Electronic Supplementary Material for Dalton Transactions

Supplementary Information

Epoxidation of olefins catalysed by vanadium-salan complexes: a theoretical mechanistic study

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Additional discussion of the FMO composition

For complex **3c**, there are other lower lying virtual MOs with a symmetry appropriate for the interaction with the HOMO of C_2H_4 (*i.e.*, LUMO+5, LUMO+6, and LUMO+7, Figure 3S). However, a contribution from the peroxo-group to these MOs is not significant. In order to check how the structural changes occurring in complex **3c** upon formation of **TS3a** affect the composition and energies of the MOs we calculated two correlation MO diagrams. For the first diagram, single-point calculations in several points along the **3c** → **TS3a** IRC path were performed with removed ethylene molecule. The results are presented in Figure 3S and demonstrate changes of the orbitals in the fragment {V(=O)(OO)LH} from **3c** to **TS3a**. The second diagram (Figure 4S) shows what changes of MOs occur in **TS3a** upon moving off the C_2H_4 molecule with other structural parameters preserved. The analysis of these diagrams indicates that the energy of the LUMO+12 of **3c** decreases significantly (by 5.53 eV) ongoing to **TS3a**. In fact, this MO becomes the first LUMO in the {V(=O)(OO)LH} fragment with geometry taken from the equilibrium structure of **TS3a** (fragment $\mathbf{\{3c\}_{TS3a}}$). The HOMO of **3c** becomes the HOMO–3 in $\mathbf{\{3c\}_{TS3a}}$ and its energy also *decreases* (by 1.39 eV). As a result, the $HOMO_{C2H4}$–$LUMO_{\mathbf{\{3c\}TS3a}}$ energy gap is smaller (by 4.45 eV) than the HOMO–$3_{\mathbf{\{3c\}TS3a}}$–$LUMO_{C2H4}$ gap and the first type of the interactions determines the reaction. At the same time it is necessary to mention that a significant mixture of virtual orbitals takes place along the reaction path. Hence, some involvement of LUMO+5, LUMO+6 and LUMO+7 of **3c** in the interaction with $HOMO_{C2H4}$ cannot be excluded.

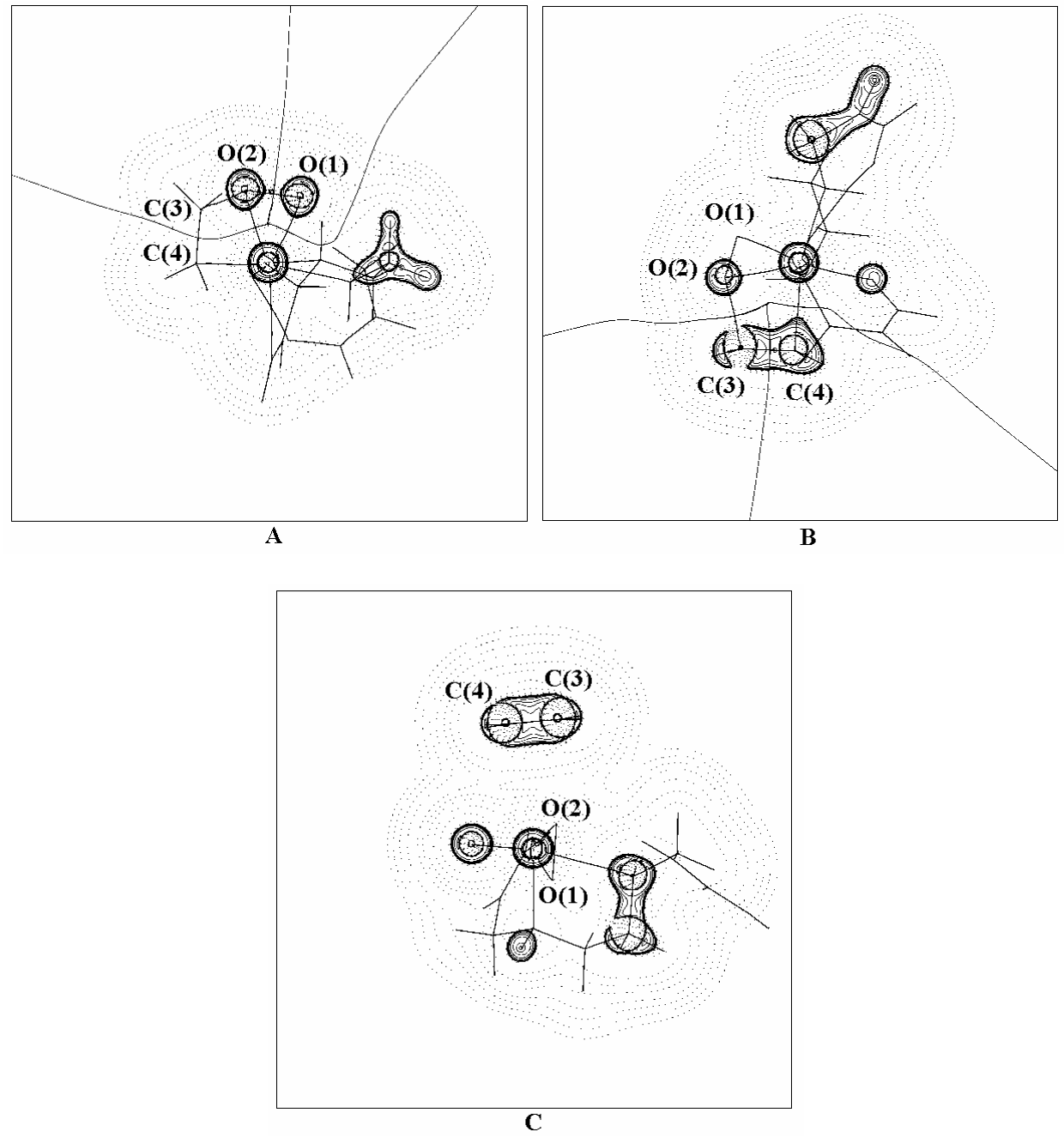
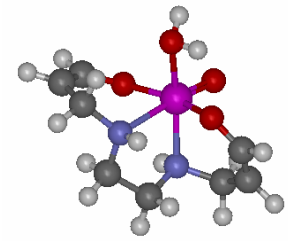


Figure 1S. Contour line diagrams of the Laplacian distribution $\nabla^2\rho(\mathbf{r})$, bond paths and selected zero-flux surfaces for transition state **TS1a** in the planes formed by V, O(1) and O(2) atoms (**A**) and V, O(2), C(3) and C(4) atoms (**B**) and for complex **4f** in the VC(3)C(4) plane (**C**). Dashed lines indicate charge depletion ($\nabla^2\rho(\mathbf{r}) > 0$), solid lines indicate charge concentration ($\nabla^2\rho(\mathbf{r}) < 0$).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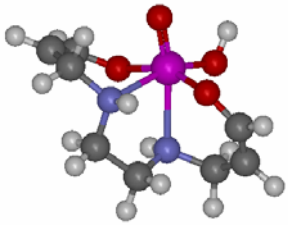
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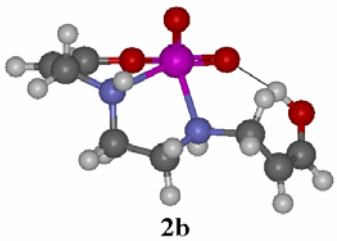
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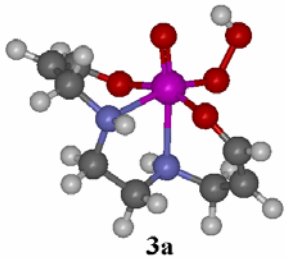
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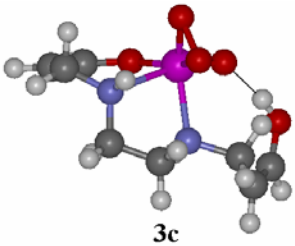
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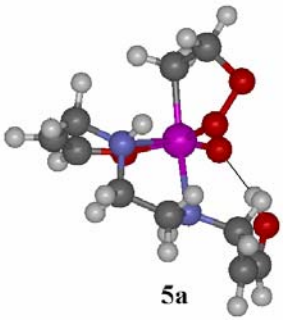
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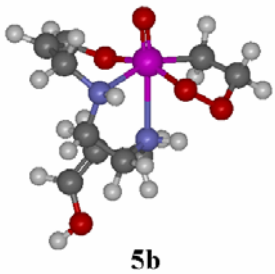
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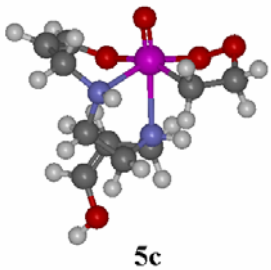
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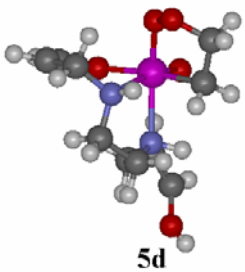
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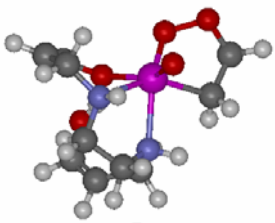
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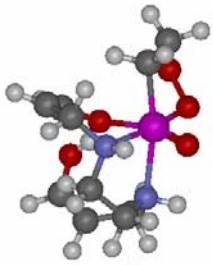
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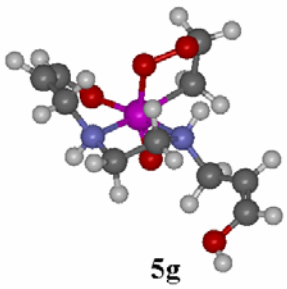
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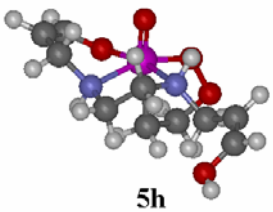
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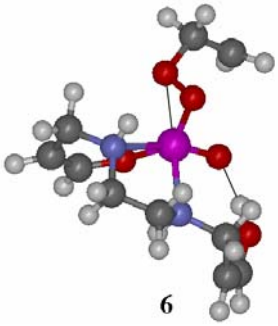
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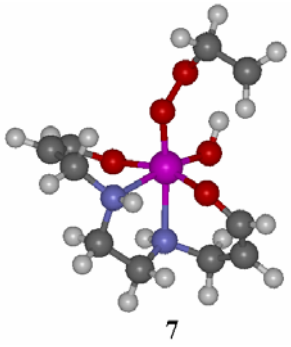
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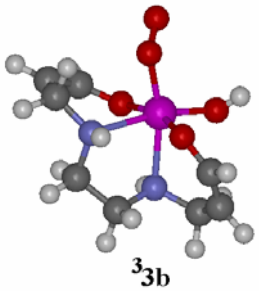
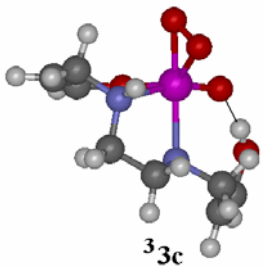

^{3}3b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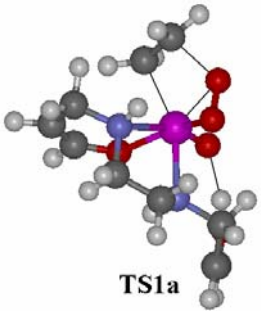
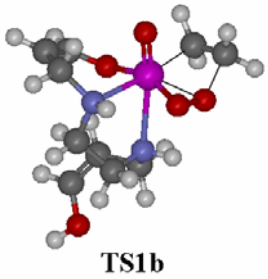

TS1a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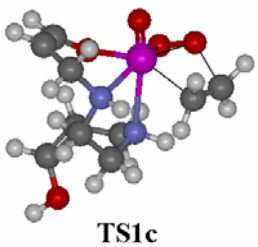
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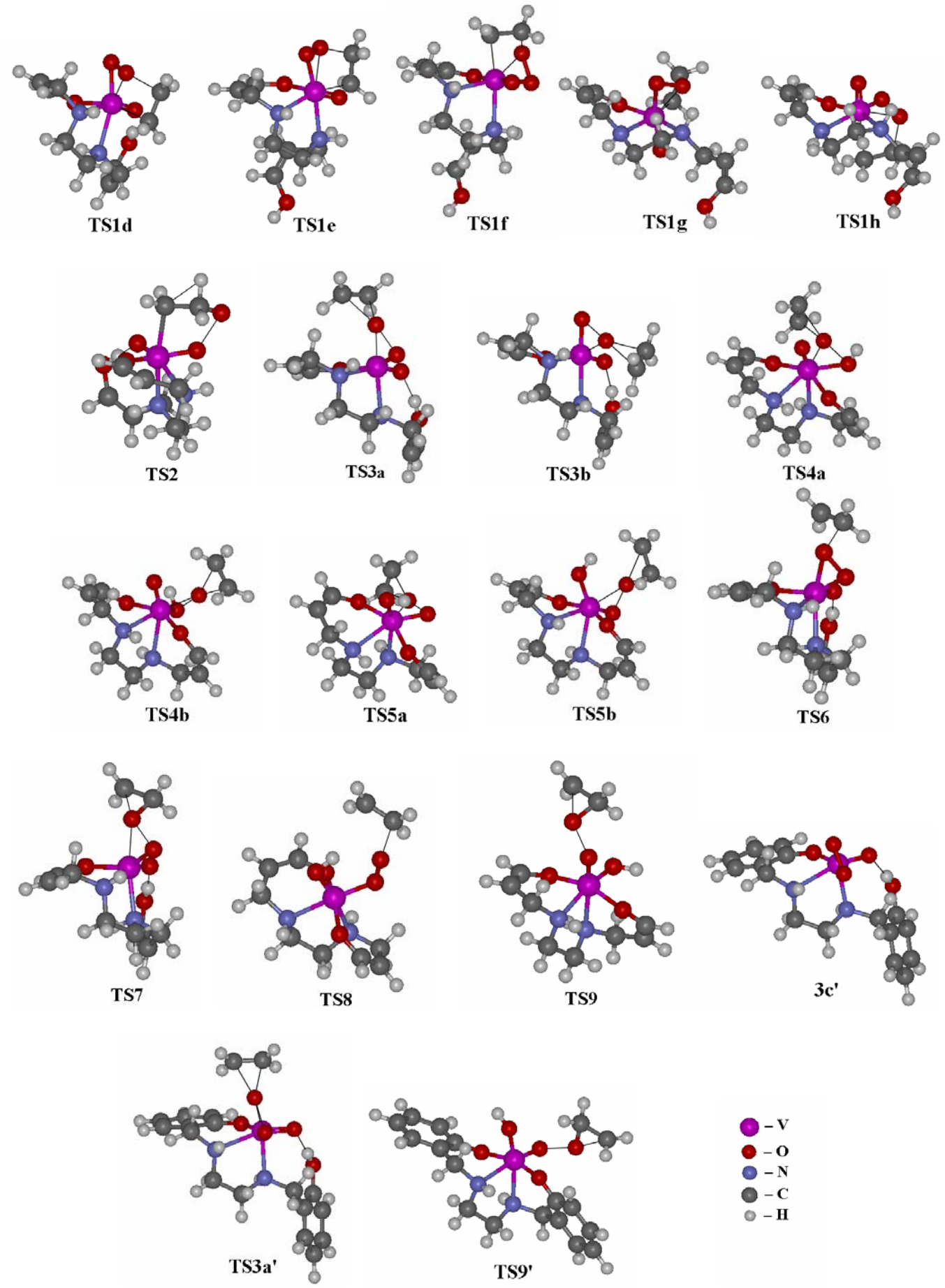
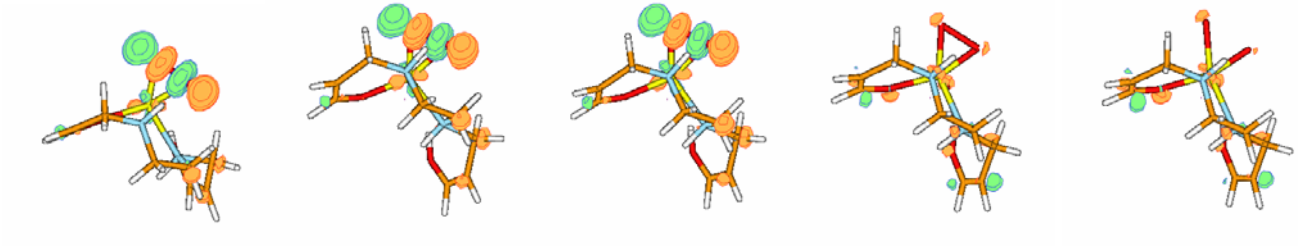
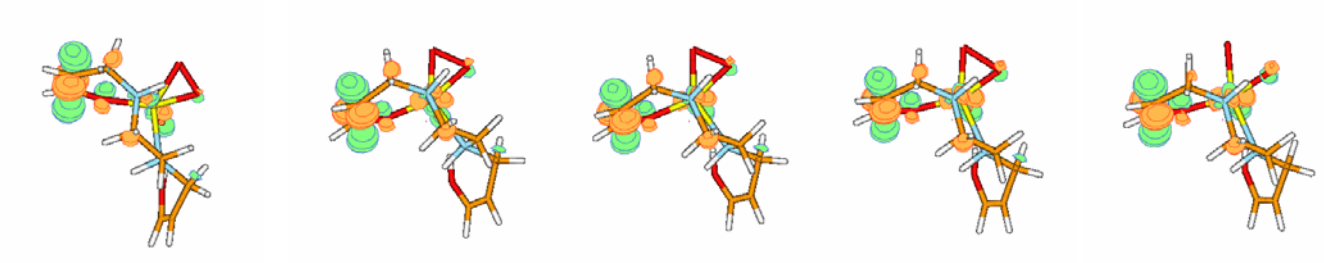


Figure 2S. General view of the main calculated equilibrium structures.

