.468770
H	2.208975	2.580963	1.686153
H	4.110088	1.219286	-3.791477
C	2.019447	2.621591	-0.652954
C	0.751782	2.041592	-0.647054
C	2.204625	3.837317	-1.322381
C	-0.296515	2.620673	-1.356861
H	0.578727	1.116976	-0.114038
C	1.149707	4.432696	-2.003316
H	3.187861	4.297127	-1.320467
C	-0.101067	3.817751	-2.037516
H	-1.268160	2.131524	-1.363965
H	1.308742	5.372471	-2.522366
H	-0.923384	4.274244	-2.579385

TS-(3+2)-B2-1R2S5S

H	-0.638730	1.143439	1.004382
P	-1.819879	-0.427520	0.083908
O	-1.485932	0.644306	1.176944
O	-0.720788	-0.972745	-0.724528
H	-6.598774	-3.236451	-2.529679
H	-7.260638	-3.415587	-0.905542
H	-4.838222	-5.349100	-1.812227
C	-6.449593	-2.956419	-1.483793
C	-4.400848	-4.560504	-1.207903
H	-7.390631	-0.971626	-1.176159
C	-6.403731	-1.432444	-1.272255
C	-5.100284	-3.387883	-0.959305
H	-5.886817	-0.960612	-2.114161
C	-3.112752	-4.700398	-0.699912
H	-2.550088	-5.608527	-0.893807
H	-7.120458	-2.271449	1.166226
H	-8.048288	-0.014828	0.864357
C	-4.542020	-2.375448	-0.172139
C	-5.538671	-1.244419	0.008010
C	-6.426179	-1.433145	1.270377
C	-7.124061	-0.071966	1.451917
C	-2.501280	-3.680699	0.037374
C	-3.248406	-2.522033	0.302739
C	-5.118010	0.204334	0.186117

C	-6.087295	0.892364	0.923790
H	-5.775648	-1.631921	2.128229
O	-2.972631	0.185465	-0.880067
H	-7.389556	0.134524	2.491941
C	-4.003002	0.889444	-0.270814
C	-0.139639	-4.278075	-0.478542
C	-1.074886	-3.779656	0.431500
C	-5.989944	2.263061	1.117435
O	-2.664948	-1.463268	0.995236
C	-1.979677	2.692611	-1.702419
C	-3.865081	2.272882	-0.074614
H	-6.750162	2.799566	1.676541
C	-4.891920	2.943624	0.599421
C	1.212266	-4.313689	-0.155258
C	-0.620985	-3.315145	1.668550
C	-0.847090	3.403151	-2.078002
C	-2.646675	3.002095	-0.508661
H	-4.815464	4.018452	0.731327
C	1.665680	-3.837632	1.067452
C	0.736274	-3.324754	1.962952
C	-0.366803	4.455867	-1.308252
C	-2.136290	4.033564	0.284781
C	-1.020573	4.757508	-0.122480
C	2.199001	-4.771144	-1.193313
F	3.373103	-5.122390	-0.644033
F	2.450486	-3.807798	-2.087337
F	1.738139	-5.830774	-1.875668
C	1.178836	-2.674057	3.238951
F	2.486961	-2.864644	3.488424
F	0.498137	-3.125362	4.299542
F	0.981519	-1.342175	3.194445
H	-0.462959	-4.603844	-1.462301
H	2.720651	-3.836640	1.308612
H	-1.323553	-2.913371	2.390555
H	-2.341501	1.895536	-2.340544
H	-2.604258	4.266090	1.236554
H	0.497215	5.024824	-1.629413
C	-0.074260	2.967641	-3.290612
F	0.801391	1.999262	-2.969413
F	0.631358	3.976328	-3.819480
F	-0.871945	2.477863	-4.245683
C	-0.494452	5.832292	0.784227
F	-1.458224	6.680044	1.165243
F	0.477772	6.549603	0.203143
F	0.023220	5.304788	1.908059
C	4.574040	-0.738978	-0.548312
C	5.376843	0.154989	-1.423796
C	6.248886	-0.524154	-2.384424
C	6.363033	-1.864039	-2.467457
C	5.620312	-2.719989	-1.574663
C	4.783864	-2.173496	-0.667153
H	6.816062	0.117086	-3.053565
H	7.023907	-2.307035	-3.206367
H	5.732595	-3.797025	-1.630157
H	4.229890	-2.813319	0.005214
C	3.740616	-0.295309	0.545749
C	5.294242	1.504217	-1.490187
H	4.649655	2.091359	-0.854185
C	1.623219	1.713078	-0.062514
O	0.687830	2.022844	0.660956
C	2.005864	0.293274	-0.326987
H	1.289918	-0.408516	0.103552
N	2.239397	-0.053757	-1.632130
N	3.010240	-0.635303	-2.244761
O	2.476640	2.587220	-0.562685
C	2.575516	3.876810	0.062668
H	2.700446	4.610918	-0.732265
H	1.689774	4.085476	0.659394
H	3.464485	3.853155	0.700079
O	3.165163	-1.341852	1.279872
H	3.446462	-1.268164	2.201478
H	5.884751	2.038131	-2.226982
C	4.083740	0.844389	1.480048
C	5.364913	1.398747	1.566602
C	3.120928	1.243044	2.419166
C	5.647243	2.379570	2.512362
H	6.137351	1.067679	0.883956
C	3.402801	2.226829	3.362765
H	2.142469	0.771551	2.416893
C	4.665931	2.809000	3.404019
H	6.646688	2.799812	2.560117
H	2.635123	2.528447	4.067711
H	4.891272	3.576253	4.137604

TS-(3+2)-B2-1S2R5R

H	0.499395	0.153467	1.834084
P	0.927002	1.238172	0.039780
O	1.313172	0.462824	1.345817
O	-0.164307	0.707815	-0.799160
H	2.619615	5.788293	-3.609644
H	2.761146	6.790942	-2.166779
H	-0.194901	6.163739	-3.281506
C	2.583244	5.767123	-2.517538
C	-0.019912	5.484335	-2.453259
H	4.595623	5.198603	-1.778026
C	3.593357	4.780354	-1.904015
C	1.267147	5.242076	-1.994152
H	3.672084	3.892676	-2.540021
C	-1.089102	4.833131	-1.844666
H	-2.102651	5.027238	-2.181787
H	3.191784	6.444603	0.159221
H	5.467221	5.550348	0.385838
C	1.488133	4.370642	-0.923310
C	2.955579	4.361327	-0.546450
C	3.283666	5.423634	0.539622
C	4.705904	5.064039	1.007458
C	-0.894685	3.914913	-0.806197
C	0.416437	3.696458	-0.364027
C	3.660810	3.147419	0.033844
C	4.738638	3.564770	0.822249
H	2.579314	5.303170	1.369124
O	2.289367	1.365280	-0.805285
H	4.899534	5.357683	2.042397
C	3.448700	1.790376	-0.156494
C	-3.062408	2.715433	-1.050190
C	-2.052135	3.198802	-0.219119

C	5.646612	2.643602	1.323355
O	0.673699	2.732049	0.609220
C	3.726056	-1.077590	-1.204601
C	4.365124	0.833605	0.306874
H	6.491023	2.966943	1.923944
C	5.470734	1.294592	1.032540
C	-4.196503	2.113899	-0.510013
C	-2.176641	3.018616	1.165359
C	3.707501	-2.438072	-1.491334
C	4.221656	-0.616474	0.020349
H	6.207491	0.574071	1.372496
C	-4.341941	1.973281	0.861499
C	-3.308039	2.409657	1.688255
C	4.199769	-3.368485	-0.588260
C	4.668185	-1.561594	0.952164
C	4.666991	-2.915232	0.640563
C	-5.213789	1.534118	-1.453691
F	-6.329108	1.159164	-0.819609
F	-4.718182	0.458791	-2.082591
F	-5.556855	2.417251	-2.403968
C	-3.444830	2.194844	3.168238
F	-2.288446	2.371162	3.817668
F	-3.860854	0.939116	3.426672
F	-4.347696	3.018360	3.715826
H	-2.957821	2.790158	-2.128390
H	-5.219750	1.489988	1.276073
H	-1.389327	3.352705	1.831081
H	3.366231	-0.376255	-1.948186
H	5.017340	-1.241063	1.927897
H	4.196248	-4.425833	-0.827836
C	3.065248	-2.898740	-2.770768
F	1.731604	-2.907889	-2.663135
F	3.452214	-4.137886	-3.102336
F	3.373294	-2.087272	-3.793781
C	5.064647	-3.926665	1.675697
F	5.840902	-3.397045	2.629204
F	5.724177	-4.958397	1.133805
F	3.979276	-4.436869	2.287653
C	-3.419222	-2.844547	-1.058500
C	-3.865111	-3.929564	-0.148429
C	-5.069669	-4.643819	-0.569404
C	-5.696723	-4.394343	-1.735923
C	-5.192091	-3.398119	-2.656941
C	-4.105976	-2.667870	-2.332741
H	-5.445610	-5.407323	0.106260
H	-6.586348	-4.957282	-2.002223
H	-5.684173	-3.255313	-3.612780
H	-3.705918	-1.925785	-3.012218
C	-2.139032	-2.213169	-0.902925
C	-3.320113	-4.203811	1.057475
H	-3.770676	-4.962023	1.689391
C	-1.997491	-0.881710	2.093825
O	-0.946064	-0.351325	2.437517
C	-2.531398	-0.851056	0.713958
H	-2.164013	0.014657	0.158509
N	-3.912612	-0.906612	0.652586
N	-4.702793	-1.443511	0.012678
O	-2.747828	-1.563201	2.944726
C	-2.295251	-1.568772	4.302435
H	-3.045493	-2.129897	4.854593
H	-1.319466	-2.052165	4.370276
H	-2.224496	-0.544080	4.670526
O	-1.881105	-1.261753	-1.851229
H	-1.041302	-0.811690	-1.654476
H	-2.441117	-3.703827	1.442182
C	-0.939325	-3.014252	-0.467088
C	0.094765	-2.435965	0.264857
C	-0.809348	-4.346076	-0.875457
C	1.198862	-3.181409	0.662032
H	0.023931	-1.394287	0.535748
C	0.299383	-5.092469	-0.491944
H	-1.594986	-4.799667	-1.470432
C	1.294775	-4.521106	0.298338
H	1.977162	-2.712657	1.257571
H	0.378540	-6.129766	-0.801006
H	2.141671	-5.112798	0.631756

TS-(3+2)-B2-1S2R5S

H	-0.238586	-1.057756	-0.949530
P	-2.000854	-0.143592	-0.146397
O	-1.218448	-1.031391	-1.173681
O	-1.286455	0.885828	0.616817
H	-7.738323	0.318172	2.062173
H	-8.289138	-0.002160	0.418957
H	-7.175757	2.942623	1.083501
C	-7.400087	0.044755	1.059421
C	-6.359894	2.405441	0.610034
H	-7.256041	-2.166660	0.972664
C	-6.617381	-1.281216	1.032103
C	-6.386033	1.020818	0.510578
H	-6.001956	-1.363826	1.933761
C	-5.251780	3.098086	0.132166
H	-5.215554	4.179304	0.223342
H	-7.470278	-1.077236	-1.494773
H	-7.271365	-3.470926	-0.961179
C	-5.348373	0.333396	-0.125620
C	-5.675893	-1.149096	-0.200146
C	-6.463641	-1.503986	-1.493244
C	-6.444566	-3.042549	-1.540462
C	-4.154671	2.434308	-0.430687
C	-4.243382	1.038928	-0.576112
C	-4.618821	-2.244417	-0.220925
C	-5.112831	-3.362444	-0.902972
H	-5.919915	-1.101333	-2.353999
O	-2.789460	-1.144980	0.864627
H	-6.522501	-3.438870	-2.556132
C	-3.337294	-2.290483	0.308490
C	-2.469095	4.141722	0.209709
C	-2.877982	3.149940	-0.686183
C	-4.377744	-4.537392	-0.969384
O	-3.193269	0.328155	-1.137184
C	-0.717368	-2.816540	1.850774
C	-2.552136	-3.453570	0.224904
H	-4.771313	-5.408751	-1.483362
C	-3.112677	-4.578291	-0.390821
C	-1.205524	4.711948	0.117102

C	-1.989593	2.777706	-1.699642
C	0.612763	-2.874722	2.247512
C	-1.140710	-3.482286	0.691502
H	-2.533004	-5.495307	-0.432466
C	-0.288623	4.273010	-0.829514
C	-0.702065	3.299340	-1.729147
C	1.552708	-3.606573	1.529624
C	-0.185260	-4.189635	-0.047852
C	1.140520	-4.254380	0.372265
C	-0.815695	5.734980	1.144159
F	0.307525	6.383711	0.812683
F	-0.609731	5.169512	2.347922
F	-1.780671	6.650946	1.315039
C	0.280211	2.666365	-2.665146
F	1.441741	3.327189	-2.729165
F	-0.196554	2.539591	-3.906925
F	0.585605	1.406242	-2.247050
H	-3.122746	4.439538	1.023610
H	0.724310	4.658573	-0.845895
H	-2.272024	2.024449	-2.425756
H	-1.423924	-2.246621	2.441551
H	-0.473132	-4.679351	-0.973253
H	2.587695	-3.653073	1.852371
C	1.080214	-2.065192	3.424434
F	1.603064	-0.890661	3.018983
F	2.044078	-2.699739	4.105971
F	0.089213	-1.784875	4.273406
C	2.133901	-5.059806	-0.418967
F	2.116719	-6.351786	-0.063989
F	3.383087	-4.614177	-0.242311
F	1.864355	-5.014962	-1.735417
C	5.394917	0.619009	-0.620835
C	6.199557	0.671335	0.618092
C	7.642950	0.569436	0.417039
C	8.211733	0.547774	-0.807764
C	7.410159	0.622966	-2.004406
C	6.061109	0.646467	-1.905148
H	8.260533	0.532926	1.310277
H	9.292281	0.487616	-0.897889
H	7.892791	0.663330	-2.974537
H	5.434632	0.702922	-2.787547
C	3.971099	0.772416	-0.578601
C	5.702933	0.691526	1.879744
H	4.650719	0.793796	2.110935
C	2.279100	-1.421957	-0.563852
O	1.156518	-0.988346	-0.348821
C	3.414634	-1.038124	0.293052
H	3.187065	-0.911157	1.348239
N	4.533083	-1.804580	0.049385
N	5.578591	-1.701029	-0.400045
O	2.594959	-2.161911	-1.610348
C	1.589078	-2.240008	-2.629451
H	2.026925	-2.838362	-3.423793
H	0.689970	-2.723075	-2.240787
H	1.353193	-1.231988	-2.977749
O	3.349701	0.655006	-1.809681
H	2.546080	1.193394	-1.803721
H	6.386061	0.644847	2.721029
C	3.341629	1.843009	0.285826
C	2.053137	1.739598	0.821254
C	4.036414	3.053320	0.423339
C	1.490416	2.810321	1.516274
H	1.467934	0.833401	0.718137
C	3.474606	4.115079	1.119839
H	5.028095	3.145374	-0.007335
C	2.203339	3.993951	1.679811
H	0.485300	2.705282	1.913004
H	4.032443	5.039746	1.228128
H	1.768344	4.820841	2.229465

