

Introducing Topology to Assess Synchronicity of Organic Reactions.

Dual Reactivity of Oximes with Alkenes as a Case Study

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Intermolecular Reactions

Nomenclature

Table S1. Nomenclature used for the different stationary points studied

oxime	nitron	alkene	TS1 ^a	TS2 ^b	TS3 ^c	Pe ^a	Pn ^{b,d}	Px ^{c,d}
(<i>E</i>)-1a	(<i>E</i>)-2a	3a	(<i>E</i>)-TS1a	(<i>E</i>)-TS2a	(<i>E</i>)-TS3a	(<i>E</i>)-4a	5a	6a
(<i>Z</i>)-1a	(<i>Z</i>)-2a	3a	(<i>Z</i>)-TS1a	(<i>Z</i>)-TS2a	(<i>Z</i>)-TS3a	(<i>Z</i>)-4a	6a	5a
(<i>E</i>)-1a	(<i>E</i>)-2a	3b	(<i>E</i>)-TS1b	(<i>E</i>)-TS2b	(<i>E</i>)-TS3b	(<i>E</i>)-4b	5b	6b
(<i>Z</i>)-1a	(<i>Z</i>)-2a	3b	(<i>Z</i>)-TS1b	(<i>Z</i>)-TS2b	(<i>Z</i>)-TS3b	(<i>Z</i>)-4b	6b	5b
(<i>E</i>)-1a	(<i>E</i>)-2a	3c	(<i>E</i>)-TS1c	(<i>E</i>)-TS2c	(<i>E</i>)-TS3c	(<i>E</i>)-4c	5c	6c
(<i>Z</i>)-1a	(<i>Z</i>)-2a	3c	(<i>Z</i>)-TS1c	(<i>Z</i>)-TS2c	(<i>Z</i>)-TS3c	(<i>Z</i>)-4c	6c	5c
(<i>E</i>)-1b	(<i>E</i>)-2b	3c	(<i>E</i>)-TS1d	(<i>E</i>)-TS2d	(<i>E</i>)-TS3d	(<i>E</i>)-4d	5d	6d
(<i>Z</i>)-1b	(<i>Z</i>)-2b	3c	(<i>Z</i>)-TS1d	(<i>Z</i>)-TS2d	(<i>Z</i>)-TS3d	(<i>Z</i>)-4d	6d	5d
1c	2c	3c	TS1e	TS2e	TS3e	4e	5e	
1d	2d	3c	TS1f	TS2f	TS3f	4f	5f	
1c	2c	3d	TS1g	TS2g	TS3g	4g	5g	
1d	2d	3d	TS1h	TS2h	TS3h	4h	5h	

^a corresponding to the ene-like reaction of oxime 1 with alkene 3. ^b corresponding to the dipolar cycloaddition (*endo* approach) of nitron 2 with alkene 3. ^c corresponding to the dipolar cycloaddition (*exo* approach) of nitron 2 with alkene 3. ^d (*Z*-*endo* and (*E*-*exo* approaches lead to the same adduct; equally, (*Z*-*exo* and (*E*-*endo* also yield the same product.

Isomerization Oxime/Nitron

The isomerization oxime/nitron has been computationally studied previously by us.¹

Isomerization of compound (*Z*)-1a into (*Z*)-2a has been calculated following a bimolecular mechanism (Figure S1). For details on the process of isomerization of oximes into nitrones the reader is reported to the original publication.¹

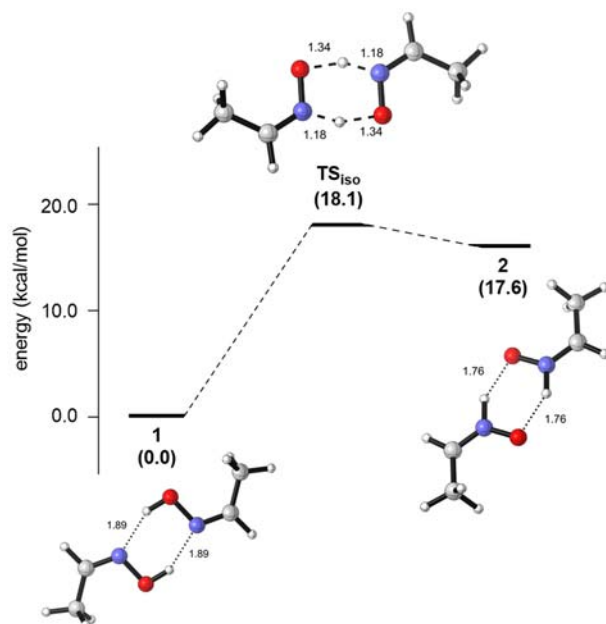


Figure S1. Isomerization of (*Z*)-1 into (*Z*)-2.

¹ D. Roca-López, A. Darù, T. Tejero and P. Merino, *RSC Adv.*, 2016, **6**, 22161-22173

Calculated energies

Table S2. Comparison of calculated absolute free energies (hartrees) for the reaction of **1a** and **2a** with **3c** at several levels of theory

	b3lyp-d3bj/def2tzvp			m062x/6-311G(d,p)			m062x/cc-pvtz		
	G	ΔG^a	$\Delta\Delta G^b$	G	ΔG^a	$\Delta\Delta G^b$	G	ΔG^a	$\Delta\Delta G^b$
(Z)- 1a	-209.188691			-209.051445			-209.076313		
(E)- 1a	-209.188886			-209.051963			-209.076656		
(Z)- 2a	-209.171841			-209.025311			-209.056693		
(E)- 2a	-209.176224			-209.030542			-209.052451		
3c	-306.546653			-306.353889			-306.390134		
(E)- TS1c	-515.691943	27.2	2.1	-515.362606	26.8	2.1	-515.421704	28.3	1.9
(Z)- TS1c	-515.695295	25.1	0.0	-515.366021	24.7	0.0	-515.424760	26.4	0.0
(E)- TS2c	-515.690229	28.3	3.2	-515.356368	30.7	6.1	-515.414465	33.9	7.5
(Z)- TS2c	-515.687746	29.9	4.7	-515.354772	31.7	7.1	-515.412805	32.8	6.5
(E)- TS3c	-515.685356	31.4	6.2	-515.350846	34.2	9.5	-515.408782	38.2	11.8
(Z)- TS3c	-515.682286	33.3	8.2	-515.348505	35.7	11.0	-515.405966	36.4	10.0
(E)- 4c	-515.728333	4.4		-515.399152	3.9		-515.458394	5.3	
(Z)- 4c	-515.736473	-0.7		-515.407606	-1.4		-515.467236	-0.3	
5c	-515.730475	3.1		-515.412963	-4.8		-515.470389	-2.3	
6c	-515.729569	3.6		-515.412740	-4.6		-515.469630	-1.8	

^a referred to the reagents (minimum value): (E)-**1a** + **3c**. ^b referred to the minimum value of TSs: (Z)-**TS1c**

We performed calculations at three levels of theory (See Table S2) for the reaction between **1** and **3c** for the purpose of comparison. Essentially, the same qualitative results were obtained. B3LYP² with empirical dispersion correction³ was used in conjunction with def2tzvp⁴ as suggested. This level gave for three products endergonic reactions and thus it was discarded. From the two basis sets used with functional M062X,⁵ 6-311G(d,p)⁶ and cc-pvtz,⁷ the latter, usually more accurate, provided higher energy barriers more in agreement with the high temperatures required for the reaction. So, we choose M062x/cc-pvtz for our calculations, that had been used also in similar processes concerning oxime/nitron tautomerism furnishing excellent results.¹ The combination M062x/cc-pvtz has also highly recommended for a variety of systems.⁸

² C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785-789.

³ S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.*, 2011, **32**, 1456-1465.

⁴ F. Weigend, *Phys. Chem. Chem. Phys.*, 2006, **8**, 227-236.

⁵ Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215-241.

⁶ V. A. Rassolov, J. A. Pople, M. A. Ratner and T. L. Windus, *J. Chem. Phys.*, 1998, **109**, 1223-1229.

⁷ D. E. Woon and T. H. Dunning Jr., *J. Chem. Phys.*, 1993, **98**, 1358-1371.

⁸ E. Papajak, J. Zheng, X. Xu, H. R. Leverentz and D. G. Truhlar, *J. Chem. Theory Comput.*, 2011, **7**, 3027-3034.

Table S3. Calculated (m062x/cc-pvtz) (m062x/cc-pvtz) absolute energies (hartrees) for the reaction of **1a** and **2a** with **3a-c**

	E_0	G	im. freq
(Z)- 1a	-209.049209	-209.076313	
(E)- 1a	-209.049956	-209.076656	
(Z)- 2a	-209.030548	-209.056693	
(E)- 2a	-209.025925	-209.052451	
3a	-117.804028	-117.828985	
3b	-193.010505	-193.037993	
3c	-306.359637	-306.390134	
(E)- TS1a	-326.809726	-326.842319	-1115.5
(Z)- TS1a	-326.812390	-326.845572	-1069.4
(E)- TS2a	-326.809277	-326.841489	-468.5
(Z)- TS2a	-326.807606	-326.839656	-494.4
(E)- TS3a	-326.810292	-326.842324	-469.3
(Z)- TS3a	-326.808488	-326.840335	-496.5
(E)- TS1b	-402.008305	-402.042481	-1090.2
(Z)- TS1b	-402.010872	-402.045486	-1047.1
(E)- TS2b	-402.022932	-402.056557	-489.3
(Z)- TS2b	-402.020844	-402.053820	-509.2
(E)- TS3b	-402.021683	-402.055501	-484.1
(Z)- TS3b	-402.020605	-402.053937	-497.4
(E)- TS1c	-515.384511	-515.421704	-305.8
(Z)- TS1c	-515.386756	-515.424760	-292.0
(E)- TS2c	-515.378605	-515.414465	-444.9
(Z)- TS2c	-515.376959	-515.412805	-473.8
(E)- TS3c	-515.372596	-515.408782	-479.0
(Z)- TS3c	-515.370120	-515.405966	-490.2
(E)- 4a	-326.865064	-326.897866	
(Z)- 4a	-326.873702	-326.906500	
5a	-326.884135	-326.915710	
6a	-326.884232	-326.915573	
(E)- 4b	-402.069409	-402.104765	
(Z)- 4b	-402.075971	-402.110908	
5b	-402.098120	-402.130975	
6b	-402.097024	-402.129954	
(E)- 4c	-515.420606	-515.458394	
(Z)- 4c	-515.428108	-515.467236	
5c	-515.434166	-515.470389	
6c	-515.433348	-515.469630	

Table S4. Calculated (m062x/cc-pvtz) absolute energies (hartrees) for the reaction of **1b** and **2b** with **3c**

	E ₀	G	im. freq
(Z)- 1b	-400.721605	-400.754238	
(E)- 1b	-400.725347	-400.757710	
(Z)- 2b	-400.706741	-400.738746	
(E)- 2b	-400.702169	-400.734504	
3c	-306.359637	-306.390134	
(E)- TS1d	-707.056136	-707.098522	-336.3
(Z)- TS1d	-707.061232	-707.103937	-272.8
(E)- TS2d	-707.055120	-707.095526	-461.5
(Z)- TS2d	-707.047451	-707.089180	-489.6
(E)- TS3d	-707.050428	-707.091297	-489.4
(Z)- TS3d	-707.041492	-707.082532	-502.1
(E)- 4d	-707.094653	-707.136634	
(Z)- 4d	-707.103784	-707.146066	
5d	-707.105246	-707.147302	
6d	-707.107933	-707.148846	

Table S5. Calculated (m062x/cc-pvtz) absolute energies (hartrees) for the reaction of **1b** and **2b** with **3c**

	E ₀	G	im. freq
1c	-631.679807	-631.719011	
1d	-483.995006	-484.032532	
2c	-631.663716	-631.702182	
2d	-483.978884	-484.016041	
3c	-306.359637	-306.390134	
3d	-345.644877	-345.677475	
TS1e	-938.016867	-938.066166	-291.2
TS1f	-790.317198	-790.364816	-298.4
TS1g	-977.301992	-977.352344	-314.0
TS1h	-829.602255	-829.650622	-811.6
TS2e	-938.004253	-938.051397	-481.5
TS2f	-790.319679	-790.363906	-479.8
TS2g	-977.275496	-977.323911	-498.5
TS2h	-829.590648	-829.636097	-490.0
TS3e	-937.996998	-938.044574	-483.0
TS3f	-790.303005	-790.347886	-459.1
TS3g	-977.284603	-977.332951	-489.5
TS3h	-829.574834	-829.620795	-530.2
4e	-938.054854	-938.103707	
4f	-790.34803	-790.394645	
4g	-977.337582	-977.388093	
4h	-829.618349	-829.662841	
5e	-938.064158	-938.111027	
5f	-790.373504	-790.418382	
5g	-977.339805	-977.387401	
5h	-829.631569	-829.676062	

Table S6. Calculated (m062x/cc-pvtz) absolute energies (hartrees) for the reaction of **1a** and **2a** with **3a-c** in toluene

	E ₀	G	im. freq
(Z)- 1a	-208.978515	-209.005188	
(E)- 1a	-209.054806	-209.081489	
(Z)- 2a	-208.962427	-208.988546	
(E)- 2a	-209.038712	-209.064840	
3a	-117.807338	-117.832281	
3b	-193.013932	-193.041516	
3c	-306.364978	-306.395476	
(E)- TS1a	-326.820288	-326.852639	-1066.8
(Z)- TS1a	-326.820094	-326.853501	-1066.5
(E)- TS2a	-326.817867	-326.849877	-488.2
(Z)- TS2a	-326.815634	-326.847662	-511.2
(E)- TS3a	-326.818658	-326.850612	-486.9
(Z)- TS3a	-326.816610	-326.849023	-512.8
(E)- TS1b	-402.017740	-402.052211	-1124.6
(Z)- TS1b	-402.019065	-402.053523	-1025.1
(E)- TS2b	-402.030583	-402.064134	-506.9
(Z)- TS2b	-402.027990	-402.061009	-523.5
(E)- TS3b	-402.029337	-402.062827	-501.5
(Z)- TS3b	-402.027818	-402.061187	-514.1
(E)- TS1c	-515.397244	-515.434623	-298.4
(Z)- TS1c	-515.398874	-515.436830	-281.2
(E)- TS2c	-515.388699	-515.424793	-477.2
(Z)- TS2c	-515.382270	-515.418015	-522.3
(E)- TS3c	-515.383350	-515.419432	-494.4
(Z)- TS3c	-515.380397	-515.416425	-532.7
(E)- 4a	-326.875850	-326.908567	
(Z)- 4a	-326.883927	-326.916842	
5a	-326.892135	-326.924008	
6a	-326.891980	-326.923199	
(E)- 4b	-402.084391	-402.119639	
(Z)- 4b	-402.086388	-402.121083	
5b	-402.105606	-402.138529	
6b	-402.104009	-402.136645	
(E)- 4c	-515.433685	-515.471583	
(Z)- 4c	-515.440538	-515.478749	
5c	-515.444191	-515.481000	
6c	-515.443017	-515.479185	

Table S7. Calculated (m062x/cc-pvtz) absolute energies (hartrees) for the reaction of **1a** and **2a** with **3a-c** in acetonitrile

	E ₀	G	im. freq
(Z)- 1a	-209.058061	-209.084762	
(E)- 1a	-208.981769	-209.008460	
(Z)- 2a	-209.044877	-209.071902	
(E)- 2a	-208.968590	-208.995605	
3a	-117.807832	-117.832767	
3b	-193.016241	-193.043874	
3c	-306.367251	-306.397733	
(E)- TS1a	-326.819768	-326.852595	-1089.0
(Z)- TS1a	-326.821571	-326.854896	-1074.2
(E)- TS2a	-326.822438	-326.854185	-534.7
(Z)- TS2a	-326.820139	-326.852069	-514.5
(E)- TS3a	-326.823422	-326.855339	-535.6
(Z)- TS3a	-326.821068	-326.853444	-513.4
(E)- TS1b	-402.020659	-402.054784	-1046.0
(Z)- TS1b	-402.022350	-402.056806	-998.9
(E)- TS2b	-402.035573	-402.069009	-547.1
(Z)- TS2b	-402.032813	-402.065993	-532.3
(E)- TS3b	-402.035271	-402.069157	-540.7
(Z)- TS3b	-402.033169	-402.066778	-531.0
(E)- TS1c	-515.403999	-515.441801	-311.3
(Z)- TS1c	-515.404960	-515.442919	-289.9
(E)- TS2c	-515.394284	-515.429932	-500.7
(Z)- TS2c	-515.390218	-515.426410	-472.3
(E)- TS3c	-515.390996	-515.427419	-530.3
(Z)- TS3c	-515.385842	-515.421734	-500.5
(E)- 4a	-326.881145	-326.914566	
(Z)- 4a	-326.888285	-326.921269	
5a	-326.896320	-326.928091	
6a	-326.896079	-326.927273	
(E)- 4b	-402.085432	-402.120168	
(Z)- 4b	-402.092007	-402.127137	
5b	-402.110499	-402.143631	
6b	-402.108979	-402.141679	
(E)- 4c	-515.442881	-515.480726	
(Z)- 4c	-515.447780	-515.485268	
5c	-515.450235	-515.486627	
6c	-515.449227	-515.485359	

Study of solvent influence considering explicit solvent molecules

We carried out a study of the ene-like reaction between (*E*)-**1a** and **3c** in the presence of two molecules of acetonitrile as reported by Fang and co-workers.⁹ Implicit solvent effects have also been considered.

Table S8. Calculated (m062x/cc-pvdz) absolute free energies (hartrees) for the reaction of (*E*)-**1a** with **3c** in acetonitrile and considering two explicit molecules of solvent.

	E_0	G	ΔG^b	im. freq
(<i>E</i>)- 1a ·2 MeCN	-209.056272	-209.009677		
3c	-306.361430	-306.296521		
Encounter pair ^a	-780.621947	-780.676619	3.7	
(<i>E</i>)- TS1c ·2 MeCN	-780.860937	-780.647521	21.9	-294.3
4c ·2 MeCN	-780.637978	-780.689232	-4.2	

^a Encounter pair in which all the reagents and solvent molecules are computed together. ^b Referred to the encounter pair (in order to keep unimolecularity).

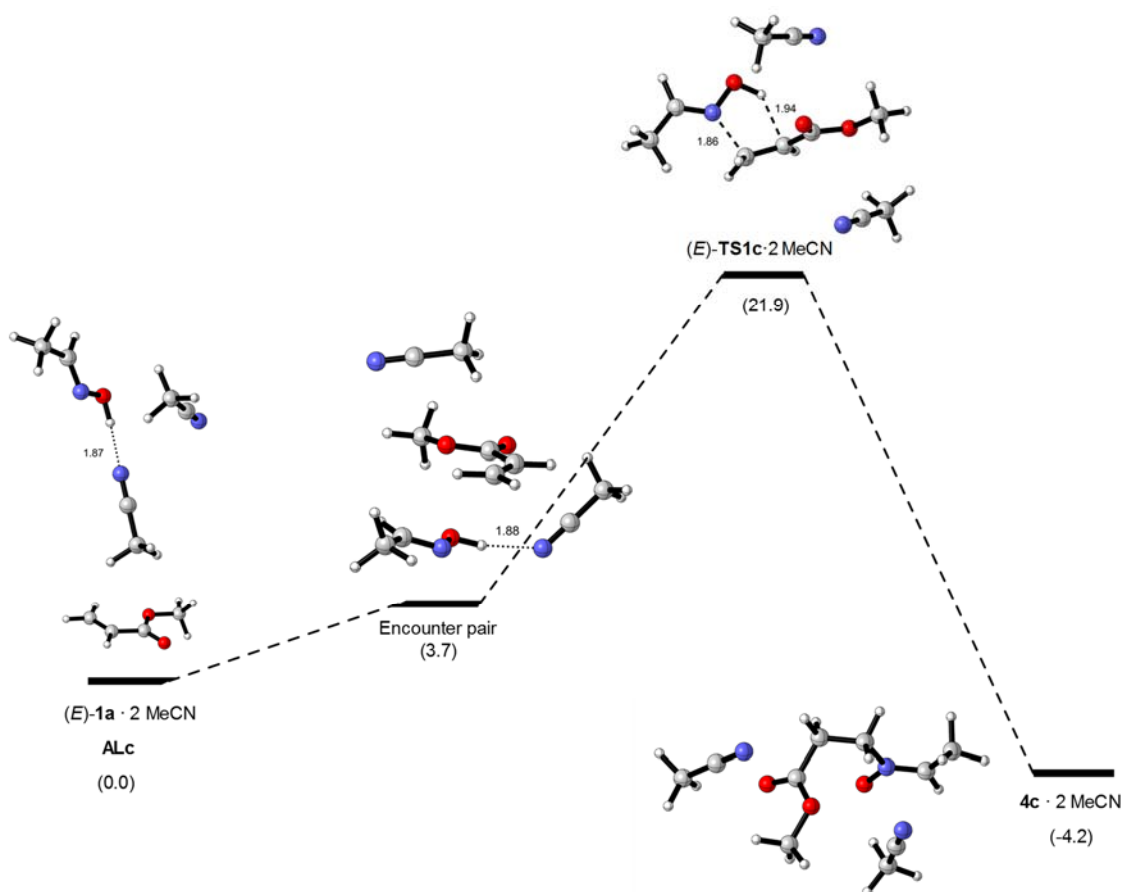


Figure S2. Free-energy (kcal/mol) diagram and geometries of stationary points corresponding to the intermolecular ene-like reaction of (*E*)-**1a** with **3c** in acetonitrile and considering two explicit molecules of solvent.

⁹ L. Zhao, S. J. Li and D. C. Fang, *ChemPhysChem*, 2015, **16**, 3711-3718.