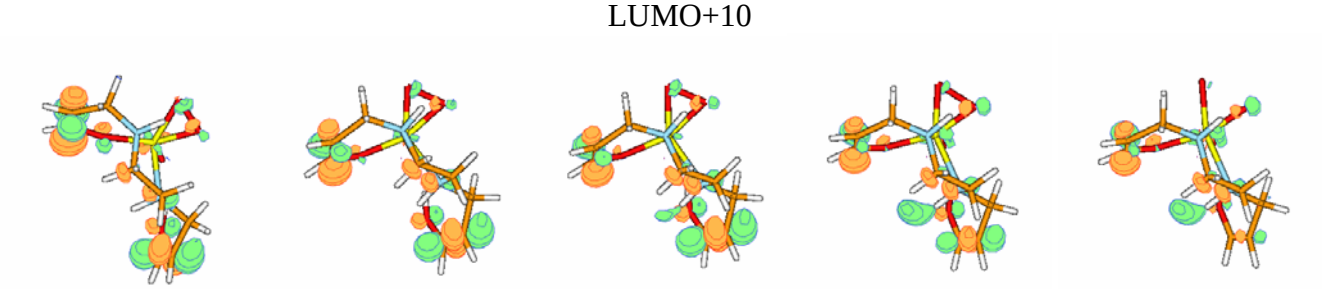


LUMO+12

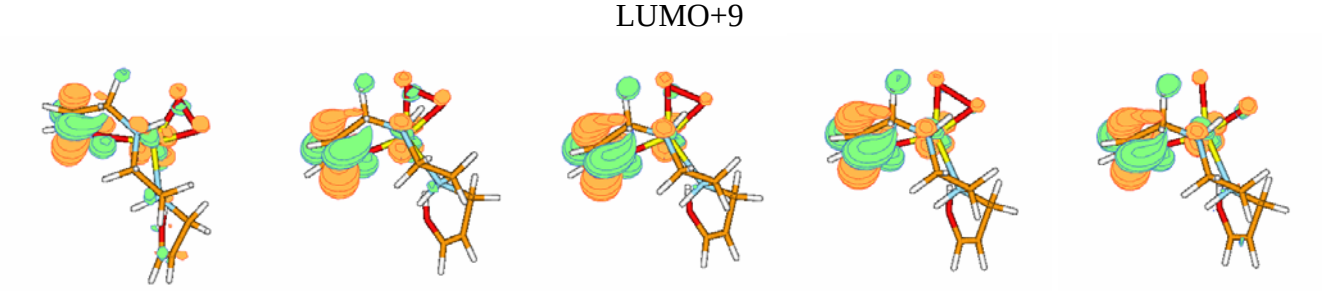
LUMO+11



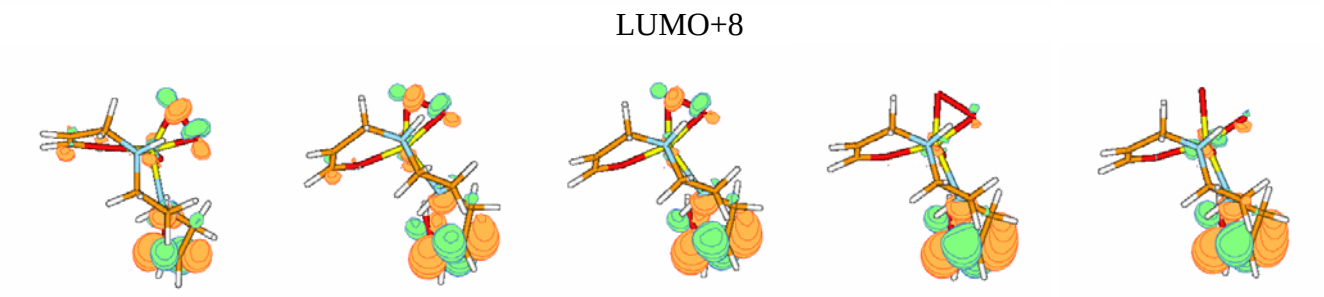
LUMO+10



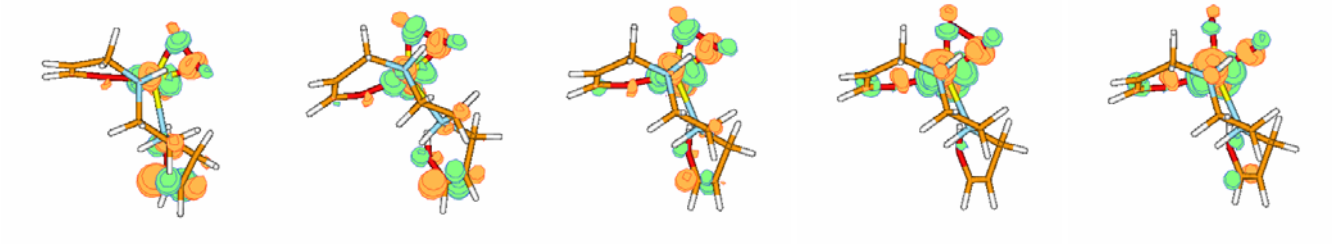
LUMO+9



LUMO+8



LUMO+7



LUMO+6

LUMO+5

LUMO+4

LUMO+3

LUMO+2

LUMO+1

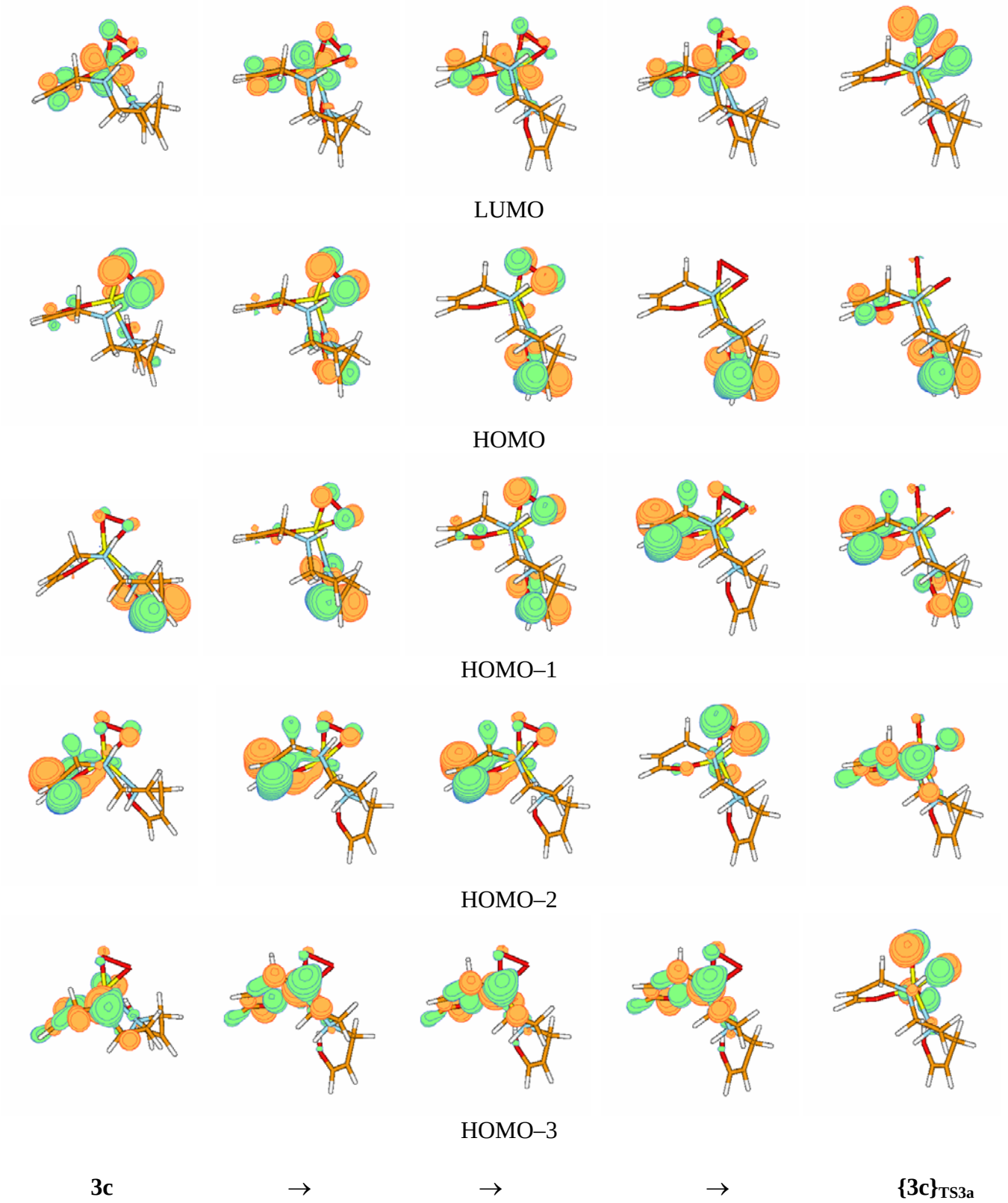
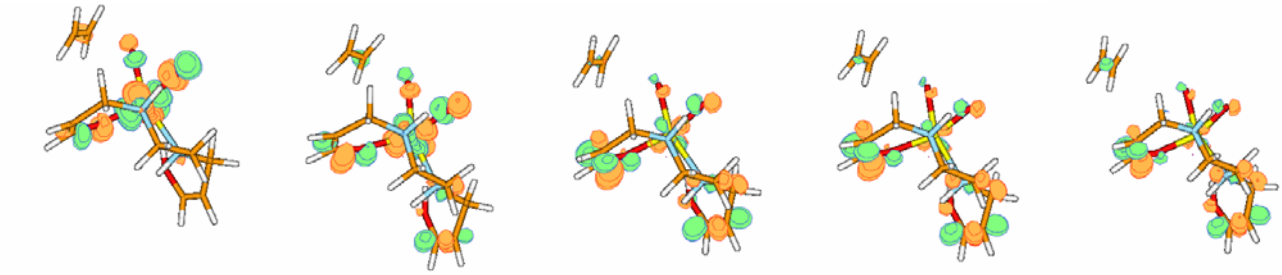
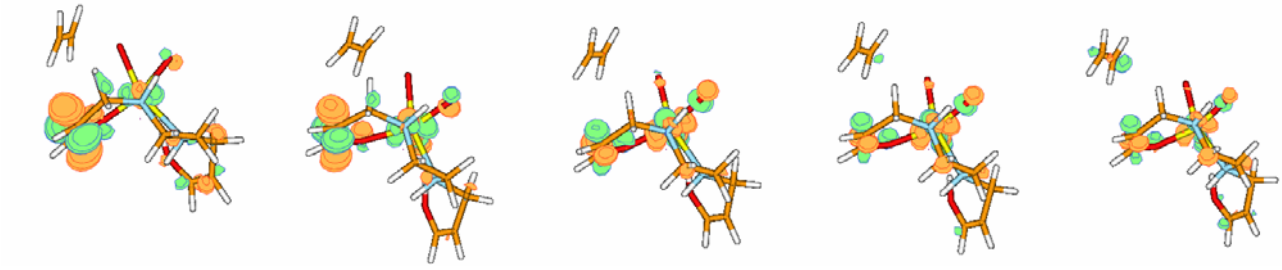


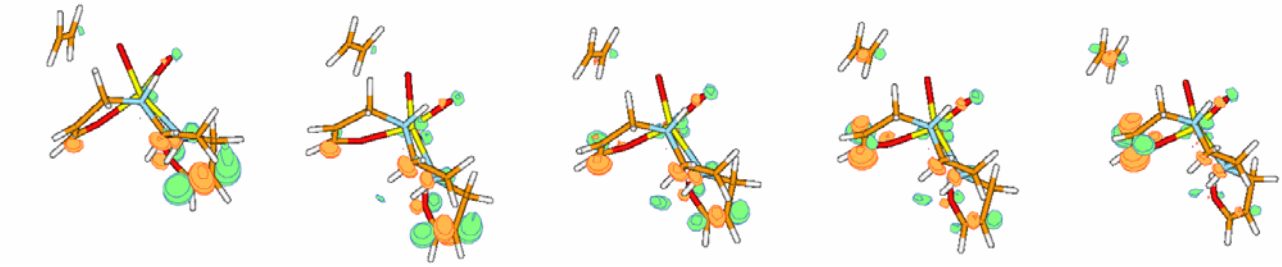
Figure 3S. Change of MO composition of the {V(=O)(OO)LH} fragment from **3c** to **TS3a** along the reaction coordinate.



LUMO+12

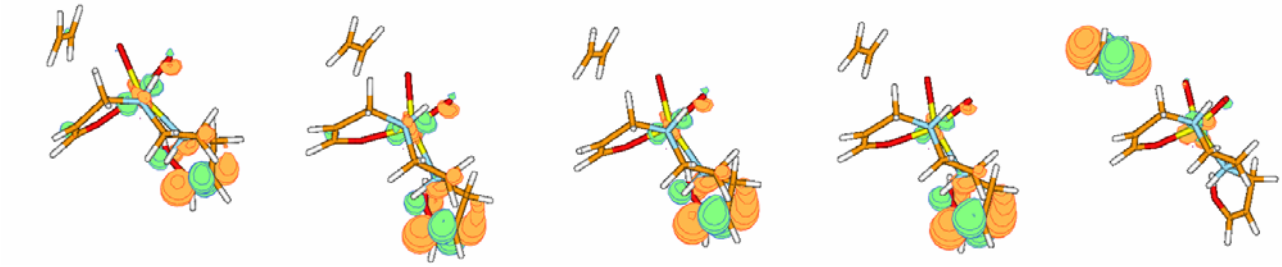


LUMO+11



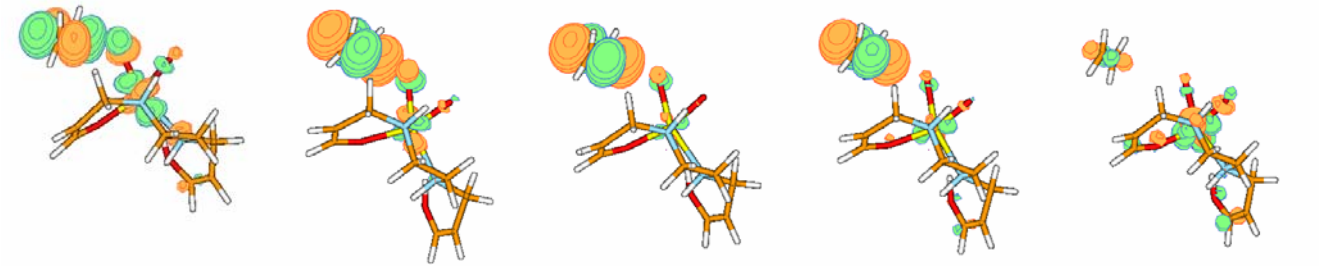
LUMO+10

LUMO+9

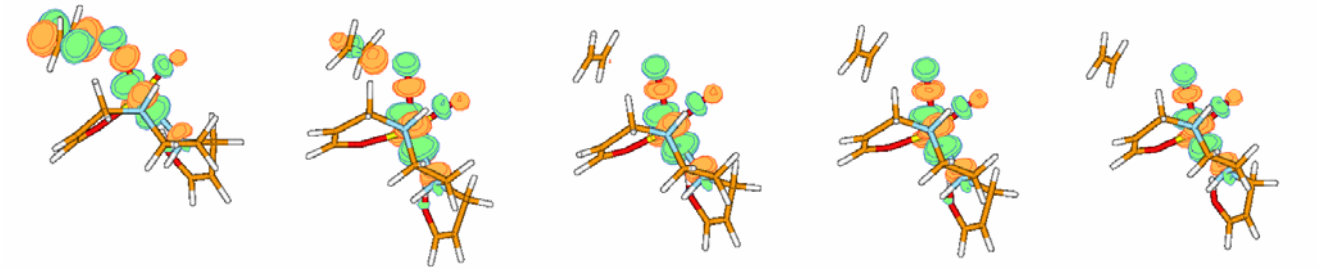


LUMO+8

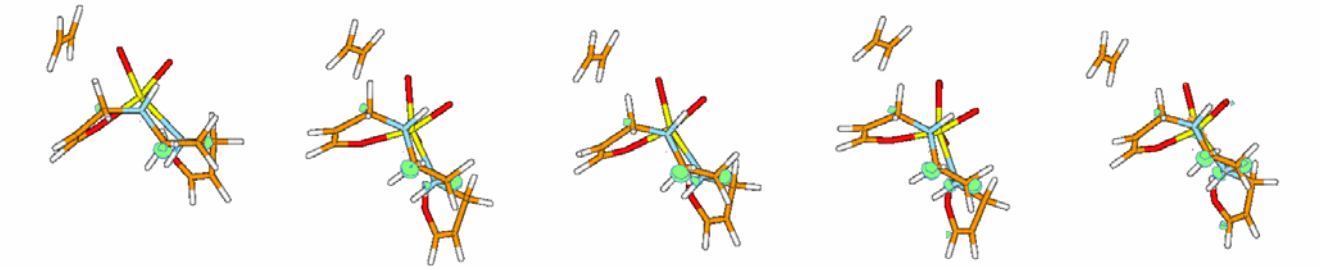
LUMO+7



LUMO+6



LUMO+5



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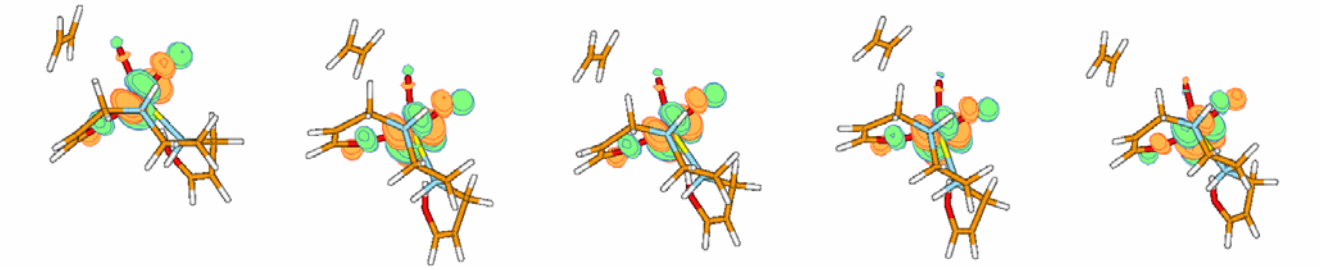
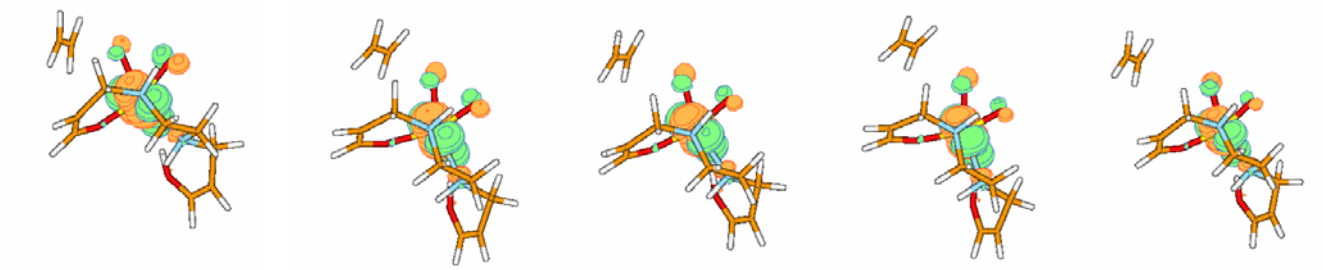
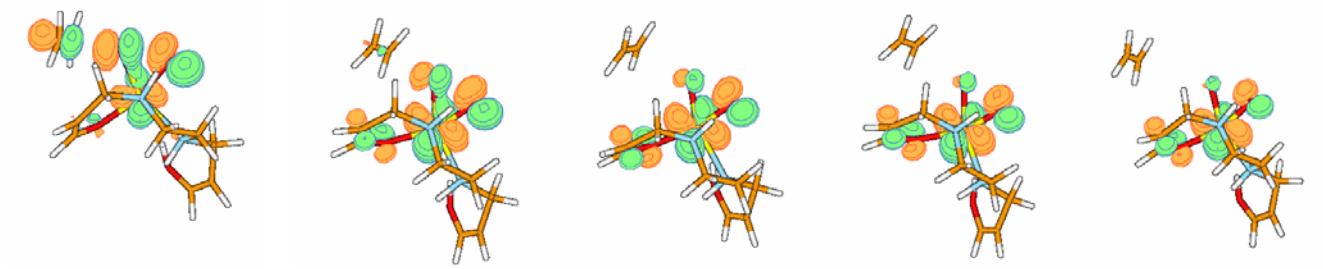


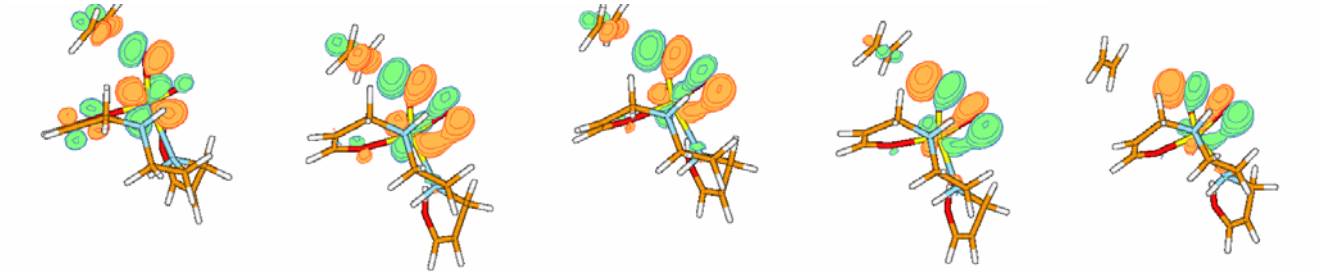
LUMO+3



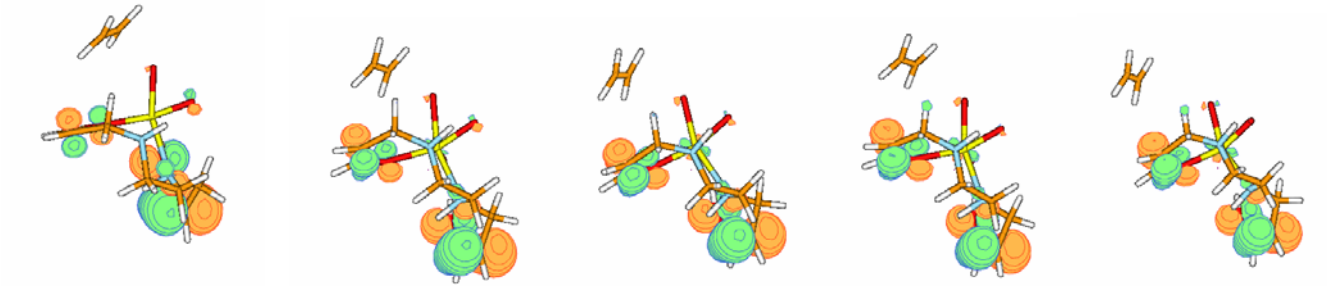
LUMO+2



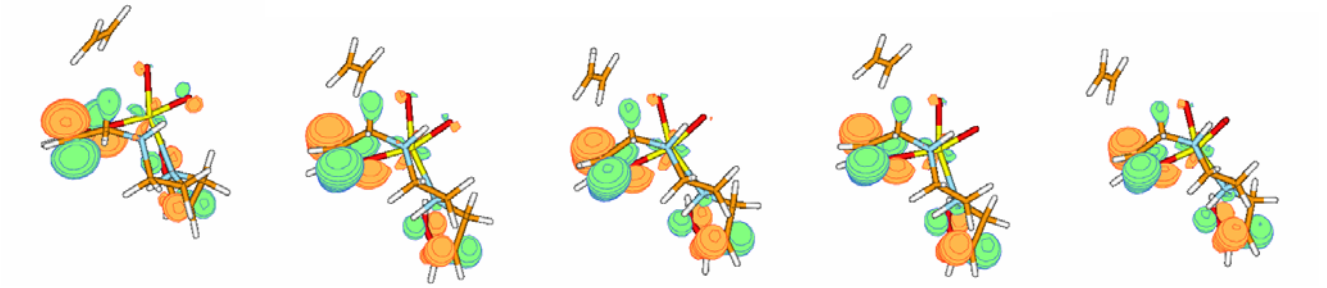
LUMO+1



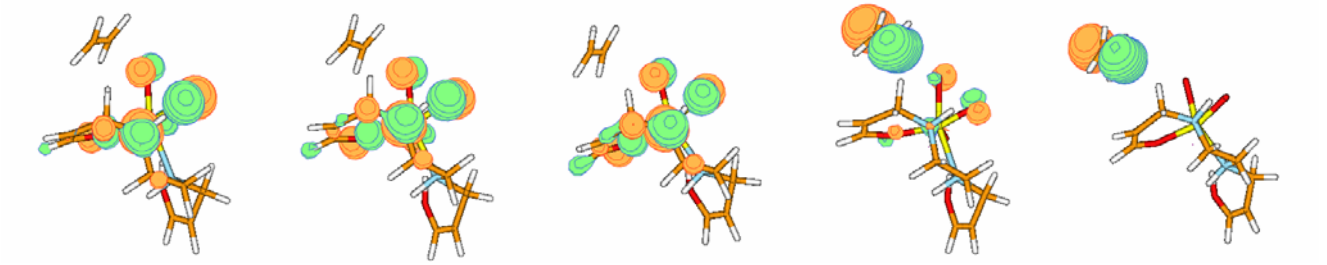
LUMO



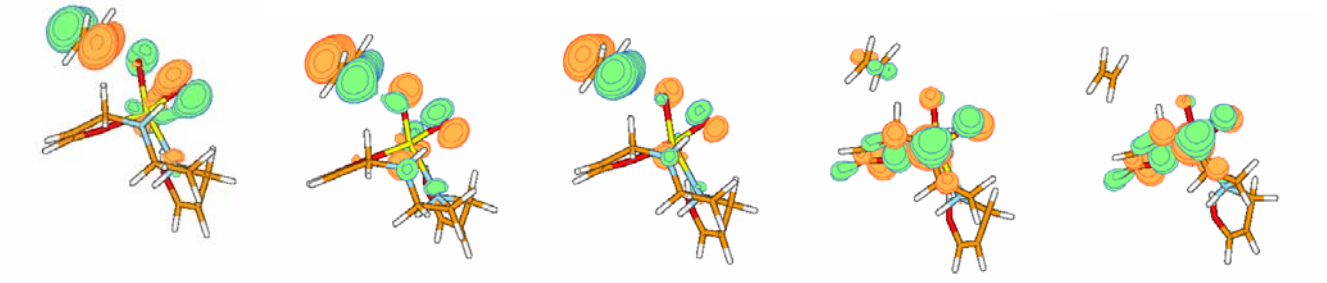
HOMO



HOMO–1



HOMO–2



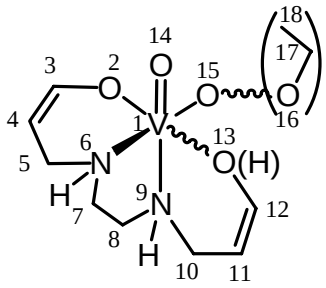
HOMO–3

HOMO–4

TS3a A B C D

Figure 4S. Change of MO composition in **TS3a** upon moving off the ethylene molecule. The O(2)C(4) distance is 2.15 Å (**TS3a**), 2.41 Å (A), 2.66 Å (B), 2.92 Å (C), 3.71 Å (D).

Table 1S. Selected calculated bond lengths (Å) of the equilibrium structures and atom numbering.