TS-(3+2)-B2-3R5R

H	0.245762	-0.094119	-1.388377
P	1.806167	0.233311	0.083123
O	0.791199	0.678262	-1.021337
O	1.296682	-0.478223	1.267031
H	7.554120	0.764219	1.960381
H	8.047690	0.366647	0.315245
H	6.952036	-1.996369	2.239398
C	7.180835	0.595245	0.947186
C	6.137957	-1.724090	1.574923
H	7.014534	2.570733	-0.048154
C	6.385932	1.793224	0.394676
C	6.161911	-0.519104	0.884987
H	5.799068	2.246137	1.200354
C	5.038387	-2.568946	1.432491
H	4.996637	-3.508086	1.976047
H	7.151766	0.628007	-1.888834
H	6.859159	3.020000	-2.376632
C	5.111394	-0.159391	0.034744
C	5.405902	1.168835	-0.640935
C	6.125826	0.987454	-2.007488
C	6.029557	2.370011	-2.680213
C	3.957373	-2.216713	0.621273
C	4.015026	-0.999709	-0.070475
C	4.311862	2.146229	-1.039172
C	4.714387	2.894401	-2.150693
H	5.571428	0.251288	-2.598572
O	2.588297	1.569209	0.527138
H	6.046149	2.313344	-3.771628
C	3.069338	2.397261	-0.480744
C	1.976476	-3.276469	1.704077
C	2.725548	-3.045582	0.548939
C	3.919000	3.920332	-2.643991
O	2.907689	-0.573844	-0.797359
C	0.722687	3.692777	1.031249
C	2.243388	3.426503	-0.952381
H	4.236051	4.499161	-3.505890
C	2.696501	4.189922	-2.031620
C	0.759396	-3.942746	1.628988
C	2.245445	-3.520047	-0.671372
C	-0.549455	3.844410	1.573505
C	0.900896	3.639111	-0.354331
H	2.067734	4.994340	-2.401742
C	0.279080	-4.425917	0.416578
C	1.042651	-4.219773	-0.726657
C	-1.671486	3.940735	0.758333

C	-0.222314	3.750323	-1.175158
C	-1.488719	3.899269	-0.619192
C	-0.080448	-4.025050	2.871795
F	-1.177256	-4.770604	2.691243
F	-0.484573	-2.800649	3.250051
F	0.604987	-4.542234	3.899947
C	0.596730	-4.779017	-2.045746
F	0.736270	-3.880408	-3.034949
F	-0.692527	-5.153034	-2.022362
F	1.315461	-5.853765	-2.397310
H	2.310237	-2.861873	2.650277
H	-0.677624	-4.932754	0.361815
H	2.801852	-3.327805	-1.583702
H	1.580217	3.605245	1.690720
H	-0.110596	3.673776	-2.252692
H	-2.662558	4.025536	1.188777
C	-0.680338	3.898727	3.071404
F	-0.267098	2.755498	3.642176
F	-1.941346	4.111101	3.461591
F	0.077591	4.879015	3.586079
C	-2.661406	4.026442	-1.546577
F	-2.685572	5.218561	-2.158517
F	-3.829997	3.879618	-0.908537
F	-2.613323	3.096826	-2.519405
C	-3.304003	0.466253	1.218223
C	-4.744152	0.126081	1.151107
C	-5.448611	0.189164	2.431421
C	-4.897818	0.707518	3.551988
C	-3.542815	1.193878	3.560637
C	-2.797034	1.054371	2.443046
H	-6.473395	-0.156913	2.444794
H	-5.490802	0.766765	4.459517
H	-3.119806	1.640100	4.454051
H	-1.751831	1.353319	2.440629
C	-2.348276	0.322115	0.192606
C	-5.456470	-0.352373	0.079742
H	-1.432575	0.901818	0.301319
C	-1.380015	-1.877127	-1.042112
O	-0.598315	-1.338344	-1.823138
C	-1.459291	-1.459948	0.361642
H	-0.508775	-1.254207	0.861431
N	-2.307993	-2.141734	1.187380
N	-3.134564	-1.998427	1.960099
O	-2.290544	-2.749232	-1.425497
C	-2.436421	-2.901617	-2.850628
H	-3.199342	-3.666396	-2.977117
H	-2.768549	-1.954220	-3.278909
H	-1.491749	-3.209546	-3.293531
H	-2.662507	0.210272	-0.838194
O	-6.670210	-0.956363	0.369328
H	-7.277396	-0.770424	-0.357546
C	-5.153982	-0.361918	-1.360269
C	-5.583558	-1.449365	-2.142404
C	-4.603423	0.748991	-2.018397
C	-5.451306	-1.430207	-3.527265
H	-6.021839	-2.310679	-1.647185
C	-4.453039	0.757411	-3.399168
H	-4.321421	1.618107	-1.434024
C	-4.879770	-0.330560	-4.162887
H	-5.790646	-2.280915	-4.111095
H	-4.027091	1.631136	-3.880435
H	-4.778491	-0.313172	-5.243223

TS-(3+2)-B2-3R5S

H	-0.917879	0.589727	1.909765
P	-1.305708	-0.938131	0.464596
O	-1.625768	-0.114933	1.751382
O	0.008071	-0.756689	-0.165443
H	-4.028698	-4.869740	-3.404042
H	-4.647442	-5.680685	-1.966616
H	-1.541861	-6.115832	-2.750770
C	-4.100249	-4.796632	-2.315847
C	-1.567021	-5.369458	-1.962935
H	-5.870675	-3.548950	-1.837339
C	-4.778549	-3.496157	-1.845930
C	-2.745945	-4.704656	-1.652718
H	-4.482135	-2.670644	-2.501275
C	-0.403229	-5.043067	-1.272491
H	0.525837	-5.549775	-1.515263
H	-5.208016	-5.075462	0.270645
H	-7.033975	-3.428983	0.212040
C	-2.776992	-3.757885	-0.625731
C	-4.190033	-3.239059	-0.427674
C	-4.978250	-4.067067	0.625833
C	-6.227087	-3.216850	0.923856
C	-0.384696	-4.051107	-0.283774
C	-1.604788	-3.434057	0.038434
C	-4.488402	-1.828449	0.056133
C	-5.706798	-1.808893	0.745204
H	-4.366671	-4.153146	1.529784
O	-2.493115	-0.655122	-0.609160
H	-6.627688	-3.386872	1.926471
C	-3.784199	-0.642090	-0.091415
C	2.014280	-3.446589	-0.531444
C	0.900948	-3.589232	0.300818
C	-6.246901	-0.618173	1.210560
O	-1.653341	-2.426800	0.994823
C	-3.370660	2.425463	-1.052671
C	-4.310965	0.575196	0.359908
H	-7.189152	-0.611966	1.749566
C	-5.551849	0.571238	0.999022
C	3.206814	-2.922734	-0.043209
C	1.020763	-3.202279	1.640101
C	-2.659049	3.616881	-1.182529
C	-3.536043	1.839191	0.202291
H	-5.956716	1.513152	1.356567
C	3.316592	-2.509248	1.276853
C	2.208225	-2.650439	2.105211
C	-2.072976	4.219887	-0.077456
C	-2.971881	2.461153	1.320655
C	-2.233428	3.628239	1.172037
C	4.375763	-2.786285	-0.979012
F	5.343603	-2.025439	-0.467210
F	3.998228	-2.247587	-2.151918
F	4.909972	-3.985335	-1.266827
C	2.245254	-2.066344	3.487090

F	3.488078	-2.008604	3.980596
F	1.489945	-2.755505	4.350194
F	1.770330	-0.800292	3.482203
H	1.937524	-3.699050	-1.585091
H	4.231855	-2.049543	1.634971
H	0.176056	-3.295383	2.313111
H	-3.806619	1.956137	-1.929229
H	-3.079668	2.004122	2.298156
H	-1.500740	5.135358	-0.187474
C	-2.610529	4.320416	-2.509701
F	-1.504539	5.069247	-2.636364
F	-3.658810	5.140774	-2.662821
F	-2.637501	3.460680	-3.540826
C	-1.607635	4.302396	2.360018
F	-2.186423	5.484113	2.614436
F	-0.301949	4.557740	2.141897
F	-1.691096	3.564456	3.472345
C	4.038298	0.829890	-0.047938
C	4.586888	0.862654	-1.431697
C	6.046350	0.858842	-1.551174
C	6.864484	0.891386	-0.481893
C	6.330771	0.927827	0.865235
C	4.997885	0.907112	1.051869
H	6.455937	0.833213	-2.553248
H	7.940498	0.884089	-0.624713
H	7.007742	0.958322	1.712493
H	4.578243	0.909908	2.056601
C	2.743462	0.426502	0.304512
C	3.869409	1.029892	-2.576419
H	2.583373	0.168498	1.349168
C	1.099366	2.188424	1.701102
O	0.132616	1.639120	2.215090
C	1.470802	2.083698	0.281323
H	0.696092	1.847100	-0.443255
N	2.388877	3.010555	-0.103849
N	3.517219	3.161559	-0.229463
O	1.988404	2.850382	2.424049
C	1.754711	2.851521	3.839001
H	2.554206	3.455649	4.261319
H	0.777983	3.285759	4.052569
H	1.793915	1.828553	4.217490
H	2.103405	-0.122567	-0.369565
O	4.565321	1.247756	-3.747794
H	3.968828	1.075250	-4.484431
C	2.399550	1.134815	-2.755904
C	1.848887	2.374548	-3.122764
C	1.561042	0.020536	-2.671921
C	0.481915	2.501708	-3.345931
H	2.505019	3.236918	-3.206840
C	0.194266	0.146620	-2.904260
H	1.985475	-0.942840	-2.406584
C	-0.347952	1.384291	-3.232012
H	0.061212	3.466911	-3.607259
H	-0.448147	-0.720601	-2.798969
H	-1.413914	1.481145	-3.403086

TS-(3+2)-B2-3S5R

H	0.514916	0.004220	-1.481283
P	1.357672	-0.862600	0.346195
O	1.193500	0.230878	-0.760848
O	0.679793	-0.709558	1.639435
H	4.467739	-5.720104	2.036379
H	4.141662	-6.428956	0.455987
H	1.757277	-6.391289	2.612450
C	4.042727	-5.512880	1.050959
C	1.578966	-5.563317	1.933419
H	5.621512	-4.576487	-0.194644
C	4.710921	-4.314737	0.351479
C	2.597816	-5.075865	1.126841
H	4.964887	-3.550826	1.093475
C	0.322366	-4.964806	1.871247
H	-0.490815	-5.335697	2.487602
H	3.701328	-5.624553	-1.751335
H	5.654106	-4.380752	-2.578336
C	2.372785	-4.002629	0.259232
C	3.607083	-3.745470	-0.584942
C	3.572097	-4.551141	-1.915225
C	4.679485	-3.919391	-2.778787
C	0.083169	-3.862413	1.046431
C	1.132568	-3.381052	0.257254
C	3.970748	-2.368709	-1.108531
C	4.663609	-2.480299	-2.318336
H	2.599078	-4.392844	-2.391737
O	2.957178	-0.994753	0.568390
H	4.490691	-4.016825	-3.851019
C	3.753637	-1.113533	-0.563373
C	-1.719025	-2.414046	2.037922
C	-1.276028	-3.248586	1.008690
C	5.192563	-1.357018	-2.938511
O	0.961228	-2.211631	-0.479390
C	4.175480	1.617184	0.787582
C	4.279908	0.039618	-1.163844
H	5.734953	-1.443920	-3.874797
C	5.011728	-0.109750	-2.346752
C	-3.025582	-1.937214	2.027284
C	-2.150886	-3.575957	-0.028423
C	4.002129	2.899404	1.303753
C	4.055996	1.386421	-0.584033
H	5.438445	0.775144	-2.809323
C	-3.909107	-2.283347	1.010504
C	-3.457902	-3.096641	-0.020853
C	3.710473	3.972954	0.475026
C	3.742809	2.465383	-1.418929
C	3.577770	3.738672	-0.891681
C	-3.527190	-1.059899	3.139728
F	-4.231410	-1.758398	4.040990
F	-4.340083	-0.098433	2.670828
F	-2.527899	-0.456546	3.798858
C	-4.428956	-3.492268	-1.096012
F	-3.816273	-4.114847	-2.119372
F	-5.074384	-2.432380	-1.601912
F	-5.364491	-4.329323	-0.627925
H	-1.028345	-2.115612	2.818118
H	-4.921752	-1.891053	1.002851
H	-1.815352	-4.223645	-0.831835
H	4.407461	0.796106	1.458021

H	3.612124	2.303607	-2.483904
H	3.580615	4.968944	0.883133
C	4.148551	3.091006	2.787740
F	3.283174	2.319107	3.462275
F	3.933754	4.359596	3.154742
F	5.376553	2.749610	3.204115
C	3.156692	4.871876	-1.783464
F	3.507707	4.663928	-3.058470
F	3.695090	6.033930	-1.392583
F	1.821025	5.035496	-1.764027
C	-3.961586	2.594253	-1.624110
C	-4.338177	3.539440	-0.535053
C	-5.687653	4.104997	-0.599795
C	-6.578162	3.756627	-1.547371
C	-6.233600	2.792617	-2.574461
C	-5.001196	2.256057	-2.598140
H	-5.954803	4.823043	0.165572
H	-7.567436	4.202955	-1.550223
H	-6.967152	2.522062	-3.326452
H	-4.721742	1.545313	-3.372647
C	-2.650415	2.239522	-1.982285
C	-3.603685	3.807471	0.579538
H	-1.801545	2.825638	-1.662228
C	-1.755635	-0.369838	-1.889750
O	-0.635636	-0.452192	-2.385908
C	-2.087911	0.580633	-0.821612
H	-1.287076	0.889504	-0.152674
N	-3.289543	0.374307	-0.221687
N	-4.371914	0.754180	-0.246837
O	-2.800182	-1.017356	-2.378117
C	-2.546593	-1.831023	-3.531605
H	-3.507057	-2.270355	-3.786367
H	-2.161227	-1.212098	-4.343313
H	-1.818781	-2.606492	-3.286863
H	-2.533092	1.788714	-2.965660
O	-4.190496	4.550275	1.577138
H	-3.506879	4.794214	2.210734
C	-2.252790	3.307538	0.936115
C	-1.097665	3.819091	0.336831
C	-2.127207	2.345051	1.950661
C	0.156855	3.332887	0.694875
H	-1.189250	4.590956	-0.422665
C	-0.872361	1.857384	2.304008
H	-3.022572	1.952160	2.424998
C	0.270550	2.347198	1.671527
H	1.040313	3.718658	0.199656
H	-0.779364	1.069058	3.041276
H	1.243313	1.951109	1.943874