Transition structures

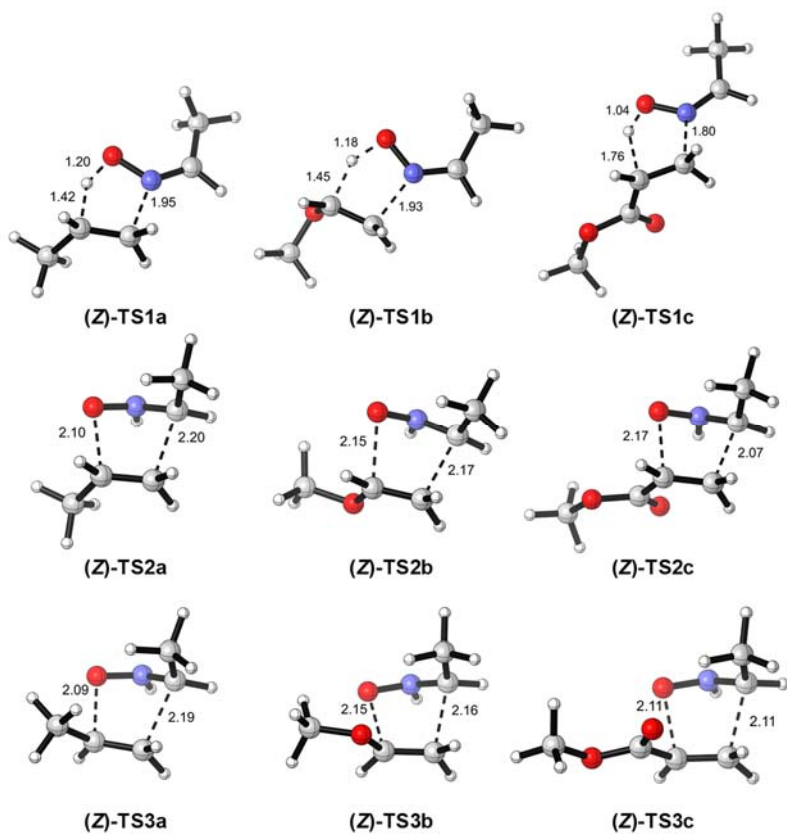


Figure S3. Transition structures corresponding to the reaction between (Z)-1a and 3a-c

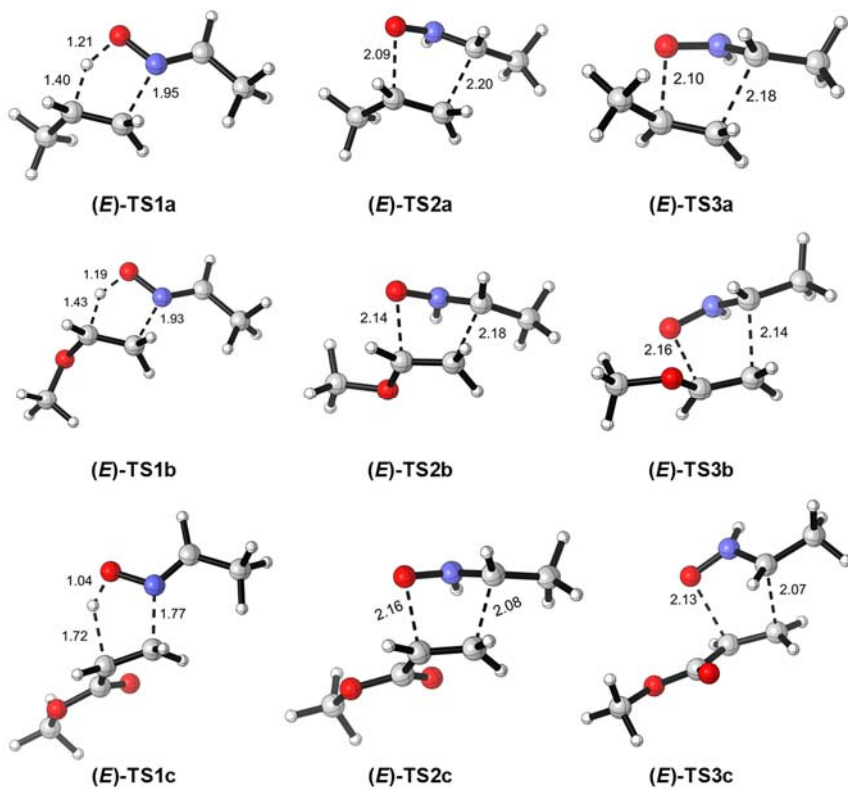


Figure S4. Transition structures corresponding to the reaction between (E)-1a and 3a-c

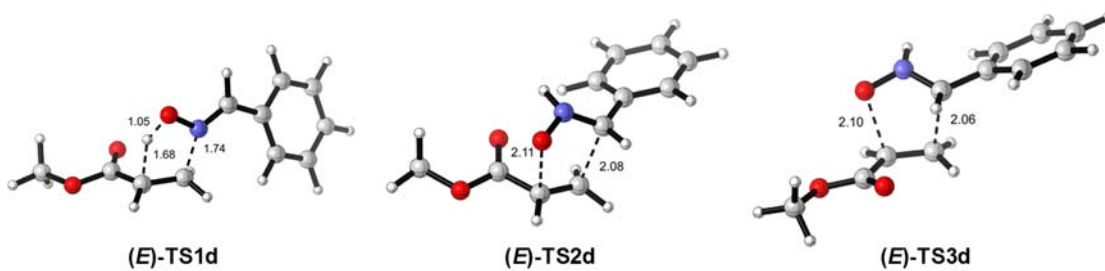


Figure S5. Transition structures corresponding to the reaction between (*Z*)-**1b** and **3c**

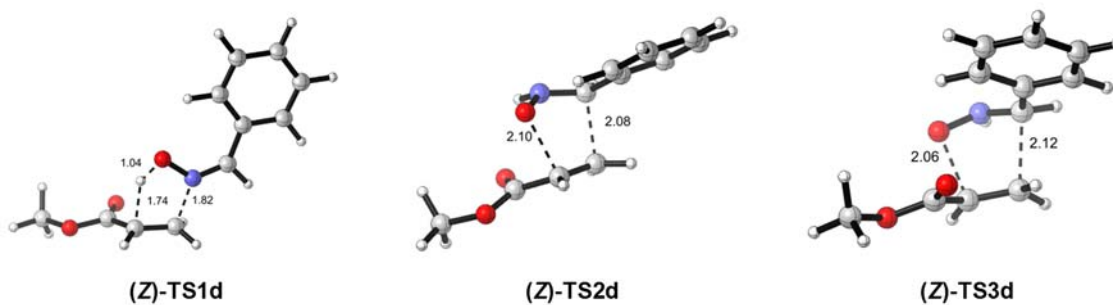


Figure S6. Transition structures corresponding to the reaction between (*E*)-**1b** and **3c**

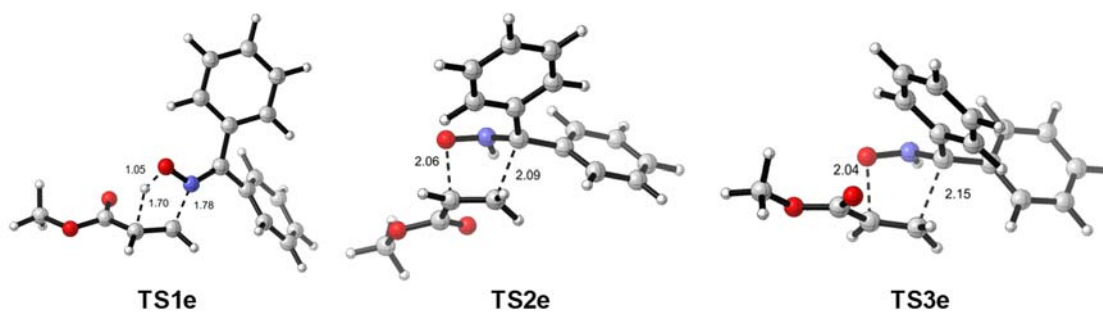


Figure S7. Transition structures corresponding to the reaction between (*E*)-**1c** and **3c**

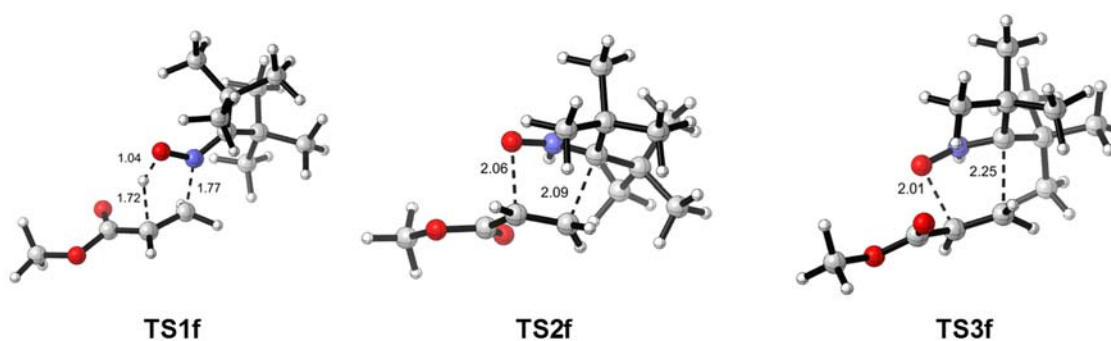


Figure S8. Transition structures corresponding to the reaction between (*E*)-**1d** and **3c**

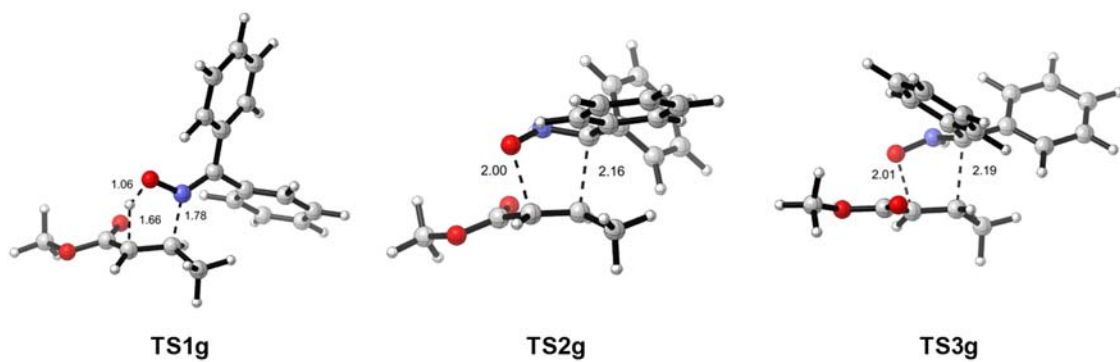


Figure S9. Transition structures corresponding to the reaction between (*E*)-1c and 3d

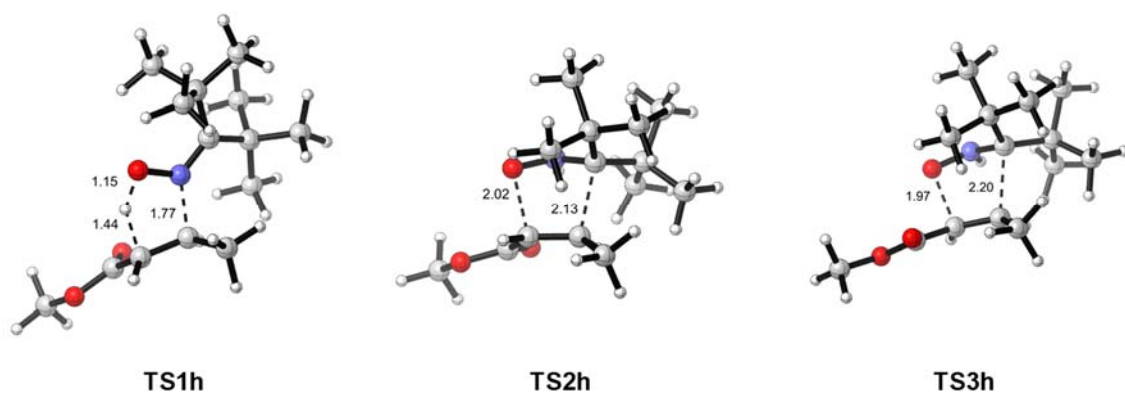


Figure S10. Transition structures corresponding to the reaction between (*E*)-1d and 3d

Topological analyses

Table S9. Electronic population of basins for the reaction between (*E*)-**1a** and **3a** (only relevant points of the IRC -25 before and 25 after the TS- are listed)

IRC	V1(C5,N3)	V2(C5,N3)	V(N3,O4)	V(N3)	V1(O4)	V2(O4)	V3(O4)	V(O4,H)	V1(C1,C2)	V2(C1,C2)	V(C2)	V(O4,H6)	V(O4,H6,C2)	V(C1)	V(C1,N3)
56	1.64	1.65	1.10	2.65	2.30	2.30	-	1.79	1.71	1.74	-	-	-	-	-
57	1.65	1.64	1.10	2.65	2.30	2.31	-	1.78	1.72	1.74	-	-	-	-	-
58	1.65	1.64	1.10	2.64	2.30	2.31	-	1.79	1.72	1.74	-	-	-	-	-
59	1.65	1.65	1.10	2.63	2.31	2.30	-	1.78	1.72	1.74	-	-	-	-	-
60	1.66	1.65	1.11	2.62	2.31	2.30	-	1.79	1.73	1.74	-	-	-	-	-
61	1.66	1.65	1.11	2.62	2.31	2.31	-	1.78	1.73	1.74	-	-	-	-	-
62	1.66	1.65	1.11	2.61	2.31	2.30	-	1.78	1.73	1.74	-	-	-	-	-
63	1.66	1.65	1.12	2.60	2.32	2.30	-	1.77	1.74	1.74	-	-	-	-	-
64	1.66	1.65	1.12	2.59	2.31	2.30	-	1.77	1.74	1.74	-	-	-	-	-
65	1.66	1.65	1.13	2.58	2.32	2.30	-	1.77	1.74	1.75	-	-	-	-	-
66	1.66	1.66	1.14	2.57	2.31	2.30	-	1.76	1.75	1.75	-	-	-	-	-
67	1.67	1.66	1.14	2.55	2.31	2.30	-	1.76	1.75	1.76	-	-	-	-	-
68	1.67	1.66	1.14	2.55	2.32	2.30	-	1.76	1.76	1.76	-	-	-	-	-
69	1.67	1.66	1.15	2.53	2.31	2.30	-	1.76	1.83	1.69	-	-	-	-	-
70	1.68	1.66	1.16	2.52	2.32	2.31	-	1.75	3.51	-	-	-	-	-	-
71	1.68	1.67	1.17	2.51	2.32	2.30	-	1.75	3.04	-	0.49	-	-	-	-
72	1.68	1.67	1.17	2.49	2.32	2.30	-	1.74	3.01	-	0.53	-	-	-	-
73	1.68	1.67	1.18	2.48	2.31	2.30	-	1.74	2.98	-	0.57	-	-	-	-
74	1.69	1.67	1.18	2.46	2.32	2.30	-	1.73	2.94	-	0.62	-	-	-	-
75	1.68	1.67	1.19	2.45	2.32	2.31	-	1.72	2.90	-	0.67	-	-	-	-
76	1.69	1.68	1.20	2.43	2.32	2.32	-	1.71	2.86	-	0.72	-	-	-	-
77	1.69	1.68	1.22	2.41	2.34	2.32	-	1.69	2.82	-	0.78	-	-	-	-
78	1.70	1.68	1.23	2.38	2.35	2.34	-	1.66	2.77	-	0.83	-	-	-	-
79	1.70	1.69	1.25	2.36	2.36	2.35	1.05	-	2.72	-	0.89	0.59	-	-	-
80	1.71	1.70	1.26	2.33	2.38	2.37	1.03	-	2.67	-	0.94	0.58	-	-	-
81	1.71	1.70	1.28	2.29	2.40	2.40	0.98	-	2.62	-	0.99	0.59	-	-	-
82	1.72	1.71	1.30	2.26	2.42	2.42	0.95	-	2.57	-	1.01	0.61	-	-	-
83	1.73	1.72	1.31	-	2.44	2.45	0.91	-	2.45	-	0.96	0.71	-	0.03	2.28
84	1.74	1.73	1.34	-	2.39	2.50	0.89	-	2.38	-	-	-	1.71	-	2.30
85	1.75	1.75	1.37	-	4.86	0.91	-	-	2.33	-	-	-	1.75	-	2.29
86	1.76	1.76	1.38	-	4.82	0.96	-	-	2.28	-	-	-	1.79	-	2.27
87	1.77	1.77	1.38	-	4.74	1.04	-	-	2.24	-	-	-	1.82	-	2.26
88	1.78	1.77	1.38	-	4.64	1.16	-	-	2.20	-	-	-	1.84	-	2.25
89	1.79	1.78	1.39	-	4.44	1.36	-	-	2.17	-	-	-	1.87	-	2.23
90	1.80	1.79	1.39	-	4.11	1.70	-	-	2.15	-	-	-	1.88	-	2.22
91	1.81	1.80	1.40	-	3.63	2.18	-	-	2.13	-	-	-	1.90	-	2.20
92	1.82	1.81	1.40	-	3.34	2.47	-	-	2.11	-	-	-	1.91	-	2.19
93	1.83	1.81	1.40	-	3.19	2.63	-	-	2.10	-	-	-	1.92	-	2.17
94	1.84	1.82	1.40	-	2.72	3.09	-	-	2.08	-	-	-	1.93	-	2.16
95	1.85	1.83	1.41	-	2.79	3.03	-	-	2.07	-	-	-	1.94	-	2.14
96	1.86	1.84	1.41	-	2.83	3.00	-	-	2.05	-	-	-	1.95	-	2.13
97	1.86	1.85	1.41	-	2.87	2.96	-	-	2.04	-	-	-	1.95	-	2.12
98	1.87	1.85	1.40	-	2.90	2.94	-	-	2.03	-	-	-	1.96	-	2.10
99	1.89	1.86	1.40	-	2.92	2.91	-	-	2.02	-	-	-	1.97	-	2.08
100	1.89	1.87	1.40	-	2.94	2.90	-	-	2.01	-	-	-	1.97	-	2.07
101	1.91	1.88	1.40	-	2.95	2.90	-	-	2.00	-	-	-	1.98	-	2.05
102	1.92	1.89	1.40	-	2.97	2.89	-	-	1.99	-	-	-	1.98	-	2.04
103	1.93	1.91	1.40	-	2.98	2.88	-	-	1.98	-	-	-	1.98	-	2.03
104	1.93	1.92	1.41	-	2.99	2.87	-	-	1.97	-	-	-	1.99	-	2.02
105	1.93	1.93	1.40	-	3.00	2.87	-	-	1.96	-	-	-	1.99	-	2.01
106	1.94	1.93	1.40	-	3.01	2.87	-	-	1.96	-	-	-	1.99	-	2.00

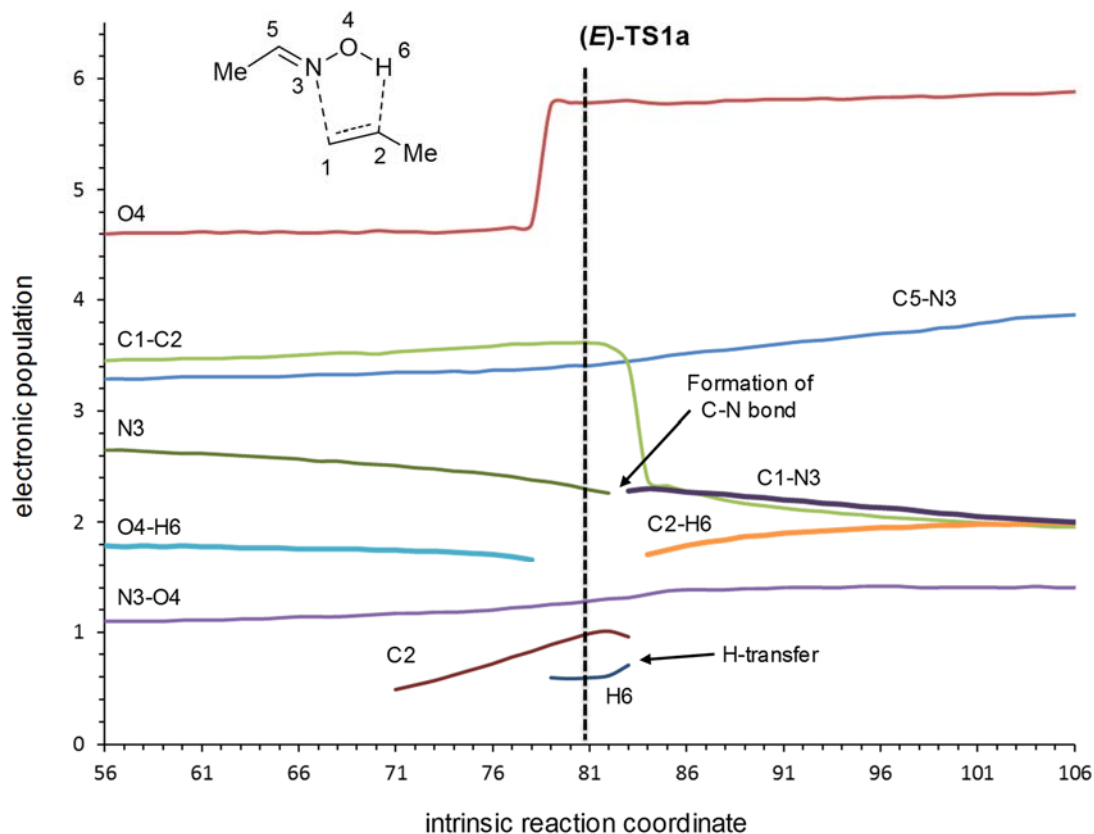


Figure S11. Graphical representation of ELF analysis for the reaction between (*E*)-**1a** and **3a**. (only relevant points of the IRC -25 before and 25 after the TS- are listed)

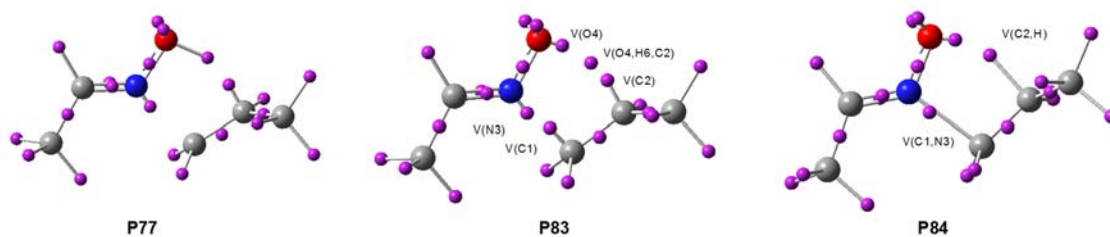


Figure S12. ELF attractor positions for the most relevant points along the reaction between (*E*)-**1a** and **3a**.

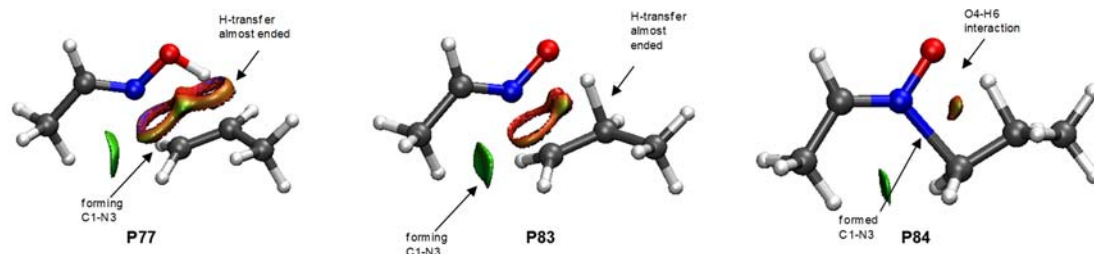


Figure S13. NCI analysis for the most relevant points along the reaction between (*E*)-**1a** and **3a**.