	1a	**2a**	**2b**	**3a**	**3b**	**3c**	**3c'**	**33b**	**33c**
VO(2)	1.962	1.888	1.836	1.893	1.920	1.826	1.820	1.898	1.890
VO(13)	1.931	1.888		1.885	1.976			1.855	
VN(6)	2.145	2.262	2.398	2.237	2.286	2.450	2.422	2.237	2.398
VN(9)	2.421	2.384	2.173	2.367	2.245	2.160	2.166	2.282	2.213
VO(14)	1.592	1.577	1.600	1.585	1.776	1.602	1.603	1.795	1.603
VO(15)	2.152	1.797	1.627	1.798	1.801	1.857	1.859	1.897	2.007
VO(16)					1.807	1.792	1.792		2.002
O(2)C(3)	1.333	1.339	1.341	1.893	1.333	1.342	1.348	1.898	1.329
C(3)C(4)	1.351	1.345	1.343	1.345	1.346	1.343	1.411	1.348	1.349
C(4)C(5)	1.507	1.504	1.503	1.504	1.498	1.504	1.510	1.505	1.503
C(5)N(6)	1.498	1.485	1.482	1.487	1.479	1.472	1.471	1.489	1.490
N(6)C(7)	1.488	1.479	1.463	1.481	1.473	1.463	1.464	1.481	1.471
C(7)C(8)	1.524	1.524	1.526	1.525	1.519	1.524	1.525	1.524	1.522
C(8)N(9)	1.469	1.470	1.486	1.474	1.480	1.484	1.486	1.478	1.482
N(9)C(10)	1.480	1.478	1.535	1.479	1.493	1.529	1.520	1.484	1.523
C(10)C(11)	1.504	1.504	1.495	1.504	1.503	1.497	1.506	1.505	1.498
C(11)C(12)	1.350	1.347	1.351	1.346	1.348	1.350	1.415	1.345	1.349
C(12)O(13)	1.328	1.338	1.336	1.339	1.337	1.339	1.355	1.341	1.339
O(15)O(16)				1.425	1.415	1.445	1.446	1.321	1.326
	5a	**6**	**7**	**TS1a**	**TS2**	**TS3a**	**TS3b**	**TS3a'**	**TS4a**
VO(2)	1.820	1.902	1.903	1.933	1.860	1.871	1.836	1.861	1.938
VO(13)			1.871						2.003
VN(6)	2.478	2.421	2.236	2.512	2.542	2.478	2.372	2.441	2.283

VN(9)	2.243	2.197	2.273	2.215	2.194	2.205	2.274	2.218	2.363
VO(14)	1.593	1.610	1.800	1.585	1.612	1.609	1.615	1.611	1.573
VO(15)	1.890	1.918	1.825	1.884	1.667	1.715	1.696	1.716	1.955
VO(16)		2.097		1.973		1.880	1.964	1.880	2.039
VC(18)	2.102			2.257	2.367				
O(2)C(3)	1.341	1.328	1.338	1.327	1.335	1.335	1.342	1.342	1.337
C(3)C(4)	1.345	1.349	1.346	1.352	1.347	1.347	1.344	1.415	1.345
C(4)C(5)	1.505	1.503	1.504	1.505	1.504	1.505	1.505	1.512	1.500
C(5)N(6)	1.472	1.485	1.486	1.477	1.471	1.471	1.478	1.469	1.476
N(6)C(7)	1.467	1.465	1.481	1.474	1.462	1.462	1.466	1.462	1.474
C(7)C(8)	1.523	1.522	1.527	1.521	1.523	1.523	1.524	1.525	1.524
C(8)N(9)	1.479	1.483	1.480	1.478	1.481	1.481	1.478	1.482	1.478
N(9)C(10)	1.520	1.522	1.482	1.517	1.527	1.524	1.516	1.516	1.485
C(10)C(11)	1.499	1.499	1.505	1.501	1.497	1.499	1.500	1.507	1.503
C(11)C(12)	1.348	1.350	1.345	1.347	1.350	1.349	1.349	1.415	1.349
C(12)O(13)	1.341	1.339	1.339	1.344	1.339	1.339	1.340	1.354	1.333
O(15)O(16)	1.453	1.472	1.454	1.419	2.024	1.826	1.783	1.827	1.763
O(16)C(17)	1.426	1.482	1.433	1.900	1.318	2.049	2.285	2.026	2.075
C(17)C(18)	1.519	1.476	1.487	1.404	1.489	1.361	1.368	1.362	1.362
O(16)C(18)						2.153	1.894	2.175	2.035
	TS5b	**TS6**	**TS7**	**TS8**	**TS9**	**TS9'**			
VO(2)	1.903	1.910	1.905	1.899	1.914	1.894			
VO(13)	1.881			1.866	1.895	1.896			
VN(6)	2.381	2.402	2.438	2.231	2.316	2.303			
VN(9)	2.329	2.215	2.225	2.276	2.252	2.249			
VO(14)	1.821	1.613	1.621	1.798	1.827	1.832			
VO(15)	1.675	1.929	1.891	1.855	1.783	1.775			
VO(16)	2.050	2.025	2.115						
O(2)C(3)	1.336	1.327	1.328	1.338	1.335	1.343			

C(3)C(4)	1.346	1.350	1.349	1.346	1.349	1.417			
C(4)C(5)	1.502	1.503	1.503	1.504	1.506	1.517			
C(5)N(6)	1.479	1.486	1.485	1.487	1.481	1.479			
N(6)C(7)	1.470	1.467	1.464	1.481	1.473	1.473			
C(7)C(8)	1.518	1.522	1.524	1.528	1.523	1.524			
C(8)N(9)	1.473	1.482	1.482	1.479	1.478	1.478			
N(9)C(10)	1.481	1.521	1.519	1.482	1.487	1.486			
C(10)C(11)	1.504	1.499	1.500	1.505	1.505	1.513			
C(11)C(12)	1.344	1.349	1.349	1.345	1.348	1.420			
C(12)O(13)	1.342	1.339	1.339	1.338	1.336	1.337			
O(15)O(16)	1.745	1.412	1.789	1.384	1.738	1.723			
O(16)C(17)	1.883	1.850	1.431	1.907	1.410	1.414			
C(17)C(18)	1.370	1.399	1.470	1.381	1.473	1.474			
O(16)C(18)	2.202		1.965		1.917	1.933			

Table 2S. Energy characteristics (in kcal/mol) of the discussed reactions calculated for the gas phase and for the CH_3CN solution (in parentheses).

Reaction	E_a	$\Delta H^{\neq}$	$\Delta G^{\neq}$	ΔE	ΔH	ΔG
1 + H_2O_2 → **2a** + H_2O + $HO^{\bullet}$				+1.4 (–4.5)	–2.5 (–8.4)	–9.6 (–12.8)
2a + H_2O_2 → **3a** + H_2O				+0.4 (+0.9)	+0.4 (+0.8)	+0.9 (+1.2)
3a → **3b**				+6.5 (+5.4)	+6.0 (+4.9)	+8.2 (+6.6)
3a → **3c**				–1.3 (–1.6)	–0.9 (–1.2)	–1.4 (–1.6)
3c + C_2H_4 → **5a** via **TS1a**	31.1 (33.8)	31.8 (34.5)	45.0 (43.6)	+9.2 (+10.6)	+11.3 (+12.6)	+23.1 (+20.7)
5a → **2b** + CH_3CHO via **TS2**	24.4 (18.8)	21.6 (16.0)	20.7 (15.3)	–70.2 (–79.2)	–71.5 (–80.5)	–85.7 (–91.0)
3c + C_2H_4 → **2b** + $\overline{CH_2CH_2O}$ via **TS3a**	21.3 (24.8)	21.6 (25.1)	32.0 (32.1)	–33.4 (–40.5)	–32.0 (–39.1)	–33.0 (–40.5)
via **TS3b**	24.5 (26.9)	24.9 (27.3)	36.1 (34.9)	–33.4 (–40.5)	–32.0 (–39.1)	–33.0 (–40.5)
2b → **2a**				–12.5 (–9.1)	–13.6 (–10.3)	–11.2 (–7.7)
3a + C_2H_4 → **2a** + $\overline{CH_2CH_2O}$ via **TS4a**	27.4 (29.9)	27.5 (30.0)	40.5 (39.0)	–47.2 (–51.2)	–46.5 (–50.5)	–45.5 (–49.7)
via **TS4b**	26.6 (30.2)	26.8 (30.4)	39.3 (39.0)	–47.2 (–51.2)	–46.5 (–50.5)	–45.5 (–49.7)
3b + C_2H_4 → **2a** + $\overline{CH_2CH_2O}$ via **TS5a**	30.7 (34.5)	30.8 (34.7)	41.1 (41.6)	–53.7 (–56.6)	–52.5 (–55.5)	–53.7 (–56.3)
via **TS5b**	24.7 (27.4)	25.2 (27.8)	35.7 (34.9)	–53.7 (–56.6)	–52.5 (–55.5)	–53.7 (–56.3)
3c → ^{3}**3c**				+14.9 (+16.2)	+14.6 (+15.9)	+12.5 (+14.2)
^{3}**3c** + C_2H_4 → **6** via **TS6**	14.6 (17.8)	14.8 (17.9)	25.6 (25.2)	+9.1 (+11.8)	+10.1 (+12.8)	+20.6 (+19.8)
6 → **2b** + $\overline{CH_2CH_2O}$ via **TS7**	13.1 (11.9)	12.4 (11.2)	12.8 (11.5)	–57.4 (–68.5)	–56.7 (–67.7)	–66.0 (–74.5)
3b → ^{3}**3b**				+10.4 (+7.9)	+9.8 (+7.2)	+6.8 (+4.9)
^{3}**3b** + C_2H_4 → **7** via **TS8**	8.7 (15.5)	9.0 (15.9)	19.6 (23.1)	–4.1 (+2.5)	–3.0 (+3.6)	+7.6 (+10.8)
7 → **2a** + $\overline{CH_2CH_2O}$ via **TS9**	17.2 (16.0)	16.8 (15.5)	17.2 (15.8)	–60.1 (–67.0)	–59.3 (–66.2)	–68.0 (–72.0)
3c' + C_2H_4 → **2b'** + $\overline{CH_2CH_2O}$ via **TS3a'**	21.6 (25.5)	21.9 (25.9)	32.5 (33.0)			
3c' + C_2H_4 → **2a'** + $\overline{CH_2CH_2O}$ via **TS8'** and **TS9'**[a]	30.7 (32.7)	29.8 (31.8)	40.7 (39.1)			

[a] Energies of **TS9'** relative to **3c'** + C_2H_4.

Table 3S. Total energies, enthalpies, Gibbs free energies (Hartree) and entropies (cal/mol•K) of the calculated structures for the gas phase and for the CH_3CN solution (for details see Computational Details section).

	E_g	E_s	H_g	H_s	S_s	G_g	G_s
C_2H_4	–78.587458	–78.612873	–78.532243	–78.557658	36.76	–78.557104	–78.575124
H_2O_2	–151.533215	–151.610735	–151.502758	–151.580278	39.47	–151.529295	–151.599031
H_2O	–76.408953	–76.463430	–76.384013	–76.438490	31.22	–76.405444	–76.453324
$HO^{\bullet}$	–75.723455	–75.765939	–75.711846	–75.754330	29.28	–75.732093	–75.768242
$\overline{CH_2CH_2O}$	–153.786262	–153.840385	–153.724522	–153.778645	41.07	–153.752045	–153.798159
CH_3CHO	–153.830121	–153.885111	–153.769464	–153.824454	44.74	–153.799253	–153.845711
1	–796.702887	–796.938164	–796.430133	–796.665410	93.30	–796.489884	–796.709740
1a	–796.703176	–796.936621	–796.430283	–796.663728	93.47	–796.490137	–796.708139
2a	–796.101492	–796.326698	–795.841075	–796.066281	87.11	–795.897006	–796.107670
2a'	–796.086918	–796.314981	–795.825874	–796.053937	86.41	–795.881371	–796.094993
2a''	–796.100287	–796.325138	–795.839353	–796.064204	86.50	–795.894908	–796.105303
2a'''	–796.077021	–796.304934	–795.816180	–796.044093	85.98	–795.871413	–796.084945
2b	–796.081569	–796.313204	–795.819359	–796.050994	93.48	–795.879222	–796.095409
3a	–871.225067	–871.472563	–870.959258	–871.206754	94.09	–871.019496	–871.251459
3b	–871.214715	–871.463956	–870.949660	–871.198901	88.48	–871.006438	–871.240941
^{3}3b	–871.198072	–871.451454	–870.934093	–871.187475	96.10	–870.995573	–871.233135
3c	–871.227091	–871.475139	–870.960624	–871.208672	95.36	–871.021648	–871.253981
^{3}3c	–871.203318	–871.449328	–870.937400	–871.183410	100.80	–871.001777	–871.231303
3c'	–1178.544386	–1178.857104	–1178.178664	–1178.491382	114.54	–1178.251519	–1178.545804
3da	–871.204709	–871.448754	–870.939435	–871.183480	97.06	–871.001504	–871.229596
3db	–871.200953	–871.444627	–870.935760	–871.179434	95.47	–870.996847	–871.224795
3dc	–871.202825	–871.451935	–870.937491	–871.186601	98.72	–871.000583	–871.233506
3dd	–871.200069	–871.448135	–870.934536	–871.182602	94.84	–870.995235	–871.227664
3de	–871.179016	–871.447760	–870.912740	–871.181484	92.60	–870.972057	–871.225481
3df	–871.196068	–871.461101	–870.930057	–871.195090	96.24	–870.991621	–871.240817
3dg	–871.194174	–871.461141	–870.928277	–871.195244	102.32	–870.993596	–871.243860
4a	–949.795748		–949.472344		122.69	–949.550228	
4b	–949.797262		–949.473443		118.48	–949.548728	
4c	–949.795892		–949.472396		119.81	–949.548508	
4d	–949.796610		–949.473826		116.47	–949.547872	
4e	–949.795748		–949.472344		122.72	–949.550249	
4f	–949.795891		–949.472392		119.74	–949.548457	
4g	–949.796444		–949.472714		121.96	–949.550148	
4h	–949.793062		–949.470637		117.06	–949.545050	
4i	–949.817122		–949.494493		117.42	–949.569127	
5a	–949.799859	–950.071136	–949.474907	–949.746184	105.16	–949.541973	–949.796149
5b	–949.784830	–950.057944	–949.460090	–949.733204	106.53	–949.528002	–949.783820
5c	–949.775899		–949.450890		105.61	–949.518236	
5d	–949.783558		–949.458231		107.49	–949.526737	
5e	–949.774702		–949.449014		102.16	–949.514232	
5f	–949.770555		–949.445389		102.38	–949.510740	
5g	–949.780490		–949.455385		105.27	–949.522520	
5h	–949.768108		–949.443284		105.46	–949.510535	
6	–949.776315	–950.043464	–949.453538	–949.720687	113.97	–949.526042	–949.774838
7	–949.792038	–950.060288	–949.471175	–949.739425	109.02	–949.540624	–949.791096
TS1a	–949.765061	–950.034145	–949.442197	–949.711281	101.60	–949.507072	–949.759554
TS1b	–949.753935	–950.024769	–949.431376	–949.702210	105.03	–949.498366	–949.752113
TS1c	–949.741508		–949.419045		104.57	–949.485749	
TS1d	–949.761043		–949.438485		101.33	–949.503191	
TS1e	–949.739195		–949.414909		107.00	–949.483110	
TS1f	–949.739584		–949.415341		106.56	–949.483272	
TS1g	–949.738386		–949.415798		106.96	–949.483980	
TS1h	–949.749268		–949.426387		104.48	–949.493038	
TS1i	–949.723486		–949.401353		102.14	–949.466557	
TS1j	–949.713892		–949.391937		102.35	–949.457274	

	E_g	E_s	H_g	H_s	S_s	G_g	G_s
TS1k	–949.721098		–949.399024		106.77	–949.467083	
TS1l	–949.722129		–949.399447		100.08	–949.463383	
TS1m	–949.715463		–949.393353		103.24	–949.459234	
TS1n	–949.730654		–949.408601		109.48	–949.478334	
TS1o	–949.737616		–949.415496		104.80	–949.482344	
TS1p	–949.731082		–949.410335		98.82	–949.473491	
TS1q	–949.725713		–949.405076		100.15	–949.469052	
TS1r	–949.725953		–949.405201		100.07	–949.469128	
TS1s	–949.730024		–949.409206		99.32	–949.472671	
TS1t	–949.711902		–949.391691		100.36	–949.455797	
TS1u	–949.737238		–949.416177		101.81	–949.481178	
TS1v	–949.725218		–949.404606		100.41	–949.468746	
TS1w	–949.718406		–949.396452		100.93	–949.460908	
TS1x	–949.727744		–949.405380		100.91	–949.469824	
TS1y	–949.728390		–949.407227		106.33	–949.475016	
TS1z	–949.745943		–949.424419		105.07	–949.491433	
TS1aa	–949.749274		–949.427104		101.35	–949.491819	
TS1ab	–949.718209		–949.397942		111.15	–949.468706	
TS2	–949.761021	–950.041182	–949.440483	–949.720644	107.62	–949.509071	–949.771778
TS3a	–949.780598	–950.048456	–949.458484	–949.726342	108.81	–949.527802	–949.777908
TS3b	–949.775484	–950.045091	–949.453268	–949.722875	106.71	–949.521291	–949.773448
TS3a'	–1257.097488	–1257.429292	–1256.675967	–1257.007771	127.62	–1256.756894	–1257.068407
TS4a	–949.768944	–950.037856	–949.447696	–949.716608	100.80	–949.512073	–949.764501
TS4b	–949.770154	–950.037329	–949.448817	–949.715992	102.09	–949.513991	–949.764379
TS5a	–949.753320	–950.021784	–949.432814	–949.701278	102.19	–949.498052	–949.749832
TS5b	–949.762785	–950.033211	–949.441823	–949.712249	101.43	–949.506590	–949.760442
TS6	–949.767451	–950.033827	–949.446131	–949.712507	113.11	–949.518107	–949.766249
TS7	–949.755466	–950.024544	–949.433796	–949.702874	112.82	–949.505589	–949.756478
TS8	–949.771746	–950.039574	–949.452004	–949.719832	108.92	–949.521391	–949.771455
TS9	–949.764597	–950.034822	–949.444459	–949.714684	107.91	–949.513222	–949.765956
TS9'	–1257.082962	–1257.417938	–1256.663383	–1256.998359	126.79	–1256.743798	–1257.058601

Table 4S. Cartesian atomic coordinates (Å) of the calculated equilibrium structures. First column – symbol of the element or its nuclear charge, second, third and fourth columns – x, y and z coordinates, respectively.

C_2H_4

C	0.044521	0.000000	0.000000
C	1.375479	0.000000	0.000000
H	–0.529650	0.923500	0.000000
H	–0.529650	–0.923500	0.000000
H	1.949650	0.923500	0.000000
H	1.949650	–0.923500	0.000000

$CH_3C(H)O$

C	–1.142215	–0.280226	0.078310
C	0.366085	–0.272276	0.079802
O	1.050856	0.686940	–0.196387
H	0.837659	–1.241820	0.361805
H	–1.509158	–1.045939	–0.617995
H	–1.530508	0.700326	–0.206446
H	–1.513459	–0.556271	1.074188

H_2O_2

O	0.039076	–0.199177	0.054026
O	1.437719	0.138093	–0.168779
H	–0.344215	0.695705	0.072822
H	1.827420	–0.234621	0.641931

H_2O

O	0.000000	0.067990	0.000000
H	–0.761819	0.666005	0.000000
H	0.761819	0.666005	0.000000

CH_2CH_2O

O	0.000000	–0.021051	0.000000
C	–0.734471	–1.248059	0.000000
C	0.734471	–1.248059	0.000000
H	–1.274780	–1.470708	0.920583
H	–1.274780	–1.470708	–0.920583
H	1.274780	–1.470708	0.920583
H	1.274780	–1.470708	–0.920583

$HO^{\bullet}$

O	0.008544	0.000000	0.000000
H	0.991456	0.000000	0.000000

1

V	1.150130	–0.623808	0.740143
O	2.257648	–0.740363	–0.875349
O	–0.477745	–0.659836	1.777556
N	–0.533728	–0.444859	–0.990165
C	3.221245	1.469679	–0.762570
N	1.020971	1.493448	0.420095
C	–2.262834	–1.531422	0.409152
C	3.118135	0.210451	–1.240103
H	–3.279348	–1.912945	0.444826
H	3.982687	2.108273	–1.200795
C	–1.608825	–1.460584	–0.942995
H	–1.138783	–2.416549	–1.215595
H	–2.369859	–1.253716	–1.715577
H	–2.280153	–1.252609	2.494036
C	0.181622	1.877491	–0.746430
H	0.830286	1.817968	–1.625767
H	–0.153317	2.919472	–0.650825
H	3.788165	–0.093365	–2.050548
C	–1.689357	–1.165392	1.575421

C	2.398680	2.075889	0.345220
H	2.848733	1.903594	1.329755
H	2.322094	3.164173	0.199213
C	–1.011189	0.942211	–0.905351
H	–1.676624	1.005770	–0.039767
H	–1.595163	1.241833	–1.791447
O	2.257018	–0.571426	1.882683
H	0.014744	–0.566681	–1.840469
H	0.571430	1.821649	1.276465
O	1.150001	–2.740917	0.352526
H	1.948984	–2.717536	–0.213650
H	1.391862	–3.199253	1.174661

1a

V	0.229934	–0.561013	–0.614958
O	1.928639	–1.275619	–0.092168
O	–0.405057	–0.733122	1.309917
N	–1.682343	0.636335	–0.711266
C	2.879562	0.617575	1.058225
N	1.038705	1.400419	–0.376788
C	–2.744605	–0.234610	1.358182
C	2.891700	–0.643147	0.571732
H	–3.625305	–0.147582	1.986867
H	3.762302	0.970746	1.581726
C	–2.903062	0.029178	–0.112458
H	–3.083084	–0.894168	–0.682689
H	–3.770050	0.685495	–0.289018
H	–1.538171	–0.758707	3.008057
C	0.004962	2.416207	–0.705155
H	–0.020406	2.505899	–1.796733
H	0.275368	3.397477	–0.292089
H	3.791466	–1.249196	0.712495
C	–1.570838	–0.585032	1.925773
C	1.720142	1.568655	0.943826
H	0.962339	1.396126	1.716839
H	2.067230	2.608095	1.035960
C	–1.365512	1.982387	–0.191800
H	–1.372362	1.916144	0.898764
H	–2.126137	2.722494	–0.484372
H	1.768313	1.430890	–1.090063
O	0.197431	–0.556104	–2.219067
O	–0.414704	–2.657926	–0.461065
H	0.379915	–3.140186	–0.750569
H	–0.367415	–2.626017	0.516987
H	–1.807885	0.685520	–1.722024

2a

V	1.359403	–0.892473	0.141362
O	2.235946	–0.443928	–1.470077
O	0.020224	–0.751867	1.465109
N	–0.500285	–0.291451	–1.224347
C	3.473198	1.520174	–0.857771
N	1.264562	1.365094	0.251210
C	–2.058453	–1.332002	0.373706
C	3.244464	0.426811	–1.607008
H	–3.088517	–1.617080	0.568383
H	4.329833	2.139838	–1.105207
C	–1.638497	–1.220159	–1.066170
H	–1.307467	–2.189671	–1.456876
H	–2.494962	–0.894462	–1.680294
H	–1.696087	–1.184558	2.444717
C	0.420208	1.945999	–0.814620
H	1.017422	1.948161	–1.730116
H	0.161995	2.990344	–0.584869
H	3.895526	0.198010	–2.453738

C	–1.270600	–1.102223	1.441322
C	2.625074	1.958882	0.304650
H	3.065447	1.649353	1.259894
H	2.546878	3.057985	0.320398
C	–0.846723	1.120232	–1.003693
H	–1.468735	1.162987	–0.104290
H	–1.441488	1.537860	–1.831300
O	2.607696	–0.920088	1.104000
H	–0.079698	–0.408458	–2.144999
H	0.806523	1.485777	1.154377
O	0.971535	–2.581591	–0.334338
H	1.555148	–3.252518	0.055514

2a'

V	0.129243	–0.835191	–0.508261
O	1.849487	–1.315969	–0.144556
O	–0.215505	–0.420970	1.368930
N	–1.612256	0.558722	–0.697918
C	2.822189	0.516127	1.059471
N	1.118660	1.220515	–0.569849
C	–2.542598	0.064692	1.548900
C	2.761113	–0.769431	0.673469
H	–3.376478	0.216800	2.226706
H	3.636427	0.810063	1.714658
C	–2.817937	0.137528	0.074727
H	–3.115814	–0.836229	–0.333857
H	–3.636911	0.844981	–0.130358
H	–1.192354	–0.247676	3.145406
C	0.148561	2.225262	–1.050188
H	0.087631	2.126342	–2.139139
H	0.478625	3.249084	–0.823294
H	3.519405	–1.483702	0.995286
C	–1.323628	–0.209237	2.059045
C	1.837922	1.583068	0.672383
H	1.087565	1.726511	1.458193
H	2.356190	2.544987	0.530109
C	–1.216209	1.957988	–0.429377
H	–1.187958	2.081799	0.655317
H	–1.963843	2.660121	–0.826207
H	1.810238	1.049583	–1.298826
O	0.111952	–0.797021	–2.117859
O	–0.892595	–2.307746	–0.285021
H	–1.055944	–2.743881	–1.138462
H	–1.807392	0.453608	–1.693688

2a''

V	0.946403	0.690748	0.548241
O	–0.547610	0.455442	1.565227
O	0.841260	–1.087009	–0.088569
N	2.186262	0.837096	–1.279043
C	–2.349502	–0.117731	0.064220
N	–0.637429	1.131800	–1.163282
C	3.028632	–1.470820	–0.983621
C	–1.795857	0.068622	1.278539
H	3.762491	–2.223166	–1.254955
H	–3.380115	–0.460508	0.043691
C	3.390583	–0.032489	–1.226869
H	4.028119	0.364741	–0.427480
H	3.949254	0.065251	–2.171279
H	1.643643	–2.937243	–0.341151
C	0.082048	1.454109	–2.406454
H	0.320700	2.521877	–2.382896
H	–0.535170	1.271778	–3.298915
H	–2.392556	–0.107223	2.174872
C	1.856512	–1.872641	–0.461330

C	–1.677033	0.094147	–1.264401
H	–1.191238	–0.827996	–1.607137
H	–2.429050	0.367668	–2.023311
C	1.373292	0.644203	–2.502309
H	1.159439	–0.422844	–2.585802
H	1.945355	0.943361	–3.392941
H	–1.045329	1.981130	–0.777649
O	0.923373	2.554578	0.346796
O	2.179126	0.598277	1.533973
H	2.468478	1.814967	–1.219440
H	1.457090	2.955114	1.051855

2a'''