TS-(3+2)-B2-3S5S

H	0.657840	1.000639	-1.041326
P	1.673425	-0.559729	0.054464
O	1.459020	0.399602	-1.156850
O	0.532896	-0.864148	0.933438
H	5.708469	-3.587295	3.387827
H	6.439439	-4.151064	1.886149
H	3.655507	-5.480611	2.839964
C	5.684680	-3.472100	2.301224
C	3.409479	-4.749384	2.076314
H	6.985180	-1.754622	1.771894
C	5.927100	-2.020236	1.847591
C	4.320209	-3.763886	1.720584
H	5.450818	-1.330983	2.552409
C	2.161367	-4.775394	1.458399
H	1.438961	-5.541230	1.724486
H	6.650584	-3.361880	-0.348068
H	7.912231	-1.249723	-0.361756
C	4.005197	-2.820666	0.737091
C	5.194638	-1.913825	0.479279
C	6.109535	-2.461972	-0.653146
C	7.028621	-1.279223	-1.010839
C	1.798516	-3.814389	0.509870
C	2.743962	-2.838743	0.164480
C	5.037317	-0.472572	0.027541
C	6.132632	-0.090213	-0.753243
H	5.483985	-2.714841	-1.515340
O	2.888996	0.036043	0.952523
H	7.386467	-1.315390	-2.042934
C	4.031092	0.446730	0.279393
C	-0.683891	-3.920680	0.753967
C	0.434935	-3.793395	-0.075415
C	6.255627	1.213880	-1.212819
O	2.374517	-1.807965	-0.697457
C	2.342782	2.846948	1.247831
C	4.116804	1.766464	-0.187660
H	7.110633	1.512543	-1.811152
C	5.254371	2.133897	-0.914849
C	-1.962165	-3.902595	0.212893
C	0.241122	-3.644889	-1.449101
C	1.332461	3.788015	1.411484
C	3.014777	2.738221	0.023397
H	5.342330	3.158991	-1.261947
C	-2.157932	-3.756508	-1.157901
C	-1.046306	-3.627858	-1.979226
C	0.968299	4.644683	0.376693
C	2.628570	3.579260	-1.022792
C	1.621759	4.521662	-0.841566
C	-3.168115	-4.090610	1.090332
F	-4.131826	-3.205347	0.799280
F	-2.868713	-3.960518	2.389601
F	-3.701423	-5.310979	0.925410
C	-1.213961	-3.441294	-3.461308
F	-2.410822	-3.882667	-3.885579
F	-0.273485	-4.102500	-4.148991
F	-1.123752	-2.151584	-3.816282
H	-0.552684	-4.002988	1.827620
H	-3.160288	-3.756089	-1.573566
H	1.095934	-3.547035	-2.109918
H	2.607874	2.194864	2.072734
H	3.104180	3.482992	-1.994224
H	0.183674	5.379504	0.518987
C	0.660645	3.927031	2.749810
F	-0.576993	4.425695	2.624518
F	1.340012	4.747244	3.561931
F	0.564224	2.744170	3.377064
C	1.218900	5.365030	-2.017628

F	2.280610	5.919026	-2.616098
F	0.386525	6.356484	-1.661074
F	0.584115	4.632812	-2.945793
C	-3.718754	-0.132947	1.602498
C	-4.971248	0.553363	1.208580
C	-5.912800	0.802166	2.297792
C	-5.816206	0.158165	3.482280
C	-4.740217	-0.766918	3.746094
C	-3.739125	-0.886801	2.846752
H	-6.746005	1.464361	2.097254
H	-6.572143	0.322107	4.244360
H	-4.727118	-1.333184	4.671000
H	-2.892991	-1.540379	3.042132
C	-2.540245	-0.177613	0.834888
C	-5.278706	1.023467	-0.034503
H	-2.557390	0.026240	-0.229065
C	-1.294800	2.260090	0.059542
O	-0.527592	2.001447	-0.859536
C	-1.404799	1.443639	1.282345
H	-0.487632	0.972786	1.626295
N	-2.141328	2.008743	2.283344
N	-3.107129	1.875101	2.878484
O	-2.173822	3.247526	-0.003639
C	-2.198174	3.999753	-1.224169
H	-3.113528	4.586382	-1.179388
H	-1.329758	4.656480	-1.277630
H	-2.200865	3.326736	-2.081798
H	-1.787516	-0.909578	1.117488
O	-6.297263	1.953107	-0.132047
H	-6.745462	1.818944	-0.976252
C	-4.672698	0.672048	-1.331534
C	-4.390818	-0.660889	-1.673534
C	-4.479339	1.666110	-2.299706
C	-3.887286	-0.973755	-2.926927
H	-4.560970	-1.438028	-0.933165
C	-3.963495	1.349653	-3.555574
H	-4.729054	2.693934	-2.050744
C	-3.658392	0.030549	-3.870394
H	-3.684123	-2.006028	-3.189812
H	-3.803295	2.136222	-4.287047
H	-3.251253	-0.224024	-4.843203

TS-(3+2)-B4-1R2S5R

H	-0.225295	0.311731	2.012192
P	-1.397115	-0.391280	0.383654
O	-1.187960	0.210957	1.825702
O	-0.189678	-0.693267	-0.398022
H	-5.549846	-1.995325	-3.753909
H	-6.465918	-2.718738	-2.432892
H	-3.838048	-4.282586	-3.518704
C	-5.586069	-2.106828	-2.667069
C	-3.547213	-3.760828	-2.611965
H	-6.639418	-0.336299	-1.841643
C	-5.632783	-0.754583	-1.929009
C	-4.328468	-2.729984	-2.106700
H	-5.005803	-0.027864	-2.455762
C	-2.364007	-4.101296	-1.958970
H	-1.740239	-4.899694	-2.349362
H	-6.690336	-2.382110	-0.082051
H	-7.666622	-0.157522	0.266177
C	-3.949169	-2.067101	-0.937274
C	-4.991290	-1.042512	-0.538890
C	-6.060091	-1.640528	0.416852
C	-6.836417	-0.416572	0.934407
C	-1.927084	-3.417988	-0.817844
C	-2.757279	-2.402659	-0.322533
C	-4.661472	0.251970	0.194225
C	-5.780287	0.665278	0.927183
H	-5.545709	-2.132846	1.248595
O	-2.360804	0.618754	-0.426670
H	-7.261531	-0.573188	1.929492
C	-3.534410	1.066599	0.175855
C	0.515604	-3.821366	-1.050992
C	-0.596291	-3.691748	-0.216908
C	-5.816145	1.912528	1.533627
O	-2.351772	-1.632107	0.764758
C	-2.540034	4.321999	-0.376589
C	-3.556341	2.349679	0.740833
H	-6.688594	2.228973	2.097313
C	-4.717905	2.758706	1.401854
C	1.794425	-4.011631	-0.526854
C	-0.418642	-3.761407	1.168878
C	-1.526752	5.268206	-0.553915
C	-2.422205	3.310248	0.577890
H	-4.735378	3.752100	1.839420
C	1.942033	-4.078777	0.858957
C	0.848091	-3.951533	1.717870
C	-0.380067	5.171178	0.231116
C	-1.268545	3.248617	1.364522
C	-0.232043	4.162844	1.185089
C	2.991437	-4.078926	-1.442552
C	1.038547	-4.036245	3.211567
H	0.387985	-3.718200	-2.125771
H	2.936121	-4.213965	1.281731
H	-1.277723	-3.653442	1.824614
H	-3.433988	4.366494	-0.994081
H	-1.184103	2.474692	2.117899
H	0.435322	5.874244	0.071151
C	-1.674255	6.368408	-1.574183
C	1.051741	4.039831	1.966719
C	5.082326	0.477260	-0.448034
C	5.097484	-0.114265	-1.800160
C	6.412084	-0.551918	-2.260333
C	7.544764	-0.344830	-1.552314
C	7.515795	0.328475	-0.279394
C	6.326369	0.708612	0.246166
H	6.452651	-1.046521	-3.227087
H	8.497258	-0.679610	-1.952773
H	8.442145	0.528710	0.247383
H	6.276560	1.219003	1.201155
C	3.868575	1.002592	0.102869
C	4.004090	-0.369977	-2.565749
H	2.999674	-0.058063	-2.310914
C	2.322204	-0.473495	1.884573
O	1.448576	0.327816	2.185651
C	2.782736	-0.698069	0.494086

H	1.983424	-0.861605	-0.232421
N	3.773689	-1.655625	0.454579
N	4.889894	-1.779397	0.266312
O	3.021936	-1.134460	2.796853
C	2.731377	-0.798388	4.157385
H	3.390577	-1.421315	4.757845
H	2.936148	0.260103	4.327111
H	1.685058	-1.010376	4.383571
O	4.008083	1.527076	1.382240
H	3.237453	2.086623	1.551497
H	4.131511	-0.877054	-3.516636
C	2.970405	1.851827	-0.767929
C	1.579291	1.844538	-0.666918
C	3.582071	2.765655	-1.636877
C	0.805114	2.691177	-1.457665
H	1.082584	1.162226	0.009229
C	2.810789	3.628634	-2.405551
H	4.664683	2.778241	-1.713931
C	1.419114	3.586308	-2.325753
H	-0.277940	2.649922	-1.375338
H	3.298255	4.328511	-3.076890
H	0.815268	4.251978	-2.935467
H	2.810816	-4.762199	-2.277000
H	3.217070	-3.093357	-1.869764
H	3.882076	-4.417860	-0.907854
H	2.017893	-3.643764	3.499836
H	0.982973	-5.073008	3.559404
H	0.267067	-3.469993	3.740535
H	-2.241774	6.028120	-2.443954
H	-0.698354	6.720705	-1.917386
H	-2.205199	7.227103	-1.150152
H	1.910358	4.156842	1.295210
H	1.118365	3.060913	2.451977
H	1.129899	4.809169	2.741671

TS-(3+2)-B4-1R2S5S

H	-0.250672	1.331727	1.294637
P	-1.377861	-0.099664	0.105236
O	-1.075143	0.771133	1.370694
O	-0.235090	-0.586779	-0.693200
H	-5.550329	-2.216670	-3.679047
H	-6.499526	-2.685725	-2.269565
H	-3.917997	-4.461477	-3.067992
C	-5.600930	-2.143891	-2.589529
C	-3.618075	-3.818790	-2.245786
H	-6.612645	-0.235073	-2.084175
C	-5.617421	-0.688614	-2.087574
C	-4.367475	-2.698486	-1.915370
H	-4.964790	-0.075612	-2.717724
C	-2.461994	-4.100470	-1.521853
H	-1.866523	-4.975825	-1.762342
H	-6.760060	-1.935827	-0.014402
H	-7.624072	0.365728	-0.018260
C	-3.977589	-1.865416	-0.861842
C	-4.999992	-0.760311	-0.661293
C	-6.095274	-1.156760	0.369149
C	-6.815007	0.165763	0.694898
C	-2.019959	-3.266192	-0.489372
C	-2.801388	-2.143874	-0.183322
C	-4.628019	0.618541	-0.145414
C	-5.703762	1.179500	0.547924
H	-5.603615	-1.539843	1.269285
O	-2.355189	0.732963	-0.871768
H	-7.257061	0.173479	1.694726
C	-3.459332	1.349445	-0.289761
C	0.415209	-3.836379	-0.472754
C	-0.758453	-3.568699	0.236552
C	-5.633294	2.483015	1.019887
O	-2.332714	-1.216695	0.756773
C	-1.291853	3.410101	-1.083893
C	-3.344938	2.662937	0.187321
H	-6.471291	2.926749	1.548820
C	-4.466473	3.215572	0.819319
C	1.596122	-4.175238	0.193655
C	-0.743661	-3.631770	1.632489
C	-0.147338	4.197276	-1.193035
C	-2.084550	3.444256	0.073280
H	-4.407624	4.241137	1.169804
C	1.572805	-4.259033	1.585203
C	0.415593	-3.990241	2.317532
C	0.202948	5.029971	-0.125524
C	-1.689833	4.264081	1.132533
C	-0.552989	5.069616	1.043222
C	2.867052	-4.429218	-0.575291
C	0.409510	-4.104858	3.820377
H	0.412411	-3.752008	-1.557841
H	2.487609	-4.514994	2.114991
H	-1.653961	-3.413849	2.185439
H	-1.583691	2.776153	-1.915136
H	-2.271954	4.265055	2.050767
H	1.091952	5.653177	-0.210870
C	0.685658	4.188978	-2.449594
C	-0.157392	5.948256	2.203434
C	4.415440	-0.288915	-1.270471
C	5.467084	0.504651	-0.592338
C	6.732053	0.605601	-1.319125
C	6.979335	-0.079847	-2.453938
C	5.988508	-0.966710	-3.021998
C	4.767938	-1.060295	-2.453143
H	7.494310	1.248986	-0.887967
H	7.943336	0.018690	-2.944212
H	6.234646	-1.555385	-3.898855
H	4.006203	-1.711687	-2.865451
C	3.166477	-0.583567	-0.624504
C	5.304151	1.202426	0.554880
H	4.406153	1.156073	1.157465
C	2.008679	2.260562	0.337486
O	1.179857	2.138022	1.229837
C	2.164895	1.305403	-0.778308
H	1.223495	0.873618	-1.117191
N	2.903532	1.794599	-1.843292
N	3.820170	1.470731	-2.453867
O	2.907920	3.239908	0.333411
C	2.980934	4.024571	1.525700
H	3.649940	4.850660	1.292318
H	1.991222	4.385021	1.805491

H	3.393020	3.417574	2.335718
O	2.305299	-1.285853	-1.422031
H	1.449477	-1.405453	-0.968824
H	6.112557	1.825431	0.923456
C	3.138069	-0.978599	0.831297
C	4.224264	-1.686117	1.364988
C	2.022604	-0.762382	1.637249
C	4.212054	-2.101721	2.691022
H	5.086925	-1.887312	0.737968
C	2.011881	-1.168176	2.968954
H	1.159302	-0.266223	1.223103
C	3.113240	-1.825591	3.504750
H	5.067235	-2.636415	3.092515
H	1.134399	-0.969843	3.576970
H	3.113631	-2.133453	4.546122
H	-0.977956	6.610877	2.493017
H	0.705640	6.570697	1.954012
H	0.098650	5.345848	3.081506
H	0.422537	5.032601	-3.096216
H	1.750235	4.269992	-2.212660
H	0.534022	3.270124	-3.021177
H	1.427762	-4.123893	4.215617
H	-0.120213	-3.264438	4.278316
H	-0.093473	-5.023233	4.140731
H	3.680188	-4.714102	0.096370
H	2.730971	-5.229764	-1.308955
H	3.169022	-3.527401	-1.116851