Table S10. Electronic population of basins for the reaction between (*E*)-**1a** and **3b** (only relevant points of the IRC -25 before and 25 after the TS- are listed)

IRC	V1(C5,N3)	V2(C5,N3)	V(N3,O4)	V(N3)	V1(O4)	V2(O4)	V3(O4)	V(O4,H)	V1(C1,C2)	V2(C1,C2)	V(C2)	V(O4,H6)	V(O4,H6,C2)	V(C1)	V(C1,N3)
56	1.64	1.65	1.09	2.65	2.34	2.28	-	1.78	1.80	1.81	-	-	-	-	-
57	1.64	1.65	1.10	2.64	2.33	2.28	-	1.78	1.81	1.81	-	-	-	-	-
58	1.64	1.65	1.11	2.64	2.33	2.28	-	1.78	1.81	1.80	-	-	-	-	-
59	1.65	1.65	1.10	2.63	2.33	2.28	-	1.78	1.81	1.81	-	-	-	-	-
60	1.65	1.65	1.11	2.62	2.27	2.34	-	1.78	1.82	1.80	-	-	-	-	-
61	1.65	1.65	1.12	2.62	2.27	2.34	-	1.78	1.82	1.80	-	-	-	-	-
62	1.65	1.66	1.12	2.61	2.28	2.33	-	1.77	1.83	1.80	-	-	-	-	-
63	1.65	1.66	1.12	2.59	2.27	2.33	-	1.77	1.84	1.80	-	-	-	-	-
64	1.66	1.66	1.12	2.58	2.28	2.34	-	1.77	1.84	1.80	-	-	-	-	-
65	1.66	1.66	1.13	2.57	2.28	2.33	-	1.77	1.84	1.80	-	-	-	-	-
66	1.66	1.66	1.14	2.57	2.28	2.33	-	1.77	1.85	1.81	-	-	-	-	-
67	1.66	1.67	1.15	2.55	2.28	2.32	-	1.76	1.85	1.81	-	-	-	-	-
68	1.66	1.67	1.15	2.54	2.28	2.33	-	1.76	1.85	1.81	-	-	-	-	-
69	1.66	1.67	1.15	2.53	2.28	2.34	-	1.76	1.84	1.83	-	-	-	-	-
70	1.67	1.67	1.16	2.52	2.28	2.34	-	1.75	1.83	1.85	-	-	-	-	-
71	1.67	1.67	1.16	2.51	2.28	2.33	-	1.75	3.11	-	0.57	-	-	-	-
72	1.67	1.67	1.17	2.50	2.28	2.33	-	1.74	3.07	-	0.61	-	-	-	-
73	1.68	1.68	1.18	2.48	2.28	2.34	-	1.73	3.05	-	0.66	-	-	-	-
74	1.68	1.68	1.19	2.46	2.28	2.35	-	1.73	3.00	-	0.72	-	-	-	-
75	1.68	1.69	1.20	2.44	2.28	2.34	-	1.72	2.96	-	0.77	-	-	-	-
76	1.69	1.69	1.21	2.42	2.28	2.34	-	1.71	2.91	-	0.83	-	-	-	-
77	1.69	1.69	1.22	2.39	2.29	2.35	-	1.69	2.86	-	0.89	-	-	-	-
78	1.69	1.69	1.23	2.37	2.29	2.37	-	1.67	2.81	-	0.95	-	-	-	-
79	1.70	1.70	1.25	2.35	2.30	2.38	1.05	-	2.75	-	1.01	0.60	-	-	-
80	1.70	1.71	1.27	2.31	2.32	2.41	1.03	-	2.70	-	1.06	0.58	-	-	-
81	1.71	1.72	1.28	2.28	2.34	2.44	0.99	-	2.66	-	1.10	0.57	-	-	-
82	1.72	1.72	1.30	2.28	2.34	2.49	0.95	-	2.54	-	1.14	0.58	-	-	-
83	1.73	1.74	1.31	-	2.33	2.54	0.91	-	2.46	-	1.15	0.61	-	-	2.31
84	1.74	1.75	1.33	-	2.20	2.72	0.88	-	2.41	-	1.04	0.76	-	-	2.29
85	1.75	1.76	1.36	-	4.88	0.90	-	-	2.36	-	-	-	1.83	-	2.27
86	1.76	1.77	1.38	-	4.84	0.93	-	-	2.31	-	-	-	1.87	-	2.25
87	1.77	1.78	1.38	-	4.78	1.01	-	-	2.27	-	-	-	1.90	-	2.23
88	1.78	1.80	1.38	-	4.65	1.14	-	-	2.24	-	-	-	1.92	-	2.21
89	1.79	1.81	1.39	-	4.43	1.36	-	-	2.21	-	-	-	1.94	-	2.20
90	1.80	1.82	1.40	-	3.97	1.82	-	-	2.18	-	-	-	1.95	-	2.18
91	1.81	1.82	1.41	-	3.47	2.32	-	-	2.16	-	-	-	1.97	-	2.17
92	1.82	1.84	1.41	-	3.22	2.59	-	-	2.14	-	-	-	1.98	-	2.16
93	1.83	1.85	1.41	-	3.09	2.71	-	-	2.12	-	-	-	1.99	-	2.14
94	1.84	1.86	1.42	-	3.03	2.78	-	-	2.11	-	-	-	2.00	-	2.13
95	1.84	1.86	1.42	-	2.98	2.83	-	-	2.09	-	-	-	2.00	-	2.11
96	1.85	1.87	1.42	-	2.95	2.87	-	-	2.08	-	-	-	2.01	-	2.09
97	1.86	1.89	1.41	-	2.93	2.90	-	-	2.07	-	-	-	2.01	-	2.08
98	1.87	1.90	1.41	-	2.91	2.93	-	-	2.06	-	-	-	2.02	-	2.06
99	1.88	1.91	1.40	-	2.91	2.94	-	-	2.05	-	-	-	2.02	-	2.05
100	1.89	1.91	1.41	-	2.90	2.96	-	-	2.04	-	-	-	2.03	-	2.04
101	1.90	1.92	1.41	-	2.87	2.98	-	-	2.03	-	-	-	2.04	-	2.02
102	1.91	1.93	1.40	-	2.87	2.99	-	-	2.02	-	-	-	2.04	-	2.01
103	1.92	1.93	1.40	-	2.86	3.00	-	-	2.02	-	-	-	2.04	-	1.99
104	1.93	1.94	1.40	-	2.85	3.01	-	-	2.01	-	-	-	2.04	-	1.99
105	1.94	1.94	1.40	-	2.86	3.02	-	-	2.00	-	-	-	2.04	-	1.98
106	1.95	1.94	1.40	-	2.86	3.02	-	-	2.00	-	-	-	2.05	-	1.97

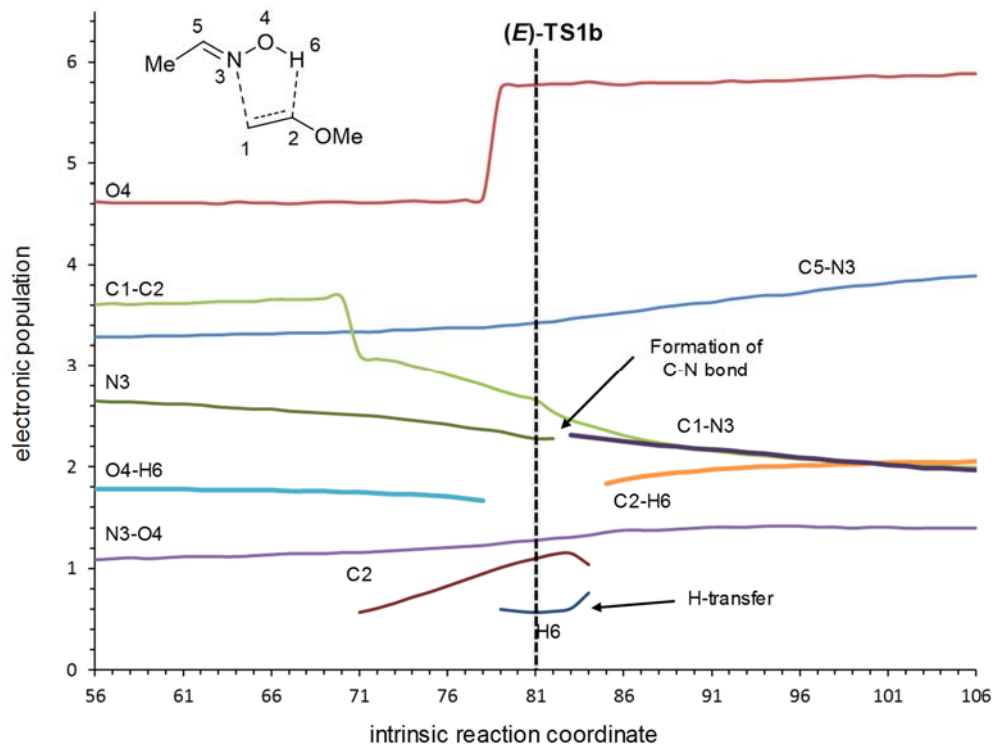


Figure S14. Graphical representation of ELF analysis for the reaction between *(E)*-1a and 3b. (only relevant points of the IRC -25 before and 25 after the TS- are listed)

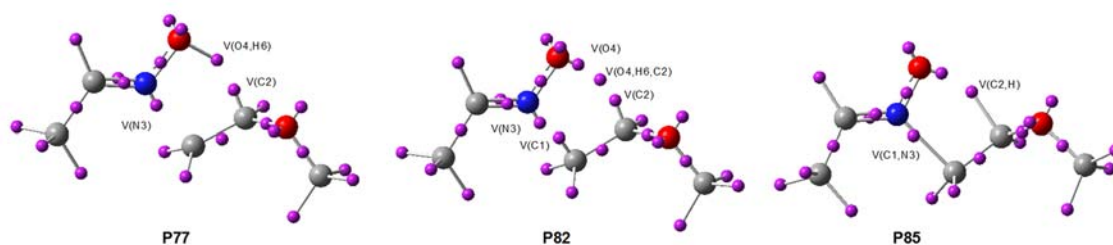


Figure S15. ELF attractor positions for the most relevant points along the reaction between *(E)*-1a and 3b.

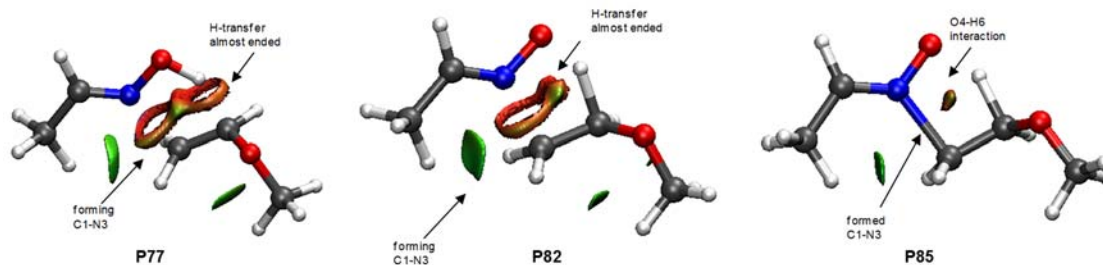


Figure S16. NCI analysis for the most relevant points along the reaction between *(E)*-1a and 3b.

Table S11. Electronic population of basins for the reaction between (Z)-1a and 3c (only relevant points of the IRC -25 before and 25 after the TS- are listed)

IRC	V1(C5,N3)	V2(C5,N3)	V(N3,O4)	V(N3)	V1(O4)	V2(O4)	V3(O4)	V(O4,H)	V1(C1,C2)	V2(C1,C2)	V(C2)	V(O4,H6)	V(O4,H6,C2)	V(C1)	V(C1,N3)
36	1.60	1.58	1.03	2.82	2.30	2.36	-	1.78	1.73	1.64	-	-	-	-	-
37	1.60	1.58	1.04	2.81	2.29	2.35	-	1.78	1.74	1.64	-	-	-	-	-
38	1.60	1.58	1.05	2.80	2.29	2.35	-	1.78	1.74	1.64	-	-	-	-	-
39	1.61	1.58	1.05	2.79	2.30	2.34	-	1.79	1.74	1.64	-	-	-	-	-
40	1.60	1.59	1.05	2.79	2.29	2.35	-	1.78	1.75	1.63	-	-	-	-	-
41	1.61	1.58	1.06	2.79	2.29	2.35	-	1.78	1.75	1.63	-	-	-	-	-
42	1.61	1.58	1.06	2.77	2.29	2.35	-	1.78	1.75	1.63	-	-	-	-	-
43	1.62	1.59	1.06	2.76	2.29	2.34	-	1.78	1.76	1.62	-	-	-	-	-
44	1.62	1.59	1.06	2.75	2.30	2.34	-	1.78	1.76	1.61	-	-	-	-	-
45	1.62	1.59	1.07	2.74	2.29	2.34	-	1.78	1.77	1.61	-	-	-	-	-
46	1.62	1.59	1.08	2.72	2.29	2.34	-	1.78	1.78	1.60	-	-	-	-	-
47	1.62	1.59	1.08	2.71	2.34	2.30	-	1.78	1.79	1.59	-	-	-	-	-
48	1.63	1.59	1.10	2.70	2.29	2.34	-	1.78	1.80	1.59	-	-	-	-	-
49	1.63	1.59	1.10	2.68	2.29	2.34	-	1.78	1.81	1.57	-	-	-	-	-
50	1.63	1.60	1.11	2.65	2.29	2.34	-	1.78	1.81	1.58	-	-	-	-	-
51	1.63	1.60	1.11	2.64	2.29	2.34	-	1.78	1.78	1.61	-	-	-	-	-
52	1.64	1.61	1.12	2.61	2.29	2.34	-	1.78	1.77	1.63	-	-	-	-	-
53	1.64	1.61	1.13	2.59	2.29	2.33	-	1.78	3.39	-	-	-	-	-	-
54	1.65	1.61	1.13	-	2.29	2.33	-	1.78	3.02	-	0.39	-	-	-	2.56
55	1.65	1.61	1.13	-	2.28	2.33	-	1.77	3.00	-	0.43	-	-	-	2.56
56	1.66	1.61	1.14	-	2.28	2.34	-	1.76	2.96	-	0.48	-	-	-	2.53
57	1.67	1.62	1.15	-	2.28	2.35	-	1.76	2.93	-	0.53	-	-	-	2.50
58	1.67	1.63	1.17	-	2.28	2.35	-	1.76	2.89	-	0.57	-	-	-	2.46
59	1.68	1.63	1.18	-	2.28	2.34	-	1.75	2.84	-	0.63	-	-	-	2.43
60	1.69	1.64	1.19	-	2.28	2.35	-	1.75	2.76	-	0.67	-	-	-	2.44
61	1.70	1.65	1.19	-	2.27	2.35	-	1.74	2.70	-	0.73	-	-	-	2.44
62	1.71	1.66	1.20	-	2.28	2.36	-	1.73	2.63	-	0.79	-	-	-	2.42
63	1.73	1.68	1.21	-	2.28	2.36	-	1.72	2.57	-	0.85	-	-	-	2.39
64	1.75	1.69	1.23	-	2.29	2.36	-	1.71	2.51	-	0.91	-	-	-	2.35
65	1.76	1.72	1.24	-	2.29	2.38	1.12	1.70	2.43	-	0.99	0.57	-	-	2.31
66	1.79	1.74	1.25	-	2.30	2.41	1.15	-	2.34	-	1.06	0.52	-	-	2.26
67	1.82	1.77	1.30	-	4.70	1.15	-	-	2.25	-	1.13	0.50	-	-	2.21
68	1.85	1.80	1.32	-	4.70	1.18	-	-	2.14	-	1.17	0.52	1.70	-	2.16
69	1.89	1.83	1.32	-	1.51	4.40	-	-	2.08	-	-	-	1.75	-	2.11
70	1.91	1.86	1.34	-	2.47	3.46	-	-	2.04	-	-	-	1.81	-	2.05
71	1.93	1.88	1.37	-	2.76	3.17	-	-	2.00	-	-	-	1.85	-	2.02
72	1.93	1.92	1.37	-	2.86	3.07	-	-	1.97	-	-	-	1.88	-	1.99
73	1.91	1.96	1.38	-	2.92	3.03	-	-	1.97	-	-	-	1.89	-	1.97
74	1.91	1.99	1.38	-	2.95	2.98	-	-	1.94	-	-	-	1.91	-	1.96
75	1.90	2.01	1.38	-	2.98	2.96	-	-	1.94	-	-	-	1.93	-	1.96
76	3.89	-	1.40	-	2.95	3.01	-	-	1.94	-	-	-	1.93	-	1.96
77	3.89	-	1.40	-	2.94	3.01	-	-	1.93	-	-	-	1.94	-	1.96
78	3.89	-	1.40	-	2.93	3.03	-	-	1.92	-	-	-	1.95	-	1.96
79	3.90	-	1.41	-	2.93	3.03	-	-	1.92	-	-	-	1.96	-	1.96
80	3.90	-	1.40	-	2.93	3.04	-	-	1.92	-	-	-	1.97	-	1.97
81	3.90	-	1.41	-	2.93	3.03	-	-	1.92	-	-	-	1.97	-	1.97
82	3.90	-	1.41	-	2.93	3.04	-	-	1.92	-	-	-	1.97	-	1.97
83	3.90	-	1.41	-	2.92	3.04	-	-	1.92	-	-	-	1.98	-	1.97
84	3.91	-	1.42	-	2.92	3.04	-	-	1.92	-	-	-	1.98	-	1.97
85	3.90	-	1.42	-	2.92	3.04	-	-	1.92	-	-	-	1.98	-	1.98
86	3.90	-	1.41	-	2.93	3.04	-	-	1.92	-	-	-	1.99	-	1.97

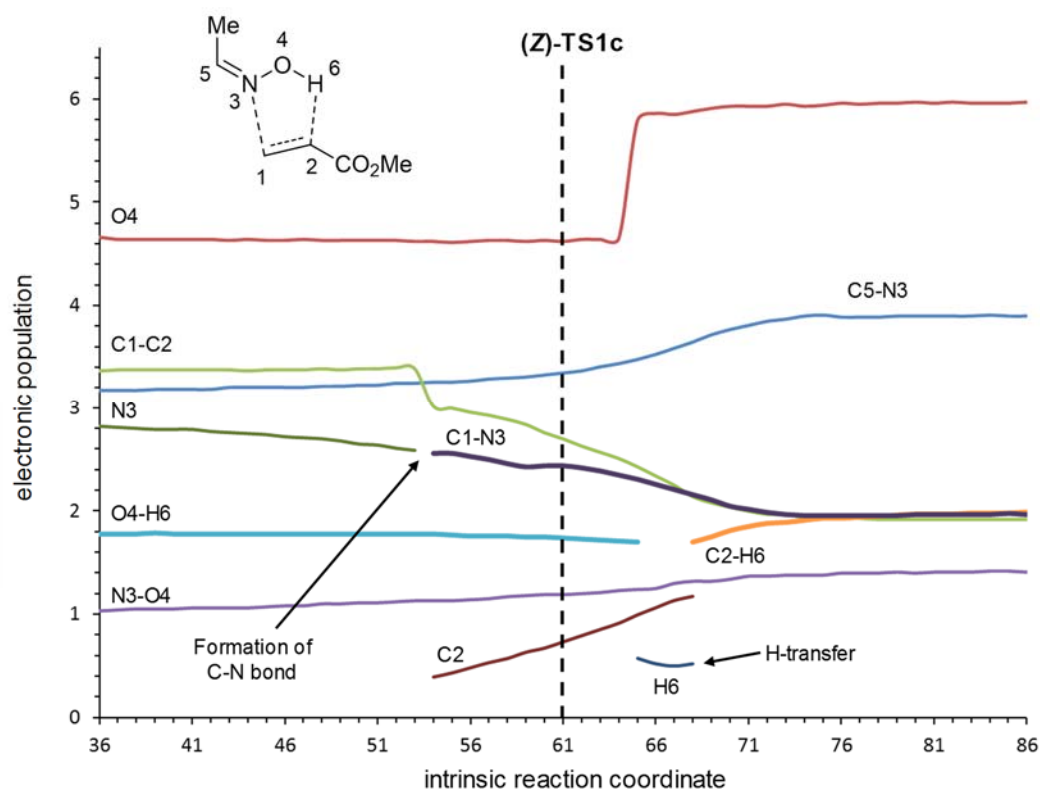


Figure S17. Graphical representation of ELF analysis for the reaction between (*Z*)-**1a** and **3c**. (only relevant points of the IRC -25 before and 25 after the TS- are listed)

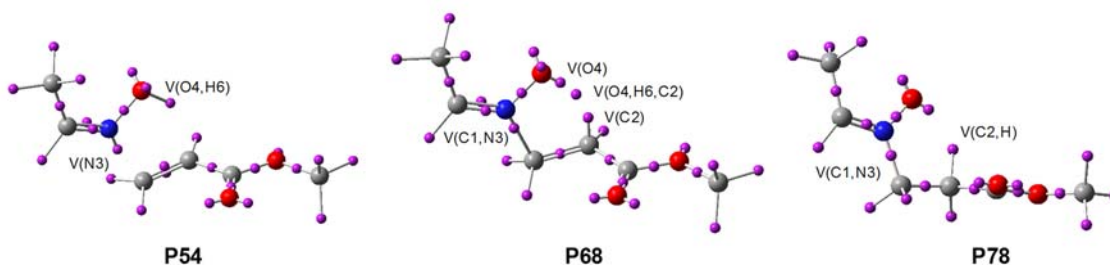


Figure S18. ELF attractor positions for the most relevant points along the reaction between (*Z*)-**1a** and **3c**.

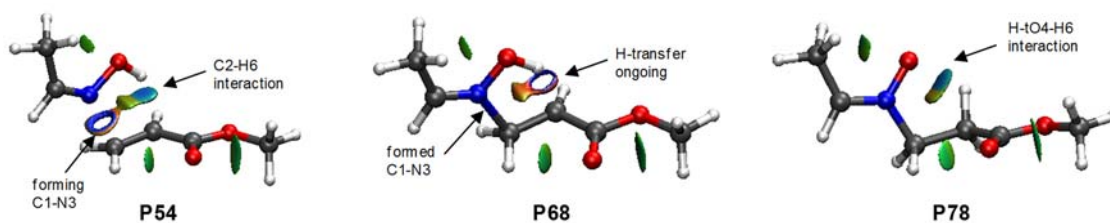


Figure S19. NCI analysis for the most relevant points along the reaction between (*Z*)-**1a** and **3c**.

Table S12. Electronic population of basins for the reaction between (*E*)-**1a** and **3c** (only relevant points of the IRC -25 before and 25 after the TS- are listed)

IRC	V1(C5,N3)	V2(C5,N3)	V(N3,O4)	V(N3)	V1(O4)	V2(O4)	V3(O4)	V(O4,H)	V1(C1,C2)	V2(C1,C2)	V(C2)	V(O4,H6)	V(O4,H6,C2)	V(C1)	V(C1,N3)
49	1.61	1.64	1.05	2.72	2.36	2.28	-	1.78	1.71	1.62	-	-	-	-	-
50	1.61	1.64	1.06	2.72	2.34	2.28	-	1.78	1.71	1.62	-	-	-	-	-
51	1.62	1.64	1.06	2.70	2.33	2.29	-	1.78	1.72	1.62	-	-	-	-	-
52	1.62	1.64	1.07	2.69	2.33	2.29	-	1.78	1.72	1.61	-	-	-	-	-
53	1.62	1.64	1.07	2.69	2.33	2.29	-	1.78	1.73	1.60	-	-	-	-	-
54	1.62	1.65	1.07	2.67	2.33	2.29	-	1.78	1.73	1.60	-	-	-	-	-
55	1.63	1.65	1.08	2.66	2.32	2.29	-	1.78	1.73	1.60	-	-	-	-	-
56	1.63	1.65	1.09	2.64	2.32	2.29	-	1.78	1.74	1.59	-	-	-	-	-
57	1.63	1.65	1.10	2.63	2.34	2.28	-	1.78	1.75	1.59	-	-	-	-	-
58	1.63	1.65	1.10	2.61	2.32	2.29	-	1.77	1.75	1.58	-	-	-	-	-
59	1.63	1.66	1.10	2.59	2.28	2.33	-	1.78	1.76	1.58	-	-	-	-	-
60	1.63	1.66	1.11	2.58	2.29	2.32	-	1.78	1.76	1.58	-	-	-	-	-
61	1.64	1.67	1.12	2.56	2.28	2.32	-	1.77	1.75	1.59	-	-	-	-	-
62	1.64	1.67	1.13	2.54	2.28	2.32	-	1.77	3.33	-	-	-	-	-	-
63	1.64	1.67	1.14	2.51	2.28	2.32	-	1.77	3.35	-	-	-	-	-	-
64	1.65	1.68	1.14	-	2.28	2.32	-	1.77	2.97	-	0.40	-	-	-	2.48
65	1.65	1.68	1.15	-	2.28	2.33	-	1.76	2.94	-	0.46	-	-	-	2.46
66	1.66	1.69	1.16	-	2.28	2.32	-	1.76	2.89	-	0.51	-	-	-	2.43
67	1.67	1.70	1.17	-	2.28	2.32	-	1.75	2.85	-	0.56	-	-	-	2.40
68	1.68	1.70	1.17	-	2.28	2.33	-	1.75	2.79	-	0.62	-	-	-	2.37
69	1.69	1.71	1.19	-	2.28	2.32	-	1.74	2.71	-	0.68	-	-	-	2.38
70	1.70	1.72	1.19	-	2.28	2.33	-	1.74	2.64	-	0.75	-	-	-	2.37
71	1.71	1.74	1.20	-	2.29	2.33	-	1.73	2.57	-	0.81	-	-	-	2.34
72	1.73	1.76	1.21	-	2.29	2.34	-	1.72	2.51	-	0.88	-	-	-	2.31
73	1.74	1.77	1.23	-	2.30	2.33	-	1.71	2.43	-	0.95	0.55	-	-	2.28
74	1.77	1.80	1.24	-	2.32	2.34	1.15	-	2.34	-	1.02	0.55	-	-	2.24
75	1.79	1.82	1.26	-	2.37	2.32	1.14	-	2.26	-	1.10	0.53	-	-	2.19
76	1.81	1.84	1.29	-	2.44	2.28	1.12	-	2.18	-	1.15	0.54	-	-	2.14
77	1.87	1.84	1.33	-	1.20	4.65	-	-	2.11	-	-	0.54	1.75	-	2.10
78	1.86	1.90	1.33	-	1.48	4.41	-	-	2.05	-	-	-	1.81	-	2.06
79	1.88	1.93	1.35	-	2.36	3.55	-	-	2.01	-	-	-	1.86	-	2.03
80	1.90	1.95	1.37	-	2.73	3.16	-	-	1.98	-	-	-	1.88	-	2.00
81	1.91	1.97	1.37	-	2.85	3.05	-	-	1.97	-	-	-	1.91	-	1.98
82	1.92	1.98	1.38	-	2.90	2.99	-	-	1.95	-	-	-	1.92	-	1.97
83	1.93	1.98	1.39	-	2.96	2.94	-	-	1.94	-	-	-	1.94	-	1.96
84	1.95	1.98	1.38	-	2.98	2.92	-	-	1.93	-	-	-	1.95	-	1.96
85	1.96	1.97	1.39	-	2.99	2.92	-	-	1.93	-	-	-	1.96	-	1.96
86	1.97	1.96	1.40	-	3.02	2.91	-	-	1.92	-	-	-	1.96	-	1.96
87	1.98	1.96	1.40	-	3.02	2.90	-	-	1.92	-	-	-	1.97	-	1.96
88	1.99	1.96	1.39	-	3.03	2.90	-	-	1.92	-	-	-	1.98	-	1.97
89	1.99	1.95	1.40	-	3.03	2.89	-	-	1.91	-	-	-	1.98	-	1.97
90	2.00	1.95	1.40	-	3.02	2.89	-	-	1.91	-	-	-	1.99	-	1.97
91	2.00	1.95	1.41	-	3.02	2.88	-	-	1.91	-	-	-	1.99	-	1.97
92	2.01	1.94	1.40	-	3.04	2.89	-	-	1.92	-	-	-	1.99	-	1.97
93	2.01	1.94	1.40	-	3.04	2.88	-	-	1.91	-	-	-	1.99	-	1.97
94	2.02	1.94	1.40	-	3.03	2.89	-	-	1.91	-	-	-	1.99	-	1.97
95	2.02	1.94	1.40	-	3.02	2.89	-	-	1.92	-	-	-	1.99	-	1.97
96	2.02	1.94	1.41	-	3.02	2.89	-	-	1.91	-	-	-	1.99	-	1.97
97	2.02	1.94	1.40	-	3.03	2.89	-	-	1.91	-	-	-	2.00	-	1.97
98	2.01	1.95	1.41	-	3.02	2.89	-	-	1.91	-	-	-	2.00	-	1.98
99	2.01	1.95	1.40	-	3.03	2.89	-	-	1.91	-	-	-	2.00	-	1.98