V	0.027785	0.143892	0.666652
O	–1.454665	–0.047224	1.712227
O	1.557069	0.021221	1.651344
N	1.343624	–0.154961	–1.033538
C	–3.122300	–1.054088	0.303836
N	–1.466302	0.187521	–1.019771
C	3.139487	1.043289	0.172131
C	–2.635306	–0.645961	1.490142
H	4.111909	1.523522	0.115001
H	–4.107170	–1.511781	0.303184
C	2.399231	0.877966	–1.128537
H	1.916548	1.815951	–1.428623
H	3.105377	0.600384	–1.926971
H	3.338107	0.787784	2.267573
C	–0.717785	0.416291	–2.274214
H	–0.476643	1.481904	–2.314783
H	–1.324674	0.170885	–3.157570
H	–3.224891	–0.762852	2.399917
C	2.712975	0.647725	1.385724
C	–2.419457	–0.942935	–1.023057
H	–1.843944	–1.850115	–1.233875
H	–3.156979	–0.805912	–1.829616
C	0.567713	–0.408211	–2.273615
H	0.328605	–1.473033	–2.284962
H	1.168828	–0.178310	–3.163581
H	1.744202	–1.040985	–0.722994
H	–1.973217	1.039169	–0.781674
O	0.079152	1.724123	0.355561
O	0.004188	–1.782951	0.266746
H	–0.419664	–2.259865	0.997656

2b

V	0.490752	1.457580	–0.020396
O	–1.172463	1.325089	–0.786413
O	3.133359	–0.704419	–2.327742
N	1.263062	–0.403899	0.819173
C	–2.896633	1.592543	0.865446
N	–0.723975	1.066931	1.972136
C	3.178264	–1.749167	–0.132883
C	–2.448319	1.436087	–0.390194
H	3.387014	–2.692991	0.362284
H	–3.970891	1.639879	1.016361
C	2.779326	–0.574942	0.703744
H	3.164323	–0.670903	1.723130
H	3.166045	0.356996	0.288673
H	3.683208	–2.602230	–1.998904
C	–0.742215	–0.373507	2.240473
H	–1.390858	–0.852816	1.498255
H	–1.140637	–0.619048	3.237430
H	–3.154161	1.346172	–1.217612
C	3.333311	–1.713703	–1.475200
C	–2.022730	1.773847	2.073859

H	–1.778094	2.834395	2.214602
H	–2.557630	1.448073	2.979760
C	0.699720	–0.856138	2.115712
H	1.305197	–0.406333	2.910777
H	0.771511	–1.946092	2.220200
H	0.880508	–1.014442	0.091187
H	–0.077985	1.516278	2.619948
O	1.489544	1.161554	–1.271400
O	0.941028	2.820110	0.686994
H	2.616587	0.046324	–1.927700

3a

V	0.404282	1.178648	–0.042759
O	–1.428014	0.741040	–0.110283
O	2.262153	0.834917	–0.158456
N	0.448950	–0.032573	–1.922586
C	–1.798674	–0.875704	1.646001
N	0.491899	–1.049580	0.751218
C	2.645120	0.945590	–2.525522
C	–2.190368	0.026696	0.726848
H	3.391512	1.113772	–3.295838
H	–2.574401	–1.346940	2.242588
C	1.248096	0.631369	–2.986279
H	0.702984	1.541778	–3.264607
H	1.280771	–0.014865	–3.878035
H	4.073573	1.233191	–0.992036
C	0.225994	–1.954545	–0.381554
H	–0.860024	–2.006488	–0.503928
H	0.581539	–2.977447	–0.183258
H	–3.255757	0.229445	0.595636
C	3.029669	1.028268	–1.239140
C	–0.379403	–1.290327	1.922126
H	0.045946	–0.715481	2.754139
H	–0.350519	–2.353163	2.214498
C	0.878815	–1.424309	–1.653512
H	1.966567	–1.407986	–1.551515
H	0.634136	–2.078040	–2.503311
O	0.427193	1.641263	1.694832
H	–0.536694	–0.026788	–2.185516
H	1.471228	–1.117526	1.024924
O	0.358024	2.577898	–0.785644
O	0.450859	3.008215	2.098254
H	0.437385	3.475056	1.236244

3b

V	–0.179558	0.736126	0.577225
O	–1.212208	0.828037	–1.104973
O	1.463744	0.504291	1.542838
N	1.353805	0.551329	–1.108233
C	–2.344110	–1.303053	–1.082713
N	–0.153210	–1.452882	0.079707
C	3.166726	1.560644	0.207358
C	–2.165402	–0.028704	–1.484980
H	4.168401	1.978507	0.223114
H	–3.164043	–1.860872	–1.524989
C	2.423114	1.573552	–1.093162
H	1.942249	2.542450	–1.272881
H	3.113551	1.391214	–1.932509
H	3.274795	1.054127	2.253488
C	0.676415	–1.781906	–1.101340
H	0.031167	–1.674774	–1.978261
H	1.018860	–2.824931	–1.064721
H	–2.829200	0.382757	–2.250123
C	2.661592	1.055955	1.348641
C	–1.533480	–2.011816	–0.033598

H	–1.990711	–1.916050	0.957058
H	–1.465809	–3.085744	–0.266805
C	1.857126	–0.829956	–1.193242
H	2.554277	–0.980092	–0.365500
H	2.408191	–0.998545	–2.130650
O	–0.784452	0.315502	2.227662
H	0.708240	0.732652	–1.877195
H	0.288939	–1.825992	0.920154
O	0.018025	2.497902	0.468090
O	–1.817247	0.450977	1.269735
H	–0.644458	2.869138	–0.144254

^{3}3b

V	1.283946	0.741959	–0.519930
O	2.549691	0.375758	0.785397
O	–0.281889	0.565636	–1.578329
N	–0.172602	0.697284	1.177172
C	3.278488	–1.876683	0.407336
N	0.926001	–1.497690	–0.270331
C	–1.932052	1.712273	–0.253343
C	3.407961	–0.644668	0.930179
H	–2.926139	2.149398	–0.276523
H	4.057641	–2.603267	0.616770
C	–1.198011	1.770546	1.059518
H	–0.662835	2.719817	1.174542
H	–1.914589	1.688484	1.892174
H	–2.095869	1.156502	–2.283725
C	0.275481	–1.730664	1.036144
H	1.062354	–1.707103	1.795098
H	–0.194290	–2.724616	1.080804
H	4.262544	–0.399741	1.562454
C	–1.464244	1.163618	–1.391987
C	2.142327	–2.324263	–0.471558
H	2.408737	–2.238329	–1.532170
H	1.911048	–3.383890	–0.277786
C	–0.766762	–0.653072	1.309647
H	–1.579958	–0.714156	0.581043
H	–1.206192	–0.797986	2.307113
O	2.436584	0.265439	–1.948898
H	0.421803	0.889987	1.983533
H	0.262142	–1.677688	–1.023251
O	1.225307	2.535679	–0.532784
O	3.607643	0.875998	–1.969507
H	1.079835	2.950891	–1.400350

3c

V	1.485200	1.116177	–0.797077
O	–0.039509	1.478889	–1.733486
O	3.654478	–0.386871	–3.897081
N	1.592231	–1.040796	–0.838574
C	–2.084841	1.387301	–0.485527
N	–0.229705	0.384523	0.792062
C	3.060841	–2.271305	–2.478017
C	–1.375481	1.530463	–1.616602
H	2.873559	–3.340830	–2.517390
H	–3.165841	1.466545	–0.554157
C	2.983179	–1.598040	–1.142913
H	3.220939	–2.312255	–0.348757
H	3.685546	–0.767818	–1.057463
H	3.475982	–2.272133	–4.548668
C	–0.404158	–1.057503	0.615669
H	–1.077412	–1.214041	–0.236207
H	–0.866696	–1.543827	1.489934
H	–1.877817	1.706867	–2.568867
C	3.386481	–1.673711	–3.643713

C	–1.476928	1.163165	0.871879
H	–1.220286	2.123323	1.338113
H	–2.208301	0.675018	1.536457
C	0.958218	–1.682007	0.340385
H	1.625708	–1.520011	1.192528
H	0.865249	–2.764798	0.182498
O	2.371948	1.020416	0.831839
H	1.022554	–1.259023	–1.660720
H	0.359325	0.565966	1.603088
O	2.585660	1.215287	–1.957147
O	1.889910	2.330659	0.457438
H	3.391028	0.204131	–3.149983

^{3}3c

V	1.817279	1.637145	0.352062
O	0.117932	1.978585	1.104842
O	–0.020692	0.969669	–3.146115
N	1.351249	–0.501071	0.022469
C	0.235422	1.706805	3.489858
N	2.202334	0.577789	2.468443
C	0.269036	–1.224092	–2.134385
C	–0.399099	1.972825	2.329274
H	–0.200394	–2.202366	–2.076334
H	–0.344075	1.748363	4.406696
C	1.555537	–1.027369	–1.391828
H	2.083032	–1.984373	–1.312699
H	2.216295	–0.326054	–1.905426
H	–1.258195	–0.577688	–3.440246
C	1.670968	–0.793615	2.437396
H	0.594650	–0.729435	2.628643
H	2.108999	–1.430772	3.220306
H	–1.467784	2.203967	2.344766
C	–0.353239	–0.304050	–2.900547
C	1.702162	1.398941	3.607344
H	2.311659	2.313471	3.605794
H	1.903750	0.884911	4.559933
C	1.927806	–1.388344	1.059863
H	3.005001	–1.466925	0.868466
H	1.507310	–2.401731	0.991799
O	3.745371	2.045279	0.731624
H	0.339039	–0.467577	0.166838
H	3.219772	0.535742	2.534574
O	1.681126	1.908296	–1.221456
O	2.990353	3.060583	1.129094
H	0.671774	1.301412	–2.523488

3c’

V	1.504241	2.224505	1.874864
O	0.229386	2.241436	0.575749
O	3.794509	0.411468	–0.689015
N	1.973520	0.120971	2.088528
C	–2.029543	1.706889	1.246249
N	–0.389407	1.278315	3.050754
C	3.906600	–1.192051	1.163579
C	–1.046332	1.938718	0.261133
C	4.186052	–2.516242	1.535163
C	–3.322833	1.372325	0.834563
C	3.458300	–0.189161	2.193981
H	3.641580	–0.571206	3.200721
H	3.990264	0.759327	2.105231
C	4.450488	–1.790256	–1.131808
C	–0.297556	–0.181872	3.007337
H	–0.707373	–0.520726	2.048191
H	–0.881114	–0.675157	3.800976
C	–1.379737	1.844179	–1.099338

C	4.045259	–0.825937	–0.195810
C	–1.697577	1.860008	2.711213
H	–1.631237	2.923032	2.973666
H	–2.506184	1.424265	3.319192
C	1.171663	–0.571370	3.130238
H	1.564437	–0.251244	4.100250
H	1.297954	–1.658772	3.050279
O	1.965761	2.397848	3.667067
H	1.667338	–0.239333	1.179983
H	–0.072252	1.622930	3.955777
O	2.833847	2.414002	0.999339
O	1.395470	3.573844	3.049518
H	3.571123	1.090087	–0.012225
C	–2.678256	1.522423	–1.484380
C	–3.657312	1.283754	–0.517020
H	–0.599923	2.031527	–1.831098
H	–4.081583	1.184393	1.591722
H	–2.924550	1.454652	–2.540497
H	–4.670979	1.027420	–0.810828
C	4.717809	–3.095270	–0.735532
C	4.589369	–3.470055	0.605574
H	4.551781	–1.481247	–2.167452
H	4.093303	–2.790666	2.584339
H	5.033391	–3.824116	–1.477420
H	4.804941	–4.486588	0.920308

3da

V	–1.074605	–0.733350	0.311635
O	0.645992	–1.066881	0.584501
O	–1.799474	0.281612	1.610795
N	–0.214016	1.454414	–0.548907
C	2.858589	–1.761661	0.211979
N	3.419856	0.444522	–0.791993
C	–1.203276	2.585193	1.423252
C	1.552582	–2.040105	0.316214
H	–1.040062	3.517746	1.953979
H	3.526118	–2.579273	–0.044703
C	–1.085597	2.558650	–0.077511
H	–2.070935	2.393657	–0.533488
H	–0.716738	3.528523	–0.442838
H	–1.627931	1.519159	3.219871
C	2.096071	0.828278	–1.278473
H	1.553550	–0.091039	–1.514936
H	2.237778	1.355758	–2.230449
H	1.133409	–3.036844	0.180562
C	–1.528671	1.499489	2.135252
C	3.441869	–0.384417	0.426929
H	2.924168	0.084780	1.280675
H	4.493906	–0.485965	0.714550
C	1.230627	1.701787	–0.336328
H	1.454069	1.482012	0.710070
H	1.460134	2.767496	–0.500539
H	–0.383971	1.330001	–1.546887
O	–1.568190	–0.537270	–1.421274
O	–1.792018	–2.141471	0.474599
O	–2.334731	–1.539595	–2.097757
H	3.987975	1.275026	–0.633991
H	–2.464337	–2.199437	–1.380247

3db

V	2.223640	0.137260	0.033315
O	0.908559	–0.501327	1.086660
O	2.587801	–1.131153	–1.173155
N	0.141910	0.580081	–1.437155
C	–0.693882	–0.540476	2.807953

N	–2.493257	0.150125	1.224509
C	0.934940	–1.266127	–2.897319
C	0.566862	–0.360614	2.383970
H	0.482881	–1.911742	–3.644402
H	–0.894353	–0.383411	3.864101
C	0.490955	0.172304	–2.814951
H	1.305017	0.834542	–3.137907
H	–0.352837	0.335725	–3.503177
H	2.211330	–2.831757	–2.223992
C	–1.675599	0.867573	0.247183
H	–0.820855	1.289232	0.782103
H	–2.268171	1.718895	–0.112629
H	1.385526	–0.094874	3.055412
C	1.891686	–1.795419	–2.122926
C	–1.828988	–0.974430	1.910318
H	–1.448778	–1.740717	1.213980
H	–2.597411	–1.460393	2.521719
C	–1.155701	0.056834	–0.965369
H	–1.007000	–0.989932	–0.691019
H	–1.902470	0.077934	–1.777825
O	3.448715	0.129730	1.028745
H	0.114105	1.599400	–1.419440
O	2.548716	1.770237	–0.856277
O	1.825217	2.211993	0.337855
H	–3.340215	–0.197977	0.777657
H	2.554646	2.530291	0.908830

3dc

V	1.993069	0.969593	–0.815233
O	1.974040	–0.215998	0.539798
O	1.373181	0.913968	–2.568975
N	–0.234598	0.957192	–0.398450
C	0.800017	–1.225865	2.322375
N	–1.246803	–2.131765	1.255178
C	–0.712236	2.106097	–2.538341
C	1.630370	–0.284303	1.841479
H	–1.466811	2.586213	–3.153707
H	0.556623	–1.195445	3.381349
C	–0.930930	2.097311	–1.052136
H	–0.549475	3.014297	–0.588228
H	–2.008214	2.047368	–0.832693
H	0.425180	1.577502	–4.243529
C	–1.671349	–0.870383	0.655181
H	–1.610994	–0.092855	1.429639
H	–2.736584	–0.980495	0.425528
H	2.078154	0.480629	2.477397
C	0.343999	1.558069	–3.156393
C	0.198879	–2.315815	1.478463
H	0.777571	–2.390579	0.545516
H	0.309777	–3.275642	1.998907
C	–0.910275	–0.361196	–0.609853
H	–0.157101	–1.094344	–0.909499
H	–1.588133	–0.245672	–1.460004
O	4.118862	1.287186	–2.400541
H	–0.223337	1.140922	0.605121
O	2.092594	2.460246	–0.321870
O	3.625054	0.394322	–1.379868
H	–1.593393	–2.914471	0.705462
H	3.433873	1.154773	–3.090794

3dd

V	–0.434961	0.908158	–0.200213
O	1.040347	1.524541	–1.047815
O	–0.890666	–0.365878	–1.468302
N	–1.036282	–0.768224	1.089456

C	2.927841	0.041670	–0.729848
N	2.305215	–2.110335	0.324416
C	–2.818178	–1.400985	–0.522637
C	2.350049	1.250589	–0.834706
H	–3.728665	–1.960541	–0.709709
H	3.996700	0.036877	–0.527834
C	–2.487425	–1.060949	0.902820
H	–3.037302	–0.175501	1.246821
H	–2.763773	–1.895031	1.565266
H	–2.295658	–1.332961	–2.582768
C	1.320027	–1.752819	1.340937
H	1.473234	–0.701687	1.603684
H	1.558277	–2.331032	2.240789
H	2.959027	2.155043	–0.772670
C	–2.044802	–1.049272	–1.560447
C	2.277514	–1.304346	–0.910792
H	1.270548	–1.185949	–1.335741
H	2.862648	–1.862223	–1.653723
C	–0.179159	–1.990416	0.980179
H	–0.273834	–2.356261	–0.043168
H	–0.612258	–2.754412	1.641160
O	0.519746	2.646621	1.623209
H	–0.905451	–0.362060	2.017459
O	–1.637413	1.908371	–0.302636
O	0.272964	1.229094	1.516939
H	2.211809	–3.094519	0.082774
H	1.388749	2.725988	1.185713

3de

V	1.411000	1.485066	–0.600375
O	2.588121	0.028455	–1.225482
O	0.035470	0.274398	–1.293769
N	–0.341620	1.766177	0.863655
C	2.642206	–1.779129	0.351540
N	0.611346	–1.622087	1.907091
C	–2.023703	1.467329	–0.905201
C	3.197890	–0.847393	–0.489818
H	–3.050669	1.591022	–1.234798
H	3.313392	–2.497847	0.817510
C	–1.541039	2.350000	0.209790
H	–1.241618	3.338630	–0.157602
H	–2.337795	2.506135	0.956986
H	–1.669710	–0.014294	–2.362371
C	0.511698	–0.159807	2.291237
H	1.457684	0.302269	1.996759
H	0.423294	–0.142302	3.381191
H	4.291323	–0.874431	–0.601582
C	–1.242232	0.577663	–1.547285
C	1.193254	–2.000249	0.465470
H	0.616246	–1.404342	–0.246584
H	0.903822	–3.056694	0.400788
C	–0.689604	0.543400	1.627491
H	–1.188104	–0.121246	0.916891
H	–1.434033	0.794639	2.398010
H	0.074037	2.453439	1.490800
O	0.919986	3.124224	–1.187381
O	2.235667	1.609750	0.778094
O	2.068423	2.578786	–1.869866
H	–0.305400	–2.070758	2.016530
H	1.240619	–2.074812	2.575810

3df

V	1.971000	0.425183	–1.232317
O	1.525737	–0.757992	0.244524
O	1.208387	–0.583255	–2.553874

N	–0.896886	0.945495	–1.105121
C	1.218128	–1.024690	2.556453
N	–1.168479	–0.184581	2.431301
C	–1.150319	–0.660101	–2.953778
C	1.981279	–0.719484	1.464787
H	–1.954255	–1.261058	–3.369825
H	1.661250	–1.019009	3.546689
C	–1.462621	0.722000	–2.439552
H	–1.007985	1.480717	–3.089386
H	–2.554593	0.891920	–2.462756
H	0.261761	–2.180751	–3.374274
C	–1.025348	0.820737	1.309498
H	0.037864	1.035906	1.192515
H	–1.531815	1.731026	1.645616
H	3.031154	–0.436419	1.598469
C	0.090295	–1.180092	–2.968758
C	–0.188689	–1.425694	2.387588
H	–0.379696	–1.884314	1.416979
H	–0.568563	–2.069883	3.186009
C	–1.607406	0.311590	–0.012632
H	–1.463360	–0.771570	–0.109435
H	–2.703310	0.490363	–0.031010
O	3.525250	0.206997	–1.389721
H	–0.727626	1.933337	–0.938793
O	1.677828	2.199588	–1.485315
O	1.670253	1.845125	–0.079190
H	–2.140403	–0.513387	2.476814
H	–0.973643	0.295508	3.314625

3dg

V	2.720700	1.099718	0.477176
O	1.864504	–0.472653	–0.272457
O	1.182313	2.068715	0.681071
N	–1.710689	1.117256	0.868743
C	1.433543	–2.719030	–0.777771
N	–1.042983	–2.364858	–0.394923
C	–0.701729	3.011104	–0.455293
C	2.228336	–1.724104	–0.283381
H	–0.973080	3.670152	–1.276468
H	1.781137	–3.746287	–0.761950
C	–1.855407	2.493180	0.368543
H	–1.988775	3.120225	1.261470
H	–2.777167	2.615127	–0.232267
H	1.328146	3.306696	–0.954920
C	–1.080616	–1.179086	0.549948
H	–0.068826	–1.025613	0.920576
H	–1.737406	–1.466289	1.377921
H	3.209824	–1.967107	0.135156
C	0.618462	2.820410	–0.278994
C	0.150559	–2.393789	–1.425989
H	0.145690	–1.398214	–1.872941
H	–0.168592	–3.136013	–2.163248
C	–1.593920	0.085755	–0.139726
H	–0.862599	0.426385	–0.877336
H	–2.539252	–0.135874	–0.686128
O	3.854657	2.327490	–0.195311
H	–2.487187	0.914463	1.494766
O	3.254917	0.569942	1.870861
O	3.897182	1.062467	–0.914273
H	–1.938899	–2.418121	–0.895473
H	–0.951113	–3.221438	0.158545

4a

23	0.729012	1.960502	0.525696
8	–1.922810	–3.613251	–0.467982

8	–0.496613	1.732599	–0.844891
7	–0.918490	1.611798	1.840234
6	–1.138111	–1.478919	–1.168089
7	0.475865	–0.656751	0.551377
6	–2.419803	2.724716	0.175093
6	–2.086144	–2.419436	–1.127186
1	–3.396063	3.164186	–0.005945
1	–1.361605	–0.556935	–1.693313
6	–1.972010	2.650432	1.612237
1	–1.543329	3.602949	1.942734
1	–2.831456	2.426753	2.261766
1	–2.111404	2.404879	–1.895872
6	–0.377306	–0.835015	1.736530
1	0.247508	–0.757488	2.632147
1	–0.857086	–1.824242	1.752197
1	–3.048388	–2.278974	–1.617767
6	–1.703188	2.317392	–0.887701
6	0.225651	–1.612195	–0.551976
1	0.371971	–2.648676	–0.213973
1	0.989128	–1.401920	–1.311561
6	–1.473649	0.227509	1.776968
1	–2.076713	0.168583	0.870005
1	–2.134619	0.068529	2.641297
1	1.449852	–0.732835	0.831182
8	1.779606	1.247197	1.886880
8	0.690993	3.530691	0.704173
1	–0.518021	1.763067	2.766993
1	–2.699985	–4.167871	–0.620806
8	2.455516	1.454679	0.634200
6	3.026951	3.229965	–1.960802
6	2.369738	2.617750	–2.946469
1	2.779863	1.748666	–3.456328
1	1.393053	2.958478	–3.281098
1	2.613760	4.093888	–1.446625
1	3.997890	2.882757	–1.616877

4b

23	0.492235	1.892658	–0.811704
8	–1.131633	–3.563123	–0.599356
8	–1.031839	1.941553	–1.891386
7	–1.286888	1.765605	0.835010
6	–0.711049	–1.458683	–1.618362
7	0.612847	–0.125415	0.063380
6	–3.047768	2.517539	–0.731412
6	–1.466508	–2.549926	–1.461062
1	–4.110785	2.709407	–0.840214
1	–1.056964	–0.693062	–2.305615
6	–2.436974	2.667322	0.631719
1	–2.058300	3.688571	0.778886
1	–3.198341	2.499098	1.410746
1	–2.836467	2.129945	–2.799524
6	–0.288312	–0.387449	1.223285
1	0.229505	–0.037024	2.124383
1	–0.461515	–1.463680	1.333506
1	–2.395969	–2.682981	–2.012208
6	–2.339478	2.204219	–1.829239
6	0.610972	–1.247564	–0.944668
1	0.925021	–2.164322	–0.433367
1	1.368277	–0.977378	–1.683678
6	–1.607431	0.359417	1.070883
1	–2.165410	–0.015321	0.209740
1	–2.229022	0.210406	1.969847
1	1.571891	–0.081237	0.423282
8	1.503747	2.413245	–2.250295

8	1.008628	2.881066	0.327370
1	–0.729469	2.125402	1.607067
1	–1.758102	–4.292390	–0.705022
8	1.957868	1.194621	–1.660414
6	3.463997	0.885197	2.010664
6	4.014199	0.271019	0.959751
1	4.579385	–0.652911	1.068017
1	3.927933	0.684687	–0.042614
1	2.916093	1.817283	1.892571
1	3.558619	0.489786	3.020481