TS-(3+2)-B4-1S2R5R

H	-0.246267	0.574303	1.799786
P	-1.284071	-0.266721	0.085669
O	-1.119589	0.670780	1.331233
O	-0.112160	-0.502213	-0.779610
H	-5.253336	-3.210951	-3.367754
H	-5.906462	-3.934592	-1.899363
H	-3.102949	-5.074655	-3.015164
C	-5.196386	-3.188240	-2.276289
C	-2.866738	-4.390070	-2.206190
H	-6.552652	-1.588002	-1.552053
C	-5.487546	-1.793154	-1.691698
C	-3.801828	-3.464866	-1.764005
H	-5.076085	-1.024097	-2.353543
C	-1.611887	-4.424209	-1.603587
H	-0.875165	-5.154012	-1.924618
H	-6.035158	-3.349054	0.417398
H	-7.421554	-1.334932	0.650718
C	-3.489584	-2.587197	-0.722632
C	-4.701102	-1.759565	-0.349222
C	-5.535138	-2.442774	0.770525
C	-6.503375	-1.347442	1.250719
C	-1.252592	-3.526058	-0.590850
C	-2.218774	-2.602725	-0.173429
C	-4.603148	-0.346469	0.199310
C	-5.699679	-0.087412	1.028459
H	-4.858808	-2.721281	1.585291
O	-2.510152	0.361908	-0.743048
H	-6.802546	-1.472036	2.294887
C	-3.684636	0.664641	-0.047296
C	1.216629	-3.708256	-0.839465
C	0.109020	-3.576273	-0.003481
C	-5.917265	1.184815	1.535663
O	-1.889065	-1.610243	0.752785
C	-2.568097	3.293800	-1.256236
C	-3.896441	1.972817	0.413593
H	-6.770391	1.388619	2.175668
C	-5.033562	2.204706	1.198392
C	2.501118	-3.876283	-0.315100
C	0.299805	-3.551042	1.385210
C	-1.900550	4.459284	-1.636714
C	-3.019288	3.118026	0.054923
H	-5.220146	3.216678	1.543121
C	2.652688	-3.914540	1.068830
C	1.568988	-3.717791	1.931258
C	-1.692916	5.454997	-0.682480
C	-2.746357	4.111610	1.002949
C	-2.085529	5.285896	0.647260
C	3.691292	-3.946166	-1.234107
C	1.797088	-3.661032	3.420268
H	1.078993	-3.662185	-1.916972
H	3.647091	-4.051132	1.489488
H	-0.557281	-3.418750	2.039420
H	-2.763917	2.524227	-1.996897
H	-3.061095	3.964934	2.032990
H	-1.197776	6.379176	-0.976716
C	-1.380181	4.620136	-3.040608
C	-1.771342	6.343082	1.675085
C	4.644051	0.218430	-0.977078
C	5.560437	1.031194	-0.143675
C	6.983879	0.814189	-0.398792
C	7.436357	0.038296	-1.404899
C	6.520089	-0.616122	-2.312624
C	5.189326	-0.521267	-2.105122
H	7.682481	1.328542	0.255681
H	8.505192	-0.078678	-1.557387
H	6.907681	-1.159446	-3.167480
H	4.481099	-0.976219	-2.788293
C	3.223631	0.410381	-0.924136
C	5.183211	1.831113	0.879445
H	5.940161	2.310457	1.491419
C	2.360282	0.090244	2.226305
O	1.241183	0.501079	2.503870
C	2.727555	-0.537057	0.937902
H	1.907080	-1.117186	0.506789
N	3.872349	-1.312785	1.023905
N	4.848119	-1.453563	0.437294
O	3.374823	0.201584	3.077334
C	3.082527	0.870429	4.306702
H	4.014083	0.866441	4.867927
H	2.753659	1.891979	4.108154
H	2.298319	0.339366	4.849314
O	2.528398	-0.459540	-1.718141
H	1.569152	-0.319541	-1.602076
H	4.149836	2.043021	1.120527
C	2.661097	1.806477	-0.868475
C	1.477443	2.105184	-0.201581
C	3.288533	2.814741	-1.610414

C	0.927188	3.381321	-0.242038
H	0.977693	1.328186	0.349339
C	2.743479	4.092955	-1.656742
H	4.208360	2.590949	-2.141355
C	1.564736	4.381634	-0.969304
H	0.001454	3.579807	0.290020
H	3.241884	4.866829	-2.231985
H	1.139031	5.380374	-1.005515
H	3.524534	-4.654472	-2.050455
H	4.596161	-4.239125	-0.697296
H	3.869918	-2.961076	-1.679867
H	2.476518	-2.837996	3.670586
H	2.257712	-4.582925	3.787418
H	0.861195	-3.507218	3.961474
H	-1.332996	5.673308	-3.328887
H	-2.007729	4.091745	-3.762026
H	-0.367386	4.207661	-3.112170
H	-0.713838	6.305889	1.957230
H	-1.971257	7.344592	1.284776
H	-2.363235	6.204547	2.582450

TS-(3+2)-B4-1S2R5S

H	-0.217704	-0.976623	-1.272721
P	-1.742732	0.066194	-0.213696
O	-1.177725	-0.795266	-1.405411
O	-0.855443	1.017073	0.466289
H	-6.662780	0.740887	3.278993
H	-7.627159	0.643633	1.806619
H	-6.019682	3.379742	2.420118
C	-6.610140	0.542235	2.205266
C	-5.433957	2.825767	1.692679
H	-6.751217	-1.653163	1.915941
C	-6.018476	-0.841887	1.881466
C	-5.654535	1.470223	1.491586
H	-5.218058	-1.073957	2.591575
C	-4.434705	3.465503	0.963607
H	-4.251606	4.526238	1.105884
H	-7.424442	-0.367457	-0.345262
H	-7.319143	-2.808346	-0.073032
C	-4.899774	0.757847	0.555027
C	-5.389345	-0.676573	0.467736
C	-6.485507	-0.856261	-0.620192
C	-6.609516	-2.381970	-0.792693
C	-3.628137	2.771848	0.054182
C	-3.884093	1.405640	-0.131019
C	-4.474009	-1.839644	0.126368
C	-5.201972	-2.852088	-0.505893
H	-6.126537	-0.407820	-1.552264
O	-2.376678	-0.965210	0.868688
H	-6.949845	-2.670713	-1.790719
C	-3.121867	-2.025202	0.370349
C	-1.645325	4.284945	0.070967
C	-2.514781	3.458387	-0.649202
C	-4.602610	-4.065275	-0.813635
O	-3.051179	0.652673	-0.957011
C	-0.414417	-2.984978	1.478931
C	-2.482692	-3.238215	0.067230
H	-5.168534	-4.856766	-1.295535
C	-3.257747	-4.253683	-0.505655
C	-0.593049	4.942079	-0.558629
C	-2.319277	3.297259	-2.020298
C	0.934894	-3.243650	1.733734
C	-1.032136	-3.450460	0.316391
H	-2.784218	-5.206479	-0.721354
C	-0.422801	4.765983	-1.935020
C	-1.274816	3.951826	-2.676957
C	1.664635	-3.988396	0.810172
C	-0.263094	-4.171985	-0.609326
C	1.079600	-4.455655	-0.372308
C	0.362919	5.810787	0.217924
C	-1.096203	3.790901	-4.165687
H	-1.776844	4.384259	1.145714
H	0.398619	5.274466	-2.436817
H	-2.988523	2.652914	-2.583752
H	-0.991422	-2.415407	2.200358
H	-0.725795	-4.511806	-1.533275
H	2.715047	-4.201926	1.002945
C	1.575506	-2.707673	2.989446
C	1.899136	-5.250330	-1.357421
C	5.644398	0.388659	-0.097400
C	6.289740	0.169462	1.212359
C	7.736679	-0.017926	1.157751
C	8.449595	0.103339	0.015704
C	7.808065	0.422845	-1.233123
C	6.459267	0.542846	-1.278298
H	8.237065	-0.243528	2.095525
H	9.527152	-0.030448	0.038659
H	8.405531	0.565737	-2.126522
H	5.950311	0.781372	-2.204982
C	4.234191	0.621646	-0.191381
C	5.643802	0.020882	2.397395
H	4.580481	0.175259	2.525482
C	2.446984	-1.472422	-0.752647
O	1.331016	-0.995495	-0.679965
C	3.475165	-1.231492	0.290189
H	3.105488	-1.224729	1.312126
N	4.569895	-2.047519	0.114976
N	5.672463	-2.013188	-0.174790
O	2.891525	-2.159879	-1.795319
C	1.981663	-2.251513	-2.896339
H	2.492989	-2.847671	-3.648942
H	1.056753	-2.738971	-2.577344
H	1.764186	-1.251538	-3.277649
O	3.759216	0.746554	-1.489974
H	2.969834	1.304117	-1.459219
H	6.214379	-0.219516	3.287925
C	3.546010	1.583891	0.752952
C	2.169620	1.528393	0.992613
C	4.277048	2.671993	1.250853
C	1.536498	2.528773	1.730712
H	1.554984	0.722936	0.604774
C	3.648513	3.656900	2.000856
H	5.341420	2.732821	1.051092
C	2.276777	3.585718	2.247328
H	0.462728	2.459531	1.869162
H	4.230299	4.488154	2.386416

H	1.788603	4.362473	2.828343
H	0.040836	5.920976	1.256358
H	0.434952	6.809345	-0.223615
H	1.367244	5.375647	0.225327
H	-0.107392	4.128214	-4.484973
H	-1.840978	4.375895	-4.715084
H	-1.215801	2.746261	-4.465259
H	1.088537	-3.108653	3.883150
H	1.482906	-1.616638	3.036433
H	2.636193	-2.968650	3.041167
H	2.850221	-4.749465	-1.564185
H	1.365767	-5.383684	-2.302223
H	2.129432	-6.244291	-0.961489

TS-(3+2)-B4-3R5R

H	0.241969	-0.024391	-1.212445
P	-1.329424	0.040869	0.227995
O	-0.454771	-0.645113	-0.885027
O	-0.663508	0.861740	1.252003
H	-6.559188	0.583771	3.064498
H	-7.350136	0.786124	1.502427
H	-5.655503	3.264625	2.702236
C	-6.394876	0.544421	1.984461
C	-5.024297	2.779071	1.964099
H	-6.642301	-1.563215	1.335542
C	-5.858905	-0.820409	1.510731
C	-5.306044	1.490366	1.531625
H	-5.167069	-1.223021	2.257728
C	-3.905034	3.438066	1.457156
H	-3.670724	4.446804	1.783979
H	-6.953002	0.119992	-0.739876
H	-7.051071	-2.332674	-0.879400
C	-4.488343	0.861681	0.587372
C	-5.055346	-0.496861	0.218426
C	-6.025102	-0.400197	-0.993917
C	-6.234390	-1.859009	-1.437987
C	-3.043364	2.818254	0.547840
C	-3.356450	1.517134	0.132862
C	-4.188793	-1.668001	-0.219052
C	-4.906482	-2.491372	-1.091672
H	-5.527196	0.159890	-1.792192
O	-2.152477	-1.150584	0.922817
H	-6.475453	-1.949537	-2.500520
C	-2.895249	-2.024373	0.134891
C	-0.886528	4.017299	0.969266
C	-1.811419	3.491297	0.061418
C	-4.366312	-3.690043	-1.536289
O	-2.447355	0.812830	-0.656226
C	-0.397401	-3.375384	1.334759
C	-2.313866	-3.226183	-0.297959
H	-4.928136	-4.336386	-2.203866
C	-3.088888	-4.053742	-1.120943
C	0.275613	4.642050	0.522593
C	-1.556715	3.589997	-1.305317
C	0.907691	-3.749790	1.656850
C	-0.923111	-3.610364	0.060475
H	-2.666509	-5.000048	-1.443736
C	0.491609	4.752420	-0.855163
C	-0.407997	4.225178	-1.779814
C	1.689339	-4.371675	0.682972
C	-0.115057	-4.239785	-0.893154
C	1.191135	-4.625988	-0.596808
C	1.294303	5.185951	1.492160
C	-0.144551	4.292979	-3.261881
H	-1.063491	3.893541	2.034737
H	1.388856	5.260227	-1.205806
H	-2.265110	3.162760	-2.010248
H	-1.012665	-2.897795	2.090047
H	-0.502676	-4.404216	-1.895921
H	2.712734	-4.655676	0.923215
C	1.454666	-3.517689	3.041463
C	2.071045	-5.263121	-1.642122
C	3.500312	-0.543182	1.751157
C	4.751759	-0.605008	0.970291
C	5.977268	-0.621849	1.765405
C	5.979627	-0.773830	3.110392
C	4.753241	-0.867017	3.852097
C	3.583501	-0.721994	3.186441
H	6.913871	-0.561712	1.227505
H	6.927283	-0.829836	3.637853
H	4.770476	-1.009997	4.926846
H	2.640418	-0.734942	3.728243
C	2.224597	-0.270330	1.231936
C	4.896876	-0.523688	-0.396363
H	1.395109	-0.316080	1.933485
C	2.086129	1.907613	-0.692595
O	1.287936	1.365226	-1.434750
C	2.092728	1.681105	0.774083
H	1.134354	1.873669	1.256050
N	3.163940	2.206468	1.433184
N	4.083839	2.030115	2.073076
O	3.043558	2.738175	-1.100045
C	3.090245	3.062704	-2.492974
H	4.144523	3.140618	-2.756371
H	2.598323	2.290568	-3.081502
H	2.594732	4.024274	-2.639266
H	1.934754	-0.545473	0.227422
O	6.170155	-0.206749	-0.853821
H	6.334125	-0.720161	-1.654745
C	3.932928	-0.713160	-1.487925
C	4.123247	-0.006252	-2.690058
C	2.894825	-1.660995	-1.448341
C	3.279634	-0.194954	-3.779761
H	4.936525	0.711152	-2.749709
C	2.037504	-1.827647	-2.529051
H	2.762513	-2.275970	-0.561939
C	2.219157	-1.091821	-3.700430
H	3.447779	0.371045	-4.692052
H	1.225788	-2.544436	-2.449933
H	1.549846	-1.229497	-4.543064
H	1.168861	4.747984	2.485650
H	2.310384	4.969416	1.148001
H	1.204901	6.272472	1.593249
H	-1.064566	4.491173	-3.817503
H	0.575224	5.078924	-3.506171
H	0.257038	3.337934	-3.618310

H	0.905611	-2.721865	3.551676
H	2.510183	-3.235320	3.008246
H	1.367939	-4.424037	3.650256
H	2.877295	-4.582228	-1.935966
H	1.502026	-5.514069	-2.540482
H	2.533213	-6.178944	-1.263106