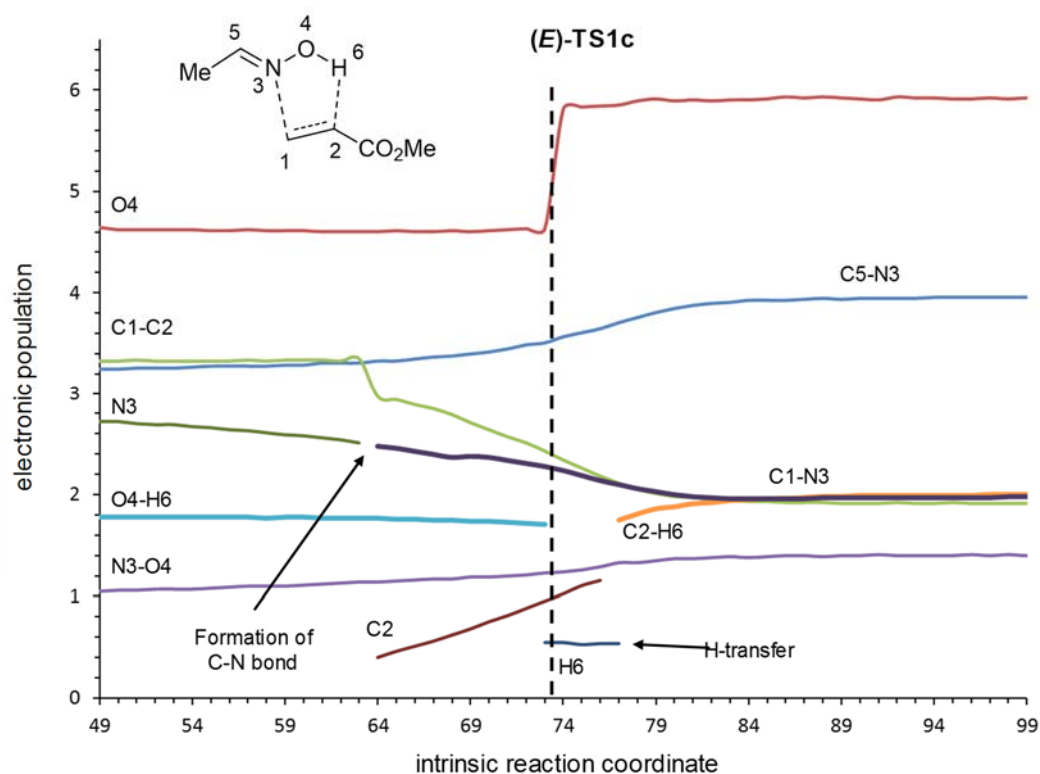


Figure S20. Graphical representation of ELF analysis for the reaction between *(E)*-1a and 3c. (only relevant points of the IRC -25 before and 25 after the TS- are listed)

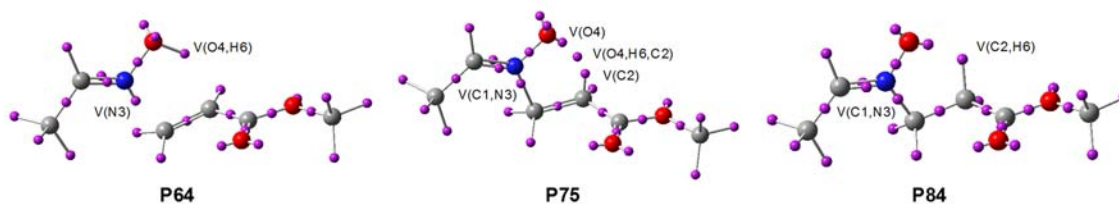


Figure S21. ELF attractor positions for the most relevant points along the reaction between *(E)*-1a and 3c.

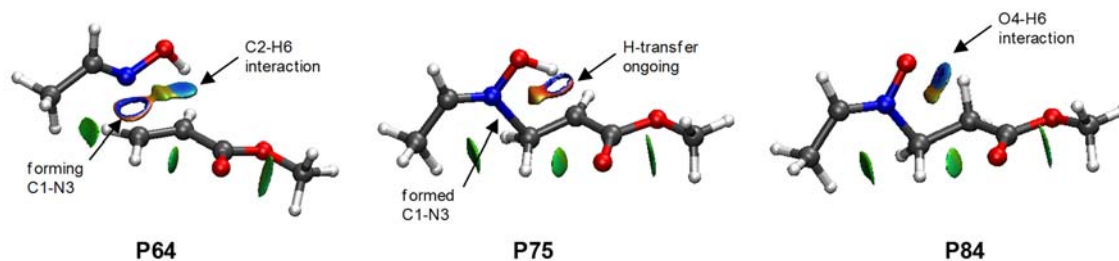


Figure S22. NCI analysis for the most relevant points along the reaction between *(E)*-1a and 3c.

Intramolecular Reactions

Calculated energies

Table S13. Calculated (m062x/cc-pvtz) absolute energies (hartrees) for oximes **6**.

	E ₀	G		E ₀	G
(E)- 6a	-364.962136	-364.996932	(E)- 6m	-495.301197	-495.338691
(Z)- 6a	-364.961293	-364.996387	(Z)- 6m	-495.301436	-495.338211
(E)- 6b	-440.167316	-440.204565	(E)- 6n	-607.675716	-607.715360
(Z)- 6b	-440.166469	-440.204009	(Z)- 6n	-607.675891	-607.714970
(E)- 6c	-553.519939	-553.559885	(E)- 6o	-608.854243	-608.896469
(Z)- 6c	-553.518712	-553.558693	(Z)- 6o	-608.853443	-608.895982
(E)- 6d	-404.241330	-404.278593	(E)- 6p	-324.459129	-324.491536
(Z)- 6d	-404.240149	-404.277466	(Z)- 6p	-324.459286	-324.491693
(E)- 6e	-479.446156	-479.485356	(E)- 6q	-363.739463	-363.773634
(Z)- 6e	-479.445356	-479.485074	(Z)- 6q	-363.739639	-363.773810
(E)- 6f	-592.798963	-592.840852	(E)- 6r	-517.355950	-517.394006
(Z)- 6f	-592.797812	-592.840013	(Z)- 6r	-517.352065	-517.389521
(E)- 6g	-364.958330	-364.993518	(E)- 6s	-721.861032	-721.901694
(Z)- 6g	-364.957282	-364.992438	(Z)- 6s	-721.857220	-721.897734
(E)- 6h	-595.917612	-595.960678	(E)- 6t	-631.838355	-631.878180
(Z)- 6h	-595.916924	-595.962095	(Z)- 6t	-631.824156	-631.863059
(E)- 6i	-702.038647	-702.079496	(E)- 6u	-517.355147	-517.392907
(Z)- 6i	-702.038021	-702.079768	(Z)- 6u	-517.354325	-517.392683
(E)- 6j	-553.520350	-553.559436	(E)- 6v	-721.859970	-721.900082
(Z)- 6j	-553.519554	-553.558713	(Z)- 6v	-721.858970	-721.899634
(E)- 6k	-592.799016	-592.840886	(E)- 6w	-631.836909	-631.875887
(Z)- 6k	-592.797780	-592.839260	(Z)- 6w	-631.835377	-631.875289
(E)- 6l	-443.516398	-443.553623			
(Z)- 6l	-443.512280	-443.548795			

Table S14. Calculated (m062x/cc-pvtz) absolute energies (hartrees) for compounds **7**.

	E ₀	G		E ₀	G
7a	-364.971276	-365.003544	7m	-495.320484	-495.354333
7b	-440.169941	-440.204104	7n	-607.683579	-607.719211
7c	-553.526965	-553.565283	7o	-608.868282	-608.906490
7d	-404.249637	-404.283273	7p	-324.488342	-324.518919
7e	-479.453319	-479.488903	7q	-363.766554	-363.797584
7f	-592.806525	-592.845185	7r	-517.378355	-517.413030
7g	-364.97162	-365.003248	7s	-721.883644	-721.921122
7h	-595.924291	-595.963109	7t	-631.860413	-631.897071
7i	-702.051272	-702.088652	7u	-517.371025	-517.406261
7j	-553.528003	-553.565056	7v	-721.875012	-721.913150
7k	-592.806055	-592.843675	7w	-721.879303	-721.916132
7l	-443.533899	-443.568632			

Table S15. Calculated (m062x/cc-pvtz) absolute energies (hartrees) for compounds **8**.

	E ₀	G		E ₀	G
8a	-364.950761	-364.982272	8m	-495.314290	-495.347796
8b	-440.164489	-440.197756	8n	-607.691631	-607.725798
8c	-553.502087	-553.538410	8o	-608.873130	-608.910960
8d	-404.257619	-404.290042	8p	-324.441937	-324.471304
8e	-479.471960	-479.506356	8q	-363.764252	-363.795397
8f	-592.809431	-592.846572	8r	-517.372720	-517.407629
8g	-364.973228	-365.003875	8s	-721.878397	-721.917270
8h	-595.929696	-595.967336	8t	-631.843783	-631.882343
8i	-702.053835	-702.090149	8u	-517.373626	-517.407789
8j	-553.504987	-553.541581	8v	-631.853196	-631.890516
8k	-592.812221	-592.849394	8w	-631.855857	-631.892277
8l	-443.534503	-443.568060			

Table S16. Calculated (m062x/cc-pvtz) absolute energies (hartrees) for nitrones **9**.

	E ₀	G		E ₀	G
(<i>E</i>)- 9a	-364.937094	-364.971640	(<i>E</i>)- 9m	-495.281357	-495.318670
(<i>Z</i>)- 9a	-364.942630	-364.977700	(<i>Z</i>)- 9m	-495.284966	-495.321642
(<i>E</i>)- 9b	-440.142678	-440.180969	(<i>E</i>)- 9n	-607.652349	-607.691385
(<i>Z</i>)- 9b	-440.148133	-440.185299	(<i>Z</i>)- 9n	-607.656377	-607.695832
(<i>E</i>)- 9c	-553.493263	-553.533268	(<i>E</i>)- 9o	-608.830389	-608.872416
(<i>Z</i>)- 9c	-553.500920	-553.541625	(<i>Z</i>)- 9o	-608.833868	-608.876854
(<i>E</i>)- 9d	-404.216516	-404.253420	(<i>E</i>)- 9p	-324.435585	-324.467982
(<i>Z</i>)- 9d	-404.221600	-404.258493	(<i>Z</i>)- 9p	-324.435742	-324.468139
(<i>E</i>)- 9e	-479.421697	-479.460906	(<i>E</i>)- 9q	-363.713491	-363.747333
(<i>Z</i>)- 9e	-479.426978	-479.466043	(<i>Z</i>)- 9q	-363.713667	-363.747509
(<i>E</i>)- 9f	-592.773110	-592.814827	(<i>E</i>)- 9r	-517.334705	-517.372174
(<i>Z</i>)- 9f	-592.779429	-592.821620	(<i>Z</i>)- 9r	-517.337119	-517.374319
(<i>E</i>)- 9g	-364.933223	-364.968129	(<i>E</i>)- 9s	-721.838651	-721.878720
(<i>Z</i>)- 9g	-364.938549	-364.973136	(<i>Z</i>)- 9s	-721.842577	-721.882338
(<i>E</i>)- 9h	-595.892653	-595.935617	(<i>E</i>)- 9t	-631.816317	-631.855458
(<i>Z</i>)- 9h	-595.899122	-595.941101	(<i>Z</i>)- 9t	-631.820564	-631.860016
(<i>E</i>)- 9i	-702.012556	-702.053512	(<i>E</i>)- 9u	-517.331066	-517.368556
(<i>Z</i>)- 9i	-702.019519	-702.060865	(<i>Z</i>)- 9u	-517.334742	-517.372616
(<i>E</i>)- 9j	-553.494751	-553.533762	(<i>E</i>)- 9v	-721.823958	-721.864945
(<i>Z</i>)- 9j	-553.501827	-553.540853	(<i>Z</i>)- 9v	-721.839907	-721.880720
(<i>E</i>)- 9k	-592.774608	-592.816159	(<i>E</i>)- 9w	-631.812296	-631.851089
(<i>Z</i>)- 9k	-592.780798	-592.819922	(<i>Z</i>)- 9w	-631.816217	-631.855270
(<i>E</i>)- 9l	-443.490735	-443.527640			
(<i>Z</i>)- 9l	-443.495287	-443.531782			

Table S17. Calculated (m062x/cc-pvtz) absolute energies (hartrees) for **TS4**.

	E_0	G	imag. freq
TS4a	-364.897207	-364.929027	-543.3
TS4b	-440.095870	-440.129668	-573.7
TS4c	-553.476455	-553.513035	-245.7
TS4d	-404.189653	-404.222906	-1101.0
TS4e	-479.388140	-479.423447	-1081.9
TS4f	-592.765027	-592.803116	-274.9
TS4g	-364.913973	-364.945044	-1010.6
TS4h	-595.871599	-595.909941	-700.3
TS4i	-702.000647	-702.037637	-394.9
TS4j	-553.462107	-553.497642	-622.7
TS4k	-592.757895	-592.795917	-1046.1
TS4l	-443.476673	-443.510856	-1013.5
TS4m	-495.265346	-495.298613	-813.8
TS4n	-607.627617	-607.663195	-972.4
TS4o	-608.810819	-608.848629	-1070.7
TS4p	-324.407239	-324.437492	-397.9
TS4q	-363.700232	-363.731271	-444.4
TS4r	-517.319650	-517.353852	-867.5
TS4s	-721.825383	-721.863755	-958.4
TS4t	-631.811741	-631.849373	-809.4
TS4u	-517.313139	-517.347365	-780.9
TS4v	-721.819984	-721.858360	-843.3
TS4w	-631.804537	-631.842131	-790.1

Table S18. Calculated (m062x/cc-pvtz) absolute energies (hartrees) for **TS5**.

	E_0	G	imag. freq.
TS5a	-364.897831	-364.929580	-591.9
TS5b	-440.110425	-440.144303	-589.1
TS5c	-553.459146	-553.494971	-568.3
TS5d	-404.193209	-404.225885	-497.4
TS5e	-479.407574	-479.441780	-501.0
TS5f	-592.755718	-592.792430	-489.3
TS5g	-364.908768	-364.939664	-504.7
TS5h	-595.873200	-595.910633	-495.4
TS5i	-701.995345	-702.031232	-473.4
TS5j	-553.465926	-553.501926	-502.6
TS5k	-592.762937	-592.799639	-431.8
TS5l	-443.469039	-443.502702	-485.0
TS5m	-495.249764	-495.283628	-479.0
TS5n	-607.629532	-607.664384	-487.5
TS5o	-608.804957	-608.842907	-464.7
TS5p	-324.367210	-324.396414	-645.2
TS5q	-363.675948	-363.706984	-544.0
TS5r	-517.304372	-517.338918	-480.1
TS5s	-721.811202	-721.850137	-471.4
TS5t	-631.795591	-631.833553	-478.8
TS5u	-517.309271	-517.343497	-486.7
TS5v	-721.817405	-721.855816	-481.8
TS5w	-631.800077	-631.837552	-489.6

Table S19. Calculated (m062x/cc-pvtz) absolute energies (hartrees) for **TS6**.

	E_0	G	imag. freq.
TS6d	-404.185019	-404.218373	-468.6
TS6e	-479.395180	-479.430495	-474.8
TS6f	-592.745451	-592.783453	-486.0
TS6g	-364.900347	-364.931548	-477.9
TS6h	-595.860702	-595.899185	-476.4
TS6i	-701.984805	-702.021414	-438.8
TS6l	-443.463086	-443.497095	-473.9

Transition structures

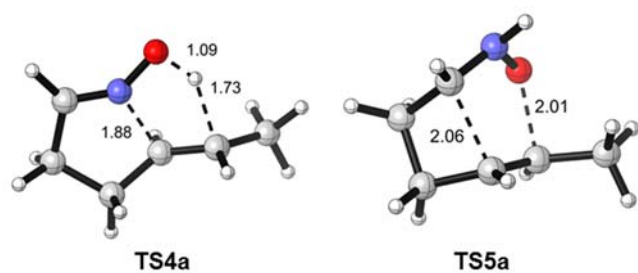


Figure S23. Transition structures corresponding to the intramolecular reactions of oxime **6a**

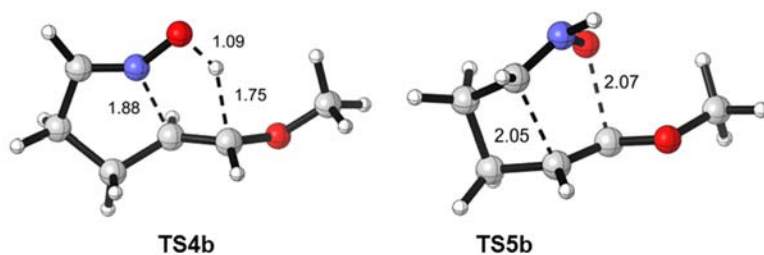


Figure S24. Transition structures corresponding to the intramolecular reactions of oxime **6b**

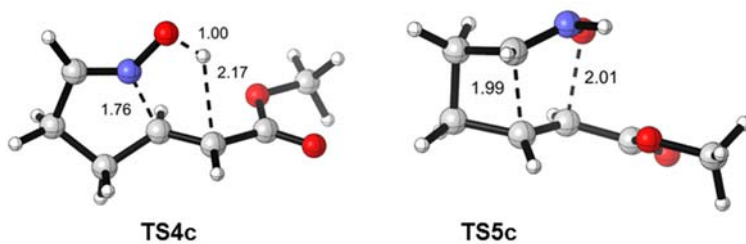


Figure S25. Transition structures corresponding to the intramolecular reactions of oxime **6c**

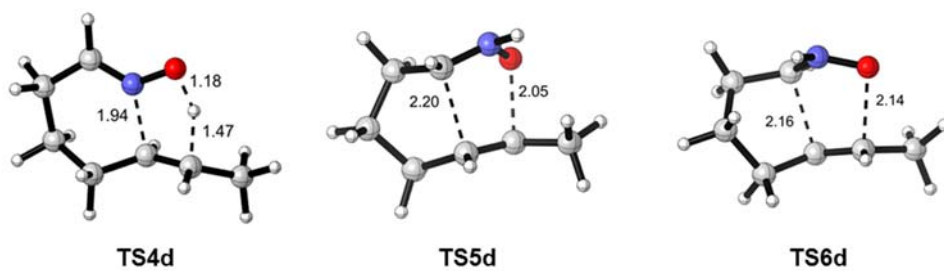


Figure S26. Transition structures corresponding to the intramolecular reactions of oxime **6d**

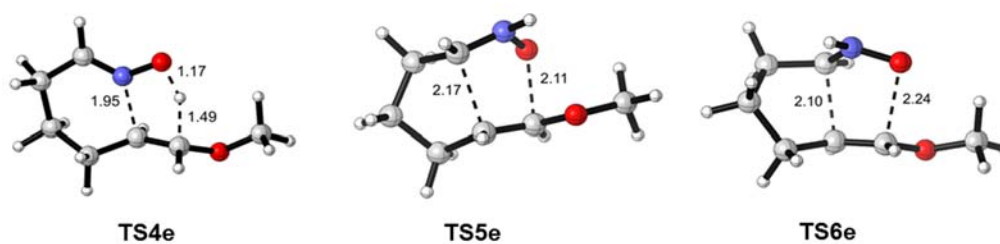


Figure S27. Transition structures corresponding to the intramolecular reactions of oxime **6e**

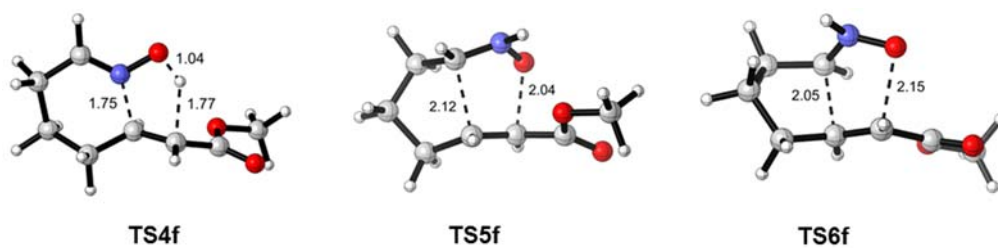


Figure S28. Transition structures corresponding to the intramolecular reactions of oxime **6f**

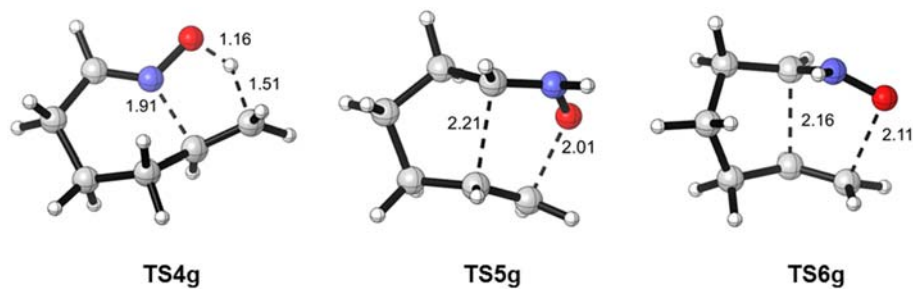


Figure S29. Transition structures corresponding to the intramolecular reactions of oxime **6g**

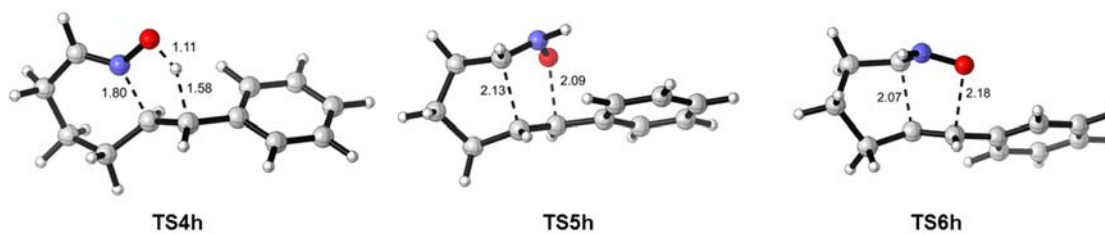


Figure S30. Transition structures corresponding to the intramolecular reactions of oxime **6h**