4c

V	1.326284	2.348196	0.331160
O	–1.171991	–3.409340	0.186701
O	0.124123	1.872040	–1.007458
N	–0.354895	2.182428	1.643816
C	–0.425325	–1.375058	–0.795904
N	1.123783	–0.237656	0.795350
C	–1.849173	2.961478	–0.199521
C	–1.349000	–2.327802	–0.641044
H	–2.833115	3.333273	–0.468875
H	–0.656374	–0.546716	–1.456414
C	–1.427390	3.141220	1.235209
H	–1.027391	4.146097	1.410403
H	–2.292350	3.004818	1.901483
H	–1.489356	2.300541	–2.177836
C	0.240357	–0.232032	1.972428
H	0.837941	0.011124	2.856449
H	–0.219622	–1.216044	2.143533
H	–2.299987	–2.289324	–1.170592
C	–1.098122	2.399110	–1.163437
C	0.922031	–1.374435	–0.131707
H	1.074420	–2.334292	0.383582
H	1.704483	–1.283906	–0.896039
C	–0.877936	0.794560	1.805956
H	–1.458420	0.566797	0.911013
H	–1.556308	0.768213	2.671243
H	2.090499	–0.241843	1.108859
O	2.303697	1.910757	1.856169
O	1.249744	3.924959	0.259278
H	0.028185	2.495119	2.536749
H	–1.938568	–3.993785	0.111561
O	3.054241	1.907992	0.634243
C	3.098588	3.261631	–2.298845
C	3.202472	1.948243	–2.515683
H	4.011883	1.363102	–2.086690
H	2.479819	1.411113	–3.124999
H	2.287502	3.849599	–2.720151
H	3.814456	3.796984	–1.681289

4d

23	0.625421	2.382619	–0.734420
8	–0.857978	–3.104521	–0.339181
8	–0.948527	2.375068	–1.738890
7	–1.066735	2.239961	1.002773
6	–0.559665	–1.014565	–1.428490
7	0.824814	0.381160	0.153975
6	–2.913837	2.939095	–0.489002
6	–1.272678	–2.122057	–1.202051
1	–3.983380	3.115770	–0.549851
1	–0.966798	–0.276054	–2.111634
6	–2.243720	3.114635	0.843285
1	–1.881360	4.145389	0.962720
1	–2.965454	2.939423	1.657846
1	–2.797902	2.530373	–2.560196

6	–0.002948	0.114523	1.365871
1	0.556239	0.488605	2.232005
1	–0.145606	–0.963706	1.498623
1	–2.228822	–2.294285	–1.693482
6	–2.254893	2.622550	–1.616470
6	0.793787	–0.752790	–0.840498
1	1.168034	–1.652941	–0.340328
1	1.494782	–0.467584	–1.627746
6	–1.344478	0.831401	1.275814
1	–1.938978	0.432168	0.450899
1	–1.914542	0.683397	2.208483
1	1.803170	0.454461	0.452229
8	1.558317	2.906060	–2.223491
8	1.170412	3.398527	0.366914
1	–0.477734	2.623465	1.739182
1	–1.468916	–3.852608	–0.389873
8	2.068560	1.707852	–1.635742
6	4.298304	0.379671	1.074700
6	3.823020	1.474737	1.673781
1	3.554687	2.364795	1.110656
1	3.690415	1.521793	2.753452
1	4.574870	–0.511620	1.634208
1	4.450460	0.350165	–0.002080

4e

23	1.380459	2.225931	0.574910
8	–1.490021	–3.257891	–0.305697
8	0.105715	2.034032	–0.755820
7	–0.236361	1.940117	1.941675
6	–0.655076	–1.154717	–1.041094
7	1.038801	–0.380810	0.623040
6	–1.749629	3.096582	0.317505
6	–1.632947	–2.061973	–0.965827
1	–2.715329	3.568734	0.164243
1	–0.863139	–0.227924	–1.564188
6	–1.260285	3.013329	1.740539
1	–0.789220	3.952016	2.052388
1	–2.106322	2.822225	2.417496
1	–1.516825	2.757038	–1.760187
6	0.217243	–0.524301	1.834959
1	0.871867	–0.464270	2.710401
1	–0.295387	–1.496370	1.870932
1	–2.604597	–1.890731	–1.427223
6	–1.080777	2.660000	–0.764624
6	0.721831	–1.332031	–0.466736
1	0.843042	–2.371395	–0.127657
1	1.468067	–1.151540	–1.250725
6	–0.840299	0.575467	1.903335
1	–1.472949	0.533227	1.015805
1	–1.479119	0.443219	2.788568
1	2.017827	–0.489160	0.873046
8	2.447894	1.483155	1.906910
8	1.401708	3.797311	0.745583
1	0.197631	2.081714	2.854770
1	–2.290319	–3.785908	–0.430909
8	3.091181	1.661602	0.632779
6	3.640137	3.410025	–1.988473
6	2.931855	2.816064	–2.949626
1	3.298026	1.933859	–3.470306
1	1.955217	3.185631	–3.252233
1	3.270883	4.287158	–1.463359
1	4.611154	3.034147	–1.676344

4f

23	–1.350102	0.031590	–0.358154

8	4.854466	–0.804513	0.111172
8	–0.517885	0.038189	1.307043
7	–0.279607	1.853444	–0.693630
6	2.612911	–0.922040	0.900432
7	1.065873	–0.758997	–1.050359
6	–0.468815	2.393303	1.737301
6	3.896657	–0.594685	1.072817
1	–0.366635	3.155050	2.504260
1	1.920914	–0.704075	1.706306
6	–0.667370	2.877393	0.324931
1	–1.717266	3.124072	0.131669
1	–0.072899	3.787006	0.151979
1	–0.269920	0.842560	3.163925
6	1.600139	0.482974	–1.631811
1	1.204705	0.591859	–2.646445
1	2.697185	0.462176	–1.703922
1	4.247861	–0.137906	1.997093
6	–0.428782	1.103091	2.115731
6	2.057478	–1.586957	–0.326722
1	2.885700	–1.878116	–0.989551
1	1.530717	–2.505027	–0.036341
6	1.200569	1.691949	–0.788673
1	1.573500	1.572011	0.229310
1	1.633393	2.612538	–1.206744
1	0.653932	–1.319274	–1.791473
8	–1.254564	–0.127730	–2.212273
8	–2.707365	0.767034	–0.020253
1	–0.635602	2.156421	–1.601002
1	5.716374	–0.539853	0.460358
8	–1.734411	–1.293125	–1.528339
6	–3.254538	–2.170177	1.185603
6	–2.170937	–2.947189	1.115326
1	–1.995057	–3.602679	0.266232
1	–1.419292	–2.951256	1.900798
1	–3.431477	–1.508373	2.029237
1	–4.000603	–2.157640	0.395848

4g

23	0.634614	2.406949	–0.829298
8	–0.637889	–3.123752	–0.327206
8	–0.967833	2.333906	–1.788994
7	–1.001553	2.254475	0.952484
6	–0.407323	–1.034084	–1.434075
7	0.932499	0.435570	0.110701
6	–2.911619	2.868444	–0.494483
6	–1.085873	–2.160423	–1.195021
1	–3.987640	3.009524	–0.524295
1	–0.840435	–0.312864	–2.120038
6	–2.202800	3.099168	0.808579
1	–1.857920	4.139871	0.885621
1	–2.892142	2.932245	1.652201
1	–2.844729	2.406594	–2.557145
6	0.122168	0.164402	1.333842
1	0.679833	0.563769	2.189527
1	0.009430	–0.915165	1.482203
1	–2.038820	–2.364748	–1.680310
6	–2.277403	2.542163	–1.633166
6	0.939262	–0.723912	–0.853366
1	1.336482	–1.600736	–0.330009
1	1.632688	–0.440297	–1.647867
6	–1.238945	0.843576	1.250079
1	–1.834127	0.416404	0.439672
1	–1.791614	0.694757	2.193067
1	1.905953	0.557381	0.408485

8	2.066671	1.750605	–1.759364
8	1.181448	3.469166	0.226089
1	–0.405990	2.662507	1.670311
1	–1.229291	–3.888056	–0.365992
8	1.505247	2.918957	–2.360106
6	3.843953	1.107949	2.220947
6	4.139878	1.566351	1.002211
1	4.780381	1.007862	0.322933
1	3.755016	2.513748	0.634975
1	3.224011	1.680761	2.907870
1	4.231272	0.161825	2.593495

4h

23	0.834679	2.104351	–1.159006
8	–1.517788	–3.335664	–0.480660
8	–0.929087	1.966567	–1.757043
7	0.020022	1.914469	0.897360
6	–1.295486	–1.207155	–1.519651
7	0.853627	–0.270249	–0.610220
6	–2.042480	3.071948	0.074114
6	–2.050556	–2.204292	–1.049550
1	–2.968879	3.560892	0.362897
1	–1.793911	–0.335307	–1.928032
6	–0.978549	2.999509	1.135160
1	–0.410850	3.934865	1.176625
1	–1.443019	2.850369	2.122060
1	–2.797301	2.763123	–1.870707
6	0.527784	–0.480297	0.811100
1	1.444434	–0.363311	1.403293
1	0.137323	–1.487958	1.001614
1	–3.138207	–2.162063	–1.086834
6	–1.949541	2.630269	–1.195052
6	0.204487	–1.226753	–1.557519
1	0.563426	–2.243771	–1.351247
1	0.553976	–0.928588	–2.550364
6	–0.494508	0.568854	1.237602
1	–1.427721	0.424131	0.689984
1	–0.709971	0.497900	2.313762
1	1.857163	–0.347717	–0.762286
8	2.474339	1.585983	–1.766293
8	1.055199	3.645398	–0.849354
1	0.834604	2.114931	1.486098
1	–2.227594	–3.971009	–0.313738
8	1.443037	1.523748	–2.781467
6	3.211188	2.504698	2.834676
6	3.390557	2.941154	1.585684
1	3.874254	2.332157	0.825014
1	3.065863	3.926983	1.263537
1	2.746080	3.125098	3.598063
1	3.550266	1.521625	3.154963

4i

23	1.557330	0.674098	0.615039
8	0.158405	0.958863	–0.520260
8	3.950567	–1.244391	–2.052194
7	1.575593	–1.473980	0.825917
6	–2.009696	1.081125	0.492012
7	–0.343791	0.189142	2.077378
6	3.147052	–2.933743	–0.497547
6	–1.178487	1.064104	–0.562282
1	2.921965	–3.994745	–0.434122
1	–3.072850	1.184981	0.296132
6	2.964803	–2.105493	0.736674
1	3.090138	–2.727442	1.628122
1	3.689611	–1.292637	0.798985

1	3.761485	–3.186580	–2.502541
6	–0.558987	–1.258400	2.051671
1	–1.148952	–1.496433	1.157807
1	–1.127683	–1.622499	2.922612
1	–1.566587	1.138611	–1.578996
6	3.608449	–2.485271	–1.684193
6	–1.558125	1.008976	1.924659
1	–1.309734	2.011575	2.296416
1	–2.375462	0.629667	2.559303
6	0.796736	–1.952461	1.995597
1	1.380585	–1.712925	2.889791
1	0.673113	–3.042818	1.952153
1	1.084717	–1.769212	–0.022525
1	0.158377	0.449576	2.924567
8	2.779303	0.609700	–0.422294
1	3.643989	–0.564092	–1.403949
8	2.266567	0.734281	2.330747
8	1.882533	2.008266	1.766666
6	2.616609	4.895259	–0.970774
6	2.511028	3.963286	–1.917364
1	2.762544	2.923759	–1.723664
1	2.164571	4.204250	–2.920368
1	2.363042	5.936926	–1.157323
1	2.964692	4.651997	0.030700

5a

V	0.637826	0.125571	0.718833
O	–0.726584	–0.072098	1.907237
O	–0.388060	3.752403	–0.769133
N	–0.579045	–0.054632	–1.156838
C	–1.209804	–2.339988	2.536813
N	0.118916	–2.283629	0.460347
C	–1.248498	2.079316	–2.315956
C	–1.400555	–1.009979	2.588854
H	–2.063099	1.915481	–3.017121
H	–1.840049	–2.957263	3.170991
C	–0.219423	0.996358	–2.194956
H	–0.120874	0.481934	–3.157249
H	0.769004	1.379475	–1.935653
H	–2.009667	4.006308	–1.917335
C	–0.885761	–2.431504	–0.598835
H	–1.870306	–2.238647	–0.155399
H	–0.911937	–3.451991	–1.014150
H	–2.172666	–0.591658	3.236440
C	–1.242426	3.270180	–1.683345
C	–0.183119	–3.039252	1.687400
H	0.759549	–3.152652	2.239035
H	–0.527797	–4.060369	1.453950
C	–0.598262	–1.427519	–1.707079
H	0.390542	–1.611342	–2.138015
H	–1.343727	–1.519671	–2.509798
H	–1.518345	0.175277	–0.824567
H	1.036481	–2.535817	0.096507
O	0.797973	1.706507	0.607030
H	0.170013	3.042713	–0.372704
O	1.944740	–0.535640	–0.475603
O	3.282065	–0.148957	–0.060925
C	3.400753	–0.712031	1.244204
C	2.185077	–0.325522	2.068444
H	2.319871	0.602571	2.632101
H	1.854455	–1.114296	2.752785
H	3.498396	–1.807454	1.165827
H	4.348120	–0.306942	1.623283

5b

23	–0.034321	0.008739	–0.079553
8	–0.351242	–6.000035	–1.693226
8	–0.190599	–0.452662	–1.851278
7	–2.114158	–0.737532	0.083945
6	0.152578	–3.695746	–2.006331
7	0.157140	–2.545992	0.214890
6	–2.479959	0.104582	–2.249646
6	–0.362875	–4.848728	–2.441880
1	–3.214468	0.348652	–3.011897
1	0.088330	–2.831767	–2.658422
6	–2.985318	0.057775	–0.828942
1	–3.039404	1.068481	–0.407725
1	–4.003928	–0.359863	–0.813106
1	–0.946858	–0.045784	–3.706957
6	–1.185637	–2.962121	0.657724
1	–1.278309	–2.749506	1.727796
1	–1.344340	–4.040762	0.518525
1	–0.823120	–4.929901	–3.425669
6	–1.213710	–0.101175	–2.650921
6	0.835880	–3.511843	–0.681417
1	0.944126	–4.488387	–0.187833
1	1.847033	–3.117097	–0.847659
6	–2.260917	–2.200978	–0.110614
1	–2.162786	–2.398683	–1.179654
1	–3.265059	–2.521889	0.205827
1	0.742215	–2.410597	1.040761
8	–0.029697	–0.299970	1.806755
8	–0.465895	1.524585	–0.099692
1	–2.353025	–0.507843	1.049540
1	–0.739679	–6.717930	–2.211450
8	1.191753	–0.922596	2.297309
6	2.234227	–0.109835	1.740371
6	2.022867	0.002357	0.242954
1	2.397218	–0.869592	–0.309589
1	2.454023	0.913720	–0.184513
1	2.209814	0.878495	2.217340
1	3.158423	–0.625401	2.037676

5c

23	1.256196	0.082078	–0.367367
8	–4.640173	–1.226849	0.267936
8	–0.022195	1.005390	–1.359163
7	0.406232	1.345471	1.266777
6	–2.745225	–0.509870	–0.978458
7	–0.772805	–1.140038	0.450238
6	0.084846	3.185567	–0.396380
6	–4.030408	–0.388647	–0.633832
1	–0.097121	4.243973	–0.556125
1	–2.333092	0.212911	–1.672271
6	0.632747	2.786739	0.948767
1	1.715609	2.949756	0.996334
1	0.171476	3.403034	1.736369
1	–0.582211	2.698377	–2.350478
6	–1.259577	–0.454799	1.663804
1	–0.723778	–0.852808	2.533112
1	–2.328620	–0.636845	1.833092
1	–4.660407	0.396644	–1.049072
6	–0.173873	2.336230	–1.405360
6	–1.839305	–1.600893	–0.486314
1	–2.444472	–2.382584	–0.007162
1	–1.310678	–2.054274	–1.332601
6	–1.018945	1.048987	1.555933
1	–1.607029	1.459333	0.734239
1	–1.330347	1.554060	2.482730

1	–0.258555	–1.973332	0.723588
8	1.564503	–1.498253	–1.212196
8	2.554998	0.966915	–0.489874
1	0.964041	1.118991	2.088872
1	–5.586598	–1.029683	0.294444
8	2.808730	–2.110110	–0.781772
6	2.599171	–2.336293	0.617921
6	2.102221	–1.059140	1.291319
1	1.877635	–3.160408	0.742796
1	3.580792	–2.688082	0.962763
1	2.929560	–0.454136	1.675730
1	1.426022	–1.292614	2.123323

5d

23	1.649717	0.986651	0.336184
8	–2.899144	2.178769	–2.738994
8	0.558672	0.302858	1.678383
7	1.898417	–1.425751	–0.043036
6	–1.599341	2.158171	–0.748322
7	0.192868	0.494337	–1.276884
6	1.116196	–1.961389	2.243518
6	–2.370172	2.796231	–1.634582
1	0.908066	–2.769872	2.938668
1	–1.196455	2.724604	0.082363
6	2.154600	–2.207397	1.184901
1	3.149779	–1.911915	1.535826
1	2.198870	–3.285369	0.955143
1	–0.305643	–0.725785	3.201245
6	0.408573	–0.846277	–1.885720
1	1.235965	–0.762191	–2.595092
1	–0.479255	–1.155258	–2.452764
1	–2.616479	3.849801	–1.515427
6	0.436909	–0.811720	2.404340
6	–1.245477	0.707138	–0.860022
1	–1.380093	0.200924	0.098174
1	–1.889495	0.227169	–1.605735
6	0.742781	–1.884115	–0.819545
1	–0.095014	–2.001498	–0.125250
1	0.909606	–2.863966	–1.296373
1	0.393310	1.203688	–1.981536
8	3.245964	0.867361	1.242887
8	1.253313	2.520333	0.304913
1	2.741106	–1.452351	–0.612136
1	–3.461615	2.805678	–3.214067
8	4.371468	0.305949	0.517689
6	4.414852	1.108630	–0.664919
6	3.047152	1.059198	–1.322618
1	2.964937	0.188170	–1.984116
1	2.845446	1.960636	–1.912025
1	4.694317	2.135231	–0.393751
1	5.229241	0.663150	–1.254890

5e

23	0.968801	0.298160	0.166887
8	–1.845393	–1.889399	–2.012090
8	–0.342727	0.192807	–1.254454
7	–0.674648	1.849336	0.857134
6	–2.484395	–1.942194	0.318747
7	–0.460786	–0.845996	1.520005
6	–1.364913	2.343058	–1.472845
6	–2.735137	–1.955077	–1.004316
1	–1.953193	2.991270	–2.114715
1	–3.346294	–2.004395	0.977347
6	–0.904338	2.900137	–0.157241
1	0.049857	3.436104	–0.265104

1	–1.636048	3.633393	0.218540
1	–1.440275	0.765423	–2.879515
6	–1.400379	0.041000	2.263438
1	–0.850920	0.456621	3.116897
1	–2.249200	–0.525821	2.663626
1	–3.756249	–2.057546	–1.369643
6	–1.066315	1.110150	–1.914465
6	–1.122479	–2.082203	0.929328
1	–1.193448	–2.817645	1.742843
1	–0.425941	–2.485033	0.191095
6	–1.872483	1.174146	1.363055
1	–2.430701	0.780332	0.512313
1	–2.531839	1.856802	1.922889
1	0.209167	–1.203987	2.198169
8	2.095433	0.114336	–1.270837
8	1.829280	1.296411	1.054437
1	–0.157963	2.262924	1.631387
1	–1.072346	–1.334197	–1.736589
8	3.456113	–0.117168	–0.827964
6	3.354169	–1.386808	–0.187638
6	2.145474	–1.395177	0.752857
1	2.424125	–1.226031	1.799397
1	1.597738	–2.339515	0.670342
1	3.248573	–2.173033	–0.949594
1	4.317987	–1.515028	0.320789

5f

23	–0.934417	0.072323	–0.705200
8	2.036493	–2.189736	1.405641
8	0.034611	–0.492940	0.948191
7	–0.178398	2.060072	0.090098
6	3.178190	–0.809671	–0.209852
7	1.196259	0.080448	–1.612981
6	–0.104097	1.365293	2.464854
6	3.076058	–1.454263	0.967322
1	0.025190	1.669309	3.499203
1	4.097282	–0.258679	–0.390175
6	–0.517052	2.430442	1.488665
1	–1.599316	2.618959	1.511532
1	–0.029150	3.385455	1.743791
1	0.484350	–0.603053	2.932092
6	1.658613	1.489308	–1.505733
1	1.178429	2.055545	–2.310005
1	2.744008	1.565093	–1.648323
1	3.899311	–1.440891	1.680952
6	0.140347	0.077315	2.149534
6	2.227921	–0.987035	–1.357509
1	2.828835	–1.081813	–2.274142
1	1.668280	–1.920759	–1.240934
6	1.291646	2.093770	–0.152596
1	1.764789	1.524814	0.648118
1	1.658706	3.129827	–0.097162
1	0.886773	–0.057794	–2.574452
8	–1.580713	–1.547011	–1.146990
8	–1.282432	0.922375	–2.013146
1	–0.626833	2.722761	–0.542072
1	1.194551	–1.800844	1.050438
8	–2.102999	–2.213337	0.034843
6	–3.176172	–1.329995	0.423464
6	–2.674566	0.114592	0.471209
1	–2.374912	0.418192	1.478214
1	–3.408952	0.817887	0.066577
1	–3.997978	–1.438841	–0.296271
1	–3.494015	–1.735136	1.392320

5g

23	–0.721574	1.774035	–0.487037
8	–1.712831	1.514798	–1.721244
8	–2.675903	–3.657664	–0.681973
8	–1.068101	3.494482	–0.026404
7	–2.016300	1.326591	1.276047
6	–0.611031	–2.730196	–1.392212
7	–0.547004	–0.475676	–0.292867
6	–1.322699	3.447872	2.354164
6	–1.367411	–3.784781	–1.073772
1	–1.340426	4.051885	3.256301
1	0.422433	–2.926536	–1.667759
6	–1.526895	1.968563	2.526153
1	–0.582133	1.479466	2.787565
1	–2.246672	1.775949	3.336609
1	–0.949986	5.152412	1.148433
6	–1.001849	–0.894299	1.053211
1	–0.207833	–0.648421	1.759795
1	–1.184384	–1.974333	1.093560
1	–0.976549	–4.800835	–1.101635
6	–1.093220	4.072827	1.187858
6	–1.090087	–1.304425	–1.406274
1	–0.799994	–0.806360	–2.334602
1	–2.179778	–1.259602	–1.357885
6	–2.271484	–0.128161	1.399127
1	–3.067207	–0.386323	0.693186
1	–2.621690	–0.383641	2.408972
1	–2.880353	1.796221	1.003435
1	0.477589	–0.504848	–0.299249
1	–3.072240	–4.536380	–0.602897
8	0.729374	1.506744	0.852419
8	1.917078	0.877686	0.306201
6	2.208210	1.664569	–0.851937
6	0.970149	1.730868	–1.722837
1	0.876289	0.884740	–2.412544
1	0.889673	2.657391	–2.305010
1	2.526600	2.665525	–0.528946
1	3.061821	1.156228	–1.322723

5h

23	–0.156395	1.314540	0.612514
8	–1.211997	0.853909	1.749616
8	–0.308949	–3.945322	–2.226067
8	–0.324121	3.133205	0.506263
7	–1.688003	1.312256	–0.948590
6	0.471069	–3.295240	–0.080634
7	–0.428453	–0.976396	0.185005
6	–2.660959	3.369936	0.026709
6	0.053645	–4.234600	–0.933990
1	–3.502629	4.055899	0.038350
1	0.718469	–3.615660	0.928572
6	–2.931662	1.977955	–0.474892
1	–3.363608	1.345105	0.308549
1	–3.654217	2.014871	–1.305255
1	–1.359532	4.863949	0.776583
6	–1.760768	–1.108889	–0.441935
1	–2.515432	–0.958976	0.334111
1	–1.909636	–2.105463	–0.875410
1	–0.026661	–5.280521	–0.641881
6	–1.470937	3.828504	0.453253
6	0.628851	–1.836288	–0.415632
1	1.585641	–1.452942	–0.048884
1	0.610654	–1.694778	–1.497860
6	–1.905231	–0.042290	–1.522876