TS-(3+2)-B4-3R5S

H	0.509969	1.028283	-2.223662
P	1.293980	-0.246718	-0.733740
O	1.405296	0.638899	-2.023248
O	-0.056497	-0.523523	-0.228028
H	5.131558	-2.816320	3.365581
H	6.034297	-3.368840	1.955220
H	3.245802	-4.851791	2.733597
C	5.195269	-2.739430	2.276976
C	3.035135	-4.177991	1.908556
H	6.400768	-0.937416	1.805231
C	5.365725	-1.290073	1.787566
C	3.916561	-3.154182	1.587940
H	4.767442	-0.620743	2.414592
C	1.857747	-4.313199	1.177342
H	1.153658	-5.102102	1.423884
H	6.430763	-2.586695	-0.304731
H	7.498084	-0.378591	-0.199653
C	3.643905	-2.291898	0.523090
C	4.766333	-1.284594	0.349191
C	5.844480	-1.739518	-0.672201
C	6.685125	-0.472871	-0.929869
C	1.530598	-3.440156	0.132019
C	2.462132	-2.439025	-0.186043
C	4.521168	0.137157	-0.129046
C	5.669324	0.634660	-0.754795
H	5.342301	-2.044652	-1.595938
O	2.199022	0.444269	0.424697
H	7.141996	-0.463158	-1.923045
C	3.418600	0.967401	0.002589
C	-0.947108	-3.663513	0.229263
C	0.209242	-3.523540	-0.543685
C	5.741936	1.961666	-1.155611
O	2.186741	-1.510896	-1.187507
C	2.078543	3.694026	1.178294
C	3.472951	2.319213	-0.359190
H	6.632497	2.342563	-1.646421
C	4.652351	2.803059	-0.927186
C	-2.213535	-3.665436	-0.356202
C	0.089074	-3.409412	-1.930534
C	0.980931	4.511093	1.465304
C	2.294824	3.202645	-0.107409
H	4.697543	3.848594	-1.216243
C	-2.302657	-3.534138	-1.742735
C	-1.164561	-3.407687	-2.540299
C	0.087305	4.807987	0.439823
C	1.402513	3.546950	-1.128550
C	0.288830	4.342610	-0.863792
C	-3.457934	-3.787405	0.486226
C	-1.288712	-3.217120	-4.031029
H	-0.857640	-3.730783	1.311711
H	-3.287290	-3.509641	-2.206968
H	0.982671	-3.300199	-2.538366
H	2.780036	3.435485	1.968940
H	1.579028	3.175421	-2.133722
H	-0.780863	5.429257	0.652988
C	0.793435	5.070616	2.853025
C	-0.677830	4.719838	-1.958500
C	-4.344520	-0.452961	-0.124849
C	-4.776134	-0.674656	1.284029
C	-6.118940	-1.229949	1.472476
C	-6.975979	-1.416923	0.450343
C	-6.602619	-1.076055	-0.909632
C	-5.362262	-0.618071	-1.161738
H	-6.410832	-1.477882	2.485663
H	-7.962692	-1.827543	0.640988
H	-7.317953	-1.210834	-1.714046
H	-5.053079	-0.388007	-2.179321
C	-3.015234	-0.450786	-0.564639
C	-4.081419	-0.327351	2.400461
H	-2.847780	-0.631689	-1.625358
C	-2.019572	1.789003	-1.969329
O	-0.971687	1.562582	-2.553732
C	-2.284578	1.518385	-0.546913
H	-1.442540	1.498168	0.140951
N	-3.417169	2.119679	-0.092162
N	-4.523764	1.921675	0.123712
O	-3.101510	2.223233	-2.617356
C	-2.949251	2.400393	-4.027498
H	-3.924018	2.722481	-4.386826
H	-2.191942	3.159414	-4.233024
H	-2.651951	1.460730	-4.496283
H	-2.203234	-0.804948	0.053870
O	-4.704063	-0.477446	3.623442
H	-4.034215	-0.385217	4.309436
C	-2.747501	0.317460	2.509460
C	-2.678725	1.676301	2.859596
C	-1.561563	-0.406789	2.375250
C	-1.447255	2.303797	3.006721
H	-3.602655	2.236187	2.977854
C	-0.327971	0.216576	2.546949
H	-1.602128	-1.457080	2.099283
C	-0.268481	1.572016	2.848681
H	-1.404964	3.363512	3.240156
H	0.584616	-0.350823	2.401559
H	0.696791	2.059217	2.940480
H	-0.668580	5.799929	-2.134321
H	-0.421605	4.217324	-2.893935
H	-1.704752	4.445287	-1.689718
H	-0.167161	5.582725	2.948162
H	1.581035	5.792762	3.089746
H	0.837892	4.283933	3.613511
H	-1.330071	-2.150975	-4.280689
H	-0.431909	-3.643068	-4.558671
H	-2.197666	-3.684364	-4.417579
H	-4.331886	-3.389854	-0.037834
H	-3.659111	-4.833648	0.740552
H	-3.359973	-3.228783	1.422135

TS-(3+2)-B4-3S5R

H	-0.330612	0.440210	1.267487
P	-1.393535	0.226780	-0.619933
O	-0.720928	1.023095	0.558899
O	-0.718358	0.218075	-1.924777
H	-6.727049	-2.644558	-1.527849
H	-6.598517	-3.266748	0.115059
H	-4.848274	-4.754766	-2.039441
C	-6.131536	-2.591710	-0.612394
C	-4.180727	-4.043915	-1.561821
H	-6.844303	-0.872249	0.592377
C	-6.014193	-1.161765	-0.057922
C	-4.686663	-2.967091	-0.848317
H	-5.962570	-0.445465	-0.884314
C	-2.801279	-4.200248	-1.654595
H	-2.379695	-5.044231	-2.191871
H	-5.451454	-2.679721	2.076145
H	-6.491486	-0.611787	2.904167
C	-3.831863	-2.052324	-0.222149
C	-4.650905	-1.148455	0.689160
C	-4.823843	-1.784563	2.099665
C	-5.397121	-0.648657	2.968014
C	-1.918277	-3.261278	-1.110571
C	-2.459901	-2.163827	-0.424891
C	-4.254384	0.260867	1.081122
C	-4.775475	0.577479	2.340092
H	-3.834808	-2.070591	2.473034
O	-2.877982	0.839110	-0.778587
H	-5.139365	-0.751051	4.025522
C	-3.533127	1.215498	0.388179
C	0.336364	-2.628071	-2.018831
C	-0.450285	-3.478989	-1.247742
C	-4.642085	1.858936	2.854791
O	-1.608571	-1.206247	0.117399
C	-2.732208	3.698522	-1.246225
C	-3.379525	2.521885	0.875442
H	-5.049280	2.109451	3.829685
C	-3.966210	2.823255	2.109144
C	1.703131	-2.870803	-2.182203
C	0.139338	-4.594421	-0.639532
C	-2.023624	4.687378	-1.934415
C	-2.595382	3.543123	0.134520
H	-3.870235	3.834526	2.492397
C	2.274298	-3.968007	-1.543060
C	1.504098	-4.841462	-0.768900
C	-1.175839	5.527069	-1.216225
C	-1.724375	4.394000	0.827815
C	-1.015611	5.393370	0.166603
C	2.515355	-1.949584	-3.056033
C	2.154460	-6.010188	-0.072563
H	-0.116262	-1.770873	-2.504627
H	3.343627	-4.146556	-1.643298
H	-0.478366	-5.264463	-0.044535
H	-3.400885	3.042091	-1.794914
H	-1.588388	4.256640	1.897850
H	-0.616893	6.297838	-1.743326
C	-2.161233	4.811155	-3.430321
C	-0.084781	6.315847	0.912928
C	4.949125	0.047714	1.553078
C	5.743382	0.915357	0.639450
C	7.190540	0.686601	0.625001
C	7.780347	-0.297775	1.330033
C	6.998966	-1.191781	2.159532
C	5.668035	-1.014947	2.251707
H	7.784405	1.346130	0.004697
H	8.857434	-0.424307	1.282380
H	7.491413	-1.984124	2.712886
H	5.069116	-1.661940	2.888920
C	3.645764	0.305175	2.007745
C	5.247530	1.789973	-0.280950
H	3.228452	1.301291	1.977405
C	1.381084	-1.245022	1.418791
O	0.463418	-0.757621	2.065643
C	2.287739	-0.413102	0.611738
H	1.840777	0.461291	0.143050
N	3.167642	-1.078419	-0.180373
N	4.274403	-1.349855	-0.277464
O	1.721813	-2.520906	1.488821
C	0.857013	-3.333562	2.292372
H	1.217340	-4.352642	2.166724
H	0.914618	-3.019608	3.336322
H	-0.169969	-3.240949	1.933812
H	3.316318	-0.283719	2.861240
O	6.128753	2.335716	-1.190979
H	5.696862	3.089045	-1.608218
C	3.835481	2.152987	-0.546902
C	3.095206	2.958553	0.325696
C	3.236609	1.719416	-1.740467
C	1.761154	3.251429	0.055857
H	3.571912	3.336513	1.225807
C	1.902112	2.013648	-2.010324
H	3.817416	1.109227	-2.428326
C	1.157686	2.769138	-1.104205
H	1.177252	3.839081	0.756979
H	1.420284	1.621791	-2.899862
H	0.106411	2.969062	-1.289818
H	2.330270	-2.156870	-4.114845
H	2.231651	-0.908771	-2.868359
H	3.586327	-2.059094	-2.868582
H	2.909460	-5.665449	0.642259
H	2.662382	-6.665372	-0.786371
H	1.419211	-6.609782	0.470242
H	-1.674978	3.968364	-3.931827
H	-3.212317	4.807724	-3.731307
H	-1.703150	5.732378	-3.796582
H	0.905283	6.333810	0.446987
H	-0.466151	7.341671	0.912589
H	0.034166	6.003020	1.953270

TS-(3+2)-B4-3S5S

H	-0.464443	1.515731	1.128077
P	-1.493504	-0.146698	0.161753
O	-1.218193	0.881897	1.305760
O	-0.384701	-0.542360	-0.725088
H	-5.644772	-3.278564	-2.881461
H	-6.362377	-3.715086	-1.331681

H	-3.629879	-5.186023	-2.235427
C	-5.596246	-3.089286	-1.805879
C	-3.351332	-4.410828	-1.527896
H	-6.838685	-1.301905	-1.376151
C	-5.789979	-1.603417	-1.450902
C	-4.229325	-3.378029	-1.229466
H	-5.307955	-0.978746	-2.209999
C	-2.096256	-4.432695	-0.923986
H	-1.401960	-5.238227	-1.142560
H	-6.502763	-2.766612	0.849603
H	-7.720886	-0.634118	0.726881
C	-3.869246	-2.379676	-0.319317
C	-5.028538	-1.420389	-0.106485
C	-5.937077	-1.858761	1.077430
C	-6.824262	-0.631185	1.358822
C	-1.683051	-3.422829	-0.047545
C	-2.599632	-2.399874	0.236587
C	-4.833343	0.048058	0.232495
C	-5.909394	0.514609	0.992184
H	-5.302045	-2.060684	1.946166
O	-2.696191	0.421603	-0.759706
H	-7.161580	-0.579821	2.397442
C	-3.815025	0.924205	-0.109396
C	0.789554	-3.723048	-0.279085
C	-0.313865	-3.434595	0.532045
C	-5.999399	1.856888	1.334986
O	-2.197602	-1.314803	1.018464
C	-2.062322	3.179557	-1.300332
C	-3.860836	2.282774	0.237210
H	-6.840328	2.225287	1.914717
C	-4.987204	2.728061	0.940852
C	2.075838	-3.800998	0.253176
C	-0.112563	-3.198942	1.893608
C	-1.054850	4.097576	-1.589675
C	-2.748342	3.219898	-0.076549
H	-5.055577	3.781614	1.193158
C	2.240939	-3.585677	1.625145
C	1.163937	-3.270605	2.452613
C	-0.735363	5.072977	-0.638896
C	-2.384108	4.187661	0.861849
C	-1.385907	5.125788	0.591022
C	3.267526	-4.118608	-0.614837
C	1.370160	-3.000823	3.921676
H	0.641694	-3.874942	-1.345580
H	3.236297	-3.678020	2.058828
H	-0.964444	-2.972794	2.528560
H	-2.330319	2.431916	-2.040014
H	-2.876078	4.200206	1.831221
H	0.043942	5.799197	-0.866430
C	-0.332966	4.069825	-2.913581
C	-1.016907	6.154229	1.630368
C	3.292236	-0.488520	-1.303818
C	4.753862	-0.486006	-1.498331
C	5.204650	-0.821579	-2.844949
C	4.379045	-1.427322	-3.729908
C	3.006788	-1.723243	-3.394102
C	2.491452	-1.271167	-2.225440
H	6.244457	-0.643100	-3.090560
H	4.758406	-1.716366	-4.705460
H	2.388007	-2.272863	-4.096306
H	1.443357	-1.413992	-1.968641
C	2.612970	0.180516	-0.273415
C	5.685197	-0.202454	-0.539198
H	3.191985	0.744651	0.452214
C	1.458098	2.700831	-0.083975
O	0.751694	2.553304	0.903492
C	1.567274	1.687278	-1.136527
H	0.658319	1.150289	-1.404009
N	2.334087	1.979330	-2.225034
N	3.183417	1.571066	-2.873558
O	2.292772	3.725373	-0.225611
C	2.364697	4.615857	0.893237
H	3.038201	5.413546	0.587136
H	1.372828	5.005354	1.125394
H	2.760392	4.088067	1.763184
H	1.694554	-0.264830	0.102358
O	6.970379	0.058289	-0.969185
H	7.582328	-0.243890	-0.286385
C	5.525531	-0.156156	0.927548
C	4.708420	-1.074585	1.608285
C	6.298281	0.734957	1.684050
C	4.645257	-1.075792	2.991438
H	4.110115	-1.775204	1.034000
C	6.235368	0.729372	3.077186
H	6.936081	1.448909	1.170736
C	5.409118	-0.171725	3.736493
H	4.003740	-1.792623	3.496013
H	6.834791	1.434838	3.644291
H	5.359771	-0.178052	4.820429
H	-0.556720	5.678225	2.503029
H	-0.312369	6.888360	1.231033
H	-1.900659	6.692940	1.983452
H	0.736399	4.258376	-2.778701
H	-0.722816	4.839605	-3.587510
H	-0.448539	3.102673	-3.409013
H	1.505205	-1.929167	4.104236
H	3.923926	-3.247372	-0.726689
H	2.957805	-4.412050	-1.619883
H	3.859073	-4.930176	-0.180543
H	2.256237	-3.518965	4.298922
H	0.508902	-3.326908	4.509890

TS-[4+2]-B2-R-2

H	1.103998	1.198524	-1.978110
P	1.794654	-0.508407	-0.103866
O	1.858230	0.545535	-1.185157
O	0.581525	-0.725404	0.716822
H	5.498109	-4.604236	2.697940
H	6.086727	-5.008609	1.086306
H	3.209944	-6.148221	1.962619
C	5.443891	-4.316880	1.644539
C	3.021256	-5.266269	1.358354
H	6.930432	-2.706690	1.303611
C	5.850859	-2.852381	1.400037
C	4.029932	-4.343929	1.113224
H	5.494122	-2.229160	2.226479