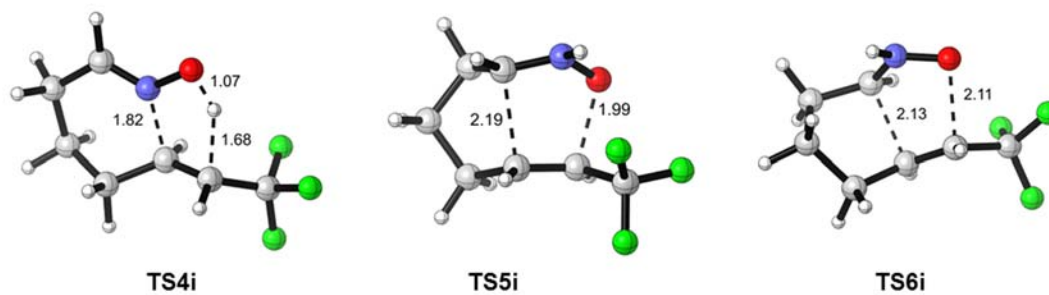


Figure S31. Transition structures corresponding to the intramolecular reactions of oxime **6i**

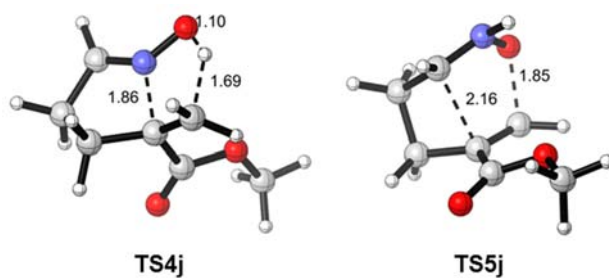


Figure S32. Transition structures corresponding to the intramolecular reactions of oxime **6j**

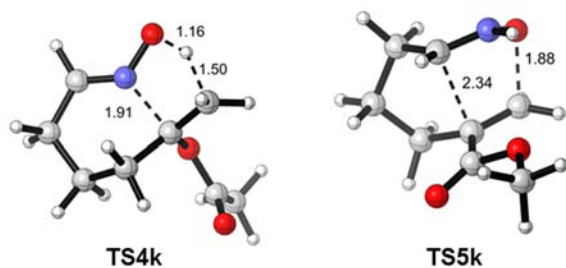


Figure S33. Transition structures corresponding to the intramolecular reactions of oxime **6k**

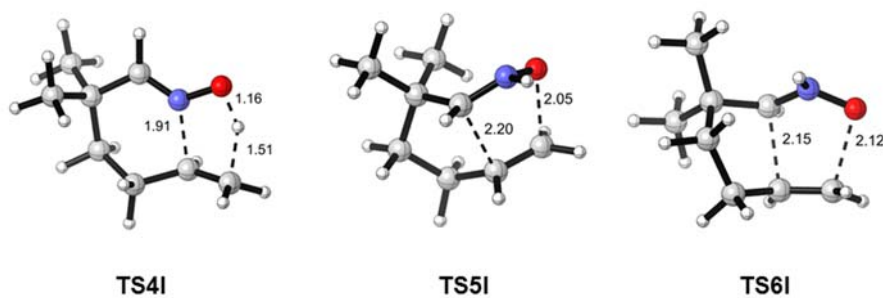


Figure S34. Transition structures corresponding to the intramolecular reactions of oxime **6l**

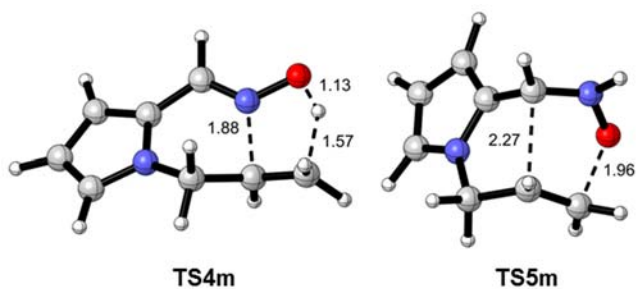


Figure S35. Transition structures corresponding to the intramolecular reactions of oxime **6m**

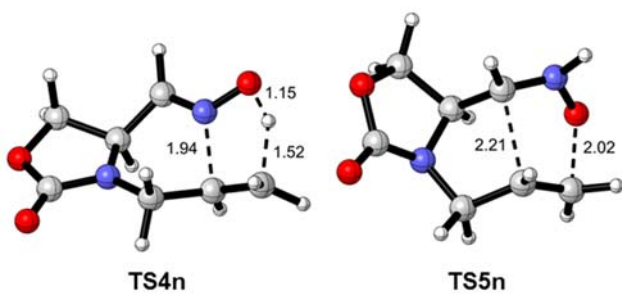


Figure S36. Transition structures corresponding to the intramolecular reactions of oxime **6n**

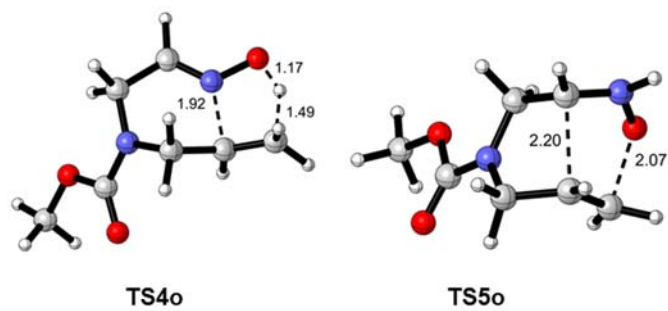


Figure S37. Transition structures corresponding to the intramolecular reactions of oxime **6o**

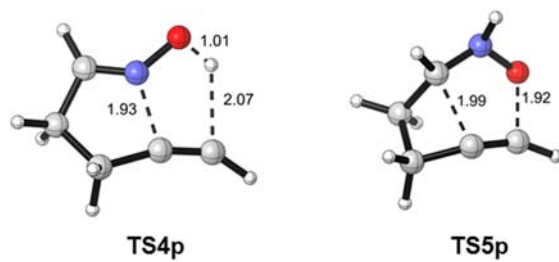


Figure S38. Transition structures corresponding to the intramolecular reactions of oxime **6p**

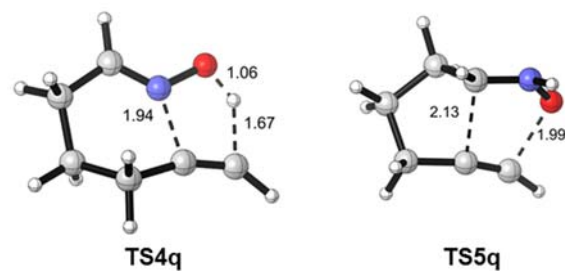


Figure S39. Transition structures corresponding to the intramolecular reactions of oxime **6q**

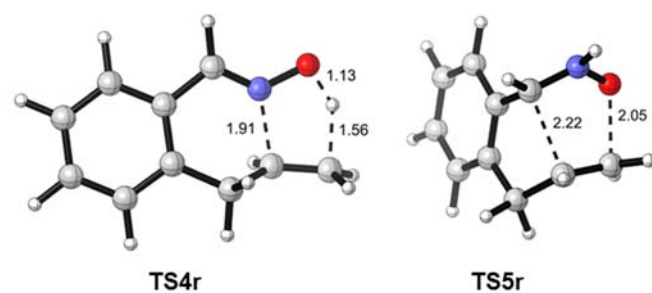


Figure S40. Transition structures corresponding to the intramolecular reactions of oxime **6r**

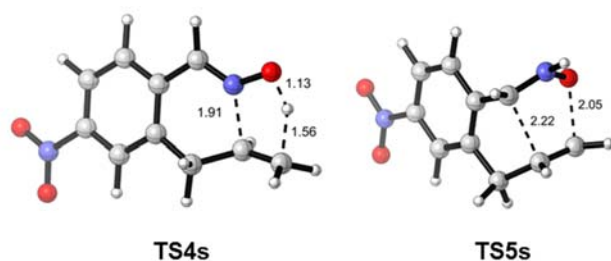


Figure S41. Transition structures corresponding to the intramolecular reactions of oxime **6s**

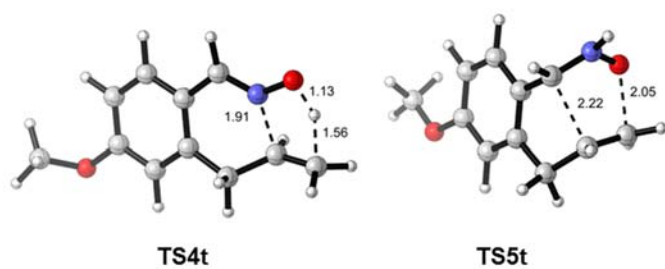


Figure S42. Transition structures corresponding to the intramolecular reactions of oxime **6t**

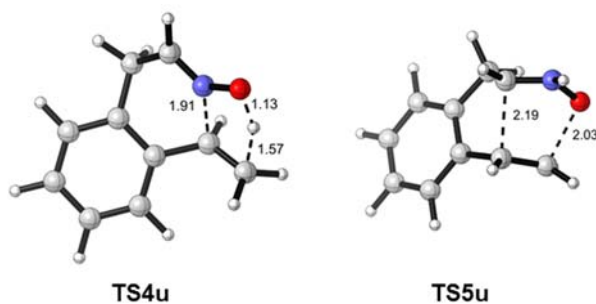


Figure S43. Transition structures corresponding to the intramolecular reactions of oxime **6u**

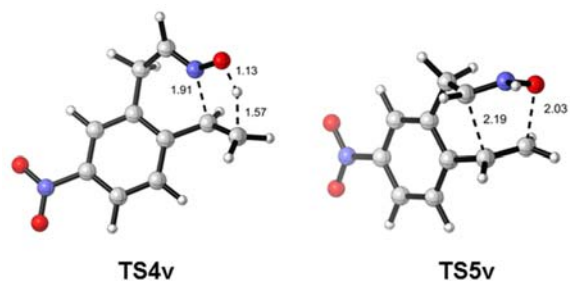


Figure S44. Transition structures corresponding to the intramolecular reactions of oxime **6v**

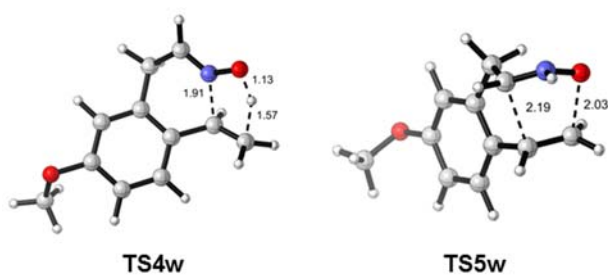


Figure S45. Transition structures corresponding to the intramolecular reactions of oxime **6w**

Topological analyses

Table S20. Electronic population of basins for the intramolecular ene-like reaction of oxime **6d** (only relevant points of the IRC -25 before and 25 after the TS- are listed)

IRC	V1(C5,N3)	V2(C5,N3)	V(N3,O4)	V(N3)	V1(O4)	V2(O4)	V3(O4)	V(O4,H)	V1(C1,C2)	V2(C1,C2)	V(C2)	V(O4,H6)	V(O4,H6,C2)	V(C1)	V(C1,N3)
36	1.67	1.65	1.09	2.62	2.20	2.41	-	1.79	1.77	1.78	-	-	-	-	-
37	1.67	1.65	1.09	2.62	2.20	2.41	-	1.78	1.77	1.78	-	-	-	-	-
38	1.67	1.65	1.10	2.61	2.20	2.42	-	1.79	1.77	1.78	-	-	-	-	-
39	1.67	1.65	1.10	2.61	2.19	2.42	-	1.78	1.77	1.79	-	-	-	-	-
40	1.67	1.65	1.10	2.60	2.20	2.41	-	1.78	1.77	1.79	-	-	-	-	-
41	1.67	1.65	1.10	2.59	2.20	2.42	-	1.78	1.76	1.80	-	-	-	-	-
42	1.68	1.65	1.10	2.58	2.20	2.42	-	1.78	1.76	1.80	-	-	-	-	-
43	1.68	1.65	1.11	2.57	2.20	2.42	-	1.78	1.76	1.81	-	-	-	-	-
44	1.68	1.65	1.12	2.56	2.20	2.42	-	1.78	1.76	1.82	-	-	-	-	-
45	1.68	1.65	1.12	2.55	2.20	2.43	-	1.77	1.77	1.81	-	-	-	-	-
46	1.68	1.65	1.13	2.54	2.19	2.43	-	1.78	1.82	1.77	-	-	-	-	-
47	1.69	1.65	1.13	2.53	2.19	2.43	-	1.76	3.57	-	-	-	-	-	-
48	1.69	1.66	1.14	2.52	2.20	2.43	-	1.76	3.58	-	-	-	-	-	-
49	1.69	1.66	1.14	2.51	2.19	2.43	-	1.76	3.59	-	-	-	-	-	-
50	1.70	1.66	1.14	2.49	2.19	2.43	-	1.75	3.08	-	0.52	-	-	-	-
51	1.70	1.67	1.15	2.48	2.18	2.43	-	1.75	3.05	-	0.56	-	-	-	-
52	1.70	1.67	1.15	2.47	2.18	2.44	-	1.75	3.02	-	0.60	-	-	-	-
53	1.70	1.67	1.16	2.45	2.18	2.45	-	1.74	2.99	-	0.64	-	-	-	-
54	1.70	1.67	1.17	2.44	2.18	2.46	-	1.74	2.96	-	0.68	-	-	-	-
55	1.71	1.67	1.18	2.43	2.18	2.47	-	1.72	2.93	-	0.72	-	-	-	-
56	1.71	1.67	1.19	2.40	2.17	2.47	-	1.72	2.89	-	0.76	-	-	-	-
57	1.72	1.67	1.20	2.39	2.18	2.47	-	1.71	2.86	-	0.81	-	-	-	-
58	1.72	1.68	1.21	2.37	2.18	2.49	-	1.68	2.82	-	0.86	-	-	-	-
59	1.72	1.68	1.22	2.34	2.17	2.52	1.05	-	2.78	-	0.90	0.62	-	-	-
60	1.73	1.69	1.24	2.32	2.18	2.56	1.04	-	2.73	-	0.95	0.59	-	-	-
61	1.74	1.69	1.25	2.30	2.18	2.62	1.00	-	2.69	-	0.99	0.58	-	-	-
62	1.75	1.69	1.26	2.28	2.16	2.70	0.95	-	2.64	-	1.03	0.58	-	-	-
63	1.76	1.71	1.27	-	2.13	2.80	0.89	-	2.52	-	1.04	0.61	-	0.03	2.28
64	1.77	1.70	1.29	-	2.07	2.93	0.83	-	2.46	-	0.99	0.62	-	-	2.32
65	1.78	1.71	1.31	-	2.72	3.12	-	1.72	2.40	-	-	-	1.73	-	2.31
66	1.80	1.71	1.32	-	3.29	2.55	-	-	2.35	-	-	-	1.76	-	2.29
67	1.81	1.72	1.34	-	3.41	2.43	-	-	2.31	-	-	-	1.80	-	2.27
68	1.80	1.75	1.35	-	3.42	2.42	-	-	2.27	-	-	-	1.83	-	2.26
69	1.79	1.77	1.37	-	3.39	2.45	-	-	2.23	-	-	-	1.86	-	2.25
70	1.77	1.80	1.38	-	3.33	2.51	-	-	2.21	-	-	-	1.88	-	2.24
71	1.75	1.84	1.38	-	3.27	2.57	-	-	2.19	-	-	-	1.89	-	2.23
72	3.57	-	1.39	-	3.22	2.62	-	-	2.16	-	-	-	1.90	-	2.23
73	3.59	-	1.40	-	3.17	2.67	-	-	2.15	-	-	-	1.91	-	2.22
74	3.60	-	1.41	-	3.13	2.71	-	-	2.13	-	-	-	1.93	-	2.21
75	3.62	-	1.41	-	3.09	2.75	-	-	2.12	-	-	-	1.93	-	2.20
76	3.64	-	1.41	-	3.06	2.80	-	-	2.11	-	-	-	1.94	-	2.18
77	3.65	-	1.41	-	3.02	2.83	-	-	2.10	-	-	-	1.95	-	2.17
78	3.66	-	1.40	-	3.00	2.85	-	-	2.08	-	-	-	1.96	-	2.16
79	3.68	-	1.40	-	2.98	2.88	-	-	2.07	-	-	-	1.96	-	2.15
80	3.69	-	1.40	-	2.96	2.91	-	-	2.06	-	-	-	1.97	-	2.14
81	3.71	-	1.40	-	2.94	2.93	-	-	2.05	-	-	-	1.97	-	2.12
82	3.73	-	1.40	-	2.93	2.95	-	-	2.04	-	-	-	1.98	-	2.11
83	3.74	-	1.40	-	2.92	2.95	-	-	2.04	-	-	-	1.98	-	2.10
84	3.75	-	1.40	-	2.92	2.97	-	-	2.03	-	-	-	1.99	-	2.09
85	3.76	-	1.40	-	2.98	2.91	-	-	2.02	-	-	-	1.99	-	2.08
86	3.78	-	1.40	-	2.99	2.90	-	-	2.01	-	-	-	1.99	-	2.07

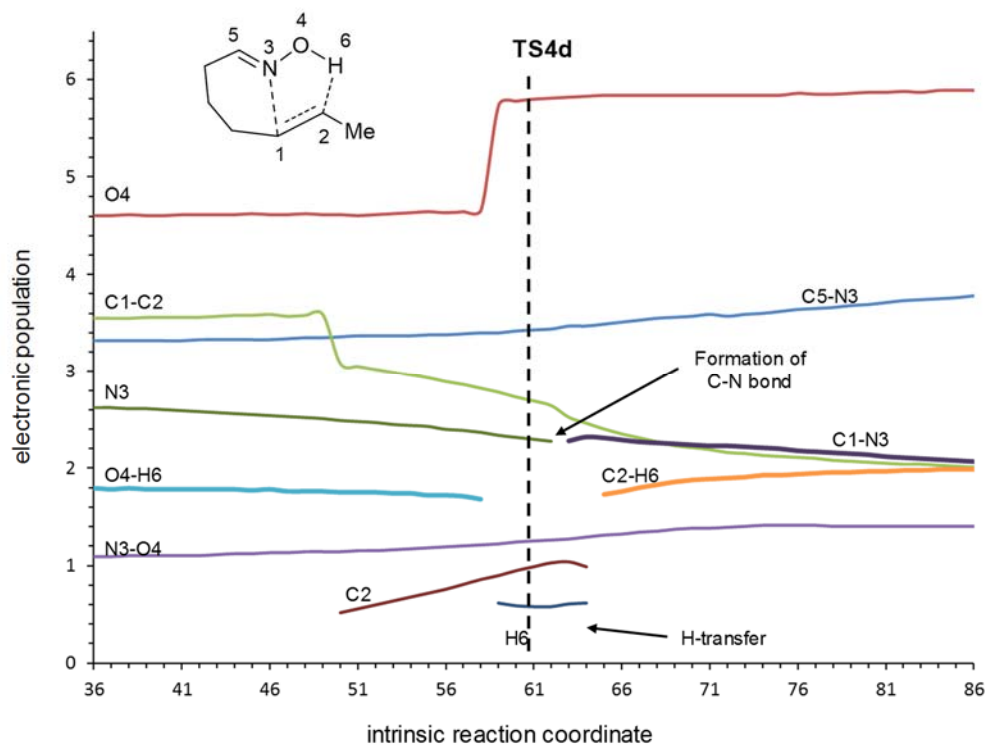


Figure S46. Graphical representation of ELF analysis for the intramolecular ene-like reaction of oxime **6d**. (only relevant points of the IRC -25 before and 25 after the TS- are listed)

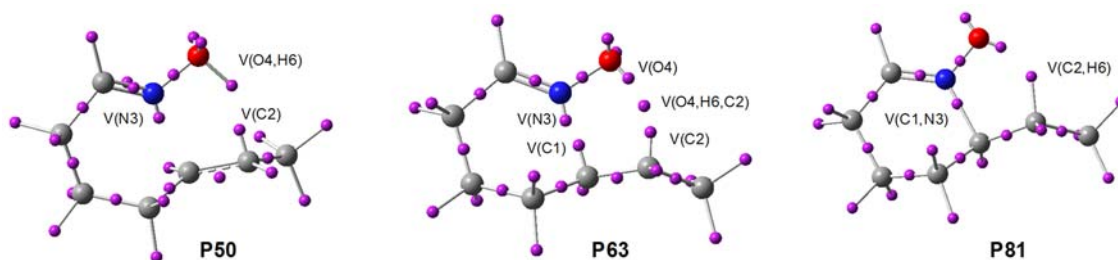


Figure S47. ELF attractor positions for the most relevant points along the intramolecular ene-like reaction of oxime **6d**.

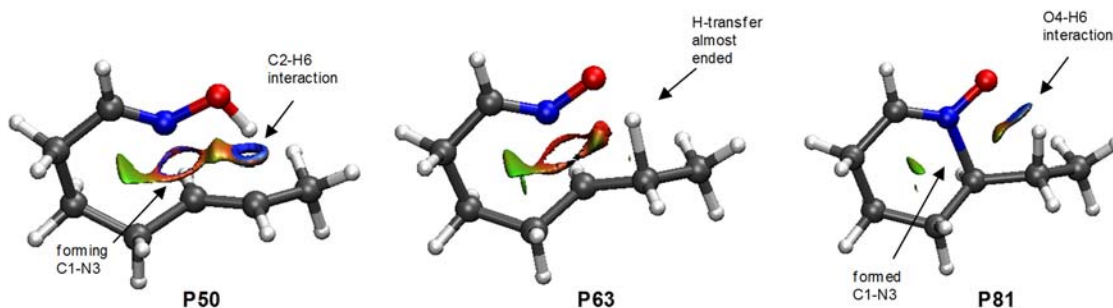


Figure S48. NCI analysis for the most relevant points along the intramolecular ene-like reaction of oxime **6d**.