1	–1.147867	–0.194273	–2.296412
1	–2.892202	–0.103477	–2.001399
1	–1.272892	1.905695	–1.665315
1	–0.512306	–1.211576	1.172583
1	–0.475345	–4.770515	–2.702382
8	1.414064	0.956451	1.419310
8	2.645786	0.793184	0.697874
6	2.523291	1.552068	–0.520351
6	1.193759	1.260450	–1.177681
1	1.229467	0.342019	–1.771156
1	0.919983	2.092577	–1.842871
1	2.623965	2.619641	–0.278218
1	3.418759	1.232302	–1.074359

6

V	0.185154	–0.695541	0.013225
O	–1.424289	–1.219744	0.881324
O	–0.995120	–2.905512	–3.087260
N	1.125403	–2.680844	–0.007919
C	–1.152518	–1.382662	3.258020
N	1.072547	–1.024509	2.242065
C	0.646378	–4.261074	–1.909966
C	–1.806029	–1.594896	2.096723
H	0.893488	–5.296272	–1.690125
H	–1.605289	–1.738568	4.178167
C	1.559424	–3.201644	–1.370905
H	2.568976	–3.611960	–1.257744
H	1.622099	–2.340910	–2.039381
H	–1.003332	–4.909368	–3.055462
C	1.632378	–2.372298	2.372740
H	0.814549	–3.036434	2.675607
H	2.414087	–2.437980	3.145654
H	–2.764278	–2.124258	2.108032
C	–0.446920	–4.054682	–2.673717
C	0.149869	–0.636211	3.339037
H	0.002770	0.447430	3.232342
H	0.623705	–0.798817	4.320204
C	2.183179	–2.813352	1.023657
H	3.023840	–2.179181	0.718528
H	2.549392	–3.848536	1.076776
H	0.336002	–3.265353	0.278464
H	1.822963	–0.338522	2.168847
O	–0.144041	–0.837975	–1.555992
H	–0.637317	–2.123305	–2.593718
O	1.551699	0.645154	0.133539
O	0.320660	1.321351	0.572406
C	–0.323859	2.178786	–1.682617
C	0.043667	2.495753	–0.288670
H	–1.353566	1.961731	–1.944349
H	0.442860	1.983916	–2.422757
H	–0.774203	2.973267	0.260587
H	0.945111	3.110050	–0.216493

7

V	–0.118234	–0.077507	0.360283
O	0.362106	1.379644	1.430276
O	0.011160	–1.346386	–1.051822
N	2.009568	–0.693829	0.665218
C	0.309202	3.292110	–0.021836
N	0.911087	1.206916	–1.206676
C	1.568037	–2.970112	–0.199873
C	0.314238	2.694394	1.183582
H	1.946179	–3.979925	–0.328395
H	0.269645	4.376949	–0.051125
C	2.163387	–2.151222	0.911777

H	1.662639	–2.353703	1.866044
H	3.229849	–2.399799	1.035300
H	0.244045	–3.211357	–1.826393
C	2.360124	1.193930	–0.907988
H	2.527946	1.922601	–0.110584
H	2.950767	1.518576	–1.778145
H	0.300926	3.299955	2.092250
C	0.601127	–2.547234	–1.035168
C	0.347111	2.571166	–1.342119
H	–0.661943	2.451506	–1.756587
H	0.932111	3.153564	–2.072814
C	2.819936	–0.194955	–0.469365
H	2.701034	–0.913056	–1.284881
H	3.889081	–0.164721	–0.211828
O	–1.752832	0.539359	–0.167927
H	2.257044	–0.183100	1.512425
H	0.731810	0.672827	–2.056281
O	–0.663446	–1.221224	1.639511
O	–2.890339	0.194285	0.670038
C	–3.745007	–1.415530	–0.953680
C	–3.959258	–0.137136	–0.225657
H	–4.588904	–2.033887	–1.241232
H	–2.752387	–1.664267	–1.312407
H	–1.639239	–1.216622	1.687355
H	–4.837593	–0.183484	0.431966
H	–4.101971	0.718856	–0.908162

TS1a

V	1.016419	0.156185	–0.508670
O	–0.628119	–0.217103	–1.453345
O	2.312070	–2.185097	–3.574277
N	0.900990	–2.032562	–0.188199
C	–2.559502	0.412725	–0.135395
N	–0.666035	–0.160441	1.328969
C	1.936181	–3.726539	–1.730991
C	–1.915627	0.043413	–1.265583
H	1.685292	–4.762237	–1.519745
H	–3.631262	0.575345	–0.205788
C	2.152188	–2.801258	–0.569611
H	2.469233	–3.370320	0.309655
H	2.933875	–2.067045	–0.772909
H	1.904334	–4.133815	–3.805788
C	–0.888971	–1.612721	1.446868
H	–1.662936	–1.879820	0.720400
H	–1.268825	–1.888921	2.443022
H	–2.507610	–0.081818	–2.177758
C	2.039340	–3.383039	–3.029846
C	–1.931992	0.592053	1.220658
H	–1.704435	1.647861	1.432213
H	–2.643486	0.276848	2.003563
C	0.387109	–2.386628	1.151283
H	1.167650	–2.144403	1.878236
H	0.188354	–3.466355	1.216849
H	0.183889	–2.248057	–0.882998
H	–0.129702	0.155230	2.135192
O	1.967566	–0.108041	–1.748702
H	2.282044	–1.460005	–2.909644
O	2.039409	–0.064930	1.057355
O	2.311240	1.223346	0.528564
C	1.044978	2.635945	0.420383
C	0.272475	2.279136	–0.696026
H	0.606501	2.605543	–1.677890
H	–0.798042	2.149868	–0.588644
H	0.624516	2.602400	1.422953

H	1.912941	3.282116	0.321654

TS1b

V	0.089606	–0.243007	0.237359
O	–0.464552	–6.053955	–1.852431
O	–0.056020	–0.572965	–1.623966
N	–2.077519	–0.819659	0.160571
C	0.186579	–3.765812	–1.931656
N	0.018409	–2.798980	0.370622
C	–2.284777	0.196201	–2.090620
C	–0.342276	–4.850540	–2.504353
H	–2.957336	0.530434	–2.874893
H	0.230247	–2.849572	–2.509146
C	–2.837347	0.129841	–0.694127
H	–2.791647	1.104937	–0.194618
H	–3.895645	–0.175333	–0.721975
H	–0.722561	–0.090964	–3.480601
C	–1.394282	–3.151600	0.610572
H	–1.600732	–3.033080	1.680034
H	–1.603715	–4.197568	0.346497
H	–0.706754	–4.830794	–3.530418
C	–1.025774	–0.137057	–2.430741
C	0.741477	–3.727201	–0.537443
H	0.749653	–4.743675	–0.119067
H	1.780263	–3.373433	–0.566621
C	–2.315685	–2.237424	–0.190523
H	–2.117589	–2.348257	–1.257253
H	–3.369123	–2.502023	–0.008640
H	0.511762	–2.803363	1.259853
O	–0.218969	–0.588467	2.110894
O	–0.254808	1.296190	0.301929
H	–2.354745	–0.670501	1.130504
H	–0.841770	–6.704700	–2.459911
O	1.162432	–0.766061	1.799812
C	2.301020	0.456618	1.306340
C	2.199103	0.270069	–0.120668
H	2.807563	–0.523341	–0.552406
H	2.096743	1.150663	–0.746370
H	1.937086	1.387386	1.736362
H	3.108407	–0.001908	1.875450

TS1c

23	1.575491	1.928160	–0.174845
8	–1.286426	–3.372267	–0.744454
8	–0.011559	1.781904	–1.233415
7	0.019952	1.736721	1.449828
6	–0.499711	–1.263261	–1.519743
7	1.187404	–0.568124	0.221911
6	–1.557517	3.073997	0.073753
6	–1.457096	–2.190242	–1.427180
1	–2.465707	3.668192	0.039149
1	–0.723484	–0.341673	–2.043258
6	–0.901213	2.910286	1.412144
1	–0.298200	3.787312	1.675378
1	–1.665151	2.785715	2.196616
1	–1.655331	2.690658	–1.999565
6	0.247764	–0.733499	1.351792
1	0.821592	–0.798972	2.284851
1	–0.328748	–1.663459	1.268625
1	–2.435344	–2.047529	–1.883942
6	–1.094012	2.540239	–1.072882
6	0.885936	–1.426180	–0.969290
1	1.050110	–2.480694	–0.709795
1	1.617770	–1.132090	–1.727737
6	–0.714084	0.448396	1.417665

1	–1.348983	0.459128	0.532461
1	–1.362280	0.359898	2.302807
1	2.110253	–0.865150	0.531640
8	2.348984	1.283939	–1.737992
8	1.557159	3.496469	–0.027701
1	0.535302	1.793283	2.326165
1	–2.055266	–3.938651	–0.897330
8	3.397020	1.795821	–0.911766
6	3.952753	1.132947	0.811671
6	2.937104	1.457495	1.713499
1	2.991256	2.410748	2.232609
1	2.437113	0.655285	2.245615
1	4.151398	0.101433	0.531329
1	4.786424	1.809778	0.650927

TS1d

23	1.929452	1.108409	0.102470
8	0.534970	0.526815	–1.042712
8	3.862942	–0.956302	–2.747967
7	1.952849	–1.186906	0.386311
6	–1.495631	1.231124	0.044292
7	0.257044	0.641427	1.701182
6	3.187996	–2.699681	–1.193122
6	–0.764015	0.844570	–1.016906
1	2.892052	–3.744198	–1.152526
1	–2.550062	1.435327	–0.115576
6	3.233601	–1.928007	0.093404
1	3.433600	–2.609208	0.928234
1	4.040846	–1.191490	0.073269
1	3.469439	–2.848097	–3.282999
6	–0.005039	–0.806074	1.805444
1	–0.701919	–1.066229	1.002915
1	–0.489697	–1.065960	2.758444
1	–1.246900	0.722314	–1.989199
6	3.491855	–2.201944	–2.407604
6	–0.963293	1.447394	1.434259
1	–0.684036	2.496010	1.593232
1	–1.741762	1.205031	2.176139
6	1.294124	–1.586786	1.642399
1	1.981652	–1.369443	2.467104
1	1.083917	–2.666964	1.664826
1	1.313423	–1.374690	–0.387232
1	0.669989	0.970846	2.570962
8	3.230023	0.932772	–0.815226
1	3.710353	–0.307370	–2.021734
8	1.436806	2.871381	–0.328398
8	1.930912	2.811782	1.007049
6	3.591874	2.450481	1.563971
6	3.407863	1.058489	1.853470
1	3.039540	0.822770	2.852187
1	4.158933	0.371249	1.480707
1	4.232261	2.737138	0.733801
1	3.512978	3.201350	2.346728

TS1e

23	1.821730	0.947838	–0.945798
8	–2.042854	–2.104374	2.305259
8	1.977170	–1.020576	–1.378714
7	–0.082295	0.814889	–2.053820
6	–0.083063	–1.940676	0.968680
7	0.311990	0.541752	0.692756
6	0.473408	–1.328768	–3.212166
6	–1.188791	–2.589253	1.345990
1	0.056672	–2.050076	–3.908189
1	0.530314	–2.377196	0.190255

6	0.067987	0.108030	–3.370606
1	0.813255	0.687578	–3.929451
1	–0.884627	0.179061	–3.916849
1	1.628114	–2.819614	–2.269480
6	–1.055218	0.835301	0.184374
1	–1.179735	1.924112	0.180971
1	–1.823035	0.407086	0.840372
1	–1.469593	–3.541601	0.899231
6	1.371597	–1.751758	–2.289837
6	0.386521	–0.659872	1.588497
1	–0.199181	–0.454956	2.493129
1	1.438016	–0.751343	1.874624
6	–1.192263	0.292028	–1.230296
1	–1.107013	–0.795842	–1.234188
1	–2.167573	0.564356	–1.660119
1	0.607014	1.333651	1.261389
8	2.820517	1.393512	–2.527057
8	1.697864	2.513426	–0.602653
1	–0.248232	1.803852	–2.245574
1	–2.737218	–2.756603	2.471848
8	3.752172	0.739865	–1.650274
6	4.229580	1.439127	–0.402102
6	3.269907	0.841895	0.604320
1	3.059092	1.460940	1.477833
1	3.531273	–0.185549	0.866397
1	4.144007	2.518510	–0.531741
1	5.280430	1.135968	–0.341770

TS1f

23	1.489813	1.399873	0.021007
8	–2.563326	–1.746090	2.854389
8	1.604812	–0.545026	–0.510706
7	–0.339964	1.392081	–1.196778
6	–0.506732	–1.561499	1.674341
7	–0.126141	0.933583	1.557722
6	0.288335	–0.640749	–2.514752
6	–1.644515	–2.208126	1.943522
1	–0.041210	–1.289431	–3.320907
1	0.155412	–1.972192	0.921990
6	–0.176834	0.787286	–2.560312
1	0.519225	1.443216	–3.097181
1	–1.142465	0.852042	–3.085902
1	1.373889	–2.219304	–1.644878
6	–1.457744	1.248692	0.987371
1	–1.601855	2.333367	1.053047
1	–2.262988	0.764567	1.553630
1	–1.905049	–3.137072	1.438662
6	1.101986	–1.158555	–1.560653
6	–0.061129	–0.317625	2.382700
1	–0.667224	–0.171385	3.285669
1	0.987853	–0.416674	2.677553
6	–1.491719	0.805357	–0.467970
1	–1.390714	–0.278967	–0.537625
1	–2.439620	1.094894	–0.944945
1	0.143871	1.696569	2.177065
8	2.722238	1.069550	1.433846
8	1.398310	2.948955	0.444287
1	–0.502640	2.392646	–1.316674
1	–3.252770	–2.413284	2.976093
8	3.498718	0.930739	0.234138
6	3.799665	2.145692	–0.627153
6	2.662107	2.061858	–1.618795
1	2.825879	1.296515	–2.380165
1	2.337383	3.014354	–2.039660

1	3.802895	3.039681	–0.002871
1	4.807807	1.919362	–0.989964

TS1g

23	1.530846	1.288890	1.633460
8	2.894593	1.056141	3.040466
8	0.394541	0.745237	0.641514
8	3.415177	0.717857	1.749183
6	3.802076	2.145997	0.568279
6	2.604524	2.294072	–0.148424
1	2.458115	1.690325	–1.039988
1	2.051766	3.222094	–0.099433
1	4.086548	2.881784	1.316211
1	4.624544	1.551446	0.177342
8	–0.825202	–4.051731	1.666155
8	1.193825	3.104697	2.005212
7	0.068685	1.099531	3.293869
6	1.445914	–3.429610	1.369180
7	1.554097	–1.060742	2.191482
6	0.755981	3.194440	4.366698
6	0.512264	–4.353456	1.614738
1	0.688119	3.844692	5.233025
1	2.482010	–3.760437	1.372716
6	0.488162	1.733478	4.568077
1	1.375507	1.200579	4.930221
1	–0.307181	1.592455	5.317252
1	1.212069	4.815899	3.091368
6	0.801395	–1.246483	3.444182
1	1.466764	–1.011209	4.278719
1	0.460981	–2.282711	3.568080
1	0.770543	–5.396106	1.795298
6	1.062955	3.737176	3.176577
6	1.167098	–1.976425	1.089706
1	1.721650	–1.646022	0.205350
1	0.109893	–1.814738	0.873120
6	–0.392462	–0.302615	3.439148
1	–1.034177	–0.522739	2.582001
1	–0.989337	–0.419565	4.355373
1	–0.698810	1.653052	2.912044
1	2.552867	–1.137475	2.369346
1	–1.332781	–4.870604	1.751043

TS1h

23	2.004998	–1.036443	1.973130
8	3.525206	–1.994105	2.443556
8	2.147427	–0.771144	0.406892
8	3.733323	–0.641193	2.839998
6	3.008614	–0.584095	4.461869
6	1.598292	–0.666248	4.283876
1	1.024090	0.232460	4.498549
1	1.119457	–1.594731	4.588384
1	3.549287	–1.456202	4.821339
1	3.466397	0.358763	4.758306
8	0.723956	4.582236	3.581065
8	1.213076	–2.738958	2.047179
7	–0.193850	–0.474862	1.845337
6	2.634863	3.739250	2.459502
7	1.988384	1.386314	1.832096
6	–0.660676	–2.531502	0.558985
6	1.838492	4.756388	2.802287
1	–1.353445	–3.079141	–0.072919
1	3.486521	3.965347	1.822657
6	–0.842085	–1.046014	0.638790
1	–0.413696	–0.540543	–0.235220
1	–1.916116	–0.798641	0.659232

1	0.312141	–4.313344	1.143286
6	0.679790	1.741542	1.241131
1	0.695281	1.449977	0.188412
1	0.495875	2.821340	1.289414
1	2.034811	5.775470	2.472704
6	0.279810	–3.224433	1.226831
6	2.439870	2.314280	2.905220
1	3.386270	1.913151	3.276946
1	1.716251	2.270408	3.721903
6	–0.416965	0.983534	1.975795
1	–0.394669	1.238292	3.038457
1	–1.406690	1.264070	1.587398
1	–0.574499	–0.949440	2.662717
1	2.690105	1.388382	1.093744
1	0.336966	5.444895	3.784994

TS1i

23	1.105979	1.947818	–1.045427
8	1.361663	–0.280570	–0.887391
8	–0.336525	1.275144	–2.073833
7	–0.495510	1.690999	0.675587
6	2.156345	–2.139762	0.315873
7	0.262563	–1.749755	2.026107
6	–2.309662	2.090329	–0.970356
6	2.321584	–1.018729	–0.485518
1	–3.377852	2.247418	–1.087393
1	3.013846	–2.722434	0.635859
6	–1.692921	2.501727	0.335958
1	–1.353238	3.543780	0.317132
1	–2.435416	2.412732	1.147016
1	–2.177478	1.278914	–2.912016
6	0.294648	–0.248860	1.945447
1	3.346023	–0.745794	–0.784969
6	–1.628370	1.561003	–2.007730
6	0.815803	–2.546205	0.682945
6	–0.809336	0.300015	1.041203
1	–0.009350	2.153721	1.442652
8	0.734519	3.489188	–1.078479
1	0.192658	0.134848	2.967447
1	1.280544	0.023453	1.565151
1	–0.868820	–0.276641	0.117261
1	–1.783034	0.244769	1.557308
1	0.058888	–2.278295	–0.055467
1	0.703133	–3.586150	1.000844
8	2.163521	2.065644	0.550206
8	3.027254	1.805099	–0.548303
6	3.306699	2.811187	–1.977974
6	2.292830	2.273110	–2.845890
1	2.535472	1.351592	–3.371546
1	1.669341	2.968000	–3.398766
1	3.212358	3.840387	–1.640044
1	4.333768	2.454339	–2.032235
1	0.885254	–2.042648	2.783091
1	–0.681582	–2.076286	2.264382

TS1j

23	1.057555	1.528719	–1.136295
8	1.402552	–0.536886	–0.558878
8	–0.521082	0.743903	–1.812283
7	–0.400958	1.322765	0.901162
6	2.316650	–2.366572	0.574098
7	0.330817	–2.129628	2.222994
6	–2.323404	1.776728	–0.600866
6	2.417094	–1.228127	–0.211944
1	–3.378932	2.029328	–0.649372

1	3.198893	–2.925549	0.866535
6	–1.585970	2.177035	0.645772
1	–1.214199	3.205288	0.576768
1	–2.269982	2.131812	1.511689
1	–2.415957	0.894215	–2.513594
6	0.333228	–0.625890	2.196525
1	3.412702	–0.898250	–0.549189
6	–1.775863	1.154823	–1.664745
6	0.989727	–2.862349	0.892594
6	–0.752007	–0.053759	1.283062
1	0.147530	1.761607	1.638258
8	0.636834	3.056284	–1.041238
1	0.206661	–0.279796	3.228957
1	1.326770	–0.347379	1.846341
1	–0.829633	–0.638896	0.365318
1	–1.724680	–0.082156	1.803223
1	0.244891	–2.628793	0.130439
1	0.935780	–3.913528	1.186700
8	1.791451	1.543584	–2.855911
8	2.842911	1.377869	–1.907147
6	3.381125	2.550913	–0.644023
6	2.594548	2.121790	0.468814
1	2.049163	2.887474	1.011469
1	3.015032	1.325242	1.081494
1	4.401023	2.196031	–0.771593
1	3.186481	3.524604	–1.085420
1	0.900487	–2.439434	3.014181
1	–0.620428	–2.483845	2.376852

TS1k

23	1.775068	0.684669	0.310041
8	0.082132	0.592599	1.432144
8	0.744971	–0.584470	–0.612832
7	–1.249923	0.793704	–2.515167
6	–1.473603	1.848026	2.651651
7	–2.883159	2.169573	0.574216
6	0.118225	–1.333142	–2.813163
6	–0.195262	1.438214	2.376192
1	0.368361	–2.097206	–3.548209
1	–1.668209	2.525367	3.476713
6	–1.059376	–0.481829	–3.220926
1	–0.925721	–0.224055	–4.280260
1	–1.983950	–1.097980	–3.186814
1	1.696592	–2.069542	–1.658065
6	–1.887652	2.062037	–0.563255
1	0.633896	1.830434	2.977347
6	0.888192	–1.333093	–1.711214
6	–2.595550	1.306623	1.869929
6	–1.950522	0.694837	–1.246360
1	–1.767832	1.416394	–3.132504
8	1.607706	2.218592	–0.061931
1	–2.151703	2.861869	–1.264840
1	–0.894778	2.257171	–0.158210
1	–1.424509	–0.035349	–0.628270
1	–3.011978	0.370928	–1.352693
1	–2.398608	0.305527	1.483800
1	–3.554764	1.326161	2.396112
8	2.663634	0.746333	1.984030
8	3.494306	0.143237	0.986076
6	4.220677	0.975194	–0.359424
6	3.261339	0.606371	–1.369438
1	3.423794	–0.352985	–1.854371
1	2.874335	1.383662	–2.019487
1	4.280026	2.015937	–0.046547

1	5.161513	0.436133	–0.261026
1	–2.902930	3.142388	0.893472
1	–3.817702	1.943452	0.212905

TS1l

23	1.587657	0.901808	–0.015446
8	–0.040753	0.652893	1.303420
8	1.358530	–1.096922	–0.026112
7	–0.086263	0.778587	–1.680576
6	–1.617650	1.935782	2.497093
7	–2.901031	2.302274	0.328781
6	–0.184207	–1.700974	–1.723753
6	–0.342465	1.489779	2.237572
1	–0.876889	–2.451005	–2.092351
1	–1.801575	2.619504	3.319063
6	0.052488	–0.454677	–2.523713
1	1.069920	–0.415252	–2.926770
1	–0.648015	–0.394939	–3.371413
1	0.329809	–2.854881	–0.022644
6	–1.702491	2.319694	–0.593698
1	0.473055	1.870150	2.869777
6	0.494303	–1.917292	–0.571362
6	–2.736302	1.459045	1.681925
6	–1.478215	0.953404	–1.239342
1	0.215487	1.583524	–2.231445
8	1.246364	2.464428	0.018313
1	–1.899078	3.095612	–1.341787
1	–0.842768	2.621138	0.005180
1	–1.668089	0.149623	–0.527390
1	–2.171109	0.822109	–2.089755
1	–2.605557	0.436374	1.325549
1	–3.719208	1.569333	2.148861
8	2.575441	0.721596	–1.625201
8	3.442177	1.078204	–0.573558
6	3.821541	0.016469	0.924869
6	2.786891	0.441809	1.793439
1	2.969871	1.321389	2.406417
1	2.116930	–0.306096	2.199633
1	3.788722	–0.984290	0.506170
1	4.802059	0.483968	0.946907
1	–3.083460	3.266250	0.621682
1	–3.732130	1.977670	–0.180334

TS1m

23	1.283743	1.634443	0.408678
8	–0.361858	1.149811	–0.700717
8	–0.032765	1.622342	1.772885
7	0.996050	–1.087499	0.748072
6	–1.666474	0.721649	–2.594812
7	–1.347138	–1.766883	–2.098570
6	–0.204358	–0.538877	2.846059
6	–0.778845	1.486259	–1.871144
1	–0.789569	–1.083376	3.581808
1	–1.997079	1.043612	–3.576179
6	0.974446	–1.236336	2.226960
1	1.918867	–0.805300	2.577111
1	0.964640	–2.303039	2.512447
1	–1.429460	1.145589	3.136287
6	0.002268	–1.685198	–1.419008
1	–0.404519	2.422555	–2.306338
6	–0.564858	0.741159	2.597188
6	–2.269503	–0.460592	–1.972698
6	–0.119673	–1.771417	0.103662
1	1.887056	–1.440359	0.401530
8	1.409943	3.178796	0.135840