C	1.750725	-5.028978	0.845072
H	0.957736	-5.745297	1.036163
H	6.283475	-3.935288	-1.007603
H	7.842313	-2.047666	-0.756288
C	3.792364	-3.226793	0.308734
C	5.083580	-2.445735	0.109153
C	5.873286	-2.930082	-1.140297
C	6.947434	-1.847728	-1.358364
C	1.454863	-3.875345	0.106043
C	2.511797	-2.991676	-0.176468
C	5.120689	-0.942605	-0.117638
C	6.240506	-0.598832	-0.883151
H	5.190621	-2.948334	-1.996051
O	3.062637	-0.281868	0.909729
H	7.269349	-1.771800	-2.400335
C	4.252267	0.056638	0.294015
C	6.528892	0.728445	-1.170634
O	2.288229	-1.850637	-0.912475
C	4.509111	1.405282	-0.002618
H	7.398451	0.988807	-1.766305
C	5.663379	1.723959	-0.719971
H	5.861699	2.766024	-0.954104
C	0.046403	-3.559180	-0.251321
C	-0.314700	-2.847576	-1.403256
C	-0.970449	-3.927931	0.635624
C	-1.641076	-2.495068	-1.627446
C	-2.297728	-3.614285	0.373276
C	-2.652395	-2.890025	-0.758413
H	-3.688811	-2.616244	-0.943887
C	3.480041	2.424550	0.326535
C	2.940656	2.525630	1.605938
C	2.939944	3.213342	-0.697261
C	1.871359	3.386776	1.854340
C	1.865296	4.050146	-0.441666
C	1.316610	4.146474	0.837303
H	0.466400	4.791625	1.029711
N	-2.474581	1.408014	-0.719487
C	-1.177873	1.279741	-1.085769
N	-3.490659	1.908884	-0.952160
H	-0.528638	0.715235	-0.439502
C	-0.732662	1.882680	-2.264377
O	0.479419	1.817778	-2.660779
O	-1.602096	2.542817	-3.003929
C	-1.098377	3.133634	-4.207937
H	-1.945023	3.661929	-4.640814
H	-0.285756	3.821765	-3.976755
H	-0.740777	2.355772	-4.884732
C	-2.998770	0.946995	1.837010
C	-4.212520	1.704916	1.650522
C	-4.427933	2.867594	2.463214
C	-3.539097	3.222282	3.431491
C	-2.333081	2.480391	3.618131
C	-2.072255	1.394191	2.843518
H	-5.335267	3.438392	2.306586
H	-3.742347	4.080099	4.064032
H	-1.612772	2.799239	4.363142
H	-1.139435	0.847264	2.942228
C	-2.567874	-0.016481	0.934006
C	-5.084251	1.468903	0.570498
H	0.444571	-2.529950	-2.106622
H	-0.723909	-4.436055	1.560668
H	3.330068	1.904513	2.406488
H	3.315395	3.106471	-1.709413
C	1.233070	4.853177	-1.539917
F	1.325760	6.171362	-1.307846
F	-0.083243	4.581611	-1.648629
F	1.784852	4.616129	-2.737153
C	1.325159	3.456444	3.251370
F	0.311065	4.327107	3.357636
F	2.269837	3.830121	4.127643
F	0.870255	2.262336	3.668987
C	-2.009658	-1.682690	-2.836819
F	-2.991813	-0.805302	-2.552163
F	-2.462530	-2.448235	-3.841823
F	-0.970256	-0.982247	-3.311961
C	-3.366085	-3.982923	1.359945
F	-2.946603	-4.889421	2.250766
F	-4.447520	-4.494358	0.745368
F	-3.790894	-2.912653	2.055987
O	-5.927973	2.472423	0.259375
H	-6.610735	2.138888	-0.336733
C	-5.484702	0.142850	0.024293
C	-5.742920	-0.916325	0.901082
C	-5.730289	-0.015334	-1.343961
C	-6.237830	-2.118939	0.412361
H	-5.538588	-0.793603	1.960084
C	-6.215789	-1.225884	-1.830276
H	-5.492341	0.795119	-2.027294
C	-6.474023	-2.276740	-0.953209
H	-6.420755	-2.939826	1.095909
H	-6.379487	-1.350026	-2.895497
H	-6.849030	-3.222062	-1.331746
H	-3.245858	-0.546337	0.281106
H	-1.573164	-0.446217	1.045103

TS-[4+2]-B2-R-3

H	-0.211505	-0.501623	-1.160169
P	-0.514922	1.290718	0.144667
O	-0.830736	0.259040	-0.986233
O	0.244501	0.859036	1.335665
H	-2.277019	6.996039	1.576914
H	-1.856674	7.412430	-0.084163
H	0.510815	6.956622	2.071664
C	-1.968648	6.575835	0.616314
C	0.449225	6.056170	1.468565
H	-3.800941	5.951383	-0.465581
C	-2.954367	5.523929	0.078632
C	-0.684609	5.786195	0.714209
H	-3.348134	4.932598	0.911683
C	1.500592	5.142809	1.462378
H	2.393562	5.331861	2.050282
H	-1.816216	6.280195	-2.228571
H	-4.079039	5.493499	-2.770745
C	-0.774921	4.622680	-0.056103
C	-2.086816	4.594634	-0.821125
C	-1.969168	5.197553	-2.248777

C	-3.273370	4.772295	-2.953311
C	1.426926	3.957726	0.725200
C	0.271204	3.712333	-0.024342
C	-2.818811	3.302516	-1.131413
C	-3.580938	3.445108	-2.296095
H	-1.111563	4.739590	-2.752185
O	-1.957350	1.861486	0.586832
H	-3.159762	4.683184	-4.036718
C	-2.859498	2.099867	-0.448261
C	-4.428525	2.429341	-2.718652
O	0.136759	2.503816	-0.703712
C	-3.718263	1.064608	-0.836267
H	-5.015798	2.540141	-3.625007
C	-4.509097	1.253158	-1.971651
H	-5.171898	0.451137	-2.283305
C	2.539430	2.968726	0.770973
C	3.343576	2.739130	-0.342780
C	2.788012	2.255794	1.947492
C	4.405664	1.839134	-0.265455
C	3.828597	1.338996	1.999471
C	4.661300	1.137231	0.903024
H	5.476535	0.424285	0.953987
C	-3.736468	-0.208552	-0.067983
C	-4.083032	-0.210907	1.286066
C	-3.381130	-1.410780	-0.680025
C	-4.102953	-1.403410	1.999038
C	-3.391042	-2.595273	0.050680
C	-3.764019	-2.607100	1.388016
H	-3.775280	-3.536407	1.948770
N	0.396360	-2.972962	-2.082291
C	-0.216647	-3.541525	-3.102809
N	0.541249	-2.020942	-1.427458
H	0.047274	-4.540758	-3.395571
C	-1.203690	-2.779371	-3.843331
O	-1.789308	-3.170408	-4.828404
O	-1.396357	-1.538496	-3.314988
C	-2.272854	-0.701805	-4.061931
H	-2.292421	0.251211	-3.531946
H	-1.903035	-0.574910	-5.081747
H	-3.275067	-1.138747	-4.109538
C	1.347685	-2.739009	1.279588
C	2.017749	-3.722009	2.018005
C	1.395927	-4.322920	3.104199
C	0.108071	-3.936564	3.471444
C	-0.559178	-2.954755	2.744860
C	0.054274	-2.357704	1.647729
H	1.922030	-5.081550	3.674019
H	-0.373337	-4.396429	4.328394
H	-1.554809	-2.643248	3.040805
H	-0.476618	-1.608043	1.068206
C	2.090570	-2.024576	0.207739
C	1.635585	-4.649912	-1.139317
H	1.534743	-5.573033	-1.703062
O	2.155059	-0.699668	0.315122
H	1.568058	-0.332204	1.010867
C	3.007514	-2.621542	-0.682721
C	4.086652	-1.814466	-1.171300
C	2.817948	-3.937887	-1.249762
C	5.003660	-2.301543	-2.049188
H	4.168691	-0.806814	-0.788492
C	3.825217	-4.408012	-2.171361
C	4.877080	-3.635275	-2.545889
H	5.831631	-1.676692	-2.365612
H	3.706015	-5.409804	-2.573324
H	5.617260	-4.022366	-3.238734
H	3.147035	3.267990	-1.270900
H	2.135089	2.388974	2.803559
H	-4.333712	0.720361	1.782654
H	-3.047748	-1.419264	-1.711998
C	-2.906754	-3.866021	-0.588502
F	-3.528501	-4.940608	-0.083941
F	-1.590588	-4.042411	-0.375876
F	-3.101777	-3.862096	-1.911827
C	-4.523719	-1.426230	3.440956
F	-3.698752	-2.197409	4.173020
F	-5.754397	-1.936857	3.587449
F	-4.527577	-0.205367	3.985627
C	5.257622	1.629976	-1.485745
F	6.207428	0.702109	-1.280400
F	5.872583	2.760109	-1.860954
F	4.522444	1.220751	-2.528564
C	3.971227	0.452736	3.202642
F	3.575831	1.063980	4.326035
F	5.236504	0.048025	3.378743
F	3.219239	-0.654637	3.069130
H	0.906226	-4.486742	-0.359022
H	3.026974	-4.003049	1.733849

TS-[4+2]-B2-S-2

H	-0.610575	-0.973466	-2.188127
P	-1.878684	-0.393185	-0.234223
O	-1.360369	-1.220831	-1.416614
O	-1.067804	0.683459	0.365016
H	-6.939509	-0.859684	3.384704
H	-7.818468	-1.061603	1.869488
H	-6.813026	1.892302	2.707515
C	-6.815038	-0.980940	2.305461
C	-6.106512	1.515330	1.974523
H	-6.495088	-3.138766	1.906192
C	-5.944653	-2.194242	1.934094
C	-6.046527	0.159347	1.680500
H	-5.130056	-2.295205	2.658610
C	-5.221812	2.383794	1.342773
H	-5.248630	3.444524	1.574133
H	-7.365188	-1.918789	-0.321104
H	-6.758388	-4.292032	-0.116098
C	-5.149370	-0.328130	0.725756
C	-5.331913	-1.828747	0.550055
C	-6.337387	-2.190031	-0.578896
C	-6.136159	-3.702830	-0.800729
C	-4.271323	1.921056	0.425744
C	-4.266452	0.551269	0.113074
C	-4.185075	-2.760083	0.195001
C	-4.666787	-3.881735	-0.489519
H	-6.054856	-1.644029	-1.484751
O	-2.301445	-1.469024	0.920423

H	-6.385964	-4.019082	-1.816862
C	-2.826882	-2.656735	0.440039
C	-3.814537	-4.917887	-0.846917
O	-3.349158	0.049900	-0.789954
C	-1.941693	-3.688299	0.089558
H	-4.191961	-5.783705	-1.382249
C	-2.456655	-4.821725	-0.539619
H	-1.776218	-5.621127	-0.818502
C	-3.212711	2.819524	-0.098660
C	-2.732265	2.719147	-1.407977
C	-2.602127	3.735089	0.759824
C	-1.626440	3.456031	-1.809936
C	-1.525927	4.503241	0.328186
C	-1.006537	4.356033	-0.951166
H	-0.140932	4.923785	-1.270201
C	-0.487960	-3.483123	0.316217
C	-0.026672	-3.070804	1.564661
C	0.429161	-3.589161	-0.736445
C	1.319173	-2.771604	1.759850
C	1.769263	-3.288232	-0.527819
C	2.232744	-2.879072	0.722109
H	3.280318	-2.630849	0.873898
N	2.824367	0.434667	-1.002130
C	1.606041	0.012452	-1.380640
N	3.917376	0.634326	-1.334921
H	0.795638	0.100680	-0.678417
C	1.400279	-0.444841	-2.701350
O	0.295464	-0.873866	-3.113670
O	2.447270	-0.414871	-3.518092
C	2.212365	-0.884781	-4.846829
H	3.161189	-0.766237	-5.366279
H	1.909918	-1.932433	-4.827391
H	1.432235	-0.290748	-5.325669
C	3.090157	1.951540	1.226817
C	4.436311	2.217720	0.778137
C	4.857846	3.582121	0.635595
C	4.037129	4.612075	0.977032
C	2.704341	4.359385	1.421963
C	2.247503	3.082958	1.519866
H	5.864781	3.768905	0.283056
H	4.394251	5.634370	0.909320
H	2.052956	5.188846	1.671545
H	1.225139	2.882655	1.825709
C	2.509021	0.692433	1.174297
C	5.286680	1.207967	0.284824
H	-3.193691	2.028515	-2.104589
H	-2.940421	3.820691	1.788207
H	-0.728263	-2.948981	2.383804
H	0.076749	-3.840297	-1.731581
C	2.755726	-3.375899	-1.656328
F	3.522124	-4.475424	-1.569548
F	3.596097	-2.327027	-1.661200
F	2.150772	-3.406139	-2.853652
C	1.734348	-2.284443	3.117676
F	3.052325	-2.041559	3.185172
F	1.440141	-3.177593	4.074083
F	1.102232	-1.147390	3.441782
C	-1.062996	3.186816	-3.175438
F	-0.133322	4.085064	-3.526805
F	-2.018842	3.201966	-4.116724
F	-0.489044	1.972772	-3.228860
C	-0.905688	5.459341	1.303321
F	-1.823882	6.262922	1.859219
F	0.022132	6.240979	0.731174
F	-0.302373	4.813779	2.320366
O	6.321512	1.629222	-0.469982
H	6.946515	0.902263	-0.584967
C	5.467441	-0.162643	0.841308
C	5.756415	-1.233225	-0.012478
C	5.502189	-0.353481	2.226493
C	6.051788	-2.487135	0.514018
H	5.697044	-1.090897	-1.087318
C	5.816490	-1.603141	2.747374
H	5.275979	0.480703	2.883835
C	6.086172	-2.672140	1.894474
H	6.237065	-3.320087	-0.156583
H	5.834821	-1.746892	3.822311
H	6.316685	-3.649224	2.306122
H	3.085227	-0.220856	1.233443
H	1.440896	0.601141	1.360184

TS-[4+2]-B2-S-3

H	-0.492956	-0.300396	-1.143000
P	0.154313	1.409499	0.074898
O	-0.537481	0.700314	-1.124159
O	0.774071	0.589353	1.139638
H	0.629635	7.155402	2.161626
H	1.059969	7.594795	0.509203
H	3.255519	6.091950	2.358759
C	0.706123	6.771182	1.141353
C	2.835734	5.346900	1.690114
H	-1.295851	6.949963	0.203107
C	-0.622519	6.194908	0.618082
C	1.632322	5.581863	1.037103
H	-1.144773	5.683337	1.433053
C	3.489937	4.131397	1.498296
H	4.429481	3.930352	2.004232
H	0.544570	6.779671	-1.721190
H	-1.880728	6.864211	-2.107198
C	1.083207	4.622288	0.181504
C	-0.203220	5.135329	-0.443252
C	0.026939	5.821332	-1.819239
C	-1.383420	5.942000	-2.431279
C	2.949524	3.140939	0.673466
C	1.736298	3.410168	0.028786
C	-1.359036	4.212787	-0.790437
C	-2.086766	4.727367	-1.868863
H	0.642290	5.161971	-2.440025
O	-0.938876	2.404186	0.722123
H	-1.371828	5.948791	-3.524183
C	-1.771964	3.028644	-0.206949
C	-3.247013	4.099039	-2.302035
O	1.134082	2.410005	-0.728549
C	-2.948342	2.376562	-0.607017
H	-3.811031	4.496295	-3.140283
C	-3.681927	2.943029	-1.652975