Table S21. Electronic population of basins for the intramolecular ene-like reaction of oxime **6e** (only relevant points of the IRC -25 before and 25 after the TS- are listed)

IRC	V1(C5,N3)	V2(C5,N3)	V(N3,O4)	V(N3)	V1(O4)	V2(O4)	V3(O4)	V(O4,H)	V1(C1,C2)	V2(C1,C2)	V(C2)	V(O4,H6)	V(O4,H6,C2)	V(C1)	V(C1,N3)
36	1.67	1.65	1.08	2.63	2.22	2.41	-	1.79	1.83	1.86	-	-	-	-	-
37	1.67	1.65	1.09	2.62	2.22	2.41	-	1.79	1.83	1.86	-	-	-	-	-
38	1.67	1.65	1.09	2.61	2.22	2.39	-	1.79	1.84	1.86	-	-	-	-	-
39	1.67	1.65	1.09	2.61	2.22	2.40	-	1.78	1.83	1.87	-	-	-	-	-
40	1.67	1.66	1.10	2.60	2.21	2.41	-	1.78	1.84	1.87	-	-	-	-	-
41	1.67	1.65	1.10	2.60	2.22	2.40	-	1.78	1.83	1.88	-	-	-	-	-
42	1.67	1.65	1.10	2.59	2.22	2.41	-	1.77	1.83	1.88	-	-	-	-	-
43	1.67	1.65	1.11	2.58	2.22	2.41	-	1.78	1.84	1.88	-	-	-	-	-
44	1.67	1.65	1.11	2.58	2.21	2.41	-	1.78	1.84	1.89	-	-	-	-	-
45	1.67	1.65	1.11	2.58	2.22	2.41	-	1.78	1.83	1.90	-	-	-	-	-
46	1.68	1.65	1.12	2.56	2.22	2.41	-	1.77	1.84	1.90	-	-	-	-	-
47	1.68	1.65	1.13	2.55	2.22	2.42	-	1.77	1.89	1.85	-	-	-	-	-
48	1.69	1.65	1.14	2.54	2.21	2.42	-	1.76	3.73	-	-	-	-	-	-
49	1.69	1.65	1.14	2.51	2.21	2.43	-	1.75	3.74	-	-	-	-	-	-
50	1.69	1.65	1.15	2.50	2.21	2.42	-	1.75	3.16	-	0.61	-	-	-	-
51	1.69	1.66	1.15	2.49	2.21	2.43	-	1.75	3.12	-	0.65	-	-	-	-
52	1.70	1.67	1.16	2.47	2.20	2.43	-	1.75	3.08	-	0.70	-	-	-	-
53	1.70	1.67	1.16	2.46	2.20	2.44	-	1.74	3.03	-	0.75	-	-	-	-
54	1.70	1.67	1.16	2.45	2.20	2.44	-	1.74	3.00	-	0.79	-	-	-	-
55	1.71	1.67	1.17	2.44	2.21	2.44	-	1.73	2.96	-	0.84	-	-	-	-
56	1.70	1.68	1.18	2.42	2.21	2.45	-	1.72	2.92	-	0.89	-	-	-	-
57	1.71	1.68	1.19	2.40	2.21	2.46	-	1.70	2.88	-	0.94	-	-	-	-
58	1.71	1.68	1.20	2.38	2.21	2.48	-	1.68	2.83	-	0.99	-	-	-	-
59	1.72	1.68	1.21	2.35	2.21	2.51	-	1.65	2.79	-	1.04	-	-	-	-
60	1.73	1.69	1.23	2.32	2.21	2.54	1.03	-	2.75	-	1.09	0.60	-	-	-
61	1.74	1.69	1.25	2.30	2.22	2.60	0.99	-	2.70	-	1.12	0.59	-	-	-
62	1.75	1.69	1.26	-	2.21	2.66	0.94	-	2.66	-	1.15	0.59	-	-	2.27
63	1.76	1.69	1.28	-	2.20	2.74	0.88	-	2.53	-	1.17	0.61	-	0.04	2.29
64	1.76	1.71	1.29	-	2.86	2.15	0.82	-	2.47	-	1.16	0.62	-	-	2.33
65	1.78	1.71	1.31	-	3.03	2.80	-	1.72	2.42	-	-	-	1.84	-	2.30
66	1.80	1.71	1.32	-	3.20	2.62	-	-	2.37	-	-	-	1.87	-	2.29
67	1.81	1.71	1.33	-	3.34	2.51	-	-	2.33	-	-	-	1.90	-	2.27
68	1.82	1.72	1.35	-	3.39	2.46	-	-	2.29	-	-	-	1.92	-	2.27
69	1.81	1.75	1.36	-	3.37	2.48	-	-	2.26	-	-	-	1.94	-	2.24
70	1.80	1.77	1.37	-	3.33	2.52	-	-	2.24	-	-	-	1.96	-	2.23
71	1.79	1.80	1.38	-	3.25	2.59	-	-	2.21	-	-	-	1.98	-	2.22
72	1.78	1.83	1.38	-	3.20	2.65	-	-	2.19	-	-	-	1.99	-	2.21
73	3.60	-	1.39	-	3.14	2.71	-	-	2.18	-	-	-	2.00	-	2.20
74	3.62	-	1.39	-	3.09	2.76	-	-	2.16	-	-	-	2.01	-	2.19
75	3.63	-	1.39	-	3.05	2.80	-	-	2.15	-	-	-	2.01	-	2.19
76	3.64	-	1.40	-	3.02	2.84	-	-	2.14	-	-	-	2.02	-	2.17
77	3.66	-	1.40	-	2.99	2.87	-	-	2.13	-	-	-	2.03	-	2.16
78	3.68	-	1.39	-	2.97	2.90	-	-	2.12	-	-	-	2.03	-	2.15
79	3.69	-	1.39	-	2.94	2.93	-	-	2.11	-	-	-	2.04	-	2.14
80	3.70	-	1.40	-	2.92	2.96	-	-	2.10	-	-	-	2.04	-	2.12
81	3.71	-	1.40	-	2.91	2.97	-	-	2.09	-	-	-	2.05	-	2.11
82	3.73	-	1.40	-	2.90	2.97	-	-	2.08	-	-	-	2.05	-	2.10
83	3.75	-	1.40	-	2.89	2.99	-	-	2.07	-	-	-	2.05	-	2.09
84	3.77	-	1.40	-	2.88	2.99	-	-	2.07	-	-	-	2.05	-	2.07
85	3.78	-	1.40	-	2.88	3.00	-	-	2.07	-	-	-	2.05	-	2.06
86	3.79	-	1.40	-	2.88	3.01	-	-	2.06	-	-	-	2.06	-	2.06

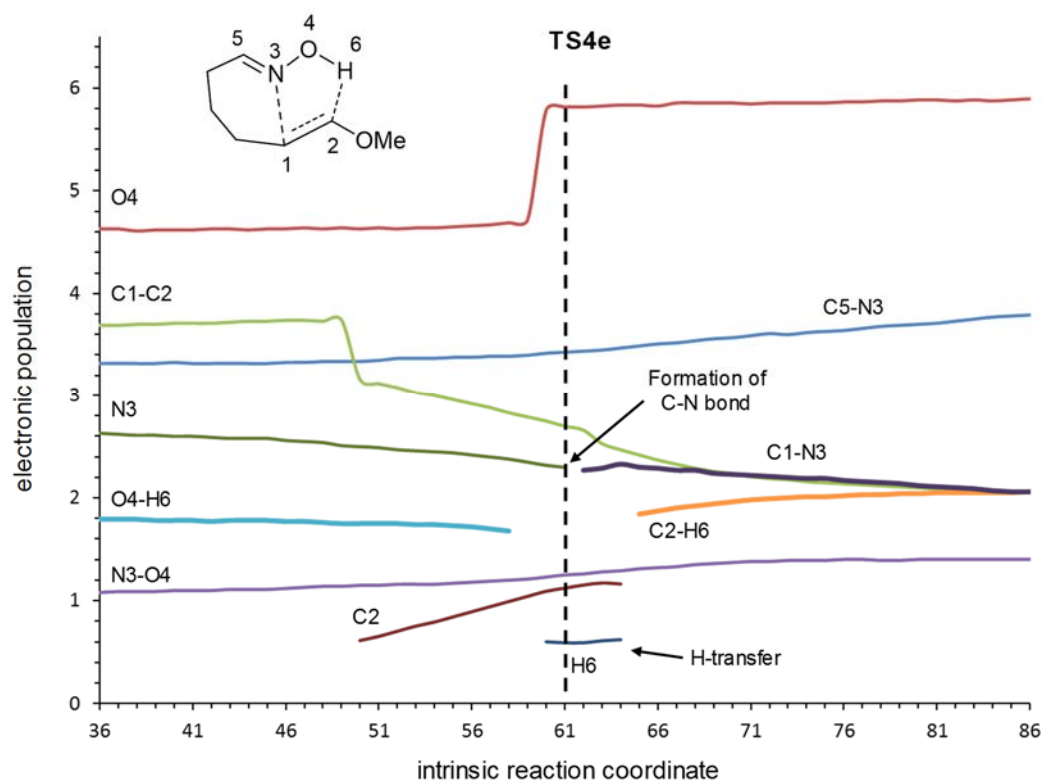


Figure S49. Graphical representation of ELF analysis for the intramolecular ene-like reaction of oxime **6e**. (only relevant points of the IRC -25 before and 25 after the TS- are listed)

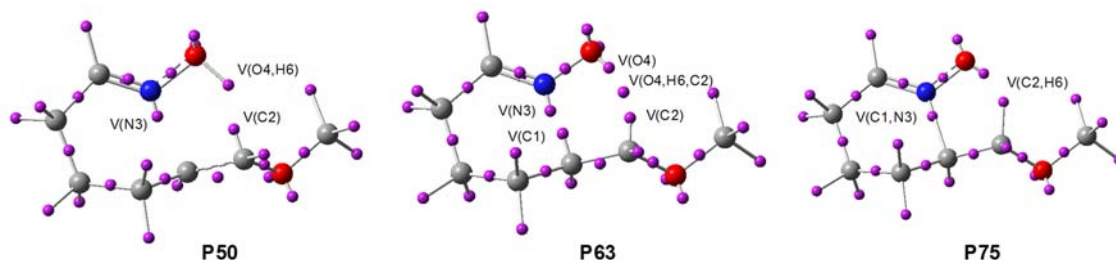


Figure S50. ELF attractor positions for the most relevant points along the intramolecular ene-like reaction of oxime **6e**.

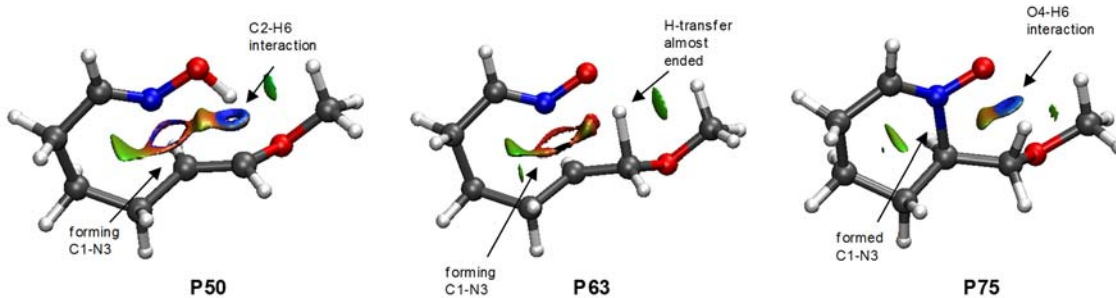


Figure S51. NCI analysis for the most relevant points along the intramolecular ene-like reaction of oxime **6e**.

Table S22. Electronic population of basins for the intramolecular ene-like reaction of oxime **6f** (only relevant points of the IRC -25 before and 25 after the TS- are listed)

IRC	V1(C5,N3)	V2(C5,N3)	V(N3,O4)	V(N3)	V1(O4)	V2(O4)	V3(O4)	V(O4,H)	V1(C1,C2)	V2(C1,C2)	V(C2)	V(O4,H6)	V(O4,H6,C2)	V(C1)	V(C1,N3)
36	1.63	1.64	1.03	2.71	2.26	2.38	-	1.78	1.76	1.65	-	-	-	-	-
37	1.63	1.64	1.03	2.71	2.26	2.38	-	1.78	1.76	1.64	-	-	-	-	-
38	1.62	1.65	1.04	2.71	2.24	2.38	-	1.78	1.76	1.64	-	-	-	-	-
39	1.63	1.65	1.05	2.70	2.24	2.37	-	1.78	1.76	1.64	-	-	-	-	-
40	1.62	1.65	1.05	2.69	2.23	2.39	-	1.79	1.77	1.63	-	-	-	-	-
41	1.63	1.65	1.05	2.67	2.24	2.38	-	1.78	1.77	1.63	-	-	-	-	-
42	1.63	1.66	1.05	2.66	2.24	2.38	-	1.78	1.77	1.62	-	-	-	-	-
43	1.63	1.66	1.06	2.66	2.23	2.38	-	1.78	1.78	1.62	-	-	-	-	-
44	1.62	1.66	1.06	2.65	2.23	2.39	-	1.79	1.78	1.61	-	-	-	-	-
45	1.62	1.66	1.07	2.64	2.23	2.39	-	1.78	1.79	1.61	-	-	-	-	-
46	1.63	1.66	1.08	2.63	2.22	2.39	-	1.78	1.79	1.61	-	-	-	-	-
47	1.63	1.66	1.08	2.60	2.22	2.39	-	1.78	1.79	1.60	-	-	-	-	-
48	1.63	1.67	1.09	2.58	2.23	2.38	-	1.78	1.77	1.63	-	-	-	-	-
49	1.64	1.68	1.09	2.56	2.22	2.39	-	1.78	1.78	1.63	-	-	-	-	-
50	1.64	1.68	1.10	2.54	2.38	2.22	-	1.79	3.38	-	-	-	-	-	-
51	1.64	1.69	1.11	2.53	2.39	2.22	-	1.78	3.40	-	-	-	-	-	-
52	1.64	1.69	1.12	2.50	2.21	2.38	-	1.78	3.04	-	0.38	-	-	-	-
53	1.65	1.69	1.12	2.47	2.22	2.38	-	1.78	3.00	-	0.43	-	-	-	-
54	1.65	1.70	1.13	2.45	2.21	2.38	-	1.78	2.96	-	0.48	-	-	-	-
55	1.65	1.70	1.14	2.44	2.20	2.39	-	1.78	2.92	-	0.53	-	-	-	-
56	1.71	1.67	1.15	-	2.21	2.39	-	1.77	2.88	-	0.58	-	-	-	2.40
57	1.71	1.68	1.15	-	2.21	2.40	-	1.77	2.81	-	0.62	-	-	-	2.41
58	1.72	1.69	1.16	-	2.22	2.40	-	1.76	2.75	-	0.67	-	-	-	2.39
59	1.73	1.71	1.17	-	2.21	2.40	-	1.76	2.69	-	0.72	-	-	-	2.37
60	1.74	1.72	1.17	-	2.20	2.41	-	1.75	2.64	-	0.77	-	-	-	2.35
61	1.75	1.75	1.18	-	2.20	2.41	-	1.75	2.57	-	0.82	-	-	-	2.32
62	1.76	1.77	1.19	-	2.43	2.19	-	1.75	2.50	-	0.88	-	-	-	2.28
63	1.79	1.78	1.21	-	2.19	2.44	-	1.74	2.32	-	0.93	-	-	-	2.25
64	1.80	1.80	1.21	-	2.17	2.47	-	1.72	2.25	-	0.99	0.56	-	-	2.22
65	1.81	1.82	1.23	-	2.15	2.52	1.15	1.72	2.20	-	1.05	0.56	-	-	2.18
66	1.82	1.85	1.24	-	2.63	2.09	1.14	-	2.16	-	1.11	0.52	-	-	2.15
67	1.84	1.88	1.27	-	2.92	1.87	1.09	-	2.12	-	1.15	0.53	-	-	2.11
68	1.89	1.86	1.30	-	4.81	1.08	-	-	2.08	-	1.10	0.65	-	-	2.09
69	1.91	1.88	1.32	-	3.50	2.41	-	-	2.05	-	-	0.65	1.79	-	2.06
70	1.92	1.90	1.34	-	3.28	2.65	-	-	2.02	-	-	-	1.84	-	2.03
71	1.92	1.92	1.36	-	3.13	2.80	-	-	2.00	-	-	-	1.88	-	2.02
72	1.93	1.93	1.37	-	3.03	2.89	-	-	1.98	-	-	-	1.90	-	2.01
73	1.94	1.93	1.38	-	2.98	2.95	-	-	1.98	-	-	-	1.91	-	2.01
74	1.94	1.94	1.38	-	2.95	2.98	-	-	1.97	-	-	-	1.93	-	2.00
75	1.95	1.94	1.39	-	2.93	3.01	-	-	1.96	-	-	-	1.94	-	2.00
76	1.96	1.94	1.39	-	2.91	3.02	-	-	1.96	-	-	-	1.95	-	2.00
77	1.97	1.94	1.38	-	2.90	3.04	-	-	1.96	-	-	-	1.96	-	2.01
78	1.97	1.94	1.39	-	2.89	3.04	-	-	1.95	-	-	-	1.97	-	2.01
79	1.96	1.95	1.40	-	2.89	3.05	-	-	1.94	-	-	-	1.97	-	2.01
80	1.96	1.96	1.40	-	2.89	3.05	-	-	1.95	-	-	-	1.97	-	2.00
81	1.95	1.96	1.40	-	2.88	3.06	-	-	1.94	-	-	-	1.98	-	2.00
82	1.94	1.98	1.40	-	2.89	3.06	-	-	1.94	-	-	-	1.98	-	2.00
83	3.89	-	1.41	-	2.89	3.05	-	-	1.94	-	-	-	1.98	-	2.01
84	3.90	-	1.41	-	2.88	3.05	-	-	1.94	-	-	-	1.98	-	2.01
85	3.90	-	1.41	-	2.89	3.05	-	-	1.94	-	-	-	1.98	-	2.01
86	3.90	-	1.42	-	2.89	3.05	-	-	1.93	-	-	-	1.99	-	2.01

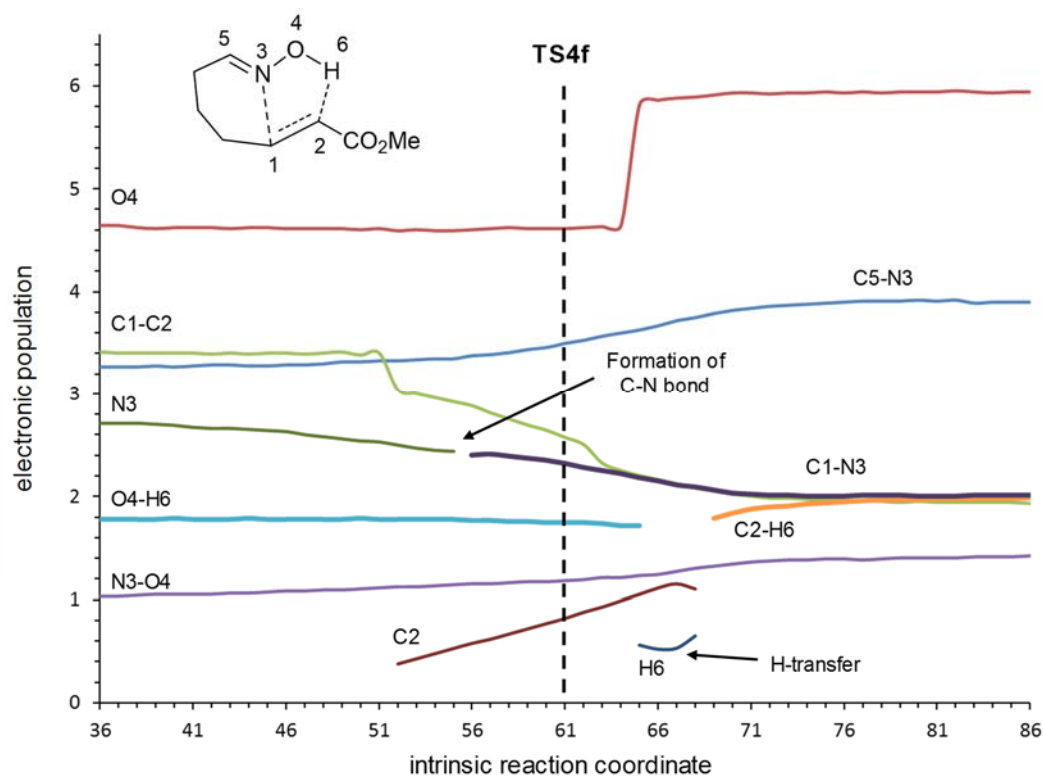


Figure S52. Graphical representation of ELF analysis for the intramolecular ene-like reaction of oxime **6f**. (only relevant points of the IRC -25 before and 25 after the TS- are listed)

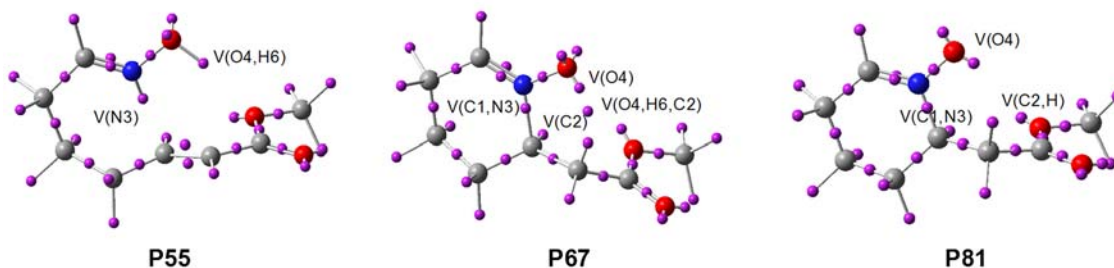


Figure S53. ELF attractor positions for the most relevant points along the intramolecular ene-like reaction of oxime **6f**.

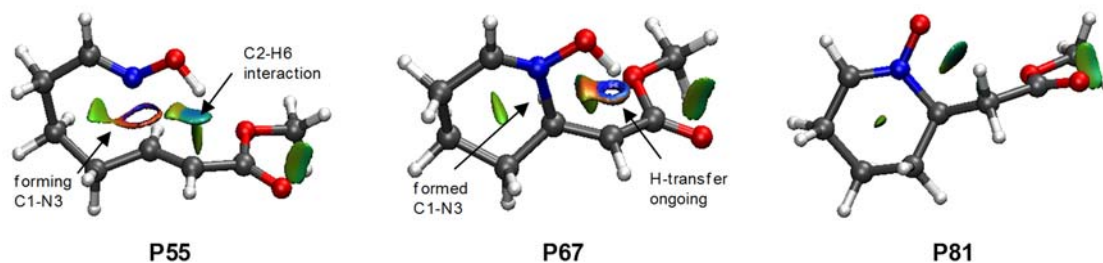


Figure S54. NCI analysis for the most relevant points along the intramolecular ene-like reaction of oxime **6f**.