1	0.608316	–2.501424	–1.827249
1	0.429814	–0.730357	–1.715279
1	–1.024772	–1.265465	0.448921
1	–0.203309	–2.833844	0.407887
1	–2.401879	–0.356048	–0.894678
1	–3.203863	–0.786687	–2.437900
8	2.580031	1.449559	1.801535
8	3.046078	0.854969	0.594351
6	3.572315	1.658799	–0.886023
6	2.381588	1.452800	–1.652937
1	2.317451	0.518671	–2.211315
1	1.947425	2.310939	–2.152804
1	3.827209	2.669612	–0.577324
1	4.431344	0.998906	–0.993070
1	–1.858228	–2.589174	–1.754450
1	–1.195614	–1.901313	–3.102006

TS1n

23	1.454383	2.062236	0.109348
8	0.011746	0.987348	–0.739062
8	1.252024	0.758576	1.463386
7	0.649684	–2.447970	1.298089
6	–1.587345	0.456539	–2.379904
7	–1.548408	–1.987301	–1.725410
6	–0.194172	–0.600469	2.768371
6	–0.541560	1.198452	–1.900840
1	–1.097281	–0.592874	3.373322
1	–1.990788	0.685243	–3.361007
6	0.575836	–1.891150	2.673422
1	1.618374	–1.743755	2.982145
1	0.130610	–2.613572	3.380177
1	–0.481881	1.449594	2.317468
6	–0.275392	–2.159118	–0.913806
1	–0.124543	2.000019	–2.515835
6	0.154304	0.568222	2.185293
6	–2.243696	–0.576894	–1.560193
6	–0.586053	–2.507483	0.545629
1	1.117201	–3.350158	1.315405
8	0.561150	3.243271	0.648601
1	0.314378	–2.942886	–1.399400
1	0.255223	–1.208440	–0.954944
1	–1.253546	–1.743983	0.957717
1	–1.116514	–3.479793	0.601468
1	–2.179733	–0.371440	–0.490424
1	–3.283116	–0.764305	–1.844477
8	2.016978	2.167774	–1.652062
8	2.639462	3.240129	–0.956956
6	4.206690	2.550196	0.097021
6	3.656960	1.724434	1.054800
1	3.455476	2.098433	2.054059
1	3.686175	0.646120	0.940838
1	4.655686	2.144215	–0.804236
1	4.452588	3.585706	0.317345
1	–2.203353	–2.743943	–1.491287
1	–1.328788	–2.067762	–2.722220

TS1o

23	1.732114	0.180436	0.920460
8	0.818876	–0.292472	2.616605
8	2.957984	0.491755	–0.454045
7	–0.060406	0.094818	–2.121911
6	–1.564072	–0.014962	2.619930
7	–1.802035	0.460449	0.165248
6	2.330004	0.157619	–2.735787
6	–0.313709	0.074968	3.152214

1	2.639317	–0.301148	–3.671942
1	–2.400963	0.319267	3.227031
6	1.026384	0.907929	–2.711937
1	1.116833	1.811625	–2.097408
1	0.775217	1.229060	–3.738370
1	4.082372	–0.555742	–1.797814
6	–2.292838	0.020892	–1.185153
1	–0.232990	0.471374	4.173812
6	3.146943	–0.000587	–1.675997
6	–1.850929	–0.601768	1.287376
6	–1.407897	0.601976	–2.292063
8	0.725136	1.413245	0.661438
1	–2.240387	–1.071506	–1.200951
1	–3.342241	0.314458	–1.285670
1	–1.103618	–1.340577	0.986740
1	–2.850568	–1.043255	1.226298
8	1.290067	–1.420245	0.241148
8	2.395586	–2.039134	0.902713
6	3.421357	–1.206445	2.169841
6	3.399753	0.241118	2.206088
1	4.216175	0.757333	1.710067
1	3.056357	0.687487	3.135107
1	2.963830	–1.726123	3.003358
1	4.284980	–1.700743	1.736735
1	0.020752	–0.868198	–2.439129
1	–1.877911	0.383372	–3.269155
1	–1.379752	1.695956	–2.201774
1	–2.314970	1.282813	0.492974
1	–0.796903	0.769885	0.112455

TS1p

23	1.189236	1.513545	–0.838373
8	1.468347	–0.265623	–0.505118
8	–0.263186	1.050282	–1.926849
7	–0.455586	1.520395	0.782114
6	2.041960	–2.140021	0.806961
7	0.067011	–1.920105	2.276108
6	–2.173125	2.085678	–0.914135
6	2.375158	–1.056343	0.083703
1	–3.216042	2.348170	–1.065469
1	2.843101	–2.696514	1.285259
6	–1.553709	2.443987	0.407157
1	–1.128501	3.453669	0.389015
1	–2.325343	2.423753	1.191928
1	–2.079793	1.170656	–2.821063
6	–0.000612	–0.462767	2.241909
1	3.411598	–0.739273	–0.043751
6	–1.537554	1.436788	–1.910749
6	0.617569	–2.556254	1.060009
6	–0.924768	0.162425	1.170946
1	0.038276	1.935096	1.572322
1	–0.854626	–2.310718	2.466274
8	0.773120	3.290118	–1.112929
1	–0.316410	–0.119904	3.236105
1	1.017318	–0.090675	2.092195
1	–0.946278	–0.451975	0.270522
1	–1.954032	0.231807	1.552111
1	0.023189	–2.346215	0.155402
1	0.572711	–3.638239	1.229183
8	2.112088	2.160062	0.643917
8	3.084470	1.756691	–0.300591
6	3.332527	2.426857	–1.987825
6	2.359592	1.668830	–2.703733
1	2.648048	0.684016	–3.063895

1	1.662419	2.199571	–3.342693
1	3.188319	3.494416	–1.854756
1	4.364458	2.089740	–1.923670
1	0.186958	3.417295	–1.878732

TS1q

23	1.264545	1.399366	–0.874255
8	1.606162	–0.331198	–0.419673
8	–0.253973	0.959512	–1.865284
7	–0.380894	1.259853	0.848162
6	2.229224	–2.278199	0.746714
7	0.176124	–2.253662	2.141871
6	–2.122857	1.978356	–0.755430
6	2.534837	–1.133597	0.108813
1	–3.155107	2.292110	–0.881508
1	3.045690	–2.862163	1.162170
6	–1.492578	2.204285	0.587955
1	–1.086591	3.217935	0.668938
1	–2.255899	2.091635	1.374238
1	–2.064583	1.223546	–2.731785
6	0.034286	–0.803473	2.199099
1	3.566747	–0.802173	–0.029100
6	–1.513616	1.392644	–1.803858
6	0.816340	–2.776560	0.916395
6	–0.838607	–0.132667	1.111106
1	0.104158	1.592084	1.679576
1	–0.732660	–2.700185	2.254516
8	0.832263	3.184792	–0.824400
1	–0.362752	–0.546907	3.190351
1	1.043793	–0.383513	2.149292
1	–0.786821	–0.685366	0.172937
1	–1.890457	–0.116751	1.430245
1	0.250333	–2.539811	0.000904
1	0.825337	–3.868005	1.013179
8	2.089290	1.603284	–2.513700
8	3.116440	1.496141	–1.524957
6	3.419103	2.614694	–0.091671
6	2.480783	2.145593	0.868031
1	1.811225	2.883677	1.295557
1	2.801017	1.344621	1.530694
1	4.439620	2.240275	–0.091364
1	3.285983	3.595922	–0.533720
1	0.503838	3.442621	–1.703819

TS1r

23	1.510933	0.589267	0.150685
8	–0.010396	0.750442	1.209555
8	1.252399	–1.172028	–0.128239
7	–0.192398	0.643011	–1.639274
6	–1.612487	2.038257	2.363486
7	–3.061325	2.154806	0.337380
6	0.197827	–1.744905	–2.188225
6	–0.341445	1.649457	2.147974
1	–0.138770	–2.568502	–2.811006
1	–1.787431	2.786044	3.132057
6	0.017685	–0.347415	–2.714878
1	0.898840	–0.039387	–3.290997
1	–0.830229	–0.330609	–3.417115
1	0.865471	–3.083263	–0.679171
6	–1.995140	2.075698	–0.656047
1	0.482820	2.046333	2.746922
6	0.764095	–2.048765	–1.007953
6	–2.796328	1.470386	1.619750
6	–1.589588	0.662796	–1.136287
1	0.044340	1.569943	–1.989902

1	–3.928602	1.788693	–0.052609
8	1.466961	2.383377	–0.267559
1	–2.306844	2.675035	–1.522308
1	–1.116877	2.571813	–0.237933
1	–1.660229	–0.055498	–0.319178
1	–2.273197	0.331326	–1.933690
1	–2.647862	0.383890	1.503239
1	–3.697945	1.600663	2.228863
8	2.446706	0.867900	1.703207
8	3.351392	0.303754	0.745659
6	3.899887	1.095359	–0.771292
6	2.858230	0.719878	–1.671917
1	2.971865	–0.234604	–2.180281
1	2.394096	1.514549	–2.244707
1	4.001968	2.137205	–0.483700
1	4.819545	0.516525	–0.719983
1	1.133401	2.886791	0.497296

TS1s

23	1.510201	0.757613	0.263846
8	0.045355	1.072762	1.334407
8	1.128181	–1.049317	0.154600
7	–0.034059	0.827182	–1.503568
6	–1.610090	2.419103	2.323290
7	–3.022297	2.327081	0.289156
6	0.338237	–1.571035	–2.034327
6	–0.321257	2.073036	2.142980
1	0.057682	–2.376909	–2.706107
1	–1.822454	3.260442	2.976899
6	0.258858	–0.167301	–2.563044
1	1.206511	0.122636	–3.032510
1	–0.517744	–0.110257	–3.340906
1	0.765393	–2.946220	–0.478869
6	–1.921306	2.247829	–0.667207
1	0.488329	2.605460	2.645326
6	0.745396	–1.902176	–0.796215
6	–2.755594	1.738636	1.619107
6	–1.456504	0.829104	–1.071057
1	0.206491	1.753029	–1.855371
1	–3.857013	1.891082	–0.100384
8	1.548152	2.572543	0.052045
1	–2.226670	2.796842	–1.568291
1	–1.074296	2.792036	–0.241605
1	–1.549969	0.139672	–0.231831
1	–2.082133	0.445400	–1.890889
1	–2.554331	0.655352	1.578332
1	–3.673701	1.868009	2.203714
8	2.612691	0.515622	–1.293909
8	3.412318	0.845242	–0.179017
6	3.671822	–0.227498	1.348488
6	2.581006	0.221087	2.129621
1	2.728503	1.094580	2.760738
1	1.858338	–0.504267	2.485853
1	3.661140	–1.226481	0.922889
1	4.655546	0.223716	1.442579
1	2.359637	2.835266	–0.417543

TS1t

23	1.092299	1.431771	0.432744
8	–0.389832	1.301696	–0.713728
8	–0.198849	1.204760	1.727182
7	1.063013	–0.904658	0.648785
6	–1.571432	0.566614	–2.631944
7	–1.485964	–1.835778	–2.005227
6	0.489501	–0.656322	3.057709

6	–0.709719	1.389617	–2.008370
1	0.387705	–1.153221	4.017386
1	–1.742463	0.725183	–3.693007
6	1.410007	–1.281695	2.047005
1	2.448209	–0.976824	2.219901
1	1.374669	–2.377961	2.142011
1	–0.853110	0.889536	3.621126
6	–0.186855	–1.784868	–1.343416
1	–0.233430	2.206529	–2.564414
6	–0.191306	0.482256	2.855960
6	–2.267554	–0.580068	–1.947463
6	–0.202891	–1.535137	0.180961
1	1.826005	–1.229017	0.055686
1	–2.047316	–2.591802	–1.615089
8	1.195362	3.188602	0.028454
1	0.334098	–2.729292	–1.552828
1	0.387363	–0.992537	–1.830988
1	–1.016783	–0.863497	0.451661
1	–0.356328	–2.484274	0.715134
1	–2.513317	–0.275295	–0.916826
1	–3.217390	–0.786552	–2.453932
8	2.248388	1.812300	1.862967
8	2.943450	1.073509	0.880071
6	3.472935	1.644428	–0.766547
6	2.365590	1.148454	–1.506510
1	2.428408	0.132163	–1.889270
1	1.850214	1.841054	–2.160301
1	3.587278	2.715785	–0.630276
1	4.391456	1.070092	–0.671161
1	0.507199	3.445459	–0.607923

TS1u

23	1.096039	1.371423	0.404760
8	–0.309089	1.180292	–0.743695
8	0.240657	1.278734	1.988931
7	0.881036	–1.111488	0.798135
6	–1.309997	0.303378	–2.700829
7	–1.688397	–1.972539	–1.842030
6	0.487482	–0.759346	3.211369
6	–0.405889	1.080388	–2.080762
1	0.281098	–1.255217	4.155066
1	–1.303401	0.289058	–3.787222
6	1.249726	–1.522040	2.166990
1	2.330938	–1.371446	2.282950
1	1.071981	–2.601305	2.301682
1	–0.509051	1.003010	3.848256
6	–0.427457	–2.049944	–1.113503
1	0.304828	1.692278	–2.639527
6	0.052156	0.501566	3.059094
6	–2.255195	–0.612905	–1.972593
6	–0.448607	–1.622414	0.372887
1	1.591977	–1.467077	0.160380
1	–2.382759	–2.583732	–1.415322
8	1.003807	3.175984	0.590784
1	–0.060966	–3.082309	–1.187178
1	0.293057	–1.422534	–1.648215
1	–1.184676	–0.833583	0.536794
1	–0.735546	–2.476643	1.004395
1	–2.517864	–0.156525	–1.004615
1	–3.186331	–0.716387	–2.541816
8	2.162692	0.482177	–0.804692
8	2.559511	1.806580	–0.944196
6	3.766821	1.997045	0.508561
6	3.094090	1.389006	1.584162

1	2.737086	2.024580	2.388603
1	3.396697	0.387350	1.872151
1	4.550596	1.471869	–0.028547
1	3.820738	3.081240	0.446835
1	1.404474	3.649974	–0.156674

TS1v

23	2.142554	–0.074283	0.446733
8	0.593224	0.003206	1.403747
8	3.420441	–0.248305	–0.886329
7	0.798401	0.451266	–1.450739
6	–1.436537	0.983108	2.102209
7	–2.607597	0.064788	0.092213
6	2.819468	1.100018	–2.756180
6	–0.095220	0.978563	2.008891
1	3.166341	1.507217	–3.701464
1	–1.897181	1.833813	2.597410
6	1.439633	1.478046	–2.311250
1	1.450191	2.407326	–1.731356
1	0.804698	1.652245	–3.193844
1	4.649176	0.068429	–2.468518
6	–1.495081	–0.351974	–0.769681
1	0.512501	1.791163	2.409978
6	3.662580	0.310160	–2.068309
6	–2.335450	–0.090539	1.537176
6	–0.604194	0.842929	–1.153750
1	–3.423066	–0.500098	–0.130420
8	2.232668	1.765636	0.409373
1	–0.879904	–1.125401	–0.288771
1	–1.913881	–0.791882	–1.684127
1	–1.895962	–1.080179	1.757154
1	–3.303456	–0.044380	2.047878
8	3.470645	–0.035757	1.728253
8	2.840456	–1.322053	1.784084
6	2.883192	–2.562735	0.556011
6	1.733909	–2.200851	–0.231915
1	0.780470	–2.606018	0.098610
1	1.874297	–2.166112	–1.307949
1	3.871622	–2.475088	0.114916
1	2.800695	–3.339788	1.313499
1	0.789657	–0.421540	–1.979532
1	–1.037950	1.346558	–2.030114
1	–0.585017	1.572727	–0.346386
1	2.897164	2.088336	1.041376

TS1w

23	–0.602840	2.310384	–0.638768
8	0.006092	0.629665	–0.129923
8	–2.050203	1.718521	–1.568103
7	–2.203895	2.217401	1.065340
6	0.517083	–1.226652	1.241158
7	–1.637526	–1.248542	2.456396
6	–3.892826	2.908674	–0.627251
6	0.865619	–0.105380	0.582725
1	–4.899196	3.277652	–0.801858
1	1.285875	–1.735353	1.816457
6	–3.299285	3.158581	0.731233
1	–2.886929	4.172773	0.788005
1	–4.089793	3.083437	1.494631
1	–3.781063	2.079305	–2.579873
6	–1.803579	0.198576	2.490931
1	1.886621	0.277584	0.600044
6	–3.279624	2.259985	–1.628610
6	–0.888515	–1.762450	1.286531
6	–2.655403	0.830667	1.363187

1	–1.724498	2.581534	1.888331
1	–2.545265	–1.709661	2.501210
8	–0.787225	3.910887	–0.670655
1	–2.235843	0.467146	3.464324
1	–0.798250	0.631487	2.460497
1	–2.571581	0.250414	0.442989
1	–3.716185	0.847987	1.652163
1	–1.384854	–1.539927	0.327829
1	–0.867435	–2.853661	1.390817
8	0.729552	2.919984	1.012637
8	1.759131	2.709249	0.005368
6	1.628227	2.960063	–1.865810
6	0.526009	2.326174	–2.488404
1	0.633600	1.290494	–2.799670
1	–0.124037	2.943299	–3.101177
1	1.672720	4.044037	–1.870420
1	2.590715	2.456426	–1.810876
1	0.601287	3.890321	0.980072

TS1x

23	0.782638	1.281243	–1.146271
8	1.408784	–0.516602	–0.908581
8	–0.814154	0.627988	–1.789042
7	–0.411260	1.276341	0.729055
6	1.964257	–2.529216	0.215696
7	0.267016	–2.233986	2.017489
6	–2.437712	1.887596	–0.594416
6	2.270815	–1.455197	–0.540446
1	–3.455555	2.264235	–0.578543
1	2.772108	–3.204617	0.484182
6	–1.561103	2.217079	0.580671
1	–1.136420	3.223238	0.484785
1	–2.153243	2.191999	1.507850
1	–2.710154	0.923145	–2.471498
6	0.264144	–0.776114	2.032403
1	3.299740	–1.320369	–0.895679
6	–2.034005	1.165220	–1.651187
6	0.573563	–2.841730	0.701801
6	–0.823127	–0.091377	1.173173
1	0.203243	1.671749	1.439560
1	–0.631274	–2.588154	2.344656
8	0.530365	2.835301	–1.382751
1	0.166094	–0.446086	3.075844
1	1.250155	–0.455943	1.688166
1	–1.025861	–0.673539	0.275256
1	–1.759361	–0.010709	1.743154
1	–0.146081	–2.548933	–0.080465
1	0.470146	–3.924638	0.837536
8	2.428588	2.422834	–3.287524
8	2.367396	1.296697	–2.374644
6	3.334621	1.771957	–0.925467
6	2.469460	1.813566	0.216750
1	2.246444	2.800399	0.613933
1	2.616944	1.029920	0.954463
1	4.036530	0.947557	–1.014748
1	3.669767	2.703681	–1.371115
1	2.916433	1.993197	–4.014666

TS1y

23	1.420542	0.244852	0.945732
8	0.177733	0.707947	2.164015
8	1.089269	–1.571893	0.648914
7	–0.278450	0.286698	–0.731123
6	–1.603120	2.079299	2.882898
7	–3.293756	1.342704	1.246922

6	0.290582	–1.979421	–1.550882
6	–0.297553	1.877328	2.648624
1	0.053367	–2.724617	–2.303038
1	–1.905494	3.052248	3.260150
6	0.129081	–0.528120	–1.899274
1	1.075688	–0.105430	–2.264693
1	–0.610951	–0.413952	–2.706715
1	0.864812	–3.442948	–0.122498
6	–2.383270	1.347227	0.108859
1	0.457624	2.638216	2.845330
6	0.751391	–2.382373	–0.356535
6	–2.668179	1.066231	2.557591
6	–1.653832	0.021453	–0.238137
1	–0.190239	1.268625	–0.986683
1	–4.054418	0.683207	1.092949
8	1.743134	1.631860	0.237740
1	–2.948446	1.688604	–0.767518
1	–1.630651	2.117100	0.313128
1	–1.581341	–0.623117	0.641018
1	–2.214482	–0.534889	–1.002107
1	–2.229573	0.057618	2.624842
1	–3.471170	1.118228	3.302476
8	3.532000	–0.498970	–0.674104
8	3.377611	–0.173961	0.758103
6	3.536139	–1.168386	2.332057
6	2.530514	–0.455036	2.991789
1	2.788374	0.416000	3.587690
1	1.613748	–0.968995	3.257698
1	3.334257	–2.169871	1.966460
1	4.584906	–0.913600	2.445209
1	3.938412	0.336117	–0.972406

TSz

23	0.984808	1.798213	0.520019
8	–0.407356	1.394321	–0.557615
8	0.172274	1.733718	2.129391
7	1.036357	–0.745867	0.840051
6	–1.720753	0.751783	–2.402603
7	–1.421833	–1.670766	–1.898058
6	0.207328	–0.424536	3.154454
6	–0.870083	1.600874	–1.800846
1	–0.205281	–1.028939	3.956626
1	–2.025009	0.986074	–3.418982
6	1.274016	–1.024854	2.278191
1	2.252598	–0.597596	2.524649
1	1.324405	–2.110131	2.456110
1	–1.010087	1.230284	3.698162
6	–0.126013	–1.587349	–1.227152
1	–0.514025	2.510146	–2.289134
6	–0.248455	0.831058	3.028009
6	–2.287390	–0.484200	–1.744944
6	–0.151336	–1.461310	0.312890
1	1.860599	–1.071667	0.334191
1	–1.931426	–2.490520	–1.571400
8	1.201315	3.355344	0.300387
1	0.453461	–2.475390	–1.513483
1	0.391367	–0.724121	–1.648047
1	–1.030983	–0.900275	0.631773
1	–0.222617	–2.464386	0.766187
1	–2.512533	–0.247292	–0.691753
1	–3.241404	–0.734348	–2.222023
8	3.166025	2.557377	2.207042
8	2.794635	1.488643	1.307422
6	3.487537	1.571642	–0.562611

6	2.364736	1.341068	–1.347254
1	2.175149	0.342125	–1.724960
1	1.953033	2.158353	–1.930731
1	3.879432	2.575238	–0.427465
1	4.171159	0.770137	–0.303255
1	2.595922	3.293067	1.899512

TS1aa

23	0.090491	1.098993	1.256549
8	–1.536053	0.984462	2.165994
8	1.545725	0.599384	0.242426
7	–0.939107	1.002268	–0.769373
6	–3.751934	1.801881	2.313980
7	–4.486604	0.453751	0.336563
6	1.217451	1.693735	–1.846597
6	–2.427033	1.956859	2.464059
1	1.694632	2.041253	–2.758100
1	–4.377635	2.662656	2.535711
6	–0.266182	1.899999	–1.743907
1	–0.501742	2.926312	–1.434215
1	–0.724981	1.756213	–2.734249
1	3.051824	0.943921	–1.086710
6	–3.229834	0.033646	–0.299441
1	–1.987391	2.899731	2.790000
6	1.985223	1.099236	–0.920454
6	–4.426559	0.546710	1.809981
6	–2.406791	1.253425	–0.755475
1	–5.210721	–0.219000	0.100057
8	0.110121	2.682220	1.153673
1	–2.628275	–0.607220	0.360000
1	–3.479760	–0.571449	–1.179424
1	–3.931928	–0.338396	2.248803
1	–5.461422	0.540884	2.169058
8	–1.176638	–1.609642	2.059196
8	–0.079187	–0.989499	1.375840
6	1.269400	–0.502734	2.941603
6	1.365863	0.876491	3.091662
1	2.259609	1.396423	2.759351
1	0.767395	1.376597	3.849284
1	0.583565	–1.094571	3.537522
1	2.033848	–1.053324	2.406125
1	–1.692045	–0.812989	2.320781
1	–0.754422	0.029633	–1.027765
1	–2.731254	1.555518	–1.760895
1	–2.598249	2.098162	–0.093542