H	-4.600135	2.456414	-1.969011
C	3.595354	1.811586	0.516541
C	3.914237	1.312928	-0.746583
C	3.844891	1.016358	1.636998
C	4.478440	0.046678	-0.879346
C	4.386643	-0.253968	1.487454
C	4.713260	-0.752185	0.231177
H	5.115176	-1.752348	0.119752
C	-3.382383	1.123439	0.062703
C	-3.332375	1.026390	1.454658
C	-3.874513	0.034096	-0.670199
C	-3.768879	-0.125541	2.101490
C	-4.319548	-1.104549	-0.008697
C	-4.271626	-1.196680	1.380298
H	-4.618548	-2.091485	1.884698
N	-1.145878	-2.642474	-1.644549
C	-2.086822	-2.834227	-2.546167
N	-0.315374	-1.944147	-1.218070
H	-2.663623	-3.740341	-2.534883
C	-2.411597	-1.752396	-3.465952
O	-3.235171	-1.818325	-4.350629
O	-1.718029	-0.624089	-3.178497
C	-2.030081	0.512004	-3.975623
H	-1.503312	1.346249	-3.512790
H	-1.699688	0.359147	-5.005791
H	-3.108703	0.692855	-3.981164
C	0.022270	-3.092311	1.149980
C	-1.007418	-4.036736	0.755286
C	-2.128573	-4.190676	1.653404
C	-2.239615	-3.480862	2.804613
C	-1.247934	-2.513546	3.156298
C	-0.173874	-2.316912	2.345558
H	-2.894631	-4.906967	1.372519
H	-3.086783	-3.638297	3.464388
H	-1.344993	-1.953337	4.078993
H	0.596956	-1.613069	2.641065
C	1.177326	-2.820890	0.381430
C	-1.085301	-4.634926	-0.489337
H	-1.969787	-5.221233	-0.720136
H	-0.238442	-4.765303	-1.146425
O	1.872812	-1.709306	0.532735
H	1.362672	-0.935071	0.887567
C	1.932815	-3.790581	-0.445013
C	2.643526	-3.315405	-1.550475
C	2.051971	-5.130209	-0.062484
C	3.447212	-4.179269	-2.285607
H	2.548029	-2.270897	-1.826725
C	2.858898	-5.989435	-0.797584
H	1.511897	-5.487384	0.809189
C	3.553908	-5.516581	-1.910758
H	3.994749	-3.801103	-3.142220
H	2.955011	-7.027347	-0.496743
H	4.184245	-6.191227	-2.481161
H	3.716245	1.912824	-1.629980
H	3.567709	1.375182	2.623657
H	-2.951860	1.855893	2.041249
H	-3.905485	0.073273	-1.755111
C	-4.920444	-2.264928	-0.752835
F	-6.188708	-2.472494	-0.362383
F	-4.257811	-3.409346	-0.501000
F	-4.930793	-2.078028	-2.073687
C	-3.748676	-0.143680	3.603532
F	-4.002633	-1.364405	4.100235
F	-4.667832	0.690004	4.112663
F	-2.561687	0.250844	4.086906
C	4.801734	-0.444999	-2.261152
F	5.407268	-1.639946	-2.246695
F	5.603145	0.409617	-2.912661
F	3.691193	-0.572281	-3.010747
C	4.504305	-1.129696	2.701526
F	4.975566	-0.446184	3.756042
F	5.318305	-2.171450	2.493908
F	3.308849	-1.622350	3.064949

TS-[4+2]-B4-R-2

H	-0.694288	-1.496043	-1.839482
P	-1.535088	0.235086	-0.527399
O	-1.465256	-0.795414	-1.674595
O	-0.312838	0.843561	0.035112
H	-5.493710	2.913412	3.309527
H	-6.553139	3.091079	1.911191
H	-3.988327	5.045871	2.229480
C	-5.611605	2.645736	2.256049
C	-3.716475	4.282450	1.506576
H	-6.558528	0.641444	2.178462
C	-5.592014	1.126702	2.016321
C	-4.450029	3.108619	1.408739
H	-4.859807	0.659705	2.683133
C	-2.600747	4.452008	0.691648
H	-2.002313	5.354991	0.768119
H	-6.940485	1.967393	-0.144607
H	-7.733650	-0.291418	0.403991
C	-4.105994	2.123474	0.476860
C	-5.091939	0.967379	0.550096
C	-6.288981	1.135120	-0.426355
C	-6.993643	-0.235857	-0.403802
C	-2.197052	3.466228	-0.215242
C	-2.984124	2.307570	-0.319771
C	-4.714122	-0.478419	0.265853
C	-5.842291	-1.184027	-0.157114
H	-5.894850	1.332365	-1.428537
O	-2.381079	-0.392199	0.707784
H	-7.519180	-0.457410	-1.336723
C	-3.504332	-1.143246	0.407870
C	-5.782748	-2.561243	-0.317200
O	-2.595789	1.280542	-1.171144
C	-3.392565	-2.531464	0.214002
H	-6.662052	-3.124222	-0.615771
C	-4.574617	-3.217872	-0.103626
H	-4.538578	-4.296951	-0.205058
C	-0.916387	3.603917	-0.956413
C	-0.821828	3.324783	-2.319785
C	0.238695	3.959175	-0.252832
C	0.406737	3.384126	-2.979125
C	1.478341	4.016999	-0.885354
C	1.545883	3.722825	-2.248986

H	2.511320	3.746545	-2.750957
C	-2.091043	-3.259709	0.272751
C	-1.002925	-2.827637	1.049572
C	-1.931672	-4.426698	-0.483474
C	0.206984	-3.520787	1.055762
C	-0.753219	-5.170499	-0.446434
C	0.313950	-4.700457	0.315887
H	1.254337	-5.249674	0.321384
N	2.934281	-1.049158	-0.334145
C	1.781685	-1.140467	-1.007222
N	3.915391	-1.584094	0.000002
H	1.087096	-0.327541	-0.910686
C	1.410055	-2.318530	-1.704696
O	0.282582	-2.465789	-2.211135
O	2.346101	-3.266054	-1.806929
C	2.001962	-4.390672	-2.614796
H	2.750969	-5.151566	-2.398696
H	1.001370	-4.744233	-2.369936
H	2.038083	-4.114315	-3.671795
C	2.906248	0.661005	1.701764
C	4.015281	-0.091436	2.227572
C	3.901201	-0.661929	3.536240
C	2.802616	-0.429787	4.309387
C	1.707759	0.331231	3.802619
C	1.748854	0.837191	2.539385
H	4.729654	-1.251473	3.910201
H	2.756575	-0.829836	5.317070
H	0.829759	0.484651	4.421538
H	0.899626	1.359577	2.108083
C	2.798208	1.005819	0.357060
C	5.112764	-0.458044	1.419579
H	-1.713132	3.032718	-2.868080
H	0.172797	4.131780	0.818969
H	-1.085008	-1.931862	1.652815
H	-2.731586	-4.757509	-1.139424
C	-0.647400	-6.453709	-1.233487
C	1.382005	-3.001925	1.846826
C	0.490238	3.082414	-4.454007
C	2.722763	4.366071	-0.106229
O	5.871705	-1.473923	1.883125
H	6.701228	-1.500673	1.390278
C	5.804803	0.430503	0.442834
C	5.945927	1.795610	0.717474
C	6.422196	-0.112395	-0.688403
C	6.678719	2.606604	-0.140441
H	5.466655	2.211674	1.598678
C	7.159599	0.702928	-1.541961
H	6.281172	-1.165418	-0.917076
C	7.287270	2.062238	-1.271076
H	6.781384	3.664635	0.077474
H	7.623615	0.277069	-2.425320
H	7.858709	2.698047	-1.939198
H	3.653961	1.163109	-0.284786
H	1.848022	1.404695	0.009920
H	0.372570	-6.846563	-1.217344
H	-0.940683	-6.304016	-2.277492
H	-1.306280	-7.222544	-0.817859
H	2.325986	-3.238729	1.345964
H	1.417304	-3.444408	2.848493
H	1.324628	-1.915355	1.964547
H	3.615717	3.948695	-0.581299
H	2.669108	3.972586	0.913479
H	2.857318	5.451002	-0.038469
H	0.062959	3.898462	-5.045719
H	-0.065358	2.173427	-4.699362
H	1.526304	2.946000	-4.772213

TS-[4+2]-B4-R-3

H	0.557567	-0.486412	-0.946087
P	-1.081079	0.272880	0.334967
O	-0.368106	-0.693604	-0.670760
O	-0.271334	0.939363	1.376526
H	-6.728316	1.784281	1.989955
H	-7.058372	2.075817	0.283170
H	-5.327641	4.276288	1.888383
C	-6.308850	1.689516	0.984913
C	-4.625052	3.670261	1.324391
H	-6.738799	-0.362032	0.257362
C	-5.910802	0.242928	0.637647
C	-4.998980	2.427392	0.831414
H	-5.508718	-0.250741	1.528373
C	-3.331224	4.130668	1.093753
H	-3.030130	5.108982	1.455510
H	-6.229428	1.246649	-1.823827
H	-6.669861	-1.165168	-1.992875
C	-4.091313	1.650491	0.107145
C	-4.764080	0.389971	-0.404089
C	-5.359488	0.583773	-1.827343
C	-5.671265	-0.844218	-2.313860
C	-2.384414	3.360118	0.407415
C	-2.794717	2.107648	-0.066997
C	-4.016540	-0.917472	-0.595471
C	-4.598932	-1.660049	-1.628327
H	-4.591522	1.031367	-2.466742
O	-2.235992	-0.635886	0.987815
H	-5.636964	-0.938753	-3.402453
C	-2.938413	-1.450115	0.092277
C	-4.148568	-2.940542	-1.919203
O	-1.870967	1.254535	-0.673681
C	-2.476003	-2.750733	-0.155183
H	-4.597205	-3.515502	-2.723755
C	-3.109242	-3.483015	-1.164719
H	-2.760108	-4.492402	-1.361986
C	-1.005439	3.869761	0.197085
C	-0.398742	3.792728	-1.057076
C	-0.319848	4.486156	1.249630
C	0.865093	4.342682	-1.277900
C	0.941871	5.040744	1.055238
C	1.511624	4.977376	-0.219180
H	2.490466	5.425660	-0.384647
C	-1.362246	-3.344884	0.628530
C	-1.397232	-3.307205	2.022205
C	-0.299796	-3.994845	-0.012885
C	-0.409872	-3.938744	2.781590
C	0.709470	-4.612615	0.721670
C	0.629086	-4.587143	2.118038

H	1.407750	-5.077985	2.700086
N	2.951314	-1.366142	-1.435693
C	2.987069	-2.562049	-1.994337
N	2.318110	-0.415588	-1.206857
H	3.885485	-3.149989	-1.942980
C	1.801879	-3.047098	-2.682275
O	1.699480	-4.147924	-3.186910
O	0.807239	-2.131450	-2.684803
C	-0.399996	-2.495090	-3.346326
H	-1.180020	-1.871707	-2.908202
H	-0.306260	-2.304542	-4.418835
H	-0.622197	-3.553198	-3.195887
C	3.200220	0.026073	1.588356
C	4.288696	0.235811	2.445964
C	4.431868	-0.525608	3.597882
C	3.490227	-1.506563	3.900109
C	2.409668	-1.719306	3.049704
C	2.255551	-0.956293	1.894658
H	5.275786	-0.353047	4.257620
H	3.598386	-2.106219	4.798279
H	1.678507	-2.486155	3.273723
H	1.418316	-1.147152	1.229925
C	3.084266	0.949112	0.424832
C	5.096768	-1.091594	-0.490680
H	5.813056	-1.764668	-0.953136
O	2.060544	1.785425	0.408190
H	1.312929	1.518293	0.997724
C	4.158532	1.231694	-0.446285
C	4.171774	2.517961	-1.083260
C	5.154264	0.248417	-0.824016
C	5.138505	2.859816	-1.975407
H	3.402780	3.224983	-0.792606
C	6.142957	0.668654	-1.792391
C	6.147543	1.912004	-2.334926
H	5.152883	3.853943	-2.410570
H	6.898124	-0.057659	-2.078231
H	6.914872	2.190466	-3.050188
H	-0.924512	3.311291	-1.876964
H	-0.776339	4.515697	2.235775
H	-2.215517	-2.795373	2.521965
H	-0.254064	-4.013623	-1.098416
C	1.876248	-5.285278	0.044658
C	-0.473614	-3.901729	4.288190
C	1.518945	4.217379	-2.629663
C	1.698232	5.668230	2.197930
H	4.549381	-1.482730	0.353709
H	5.019828	0.997830	2.194911
H	1.902687	3.201318	-2.773511
H	0.809335	4.423068	-3.435488
H	2.360984	4.907682	-2.729729
H	2.456556	4.978144	2.582102
H	2.213467	6.578436	1.879576
H	1.031148	5.922844	3.024451
H	2.805755	-4.754257	0.276806
H	1.761029	-5.296648	-1.041197
H	1.990259	-6.314950	0.396964
H	0.363204	-4.445637	4.733427
H	-0.444259	-2.870844	4.655879
H	-1.401116	-4.351477	4.654434