Table S23. Electronic population of basins for the intramolecular ene-like reaction of oxime **6i** (only relevant points of the IRC -25 before and 25 after the TS- are listed)

IRC	V1(C5,N3)	V2(C5,N3)	V(N3,O4)	V(N3)	V1(O4)	V2(O4)	V3(O4)	V(O4,H)	V1(C1,C2)	V2(C1,C2)	V(C2)	V(O4,H6)	V(O4,H6,C2)	V(C1)	V(C1,N3)
36	1.63	1.63	1.05	2.72	2.25	2.37	-	1.78	1.78	1.73	-	-	-	-	-
37	1.63	1.64	1.05	2.71	2.26	2.37	-	1.78	1.78	1.73	-	-	-	-	-
38	1.62	1.64	1.06	2.71	2.24	2.37	-	1.78	1.79	1.72	-	-	-	-	-
39	1.62	1.65	1.06	2.70	2.25	2.38	-	1.78	1.79	1.73	-	-	-	-	-
40	1.62	1.65	1.07	2.69	2.24	2.37	-	1.78	1.80	1.72	-	-	-	-	-
41	1.63	1.65	1.07	2.68	2.24	2.38	-	1.77	1.80	1.72	-	-	-	-	-
42	1.62	1.65	1.07	2.67	2.23	2.38	-	1.78	1.79	1.73	-	-	-	-	-
43	1.62	1.65	1.07	2.66	2.23	2.38	-	1.78	1.80	1.73	-	-	-	-	-
44	1.62	1.65	1.08	2.65	2.23	2.38	-	1.78	1.79	1.73	-	-	-	-	-
45	1.62	1.66	1.09	2.64	2.38	2.23	-	1.78	1.80	1.73	-	-	-	-	-
46	1.62	1.66	1.09	2.63	2.22	2.38	-	1.78	1.80	1.73	-	-	-	-	-
47	1.63	1.66	1.10	2.62	2.22	2.39	-	1.77	1.79	1.75	-	-	-	-	-
48	1.63	1.66	1.10	2.60	2.22	2.38	-	1.78	1.79	1.75	-	-	-	-	-
49	1.63	1.67	1.11	2.59	2.21	2.39	-	1.78	3.53	-	-	-	-	-	-
50	1.63	1.67	1.12	2.57	2.22	2.39	-	1.77	3.54	-	-	-	-	-	-
51	1.64	1.67	1.12	2.55	2.21	2.40	-	1.77	3.03	-	0.54	-	-	-	-
52	1.63	1.68	1.13	2.53	2.21	2.39	-	1.76	3.00	-	0.58	-	-	-	-
53	1.64	1.67	1.14	2.52	2.21	2.40	-	1.76	2.96	-	0.63	-	-	-	-
54	1.64	1.68	1.14	2.49	2.21	2.40	-	1.76	2.92	-	0.68	-	-	-	-
55	1.65	1.68	1.15	2.47	2.21	2.40	-	1.76	2.88	-	0.72	-	-	-	-
56	1.65	1.69	1.16	2.44	2.20	2.41	-	1.75	2.85	-	0.77	-	-	-	-
57	1.66	1.69	1.17	2.42	2.20	2.41	-	1.75	2.82	-	0.82	-	-	-	-
58	1.67	1.70	1.18	-	2.20	2.42	-	1.74	2.77	-	0.87	-	-	-	2.39
59	1.68	1.70	1.19	-	2.20	2.43	-	1.73	2.74	-	0.92	-	-	-	2.36
60	1.69	1.71	1.20	-	2.19	2.43	-	1.72	2.65	-	0.97	-	-	-	2.38
61	1.70	1.72	1.21	-	2.19	2.44	-	1.71	2.59	-	1.03	-	-	-	2.37
62	1.72	1.73	1.22	-	2.19	2.46	-	1.69	2.53	-	1.08	-	-	-	2.35
63	1.74	1.74	1.24	-	2.16	2.50	1.09	-	2.46	-	1.14	0.58	-	-	2.32
64	1.75	1.76	1.26	-	1.10	2.13	2.58	-	2.39	-	1.19	0.62	-	-	2.29
65	1.78	1.77	1.28	-	2.73	2.04	1.05	1.72	2.32	-	1.22	0.54	-	-	2.25
66	1.80	1.80	1.31	-	3.08	1.75	1.01	-	2.25	-	1.22	0.58	-	-	2.21
67	1.83	1.81	1.33	-	4.78	1.08	-	-	2.19	-	-	-	1.83	-	2.18
68	1.83	1.86	1.34	-	3.49	2.38	-	-	2.14	-	-	-	1.87	-	2.14
69	1.85	1.88	1.36	-	3.28	2.59	-	-	2.10	-	-	-	1.90	-	2.11
70	1.88	1.88	1.38	-	3.13	2.73	-	-	2.07	-	-	-	1.92	-	2.07
71	1.92	1.88	1.39	-	3.06	2.80	-	-	2.05	-	-	-	1.93	-	2.05
72	1.95	1.88	1.39	-	3.00	2.88	-	-	2.02	-	-	-	1.95	-	2.03
73	1.98	1.87	1.39	-	2.97	2.91	-	-	2.01	-	-	-	1.96	-	2.02
74	2.00	1.87	1.38	-	2.94	2.95	-	-	2.00	-	-	-	1.96	-	2.01
75	2.01	1.88	1.39	-	2.93	2.97	-	-	1.99	-	-	-	1.97	-	2.00
76	2.01	1.89	1.40	-	2.90	2.98	-	-	1.98	-	-	-	1.98	-	1.99
77	2.01	1.90	1.40	-	2.90	3.00	-	-	1.97	-	-	-	1.98	-	1.99
78	2.01	1.91	1.40	-	2.88	3.02	-	-	1.96	-	-	-	1.99	-	1.99
79	2.00	1.92	1.41	-	2.88	3.02	-	-	1.95	-	-	-	1.99	-	1.99
80	2.00	1.93	1.40	-	2.89	3.03	-	-	1.95	-	-	-	1.99	-	1.99
81	1.99	1.94	1.40	-	2.89	3.03	-	-	1.95	-	-	-	2.00	-	2.00
82	1.98	1.95	1.40	-	2.89	3.03	-	-	1.94	-	-	-	2.00	-	2.00
83	1.98	1.96	1.39	-	2.89	3.04	-	-	1.94	-	-	-	2.00	-	2.00
84	1.96	1.97	1.40	-	2.89	3.03	-	-	1.94	-	-	-	2.00	-	2.00
85	3.91	-	1.41	-	2.89	3.03	-	-	1.94	-	-	-	2.00	-	2.01
86	3.91	-	1.41	-	2.89	3.03	-	-	1.94	-	-	-	2.01	-	2.00

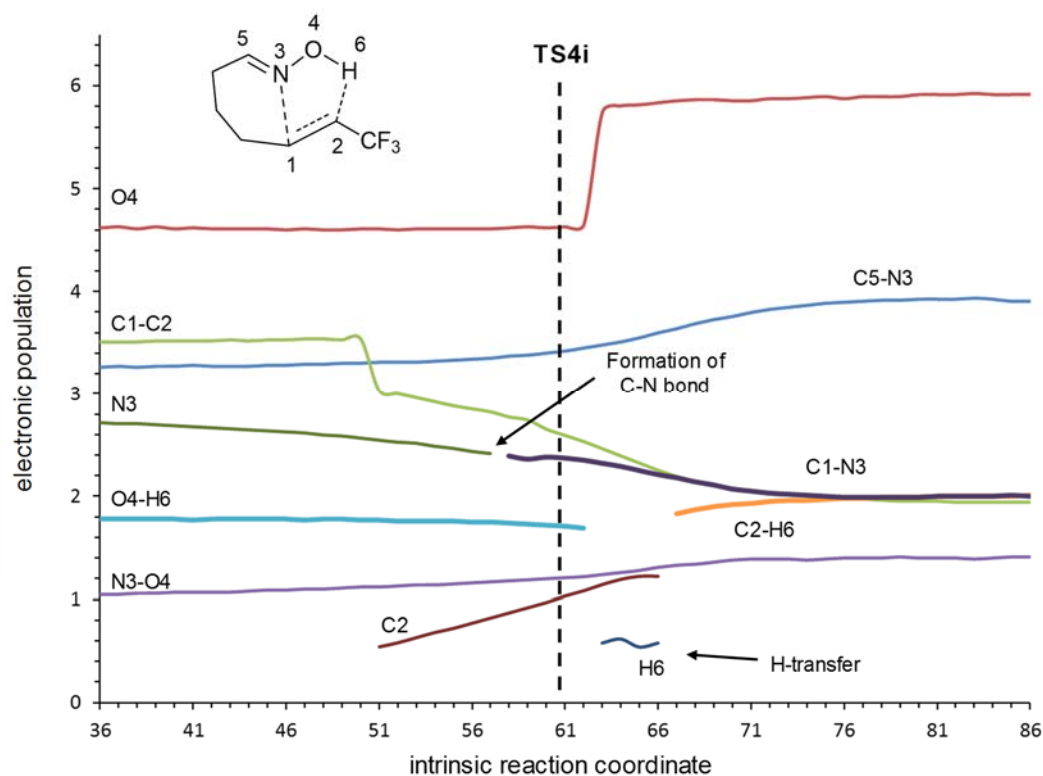


Figure S55. Graphical representation of ELF analysis for the intramolecular ene-like reaction of oxime **6i**. (only relevant points of the IRC -25 before and 25 after the TS- are listed)

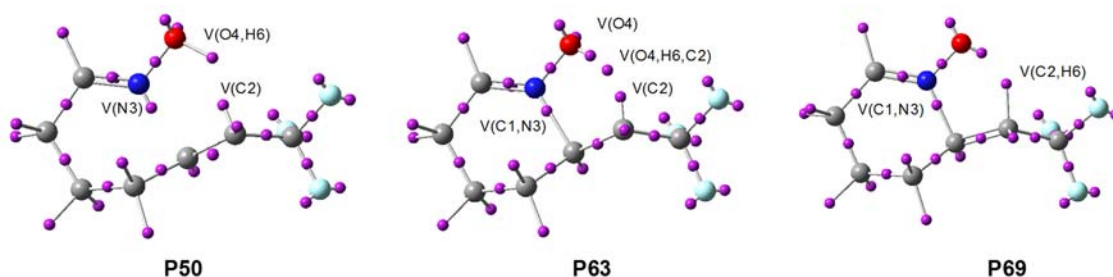


Figure S56. ELF attractor positions for the most relevant points along the intramolecular ene-like reaction of oxime **6i**.

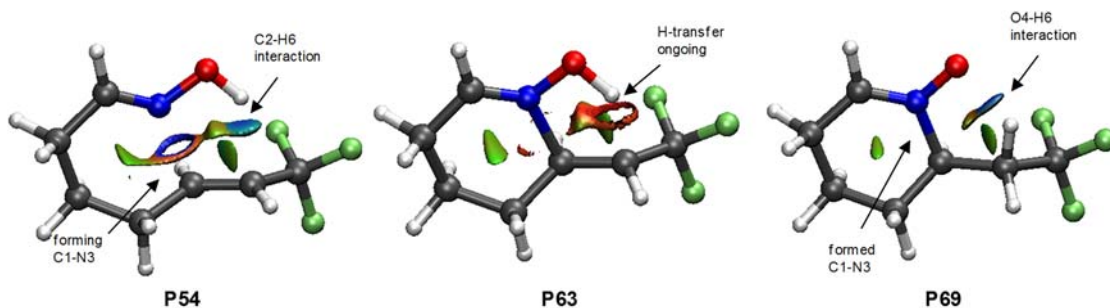


Figure S57. NCI analysis for the most relevant points along the intramolecular ene-like reaction of oxime **6i**.

Table S24. Electronic population of basins for the intramolecular ene-like reaction of oxime **6r** (only relevant points of the IRC -25 before and 25 after the TS- are listed)

IRC	V1(C5,N3)	V2(C5,N3)	V(N3,O4)	V(N3)	V1(O4)	V2(O4)	V3(O4)	V(O4,H)	V1(C1,C2)	V2(C1,C2)	V(C2)	V(O4,H6)	V(O4,H6,C2)	V(C1)	V(C1,N3)
36	1.64	1.61	1.11	2.64	2.32	2.23	-	1.80	1.70	1.71	-	-	-	-	-
37	1.64	1.62	1.11	2.63	2.33	2.24	-	1.80	1.70	1.71	-	-	-	-	-
38	1.64	1.62	1.11	2.62	2.32	2.23	-	1.80	1.70	1.71	-	-	-	-	-
39	1.64	1.62	1.12	2.61	2.32	2.23	-	1.80	1.70	1.71	-	-	-	-	-
40	1.65	1.62	1.12	2.60	2.33	2.22	-	1.80	1.70	1.71	-	-	-	-	-
41	1.66	1.61	1.12	2.60	2.34	2.22	-	1.80	1.70	1.71	-	-	-	-	-
42	1.66	1.61	1.13	2.59	2.34	2.22	-	1.80	1.70	1.71	-	-	-	-	-
43	1.66	1.61	1.14	2.58	2.34	2.22	-	1.80	1.71	1.72	-	-	-	-	-
44	1.66	1.61	1.14	2.57	2.35	2.21	-	1.80	1.71	1.72	-	-	-	-	-
45	1.67	1.61	1.14	2.56	2.35	2.21	-	1.80	1.71	1.72	-	-	-	-	-
46	1.67	1.62	1.15	2.54	2.36	2.21	-	1.80	1.71	1.72	-	-	-	-	-
47	1.67	1.62	1.15	2.53	2.36	2.20	-	1.79	1.71	1.73	-	-	-	-	-
48	1.67	1.62	1.16	2.52	2.36	2.19	-	1.79	1.70	1.74	-	-	-	-	-
49	1.68	1.62	1.17	2.51	2.37	2.19	-	1.79	1.74	1.71	-	-	-	-	-
50	1.68	1.62	1.17	2.50	2.37	2.19	-	1.78	3.43	-	-	-	-	-	-
51	1.68	1.63	1.17	2.49	2.37	2.19	-	1.78	3.45	-	-	-	-	-	-
52	1.68	1.63	1.18	2.48	2.38	2.18	-	1.77	3.46	-	-	-	-	-	-
53	1.68	1.63	1.19	2.45	2.38	2.17	-	1.77	3.02	-	0.46	-	-	-	-
54	1.68	1.63	1.19	2.44	2.40	2.17	-	1.76	2.98	-	0.51	-	-	-	-
55	1.69	1.63	1.20	2.43	2.40	2.16	-	1.76	2.95	-	0.56	-	-	-	-
56	1.69	1.64	1.21	2.41	2.40	2.16	-	1.75	2.91	-	0.61	-	-	-	-
57	1.69	1.65	1.22	2.39	2.40	2.16	-	1.74	2.87	-	0.66	-	-	-	-
58	1.69	1.65	1.22	2.37	2.41	2.16	-	1.74	2.83	-	0.71	-	-	-	-
59	1.70	1.66	1.23	2.35	2.43	2.15	-	1.73	2.78	-	0.77	-	-	-	-
60	1.70	1.66	1.24	2.34	2.46	2.15	-	1.69	2.73	-	0.84	-	-	-	-
61	1.69	1.68	1.26	2.31	2.51	2.12	1.10	-	2.68	-	0.90	0.58	-	-	-
62	1.70	1.69	1.28	-	2.59	2.08	1.09	-	2.61	-	0.95	0.56	-	-	2.30
63	1.69	1.70	1.29	-	2.70	1.99	1.07	-	2.50	-	1.00	0.56	-	-	2.33
64	1.69	1.71	1.32	-	4.70	1.06	-	-	2.43	-	1.03	0.56	-	-	2.32
65	1.70	1.71	1.33	-	4.71	1.06	-	-	2.37	-	0.99	0.66	-	-	2.31
66	1.74	1.69	1.34	-	4.69	1.09	-	-	2.32	-	-	-	1.69	-	2.30
67	1.78	1.66	1.36	-	4.59	1.19	-	-	2.27	-	-	-	1.74	-	2.29
68	3.44	-	1.38	-	4.33	1.46	-	-	2.22	-	-	-	1.77	-	2.28
69	3.46	-	1.39	-	3.48	2.31	-	-	2.18	-	-	-	1.81	-	2.27
70	3.47	-	1.41	-	3.31	2.49	-	-	2.15	-	-	-	1.84	-	2.25
71	3.48	-	1.42	-	3.18	2.61	-	-	2.12	-	-	-	1.86	-	2.24
72	3.50	-	1.42	-	3.10	2.70	-	-	2.10	-	-	-	1.89	-	2.23
73	3.51	-	1.42	-	3.03	2.75	-	-	2.08	-	-	-	1.90	-	2.22
74	3.53	-	1.43	-	2.98	2.79	-	-	2.07	-	-	-	1.91	-	2.20
75	3.56	-	1.43	-	2.95	2.82	-	-	2.05	-	-	-	1.92	-	2.19
76	3.57	-	1.43	-	2.93	2.85	-	-	2.04	-	-	-	1.93	-	2.18
77	3.58	-	1.43	-	2.92	2.89	-	-	2.02	-	-	-	1.94	-	2.16
78	3.61	-	1.44	-	2.91	2.90	-	-	2.01	-	-	-	1.94	-	2.15
79	3.62	-	1.44	-	2.89	2.92	-	-	2.00	-	-	-	1.95	-	2.14
80	3.63	-	1.44	-	2.89	2.92	-	-	1.99	-	-	-	1.96	-	2.13
81	3.65	-	1.43	-	2.88	2.93	-	-	1.98	-	-	-	1.96	-	2.11
82	3.67	-	1.43	-	2.88	2.94	-	-	1.97	-	-	-	1.96	-	2.09
83	3.69	-	1.43	-	2.87	2.95	-	-	1.97	-	-	-	1.97	-	2.08
84	3.71	-	1.43	-	2.87	2.96	-	-	1.96	-	-	-	1.97	-	2.07
85	3.73	-	1.43	-	2.87	2.96	-	-	1.95	-	-	-	1.98	-	2.06
86	3.74	-	1.43	-	2.86	2.96	-	-	1.95	-	-	-	1.98	-	2.05

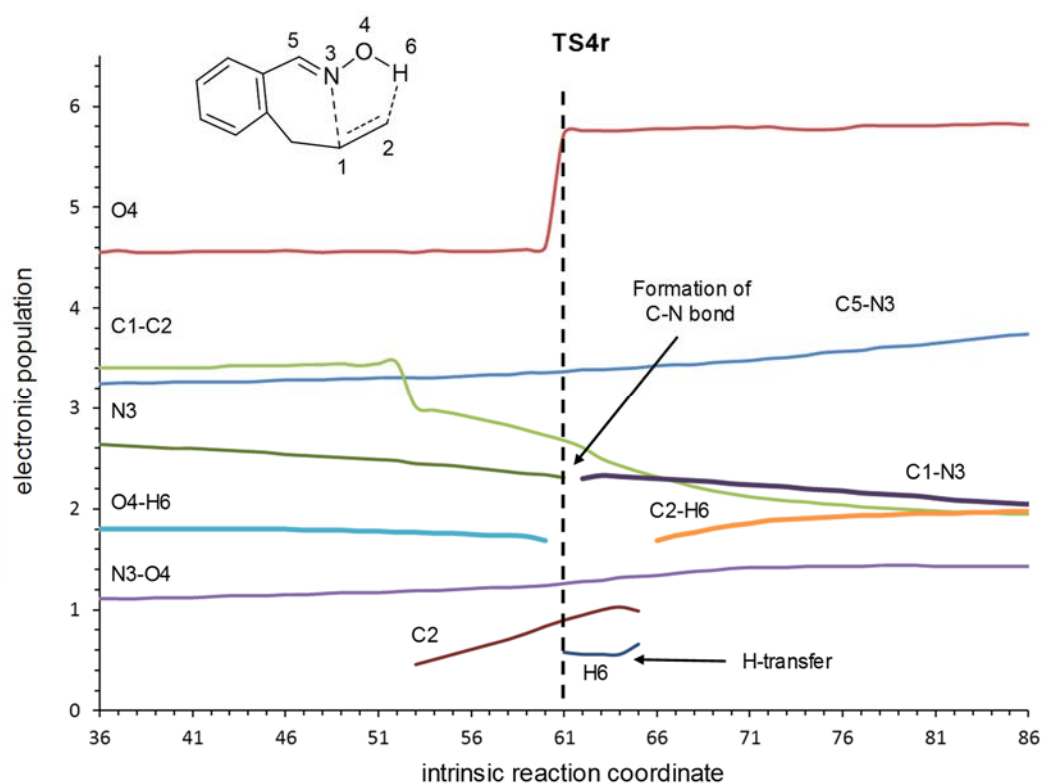


Figure S58. Graphical representation of ELF analysis for the intramolecular ene-like reaction of oxime **6r**. (only relevant points of the IRC -25 before and 25 after the TS- are listed)

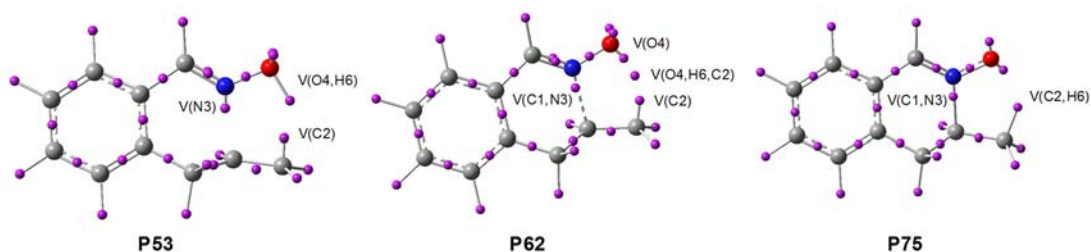


Figure S59. ELF attractor positions for the most relevant points along the intramolecular ene-like reaction of oxime **6r**.

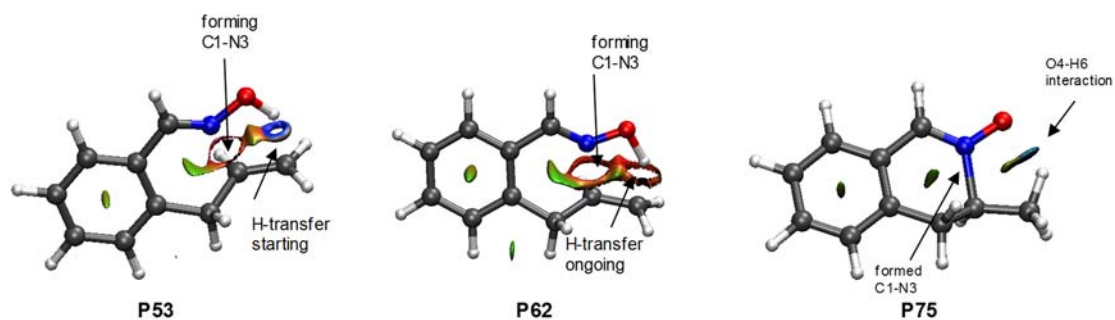


Figure S60. NCI analysis for the most relevant points along the intramolecular ene-like reaction of oxime **6r**.

Table S25. Electronic population of basins for the intramolecular ene-like reaction of oxime **6u** (only relevant points of the IRC -25 before and 25 after the TS- are listed)

IRC	V1(C5,N3)	V2(C5,N3)	V(N3,O4)	V(N3)	V1(O4)	V2(O4)	V3(O4)	V(O4,H)	V1(C1,C2)	V2(C1,C2)	V(C2)	V(O4,H6)	V(O4,H6,C2)	V(C1)	V(C1,N3)
35	1.64	1.70	1.10	2.61	2.28	2.32	-	1.79	1.74	1.65	-	-	-	-	-
36	1.64	1.70	1.10	2.60	2.27	2.32	-	1.79	1.74	1.65	-	-	-	-	-
37	1.64	1.71	1.10	2.58	2.25	2.32	-	1.80	1.74	1.65	-	-	-	-	-
38	1.65	1.71	1.11	2.58	2.26	2.32	-	1.79	1.74	1.65	-	-	-	-	-
39	1.65	1.71	1.11	2.57	2.26	2.32	-	1.79	1.74	1.65	-	-	-	-	-
40	1.65	1.71	1.12	2.56	2.26	2.32	-	1.79	1.74	1.65	-	-	-	-	-
41	1.65	1.71	1.12	2.55	2.26	2.32	-	1.79	1.74	1.65	-	-	-	-	-
42	1.66	1.71	1.12	2.54	2.26	2.32	-	1.79	1.74	1.64	-	-	-	-	-
43	1.66	1.72	1.13	2.53	2.25	2.32	-	1.79	1.75	1.64	-	-	-	-	-
44	1.66	1.72	1.13	2.52	2.25	2.33	-	1.78	1.75	1.65	-	-	-	-	-
45	1.66	1.72	1.13	2.51	2.25	2.33	-	1.78	1.76	1.64	-	-	-	-	-
46	1.66	1.72	1.14	2.50	2.25	2.33	-	1.78	1.76	1.64	-	-	-	-	-
47	1.66	1.72	1.14	2.49	2.25	2.34	-	1.78	1.76	1.66	-	-	-	-	-
48	1.67	1.72	1.15	2.48	2.25	2.34	-	1.78	3.40	-	-	-	-	-	-
49	1.67	1.73	1.16	2.46	2.25	2.34	-	1.78	3.40	-	-	-	-	-	-
50	1.68	1.73	1.16	2.44	2.25	2.34	-	1.77	3.41	-	-	-	-	-	-
51	1.68	1.73	1.17	2.43	2.25	2.34	-	1.77	3.42	-	-	-	-	-	-
52	1.68	1.73	1.17	2.41	2.25	2.34	-	1.76	3.43	-	-	-	-	-	-
53	1.68	1.74	1.18	2.40	2.25	2.34	-	1.75	3.02	-	0.43	-	-	-	-
54	1.73	1.69	1.18	2.39	2.26	2.34	-	1.75	2.98	-	0.48	-	-	-	-
55	1.74	1.69	1.19	2.36	2.26	2.35	-	1.74	2.95	-	0.53	-	-	-	-
56	1.74	1.69	1.20	2.35	2.26	2.35	-	1.74	2.92	-	0.58	-	-	-	-
57	1.75	1.70	1.21	2.33	2.26	2.35	-	1.73	2.87	-	0.63	-	-	-	-
58	1.75	1.70	1.21	2.31	2.27	2.36	-	1.72	2.84	-	0.69	-	-	-	-
59	1.76	1.70	1.22	2.29	2.27	2.37	-	1.70	2.79	-	0.75	-	-	-	-
60	1.76	1.71	1.23	2.26	2.28	2.38	-	1.68	2.74	-	0.81	-	-	-	-
61	1.77	1.71	1.25	-	2.28	2.41	1.06	1.67	2.69	-	0.88	0.59	-	-	2.24
62	1.78	1.72	1.26	-	2.28	2.44	1.06	-	2.58	-	0.94	0.57	-	0.02	2.24
63	1.79	1.73	1.28	-	2.26	2.51	1.03	-	2.50	-	0.99	0.56	-	-	2.26
64	1.80	1.74	1.30	-	2.24	2.58	0.98	-	2.43	-	1.03	0.56	-	-	2.25
65	1.80	1.75	1.31	-	2.08	2.77	0.95	-	2.37	-	1.00	0.66	-	-	2.24
66	1.82	1.76	1.34	-	4.82	0.97	-	-	2.31	-	-	-	1.70	-	2.22
67	1.83	1.76	1.37	-	4.77	1.02	-	-	2.26	-	-	-	1.74	-	2.20
68	1.84	1.77	1.38	-	4.66	1.16	-	-	2.20	-	-	-	1.78	-	2.18
69	1.85	1.78	1.39	-	4.37	1.44	-	-	2.16	-	-	-	1.82	-	2.17
70	1.86	1.79	1.40	-	2.19	3.63	-	-	2.13	-	-	-	1.85	-	2.15
71	1.87	1.80	1.40	-	2.48	3.34	-	-	2.11	-	-	-	1.87	-	2.14
72	1.88	1.80	1.41	-	2.65	3.18	-	-	2.09	-	-	-	1.89	-	2.13
73	1.89	1.81	1.41	-	2.73	3.09	-	-	2.06	-	-	-	1.90	-	2.11
74	1.90	1.82	1.41	-	2.80	3.03	-	-	2.05	-	-	-	1.92	-	2.10
75	1.91	1.82	1.42	-	2.85	2.98	-	-	2.03	-	-	-	1.93	-	2.09
76	1.92	1.83	1.42	-	2.89	2.95	-	-	2.02	-	-	-	1.94	-	2.08
77	1.93	1.84	1.42	-	2.91	2.94	-	-	2.01	-	-	-	1.94	-	2.07
78	1.93	1.85	1.42	-	2.93	2.93	-	-	1.99	-	-	-	1.95	-	2.06
79	1.93	1.87	1.42	-	2.94	2.92	-	-	1.99	-	-	-	1.96	-	2.05
80	1.93	1.89	1.41	-	2.95	2.91	-	-	1.98	-	-	-	1.96	-	2.04
81	1.91	1.93	1.41	-	2.97	2.90	-	-	1.97	-	-	-	1.97	-	2.03
82	1.93	1.92	1.41	-	2.98	2.89	-	-	1.96	-	-	-	1.97	-	2.02
83	1.93	1.93	1.41	-	2.98	2.89	-	-	1.95	-	-	-	1.98	-	2.01
84	1.93	1.94	1.41	-	2.99	2.89	-	-	1.95	-	-	-	1.98	-	2.01
85	1.96	1.92	1.42	-	3.00	2.88	-	-	1.94	-	-	-	1.98	-	2.00