TS1ab

23	–0.378643	–2.316888	0.305943
8	0.675159	–0.925953	–0.049397
8	–1.709007	–2.126767	–0.861899
7	–3.113898	0.117428	0.732649
6	–4.036019	–1.940279	–0.289139
1	–5.031252	–2.233034	–0.617869
6	–3.906264	–1.093609	0.958643
1	–4.913770	–0.862965	1.342804
1	–3.405042	–1.682471	1.736074
1	–3.203766	–2.941935	–1.967054
6	–3.019972	–2.369572	–1.057660
8	–0.993458	–2.114817	1.743385
8	–0.669435	–4.374187	–0.121062
8	0.371636	–3.919811	–1.046938
6	1.952169	–3.893046	0.120092
6	1.539161	–3.340059	1.328891
1	1.908069	–2.364181	1.624556
1	1.244635	–3.985500	2.152413

1	2.057452	–4.967934	–0.008666
1	2.523111	–3.300872	–0.590100
1	–0.217251	–5.004360	0.473972
6	–3.868123	1.341176	0.501616
6	–2.954772	2.446569	–0.064695
7	–1.630729	2.436748	0.577928
6	–0.619786	1.730366	–0.230117
6	0.600324	1.375568	0.570681
6	1.143542	0.154902	0.633627
1	–2.463523	0.273759	1.496004
1	–4.365674	1.706466	1.421221
1	–4.662574	1.133815	–0.226367
1	–3.433171	3.418801	0.105848
1	–2.863952	2.322006	–1.156162
1	–1.321246	3.391344	0.741458
1	–0.321544	2.323782	–1.118007
1	–1.082826	0.814977	–0.599617
1	1.099146	2.163133	1.132883
1	2.048274	–0.047878	1.208304

TS2

V	1.187057	1.403628	–0.272056
O	–0.638752	1.690630	–0.066013
O	1.218855	–1.219960	–3.403390
N	1.401356	–0.704048	0.299300
C	–1.342744	2.437718	2.108747
N	0.861785	1.305412	2.246776
C	1.749626	–2.519859	–1.416400
C	–1.525756	2.189268	0.797776
H	1.678422	–3.526507	–1.013436
H	–2.195304	2.824234	2.661374
C	2.397894	–1.468973	–0.569216
H	3.125280	–1.926724	0.108193
H	2.931764	–0.731274	–1.169451
H	0.878812	–3.185818	–3.221572
C	0.622895	–0.100822	2.565495
H	–0.417569	–0.336304	2.308971
H	0.750875	–0.325499	3.638045
H	–2.506219	2.371091	0.350853
C	1.275387	–2.336723	–2.667120
C	–0.065879	2.253277	2.882184
H	0.459958	3.213131	2.975942
H	–0.302106	1.940457	3.914071
C	1.582918	–0.955046	1.747911
H	2.616973	–0.690293	1.993865
H	1.444045	–2.020661	1.977221
H	0.476998	–1.053126	0.033000
H	1.823643	1.552737	2.469874
O	1.301980	0.986411	–1.825292
H	1.370549	–0.403056	–2.864072
O	2.702451	1.831849	0.275880
O	3.325954	3.750519	0.439946
C	2.107677	4.246929	0.366850
C	1.207289	3.731145	–0.700956
H	1.658943	3.619367	–1.685700
H	0.195244	4.135476	–0.720331
H	1.574383	4.415546	1.324272
H	2.239497	5.263399	–0.115922

TS3a

V	–0.062353	1.208289	0.520795
O	–1.574589	1.400234	–0.563440
O	1.667788	–1.091556	–2.320353
N	–0.274443	–0.960796	0.853701
C	–3.616234	1.818261	0.636599

N	–1.893784	0.943341	2.168795
C	0.929872	–2.636024	–0.590276
C	–2.887893	1.623591	–0.479697
H	0.605630	–3.663652	–0.450135
H	–4.682492	1.989117	0.516976
C	1.004559	–1.756510	0.621006
H	1.173786	–2.367193	1.513634
H	1.823325	–1.038191	0.555032
H	1.213815	–3.014814	–2.647536
C	–2.215393	–0.477157	2.290824
H	–2.920578	–0.729784	1.489437
H	–2.705838	–0.727157	3.246205
H	–3.384771	1.629204	–1.453584
C	1.256634	–2.275875	–1.848992
C	–3.054504	1.836550	2.032415
H	–2.707008	2.843940	2.297879
H	–3.844387	1.576760	2.757137
C	–0.934554	–1.287959	2.138926
H	–0.228711	–1.035371	2.937580
H	–1.149620	–2.363714	2.203594
O	0.752868	1.459088	2.008241
H	–0.909600	–1.221527	0.095478
H	–1.302766	1.242576	2.941752
O	1.050142	0.930811	–0.608641
O	0.140020	2.961096	1.169612
H	1.539674	–0.360027	–1.665324
C	0.146432	4.418940	–0.270654
C	–1.031954	4.589535	0.389462
H	–1.948977	4.124552	0.044878
H	–1.092187	5.220499	1.270174
H	1.049221	4.932528	0.040327
H	0.205339	3.834442	–1.182709

TS3a'

V	2.170949	1.149910	1.455583
O	0.897930	1.181697	0.099149
O	4.014665	–1.037036	–1.165526
N	2.256876	–1.056208	1.672490
C	–1.412179	1.143477	0.831276
N	0.146330	0.490503	2.649355
C	3.899205	–2.670627	0.662043
C	–0.415690	1.144336	–0.173664
C	3.959887	–4.030276	1.003926
C	–2.754833	1.065975	0.446048
C	3.659900	–1.628326	1.724236
H	3.802084	–2.063822	2.716504
H	4.353079	–0.789957	1.635056
C	4.272207	–3.308296	–1.656961
C	–0.005201	–0.963803	2.637561
H	–0.484619	–1.246123	1.692615
H	–0.648066	–1.337885	3.450738
C	–0.800730	1.079425	–1.526275
C	4.061527	–2.306548	–0.695844
C	–1.049493	1.266427	2.293964
H	–0.813927	2.308732	2.540050
H	–1.917632	0.977012	2.908487
C	1.379439	–1.593563	2.739208
H	1.842459	–1.332277	3.696783
H	1.314120	–2.688313	2.678745
O	2.625541	1.449209	3.083316
H	1.855514	–1.339052	0.774607
H	0.515127	0.807210	3.544241
O	3.515794	1.056845	0.573162
O	2.001361	2.888832	2.148337

H	3.910539	–0.338585	–0.476997
C	2.165974	4.402320	0.811370
C	0.829834	4.372662	1.073600
H	0.144195	3.803803	0.455873
H	0.408841	4.937886	1.898624
H	2.840819	5.027739	1.384817
H	2.587412	3.888170	–0.046082
C	4.324759	–4.647437	–1.289046
C	4.169908	–5.021079	0.049329
H	4.396522	–3.000349	–2.690499
H	3.849992	–4.305962	2.051155
H	4.217599	–6.065376	0.343017
H	4.492323	–5.404291	–2.051000
C	–2.143948	1.015665	–1.883032
C	–3.132004	1.008417	–0.895221
H	–0.015080	1.077363	–2.276005
H	–2.419350	0.966045	–2.933219
H	–4.182654	0.952242	–1.164692
H	–3.519534	1.054169	1.220699

TS3b

V	0.946945	1.568224	–0.497183
O	–0.617791	1.149186	–1.361063
O	2.634085	–1.036651	–3.054474
N	1.170684	–0.560067	0.273291
C	–2.461257	1.840800	0.018475
N	–0.463919	1.368109	1.398643
C	2.360997	–2.354575	–1.028666
C	–1.916288	1.396709	–1.127066
H	2.197128	–3.372091	–0.685583
H	–3.537653	1.985829	0.035797
C	2.482333	–1.270114	–0.000026
H	2.837063	–1.689628	0.947193
H	3.199672	–0.510174	–0.317164
H	2.393972	–3.025779	–3.031664
C	–0.683046	–0.028918	1.784786
H	–1.450355	–0.439232	1.118607
H	–1.057848	–0.128041	2.815634
H	–2.548307	1.180513	–1.989604
C	2.453645	–2.169394	–2.362128
C	–1.699374	2.169358	1.274128
H	–1.391511	3.220853	1.276312
H	–2.347691	2.018153	2.152539
C	0.622920	–0.798444	1.625146
H	1.360056	–0.441520	2.350297
H	0.461748	–1.869909	1.811826
O	0.862702	3.241059	–0.231423
H	0.505127	–0.951480	–0.397934
H	0.176689	1.824640	2.047014
O	2.057415	1.214531	–1.615039
O	2.031686	2.468301	0.870730
H	2.506810	–0.223941	–2.501744
C	3.523090	1.510021	2.312865
C	3.879693	2.200620	1.187676
H	4.166392	1.689439	0.274693
H	4.141120	3.251405	1.240134
H	3.349869	2.018197	3.255755
H	3.409718	0.431663	2.301330

TS4a

V	1.602403	0.751713	–0.317156
O	2.641699	0.629618	1.390396
O	–0.065822	0.273241	–1.178724
N	0.124751	0.459683	1.398624
C	3.797592	–1.490465	1.197717

N	1.602045	–1.578998	0.074649
C	–1.722188	1.438640	0.118630
C	3.595349	–0.251483	1.692465
H	–2.714918	1.877642	0.104698
H	4.632353	–2.060868	1.595011
C	–0.958312	1.461891	1.409867
H	–0.490852	2.437093	1.592066
H	–1.637429	1.262571	2.255509
H	–1.882107	0.835718	–1.897877
C	0.814929	–1.901465	1.282798
H	1.500029	–1.829070	2.131645
H	0.436400	–2.934389	1.256059
H	4.263663	0.109564	2.481343
C	–1.250064	0.870004	–1.004588
C	2.974190	–2.144857	0.123588
H	3.414197	–1.988694	–0.869217
H	2.931206	–3.233838	0.295132
C	–0.348842	–0.934511	1.466634
H	–1.096306	–1.066714	0.682547
H	–0.841233	–1.131740	2.431534
O	2.228931	0.671887	–2.255347
H	0.794655	0.642707	2.145542
H	1.115470	–1.922568	–0.752226
O	1.407585	2.307185	–0.187041
O	3.424908	0.485018	–0.973442
C	0.974978	0.294245	–3.865447
C	1.041257	1.629001	–3.602974
H	1.677036	–0.177355	–4.545351
H	0.202690	–0.323139	–3.426121
H	0.313098	2.121053	–2.970401
H	1.781746	2.259839	–4.083203
H	3.840623	1.365159	–1.009146

TS4b

V	0.511223	0.538248	–0.162057
O	1.524361	0.064930	1.393133
O	–1.163899	0.506228	–1.148924
N	–1.080626	0.452063	1.528768
C	2.123054	–2.264116	1.103721
N	–0.089664	–1.781252	0.149597
C	–2.629807	1.844732	0.220468
C	2.253249	–1.033526	1.631679
H	–3.525554	2.458686	0.209363
H	2.817917	–3.028627	1.439516
C	–1.935447	1.657793	1.538977
H	–1.282948	2.507298	1.772838
H	–2.677587	1.580318	2.350837
H	–2.809419	1.463492	–1.845535
C	–0.911615	–1.988690	1.347269
H	–0.228351	–2.079050	2.197448
H	–1.493250	–2.922898	1.296058
H	3.029121	–0.861344	2.383560
C	–2.220515	1.298389	–0.938806
C	1.091224	–2.666152	0.085401
H	1.486973	–2.593713	–0.933364
H	0.798510	–3.717932	0.246058
C	–1.847665	–0.805390	1.546790
H	–2.580938	–0.748816	0.738499
H	–2.403311	–0.918227	2.490809
O	1.004850	–0.398649	–1.860296
H	–0.433854	0.474818	2.316181
H	–0.651889	–1.883316	–0.693025
O	0.426073	2.103884	0.047226
O	2.240521	0.660807	–1.148329

C	3.269965	2.384858	–0.927526
C	3.803412	1.550368	0.005882
H	3.403433	1.510045	1.011048
H	4.640389	0.901402	–0.229076
H	3.694626	2.458339	–1.923494
H	2.464927	3.066829	–0.678836
H	0.699222	0.182430	–2.579000

TS5a

V	0.462723	0.605979	0.552478
O	–1.300491	0.220937	–0.265968
O	2.352618	0.724951	0.304759
N	0.782628	–0.006836	–1.737435
C	–1.917738	–1.768008	0.934107
N	0.526332	–1.622941	0.531980
C	2.826106	1.321510	–1.982721
C	–2.179554	–0.661983	0.209964
H	3.588734	1.716764	–2.647125
H	–2.751059	–2.400681	1.224445
C	1.488474	0.982972	–2.565177
H	0.846101	1.871828	–2.604386
H	1.602350	0.612205	–3.597903
H	4.133958	1.441387	–0.335986
C	0.554412	–2.241482	–0.812926
H	–0.485413	–2.344955	–1.135105
H	0.989915	–3.249548	–0.768120
H	–3.210730	–0.444247	–0.082249
C	3.128481	1.180222	–0.679741
C	–0.550736	–2.180576	1.401386
H	–0.339052	–1.817134	2.412963
H	–0.468663	–3.279052	1.415593
C	1.324997	–1.366559	–1.793606
H	2.385239	–1.315703	–1.527811
H	1.260546	–1.800001	–2.805212
O	1.171332	0.259594	2.449320
H	–0.211553	–0.010430	–1.959434
H	1.419616	–1.764811	1.001883
O	0.338466	2.286674	–0.089320
O	–0.440408	0.722241	1.956376
C	3.053842	–0.685427	2.965816
C	2.885552	0.655061	3.175786
H	–0.543049	2.646123	0.113147
H	2.793947	–1.415988	3.724731
H	3.467953	–1.047125	2.030664
H	3.240580	1.379051	2.454417
H	2.578333	1.034002	4.144649

TS5b

V	1.122459	0.367084	–0.563260
O	1.959458	–0.136384	1.044209
O	–0.333049	0.377601	–1.789448
N	–0.741810	0.249958	0.913474
C	2.664863	–2.407123	0.651246
N	0.510042	–1.875570	–0.420186
C	–2.148043	1.508324	–0.660670
C	2.727969	–1.213867	1.266797
H	–3.093497	2.016250	–0.829420
H	3.362453	–3.176610	0.968821
C	–1.678629	1.384079	0.760505
H	–1.146270	2.284914	1.080070
H	–2.542113	1.249064	1.433507
H	–1.945631	1.151737	–2.728348
C	–0.395309	–2.161885	0.706004
H	0.222471	–2.229684	1.605890
H	–0.897838	–3.132555	0.576899

H	3.448632	–1.057857	2.073138
C	–1.495848	1.034172	–1.738770
C	1.690231	–2.770389	–0.435436
H	2.148909	–2.690412	–1.425497
H	1.361420	–3.814908	–0.308992
C	–1.420924	–1.051835	0.843233
H	–2.076591	–1.025019	–0.032174
H	–2.057088	–1.230735	1.724157
O	2.098469	–0.327779	–1.734163
H	–0.234546	0.332754	1.793502
H	0.006347	–1.945320	–1.303816
O	0.809835	2.115739	–0.162151
O	2.901728	1.136954	–1.230270
C	3.871165	3.052161	–0.740701
C	4.164115	1.900358	–0.060203
H	3.719476	1.694415	0.907116
H	5.014009	1.288622	–0.341501
H	4.374125	3.308908	–1.666471
H	3.129072	3.752810	–0.369936
H	1.404089	2.659689	–0.703158

TS6

V	–2.856505	0.531486	–0.016028
O	–4.301132	–0.715338	–0.091506
O	–1.539192	–1.123059	–3.401398
N	–1.325953	–1.036097	0.308621
C	–5.192374	–1.085062	2.109018
N	–2.970519	–0.008084	2.321374
C	–0.193597	–2.142794	–1.650795
C	–5.111068	–1.303454	0.779239
H	0.330417	–3.062771	–1.406200
H	–5.920705	–1.654927	2.677596
C	–0.146030	–1.026242	–0.651237
H	0.767161	–1.108318	–0.051791
H	–0.136448	–0.049201	–1.138751
H	–0.742091	–2.958412	–3.519361
C	–2.158338	–1.194271	2.611612
H	–2.770479	–2.072705	2.379361
H	–1.870575	–1.263278	3.672365
H	–5.766809	–2.051620	0.322248
C	–0.813615	–2.103792	–2.848432
C	–4.360664	–0.070781	2.843018
H	–4.764490	0.945618	2.732548
H	–4.355404	–0.294686	3.921889
C	–0.919126	–1.166378	1.727629
H	–0.291666	–0.300845	1.972270
H	–0.311889	–2.069583	1.883751
H	–1.880885	–1.860510	0.066141
H	–2.516543	0.823527	2.698131
O	–2.372362	0.674152	–1.547936
H	–1.780263	–0.419457	–2.745202
O	–2.377901	2.200893	0.824162
O	–3.757134	2.261866	0.526424
C	–5.015604	2.778924	–1.711300
C	–4.072565	3.407093	–0.891367
H	–4.386062	4.243115	–0.273557
H	–3.037279	3.429768	–1.215598
H	–6.080688	2.890064	–1.531443
H	–4.700894	2.067136	–2.466852

TS7

V	–1.517302	0.590937	0.526073
O	–3.145236	–0.375681	0.313821
O	–1.203083	0.025827	–3.345863
N	–0.143049	–1.086578	0.027252

C	–3.562194	–1.859736	2.140844
N	–1.351901	–0.819441	2.507364
C	0.345211	–1.587375	–2.388867
C	–3.725729	–1.432407	0.871678
H	0.768261	–2.571605	–2.571811
H	–4.118961	–2.728680	2.477076
C	0.786961	–0.860830	–1.152843
H	1.783598	–1.210574	–0.861192
H	0.844414	0.217519	–1.313023
H	–0.737234	–1.729526	–4.195206
C	–0.479877	–1.974367	2.283500
H	–1.109206	–2.793928	1.917237
H	0.015273	–2.324029	3.202782
H	–4.407081	–1.966579	0.201178
C	–0.523204	–1.127078	–3.313522
C	–2.668780	–1.140951	3.112913
H	–3.098935	–0.174200	3.411856
H	–2.543171	–1.732859	4.033152
C	0.554023	–1.613418	1.224213
H	1.231576	–0.831551	1.587371
H	1.164993	–2.491721	0.970162
H	–0.814815	–1.795731	–0.276433
H	–0.879114	–0.117854	3.075943
O	–1.210741	1.223334	–0.934343
H	–1.159680	0.506763	–2.476619
O	–0.724736	1.709544	1.827948
O	–2.364121	2.305511	1.430525
C	–3.712515	3.284137	0.389505
C	–2.310970	3.557406	0.738704
H	–4.511539	3.541649	1.075155
H	–3.937387	2.658334	–0.466238
H	–1.599364	3.536101	–0.087283
H	–2.132855	4.380037	1.433924

TS8

V	0.961979	–0.034504	–0.094406
O	1.726604	–0.761478	1.444090
O	–0.193203	0.105157	–1.594835
N	–0.980852	–0.287040	0.972573
C	2.511270	–2.950213	0.856077
N	0.562152	–2.239645	–0.489193
C	–2.158468	1.139861	–0.675015
C	2.447210	–1.869213	1.654163
H	–3.071987	1.672729	–0.921553
H	3.149344	–3.773544	1.162589
C	–1.895186	0.870002	0.781204
H	–1.406827	1.726509	1.260795
H	–2.844976	0.687414	1.309114
H	–1.635491	0.999522	–2.716074
C	–0.506695	–2.666901	0.439920
H	–0.031200	–2.865162	1.404349
H	–0.976317	–3.605366	0.107795
H	3.008250	–1.845404	2.590553
C	–1.347306	0.776323	–1.685597
C	1.769395	–3.098745	–0.444386
H	2.396114	–2.797111	–1.293713
H	1.493468	–4.154120	–0.602012
C	–1.577268	–1.585886	0.583245
H	–2.089539	–1.426307	–0.369098
H	–2.333547	–1.910834	1.312999
O	2.497804	–0.047504	–1.134628
H	–0.690073	–0.323081	1.949441
H	0.196969	–2.207738	–1.440378
O	1.018312	1.712492	0.326306

O	3.249198	1.112854	–1.204870
C	2.207338	2.664986	–3.048946
C	3.239847	1.748745	–3.003007
H	4.267326	2.098402	–2.959853
H	3.103526	0.756632	–3.420495
H	2.367876	3.709297	–2.796805
H	1.184011	2.344662	–3.216081
H	1.802693	2.095620	–0.120862

TS9

V	0.327765	0.737960	–0.090580
O	1.337485	0.504615	1.495833
O	–1.133736	0.549414	–1.312469
N	–1.430147	0.455087	1.390288
C	2.262262	–1.706473	1.216607
N	0.090166	–1.497400	0.050275
C	–2.978169	1.592197	–0.177856
C	2.180501	–0.489397	1.789570
H	–3.958871	2.037754	–0.319850
H	3.011160	–2.394970	1.597154
C	–2.473814	1.494835	1.238226
H	–2.021282	2.437777	1.566394
H	–3.316729	1.284595	1.917944
H	–2.807191	1.230314	–2.251561
C	–0.789362	–1.897216	1.169050
H	–0.173998	–1.889154	2.073536
H	–1.166468	–2.921970	1.035587
H	2.849506	–0.249902	2.620890
C	–2.327285	1.145858	–1.271996
C	1.406553	–2.188734	0.076582
H	1.879510	–1.988999	–0.891591
H	1.253386	–3.277307	0.153910
C	–1.949647	–0.920317	1.304936
H	–2.597587	–0.966859	0.424982
H	–2.563242	–1.182886	2.180720
O	1.578781	0.547601	–1.346917
H	–0.939459	0.590812	2.273430
H	–0.378621	–1.687092	–0.835840
O	0.132471	2.544841	0.099377
O	3.036673	1.324777	–0.806806
C	4.052152	2.853116	–0.251958
C	3.088503	2.627606	–1.343352
H	5.098241	2.594197	–0.366623
H	3.682195	3.124454	0.728903
H	2.143234	3.164130	–1.224930
H	3.468470	2.664511	–2.369761
H	–0.443056	2.922044	–0.589299

TS9’

V	–0.277594	0.791638	–0.048087
O	1.376121	0.583328	0.855551
O	–2.052005	0.478871	–0.631436
N	–1.082414	–0.567852	1.627240
C	2.566313	–1.173741	–0.332986
N	0.114660	–1.301707	–0.770880
C	–3.408571	0.338678	1.370109
C	2.451473	–0.192987	0.687111
C	–4.698121	0.405067	1.912889
C	3.733252	–1.942285	–0.404337
C	–2.246219	0.048430	2.300827
H	–1.874214	0.978317	2.742752
H	–2.597104	–0.597150	3.121360
C	–4.373741	0.881490	–0.799078
C	–0.163277	–2.350162	0.233313
H	0.742733	–2.467018	0.836071

H	–0.368107	–3.321693	–0.238397
C	–3.241258	0.579147	–0.016501
C	1.476420	–1.384617	–1.360331
H	1.515100	–0.607064	–2.129185
H	1.623211	–2.358775	–1.849955
C	–1.329681	–1.928825	1.119556
H	–2.259250	–1.898880	0.545110
H	–1.468252	–2.654293	1.935537
O	0.264609	1.429146	–1.613439
H	–0.295144	–0.572654	2.275407
H	–0.577003	–1.348546	–1.519621
O	–0.687690	2.267672	0.956988
O	1.864096	2.067448	–1.667296
C	3.370469	3.067412	–0.983157
C	1.920143	3.326199	–1.025284
H	4.004053	3.310683	–1.828504
H	3.782172	2.474120	–0.175946
H	1.420777	3.325305	–0.052444
H	1.580213	4.150176	–1.661632
H	–1.514907	2.686873	0.661618
C	4.795221	–1.759602	0.480947
C	3.523530	–0.029831	1.590113
C	4.681215	–0.794313	1.484260
H	5.492564	–0.641711	2.191870
H	5.690670	–2.368169	0.394757
H	3.412217	0.718573	2.370131
H	3.809490	–2.700382	–1.182151
C	–5.639417	0.959077	–0.229806
C	–5.810990	0.719691	1.136791
H	–6.495444	1.200817	–0.854906
H	–6.797262	0.769446	1.588979
H	–4.220619	1.054291	–1.860480
H	–4.825473	0.206001	2.976018