TS-[4+2]-B4-S-2

P	1.572191	-0.136896	-0.414328
O	0.435623	-0.912222	0.120669
O	2.124577	0.831474	0.770312
O	2.876931	-1.019613	-0.797084
C	3.145932	1.718633	0.469292
C	4.455976	1.268169	0.563823
C	3.341001	-1.858286	0.209603
C	4.277539	-1.355054	1.102474
C	5.504809	2.099132	0.161916
C	5.252979	3.407944	-0.221090
C	4.687858	-2.136834	2.186545
C	4.231971	-3.438722	2.328848
C	3.939399	3.862714	-0.242829
H	3.743869	4.895141	-0.510632
C	2.849995	3.029101	0.053108
C	3.327586	-3.940298	1.399431
H	2.975764	-4.962520	1.492702
C	2.831625	-3.161148	0.344835
O	1.437214	0.698842	-1.705921
H	0.591863	1.271687	-1.973897
C	1.463413	3.549869	-0.114793
C	0.380212	3.112180	0.664785
C	1.227658	4.545020	-1.069240
C	-0.893132	3.653765	0.497652
C	-0.026824	5.133225	-1.223251
C	-1.081147	4.673183	-0.439239
H	-2.074543	5.099813	-0.570729
C	1.779831	-3.721985	-0.544129
C	0.810709	-4.569256	0.001158
C	1.751338	-3.469383	-1.920418
C	-0.155769	-5.181131	-0.797622
C	0.777059	-4.042656	-2.735214
C	-0.163782	-4.903215	-2.163833
H	-0.910625	-5.373918	-2.801031
N	-3.105719	0.595505	-0.602410
C	-1.869383	0.826189	-1.061527
N	-4.234596	0.885358	-0.659799
H	-1.084913	0.167628	-0.736319
C	-1.606730	1.854484	-2.001910
O	-0.475506	2.062273	-2.477749
O	-2.656171	2.594379	-2.371490
C	-2.405467	3.538249	-3.411134
H	-2.187071	3.018382	-4.346924
H	-3.320500	4.121123	-3.505929
H	-1.560158	4.175131	-3.150709
C	-3.539752	-1.822713	0.364414
C	-4.942407	-1.565928	0.167722
C	-5.697136	-2.462633	-0.655967
C	-5.118972	-3.567476	-1.205365
C	-3.726450	-3.819865	-1.026163
C	-2.965812	-2.972761	-0.281128
H	-6.749016	-2.252610	-0.808224
H	-5.717904	-4.256804	-1.791450
H	-3.266186	-4.679919	-1.503348
H	-1.893685	-3.127690	-0.176836

C	-2.674040	-0.881477	0.912712
C	-5.536599	-0.347965	0.565365
H	6.064831	4.070455	-0.505889
H	4.562975	-4.055591	3.158987
C	5.021000	-0.030187	1.115208
C	6.818091	1.353183	0.205234
C	6.355617	-0.110785	0.321916
C	5.328454	0.099486	2.635202
C	5.594821	-1.343452	3.097244
H	7.085977	-0.765745	0.805351
H	6.142454	-0.512385	-0.674059
H	7.415568	1.654373	1.074495
H	7.428066	1.536785	-0.683488
H	6.156262	0.786184	2.833063
H	4.435427	0.488011	3.135604
H	6.645366	-1.622595	2.948870
H	5.365078	-1.502067	4.154400
H	2.032830	4.860119	-1.726499
H	0.528422	2.339012	1.409943
H	2.500694	-2.820464	-2.362011
H	0.802592	-4.751063	1.072773
C	-0.221479	6.242856	-2.226928
C	-2.064287	3.154111	1.306324
C	0.732843	-3.725632	-4.208356
C	-1.165596	-6.117108	-0.180215
H	-1.603557	-1.069370	0.872835
H	-3.000063	-0.122347	1.610173
C	-5.304293	0.357252	1.858555
C	-5.378069	1.752428	1.924099
C	-5.131692	-0.380587	3.034623
C	-5.254094	2.402557	3.148490
H	-5.487280	2.323000	1.005650
C	-5.007987	0.272921	4.254722
H	-5.081656	-1.463747	2.977903
C	-5.065859	1.664657	4.313894
H	-5.293064	3.486192	3.188351
H	-4.869194	-0.304951	5.162324
H	-4.963839	2.172037	5.267470
O	-6.714341	-0.050239	-0.023561
H	-7.136332	0.671156	0.459441
H	0.309012	7.148413	-1.916143
H	-1.278562	6.498383	-2.337268
H	0.167337	5.959495	-3.210052
H	-2.346106	3.869351	2.087065
H	-2.938045	3.004420	0.662382
H	-1.833654	2.200479	1.788802
H	-1.892656	-5.570785	0.430244
H	-1.718344	-6.664514	-0.948360
H	-0.676086	-6.849093	0.468281
H	0.143990	-2.820678	-4.389527
H	0.276181	-4.539439	-4.777033
H	1.735449	-3.548827	-4.604841

TS-[4+2]-B4-S-3

H	0.483931	-0.629451	-0.980342
P	-1.080623	0.296649	0.219325
O	-0.505137	-0.633029	-0.893369
O	-0.144253	0.882729	1.208013
H	-6.452586	2.076716	2.450485
H	-6.927961	2.414637	0.787022
H	-4.923951	4.480961	2.260813
C	-6.137064	1.976887	1.408580
C	-4.315655	3.852306	1.617481
H	-6.748112	-0.036853	0.704610
C	-5.854677	0.516681	1.007193
C	-4.808978	2.645737	1.137803
H	-5.394438	-0.012046	1.848259
C	-3.022775	4.244121	1.276047
H	-2.626404	5.189074	1.635242
H	-6.363806	1.565121	-1.401836
H	-6.936460	-0.820548	-1.548722
C	-4.023565	1.835065	0.314141
C	-4.809950	0.618568	-0.141997
C	-5.532108	0.861267	-1.497713
C	-5.960513	-0.543136	-1.965731
C	-2.196684	3.438523	0.484034
C	-2.725946	2.225702	0.025216
C	-4.152179	-0.722253	-0.420329
C	-4.865189	-1.419111	-1.401059
H	-4.809671	1.280530	-2.205695
O	-2.218724	-0.542417	0.980233
H	-6.040621	-0.621505	-3.053188
C	-3.036622	-1.313988	0.147361
C	-4.497363	-2.709884	-1.756012
O	-1.908788	1.344310	-0.682120
C	-2.648157	-2.625193	-0.167163
H	-5.046565	-3.250391	-2.521156
C	-3.409696	-3.309149	-1.121008
H	-3.126275	-4.327253	-1.371119
C	-0.802241	3.841067	0.164104
C	-0.333871	3.807464	-1.149387
C	0.056898	4.263233	1.184746
C	0.970208	4.204048	-1.455557
C	1.366291	4.642068	0.905904
C	1.803500	4.619530	-0.421024
H	2.830652	4.901980	-0.645639
C	-1.477966	-3.262801	0.491196
C	-1.322792	-3.155454	1.874664
C	-0.544750	-4.005145	-0.244550
C	-0.262311	-3.778249	2.532000
C	0.523198	-4.638529	0.391901
C	0.652076	-4.508252	1.777421
H	1.489022	-4.992682	2.277460
N	2.708512	-1.590871	-1.263601
C	2.643951	-2.712189	-1.963505
N	2.216248	-0.557796	-1.032638
H	3.341974	-3.502764	-1.759616
C	1.511089	-2.923601	-2.846648
O	1.243657	-3.984009	-3.379610
O	0.754122	-1.814974	-2.986797
C	-0.485055	-1.994432	-3.666328
H	-0.894782	-0.994700	-3.799232
H	-0.326679	-2.489934	-4.625394
H	-1.170051	-2.588565	-3.054243
C	3.246069	-0.337513	1.438690
C	4.009070	-1.527536	1.126285

C	3.940365	-2.615021	2.069353
C	3.183410	-2.549976	3.195995
C	2.394415	-1.393938	3.468414
C	2.409058	-0.342279	2.603955
H	4.523811	-3.504632	1.849404
H	3.176526	-3.382801	3.893114
H	1.799494	-1.346417	4.373903
H	1.820955	0.541555	2.823830
C	3.208217	0.813734	0.610672
C	4.614543	-1.760869	-0.101227
H	5.070625	-2.732163	-0.269513
H	4.916171	-0.972746	-0.775067
O	2.233403	1.691191	0.675468
H	1.340510	1.326523	0.959799
C	4.350269	1.353482	-0.168483
C	4.084735	2.066372	-1.340782
C	5.660156	1.260990	0.309860
C	5.127962	2.654235	-2.047000
H	3.056982	2.141042	-1.682162
C	6.698676	1.859537	-0.393366
H	5.855347	0.717466	1.229511
C	6.434905	2.551825	-1.574429
H	4.922268	3.191211	-2.967648
H	7.714184	1.791233	-0.017685
H	7.248470	3.014367	-2.123989
H	-0.996013	3.473226	-1.943956
H	-0.296259	4.251780	2.213022
H	-2.045586	-2.583362	2.449443
H	-0.640632	-4.087652	-1.325737
C	1.509764	-5.481920	-0.375393
C	-0.148921	-3.693042	4.032569
C	1.457214	4.176970	-2.882869
C	2.328062	4.990340	2.010753
H	1.436013	-5.313195	-1.451878
H	2.533264	-5.259665	-0.055943
H	1.333360	-6.545408	-0.181303
H	-0.840959	-4.391086	4.515367
H	0.860449	-3.942709	4.369263
H	-0.393059	-2.688665	4.388814
H	2.996021	4.142597	2.197889
H	2.949988	5.848963	1.743875
H	1.804049	5.220152	2.941247
H	1.321876	3.185727	-3.327303
H	0.904440	4.889374	-3.503073
H	2.517833	4.435718	-2.940357

^{1}INT0

C	-3.447441	-1.468426	0.146863
C	-2.280260	-1.999788	0.684687
C	-1.126307	-1.225409	0.699583
C	-1.131107	0.082334	0.202340
C	-2.315586	0.636233	-0.321861
C	-3.455330	-0.169276	-0.352287
H	-4.354712	-2.063506	0.115597
H	-2.265762	-3.007582	1.085659
H	-0.209252	-1.629242	1.117735
H	-4.370937	0.238034	-0.771953
C	0.111637	0.914631	0.310960
C	1.452056	0.277152	0.081907
C	2.570742	0.903680	0.639703
C	1.622614	-0.857053	-0.716958
C	3.841485	0.386697	0.425806
H	2.416768	1.797387	1.235275
C	2.898987	-1.364322	-0.943798
H	0.759920	-1.331093	-1.174123
C	4.006404	-0.748974	-0.366708
H	4.705705	0.869001	0.870727
H	3.028410	-2.238869	-1.572842
H	5.000048	-1.150587	-0.538609
O	0.047108	2.098314	0.588156
C	-2.391631	2.047384	-0.847265
H	-2.385491	2.765266	-0.024363
H	-1.533453	2.293260	-1.476644
H	-3.305683	2.182233	-1.429538

^{3}INT0

C	3.514577	-1.446961	-0.137165
C	2.323222	-2.039138	-0.550482
C	1.154884	-1.295715	-0.573192
C	1.141103	0.053399	-0.160217
C	2.356744	0.665148	0.242873
C	3.514918	-0.108699	0.247152
H	4.436586	-2.018136	-0.118890
H	2.306502	-3.075022	-0.872964
H	0.236132	-1.743444	-0.936256
H	4.443353	0.354200	0.570214
C	-0.116021	0.781916	-0.198721
C	-1.455538	0.250715	-0.057895
C	-2.553723	0.972111	-0.574888
C	-1.707471	-0.943874	0.650234
C	-3.846448	0.497276	-0.411643
H	-2.375044	1.891809	-1.122173
C	-3.004011	-1.411312	0.793091
H	-0.881424	-1.482977	1.101098
C	-4.082142	-0.698682	0.264569
H	-4.677434	1.060965	-0.823661
H	-3.178897	-2.333868	1.337542
H	-5.094221	-1.069597	0.384917
O	-0.065275	2.091712	-0.421953
C	2.423477	2.100186	0.699479
H	2.270135	2.798032	-0.129425
H	1.654506	2.315457	1.446882
H	3.400582	2.310656	1.139182

^{3}TS1

C	3.575366	-1.411211	-0.207697
C	2.362478	-2.075216	-0.399557
C	1.160839	-1.391873	-0.323449
C	1.132171	-0.009339	-0.028859
C	2.372462	0.662457	0.146250
C	3.567528	-0.041657	0.046521
H	4.514997	-1.948197	-0.275043
H	2.356118	-3.134080	-0.637721
H	0.236123	-1.912220	-0.541468
H	4.504547	0.492590	0.178179
C	-0.084397	0.758926	0.005336

C	-1.448559	0.238774	0.013099
C	-2.479037	0.994812	-0.577467
C	-1.786862	-0.966833	0.655460
C	-3.789084	0.538312	-0.560782
H	-2.231062	1.934809	-1.058260
C	-3.100118	-1.417405	0.661906
H	-1.022051	-1.528310	1.180778
C	-4.107526	-0.673714	0.049883
H	-4.567702	1.130190	-1.031489
H	-3.341472	-2.348506	1.164915
H	-5.132197	-1.029905	0.058841
O	-0.040530	2.100550	0.008572
C	2.354906	2.123951	0.430040
H	3.040892	2.729540	-0.164451
H	1.209616	2.432157	0.104697
H	2.375433	2.397628	1.488352

^{3}INT1

C	3.629224	-1.238576	-0.068945
C	2.551294	-1.850841	-0.706035
C	1.325780	-1.186531	-0.785639
C	1.143634	0.072928	-0.219376
C	2.238503	0.702163	0.458788
C	3.474214	0.016407	0.498762
H	4.587979	-1.743254	-0.010839
H	2.663205	-2.832756	-1.153043
H	0.491403	-1.646109	-1.307045
H	4.307159	0.485881	1.014564
C	-0.143141	0.770161	-0.368765
C	-1.430814	0.221562	-0.109232
C	-2.597405	0.934926	-0.481542
C	-1.595689	-1.024221	0.545637
C	-3.854318	0.414215	-0.225225
H	-2.489023	1.892372	-0.977363
C	-2.860479	-1.529822	0.792905
H	-0.720299	-1.575446	0.872423
C	-4.001041	-0.821359	0.408599
H	-4.734124	0.975649	-0.524629
H	-2.961414	-2.484676	1.299600
H	-4.988897	-1.224027	0.604687
O	-0.118591	2.053038	-0.832557
C	2.103289	1.952929	1.114898
H	2.958444	2.391584	1.613836
H	0.784517	2.272712	-1.092932
H	1.151469	2.460121	1.192218

^{3}INT2

C	3.829432	-0.551807	-0.429091
C	3.432388	0.677302	-0.951625
C	2.136545	1.138364	-0.714802
C	1.222919	0.401866	0.040476
C	1.633209	-0.845605	0.612223
C	2.944434	-1.295918	0.335903
H	4.831714	-0.925266	-0.611735
H	4.117766	1.269907	-1.547941
H	1.812703	2.081345	-1.147691
H	3.263014	-2.241830	0.764869
C	-0.110054	0.978929	0.276804
C	-1.365959	0.362222	0.010767
C	-2.572501	1.013485	0.367653
C	-1.453592	-0.897645	-0.631315
C	-3.795874	0.418772	0.111684
H	-2.520560	1.982660	0.849892
C	-2.686611	-1.479017	-0.876737
H	-0.545166	-1.399953	-0.946867
C	-3.866907	-0.831851	-0.506847
H	-4.708458	0.932734	0.397783
H	-2.730393	-2.443703	-1.372713
H	-4.829131	-1.292199	-0.703742
O	-0.153430	2.294984	0.631453
C	0.794838	-1.602218	1.468465
H	1.152665	-2.538064	1.879499
H	0.719278	2.553301	0.953020
H	-0.189600	-1.260077	1.752642

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