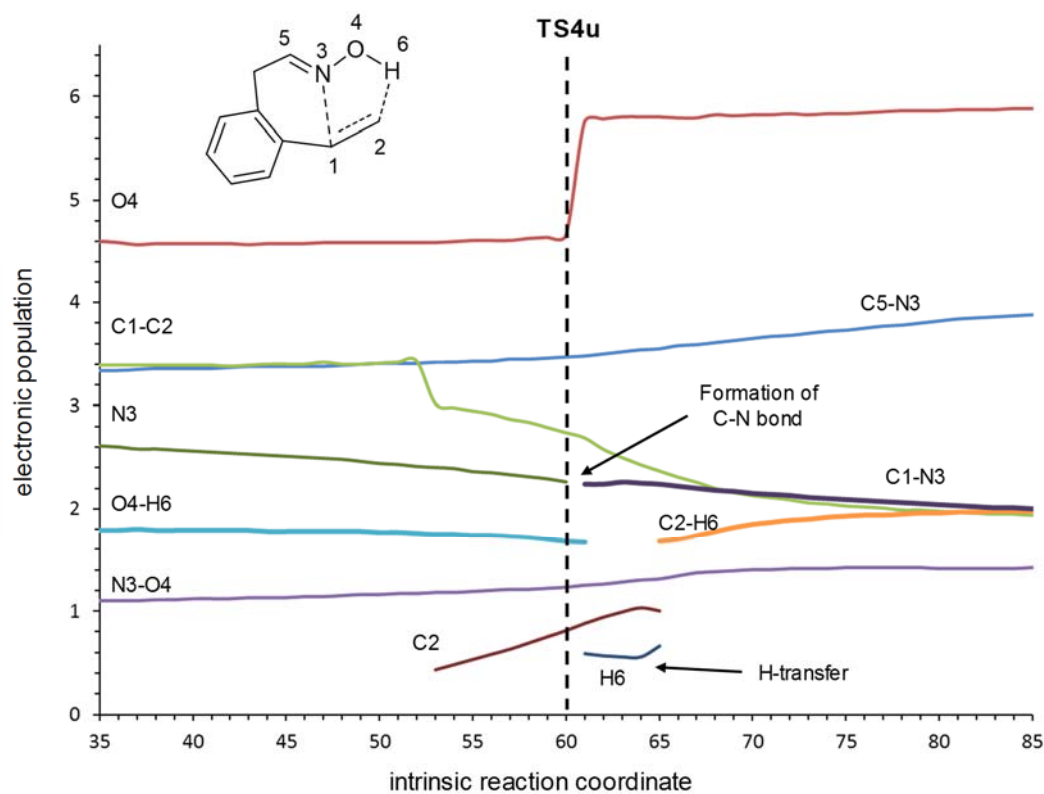


Figure S61. Graphical representation of ELF analysis for the intramolecular ene-like reaction of oxime **6u**. (only relevant points of the IRC -25 before and 25 after the TS- are listed)

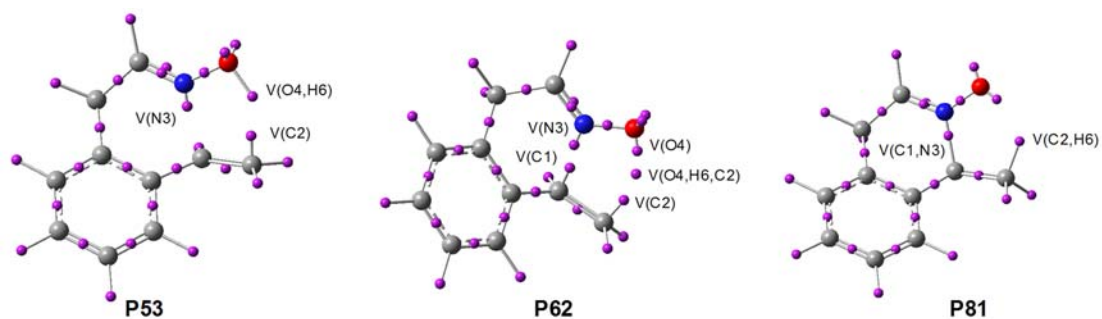


Figure S62. ELF attractor positions for the most relevant points along the intramolecular ene-like reaction of oxime **6u**.

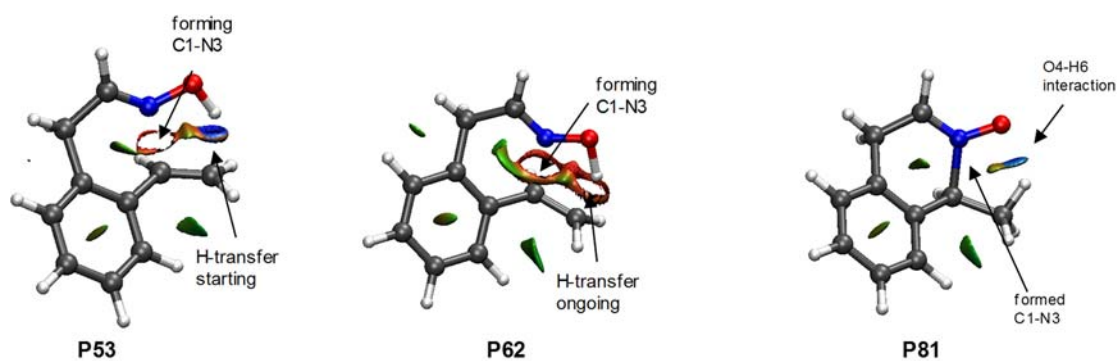


Figure S63. NCI analysis for the most relevant points along the intramolecular ene-like reaction of oxime **6u**.

Cartesian coordinates

Intermolecular reactions

1aE

0 1

N	-1.2894668804	-0.7996060099	0.0518462114
O	-0.9303013359	-1.9299577826	-0.6741134407
H	-0.0220034117	-2.0848305659	-0.4054664968
C	-2.4807966349	-0.4549296924	-0.1903362832
C	-3.0663032376	0.73636014	0.4860719994
H	-3.0780329452	-1.0319958714	-0.8954343505
H	-3.9472026498	0.4532552228	1.0637217795
H	-2.3326733611	1.1860592388	1.1504588112
H	-3.384288541	1.4758593246	-0.2500242355

1aZ

0 1

N	-0.5446926631	-0.481640432	-0.0002837553
O	-1.0604936914	-0.8109886322	1.249279632
H	-1.7625660849	-1.4284293065	1.0333283499
C	0.4313006404	0.3219836702	0.0760682619
C	1.0345504337	0.9014921625	1.3128368639
H	0.8392221233	0.5958522895	-0.8908019091
H	0.7488824875	1.9506385157	1.40890204
H	0.701585743	0.3686339147	2.1974055403
H	2.1213654615	0.8651867882	1.2486911464

1bE

0 1

N	-1.3012769724	0.7246446208	-0.1373097029
O	-0.277171342	1.6080975502	-0.4287817407
C	-2.4368405074	1.26339598	-0.298454578
H	0.5164782851	1.0908457502	-0.2713698462
C	-3.6772453496	0.5212757896	-0.0500120743
C	-4.8955701016	1.1651778329	-0.2438955046
C	-3.6683594813	-0.8084900732	0.3740734171
C	-6.0904872128	0.4962766058	-0.0192366479
H	-4.90527688	2.1969659373	-0.5729285558
C	-4.8599474655	-1.4731658075	0.5973572562
H	-2.7199097819	-1.3052524699	0.5235661655
C	-6.0747704925	-0.8238842989	0.4017269233
H	-7.0310673828	1.0071122726	-0.1732994839
H	-4.8462080853	-2.5035318658	0.9258976825
H	-7.0039791239	-1.3483664973	0.5778091359
H	-2.505390106	2.2993636732	-0.6282714464

1bZ

0 1

N	-1.3085931002	0.6855911958	-0.3963663695
O	-0.4182923245	0.6664769305	0.6621465769
C	-2.4414626879	1.1903974584	-0.1166112619
H	0.362795469	0.2618980434	0.2775678655
C	-3.0050538456	1.7639822805	1.1143408604
C	-4.3211483075	2.2271765493	1.0216354925
C	-2.341920164	1.8789864098	2.3410100164
C	-4.9636260581	2.7882869371	2.1108625324
H	-4.8433637482	2.1428219922	0.0767350581

C	-2.9898106167	2.441952861	3.4297574659
H	-1.3289682739	1.5305672235	2.4398328364
C	-4.2959226441	2.8971656771	3.3225417017
H	-5.9818323784	3.1397304436	2.0156878162
H	-2.4657009893	2.5248638196	4.3722511656
H	-4.7908736178	3.3345542123	4.1790250916
H	-3.1074405529	1.185500186	-0.9734892781

1c

0 1

N	-0.466828802	-0.5231560268	0.1879865698
O	-1.7553244814	-0.0463644244	0.3556460665
H	-2.2721253654	-0.8526872163	0.4249851276
C	0.4088198368	0.3996016025	0.0924099909
C	0.1091615106	1.8561731365	0.1121163133
C	0.7937099189	2.68690043	0.9953979712
C	-0.8267568226	2.4092164786	-0.7573249146
C	0.5370064558	4.0492459572	1.0192504976
H	1.5296747403	2.259937404	1.6647751056
C	-1.0688240113	3.7738649272	-0.7455500108
H	-1.3627663953	1.7645890564	-1.439066325
C	-0.3913112206	4.5957203934	0.1447347504
H	1.0660165154	4.6844601805	1.7165998927
H	-1.7904103364	4.1966441557	-1.4312823598
H	-0.5857010749	5.6596473744	0.155529682
C	1.8181148358	-0.0505801351	-0.0464266214
C	2.7588333237	0.761218018	-0.6765647998
C	2.2143570643	-1.2997151326	0.4322579613
C	4.067399895	0.3284831969	-0.8357921686
H	2.4623114438	1.7313741869	-1.0520918403
C	3.5209363494	-1.7276812528	0.2749999832
H	1.4845029482	-1.9242651484	0.9271947367
C	4.4523758666	-0.9153366766	-0.3602614208
H	4.7859643905	0.9653029269	-1.3336280139
H	3.8176575079	-2.6961539418	0.6544351567
H	5.4735831069	-1.2508760304	-0.4803632806

1d

0 1

N	0.1595500182	1.9234305921	0.7838884842
O	-1.0280184749	2.4940517958	1.2319195929
H	-0.7171936772	3.2911417808	1.6666888734
C	0.0524229379	0.8193355417	0.1559911218
C	-1.2985268369	0.1227512496	-0.1107166526
C	-1.2422229621	-1.1246807249	-1.0041790849
C	-1.8793592297	-0.3155306921	1.2456257803
C	-2.2675888795	1.0820313942	-0.8294521253
H	-1.0047874756	-0.8749093805	-2.0363964717
H	-0.5488709097	-1.8860399147	-0.657865284
H	-2.2380669166	-1.5701972115	-1.0010445016
H	-1.9665235864	0.5190963758	1.934967072
H	-2.871145951	-0.7444448566	1.0902028549
H	-1.2486615954	-1.0814558234	1.7006813959
H	-3.1679200814	0.5272803005	-1.0998461169
H	-2.5524684908	1.9285629713	-0.2177954974
H	-1.8167513371	1.4544034806	-1.7511960378
C	1.4314773955	0.22547467	-0.1954569896
C	1.6964008167	-0.9888522532	0.7085355029
C	1.5539833551	-0.1687713678	-1.6780610076
C	2.5465785495	1.2423475494	0.0840747156

H	1.7172470948	-0.6796812981	1.7543837986
H	0.9496238694	-1.772391774	0.6033594027
H	2.6682363859	-1.4201296634	0.4607882819
H	1.1151977739	0.5926671653	-2.3256220297
H	2.6108886138	-0.2499637383	-1.9339657329
H	1.0947127982	-1.1245631739	-1.9072361567
H	3.5045827367	0.7775273099	-0.1530051043
H	2.4300284632	2.1337443283	-0.5314540781
H	2.5578003856	1.5545216375	1.1248317644

2aE

0 1

N	0.7603121908	0.399339219	-0.1731196548
O	1.2805309744	-0.7454275574	-0.1162317782
C	-0.4240589602	0.7696835553	0.1853687692
H	1.3566916472	1.1443864793	-0.5569315482
C	-0.875546924	2.1795421825	0.0452293235
H	-1.151082457	2.6030640128	1.0120412526
H	-0.088103135	2.8010163534	-0.3824522928
H	-1.7501422344	2.2507454385	-0.6028605846
H	-1.051537302	-0.0120159734	0.5887097634

2aZ

0 1

N	0.686075082	0.1771726911	-0.0522203276
O	0.3651420397	-0.9967163971	-0.3847454582
C	1.8737528664	0.6011791031	0.2302239529
H	1.9606710202	1.6433239382	0.4954813872
C	3.005808591	-0.3534122439	0.1707629458
H	3.0747922897	-0.7847099369	-0.8300846512
H	3.9430143481	0.1305797574	0.42858791
H	2.8219709653	-1.1893233512	0.8489646781
H	-0.0745627725	0.8618968194	-0.0018517071

2bE

0 1

N	1.1401525554	-0.9031083817	-0.4005986603
O	0.0414983551	-1.4982216542	-0.5231562089
C	2.2856091422	-1.3971053821	-0.0449703994
H	1.1333781818	0.0994411291	-0.6227187708
C	3.4892493761	-0.5858537075	0.075212258
C	4.7313763145	-1.2180920104	-0.0119304712
C	3.4568597849	0.7963779087	0.2839291415
C	5.9050595822	-0.4886218966	0.0767126795
H	4.7687374653	-2.2895772271	-0.1612300333
C	4.6319043622	1.5241671283	0.361046373
H	2.5132839706	1.3088302768	0.4232481807
C	5.8608786955	0.88672535	0.2552201142
H	6.8575359692	-0.9954176388	0.0033682926
H	4.5886122212	2.5923055379	0.5243142106
H	6.7768756292	1.4565983397	0.3243931686
H	2.2983183947	-2.4637077721	0.1275661251

2bZ

0 1

N	1.0826748836	-0.9440787517	-0.3565151004
O	0.1029108366	-0.7438036527	0.409354633
C	2.2945616346	-1.3145328993	-0.0666111919
H	0.9025646269	-0.7943416541	-1.3540081335
C	2.810074497	-1.5914552559	1.2588004973

C	4.1529915105	-1.9788458613	1.3503697721
C	2.0501455954	-1.4939307026	2.4310388211
C	4.726878436	-2.2621657513	2.5746043735
H	4.7456283987	-2.0560211081	0.4470860494
C	2.636437576	-1.7806932919	3.6546259621
H	1.0167085412	-1.1962778098	2.3651523397
C	3.9670119831	-2.163373922	3.734190455
H	5.7650693584	-2.5598776209	2.6278577878
H	2.043145054	-1.7031324229	4.5555944452
H	4.4123688254	-2.3842642958	4.6946896838
H	2.9468474527	-1.4136598696	-0.9220314143

2c

0 1

N	0.8272245625	0.4634662264	0.1978127985
O	1.4731961513	-0.6188168081	0.1961725061
C	-0.4579889972	0.6730663127	0.0758497704
H	1.3857108127	1.3154016914	0.3186649742
C	-0.878823112	2.090950792	0.0870747007
C	-1.9378109876	2.504176785	0.8976232358
C	-0.2116292462	3.0410087814	-0.685438495
C	-2.3052954385	3.837483207	0.945810439
H	-2.4632045729	1.7708447054	1.4953814492
C	-0.5774253169	4.3788953725	-0.6302916858
H	0.5775106893	2.7258154683	-1.3567416053
C	-1.6235474206	4.7800796823	0.1852107102
H	-3.1219397186	4.145406445	1.5844027542
H	-0.0537104863	5.1032016011	-1.2389622446
H	-1.9133795049	5.8210814137	0.224864753
C	-1.4210454998	-0.4257647942	-0.0515374974
C	-2.659039932	-0.1728436046	-0.6528521528
C	-1.1489019319	-1.7176033498	0.4123433822
C	-3.5995096307	-1.1786182945	-0.7876524936
H	-2.8786871982	0.8180311164	-1.0264976412
C	-2.1034545941	-2.7149951012	0.2872485201
H	-0.1899069931	-1.9306145944	0.8556032408
C	-3.3263274721	-2.454479919	-0.3129750752
H	-4.5464687041	-0.9656943759	-1.2645534856
H	-1.883309754	-3.7074248363	0.656725999
H	-4.0614202638	-3.2414544623	-0.4138949968

2d

0 1

N	-0.0937961393	2.0663126138	-0.3256295133
O	-1.1149298867	2.8284631727	-0.3540801539
C	-0.0084020618	0.7874491853	-0.1018251634
H	0.7848852758	2.5507665718	-0.4969463559
C	1.4069576	0.2073968178	-0.0066009258
C	1.7173773187	-0.1373221857	1.460227197
C	1.5827414681	-1.0404910624	-0.8904260904
C	2.4807576301	1.2111039429	-0.4591150919
H	1.695819547	0.7632036939	2.0752746984
H	1.0096568079	-0.8468921395	1.8802365374
H	2.7140693883	-0.5773249644	1.5298436903
H	1.1796120119	-0.8730615692	-1.8903701714
H	2.6464168975	-1.2607904814	-0.9888859884
H	1.1100365597	-1.921312999	-0.4698344255
H	3.4543273661	0.7294145168	-0.3812742996
H	2.3461629973	1.5142546956	-1.499325454
H	2.5236101263	2.0992485899	0.1742857484

C	-1.3253350254	0.0518332589	0.1608961116
C	-2.29058104	0.2937972379	-1.0150882624
C	-1.2232645381	-1.4703987443	0.3093878963
C	-1.9181217697	0.6134508598	1.4662918952
H	-2.4929185753	1.3494508537	-1.1590463352
H	-1.8716041887	-0.1186687192	-1.9350779294
H	-3.2280422479	-0.226827695	-0.8121710637
H	-0.5286656965	-1.7957286242	1.0804272916
H	-2.211853577	-1.8320283197	0.5947968736
H	-0.9631086955	-1.9547838342	-0.6296937513
H	-2.9070091335	0.1813361655	1.6279943453
H	-1.2885372049	0.3443395789	2.316782478
H	-2.0127489443	1.695376433	1.4166465222

3a

0 1

C	2.3102493999	-0.64311363	1.0198089203
C	2.6149879626	0.0759193219	-0.0487872598
H	2.8315673903	-1.5612828489	1.2533819747
C	1.9408048336	1.3533513686	-0.4372528125
H	2.6585879783	2.1742700869	-0.4850100244
H	1.4883260816	1.2701670511	-1.4270734129
H	1.1618248147	1.6179847841	0.2764501265
H	1.5245408908	-0.3339170105	1.699088491
H	3.4088626479	-0.2684311232	-0.7044740028

3b

0 1

C	2.3721011913	1.3681006654	-0.683619755
C	2.2071990723	0.2499281466	0.0038734775
H	2.9367480428	2.1803234763	-0.255237448
H	1.9545839833	1.4797175974	-1.6736726331
H	2.6170193355	0.1190497424	1.0021942607
O	1.533533877	-0.8172201756	-0.487597695
C	1.296889103	-1.8535949276	0.4423320332
H	0.638374569	-1.5172771721	1.2467908088
H	0.8159561489	-2.6631600254	-0.0990092059
H	2.2340216769	-2.2165113272	0.872070157

3c

0 1

C	1.9326332324	-1.3859255956	1.3317278785
C	2.0057547276	-0.9723622911	0.0763079367
H	2.3318119022	-2.3465163611	1.6268771802
H	1.4716573677	-0.7733746266	2.094296883
H	2.4613406947	-1.5655026547	-0.7045503308
C	1.479748255	0.3308443914	-0.3957230954
O	1.5503640994	0.6987822204	-1.5382539493
O	0.9168550692	1.0594690342	0.578437881
C	0.3986951884	2.3210222534	0.1628086856
H	-0.0165545897	2.7811771193	1.0533383076
H	1.1930322954	2.937956167	-0.2534314738
H	-0.3721582424	2.1831323435	-0.5932379033

3d

0 1

C	0	-2.153381	-0.760643	0.
C	0	-1.488656	0.384172	0.
H	0	-1.631851	-1.707868	0.000001
H	0	-1.986163	1.344172	-0.000002

C	0	-0.009243	0.479986	0.000001
O	0	0.586671	1.524318	0.
O	0	0.599265	-0.714355	0.000002
C	0	2.024096	-0.663244	-0.000001
H	0	2.35977	-1.69501	-0.000011
H	0	2.38419	-0.142272	-0.8853
H	0	2.384196	-0.14229	0.885307
C	0	-3.69318112	-0.78545439	-0.00000142
H	0	-4.05792966	-0.28669455	-0.87355573
H	0	-4.03354801	-1.79987557	-0.00019639
H	0	-4.05792635	-0.28703209	0.8737469

4aE

0 1

C	-0.3740148798	-0.5953029772	1.0272375965
C	-1.8044976434	-0.3972326197	0.5502832833
H	-0.3109146192	-0.543031524	2.1129509622
N	0.476315922	0.5082664656	0.5275104682
O	0.0687587957	1.6656995531	0.8549419746
H	-2.1901587987	0.5164187448	0.9976821858
C	1.5264621621	0.288809777	-0.1956086617
C	-1.8980743311	-0.317536321	-0.9670041241
H	-1.4767970445	-1.2081092749	-1.4384442714
H	-2.9340266023	-0.2276442488	-1.2897058643
H	-1.3576958192	0.5554911484	-1.3338751527
C	2.0316956577	-1.0576404889	-0.6045858031
H	2.0383681963	1.1928178862	-0.492701114
H	2.9537956971	-0.9296289125	-1.1660976178
H	2.2551307747	-1.6972517801	0.2505562858
H	1.3276246934	-1.5888231507	-1.2477618903
H	0.0281494584	-1.545658466	0.6852701098
H	-2.3951466192	-1.2322878111	0.9301876329

4aZ

0 1

C	-0.4003095183	0.030906573	1.0199277395
C	-1.7938222434	-0.2028959314	0.4603603706
H	-0.4354157945	0.6625818649	1.9061336085
N	0.4232876784	0.7582747576	0.0326365573
O	-0.0526011545	1.8678053989	-0.3593850155
H	-2.2615485222	0.7675075355	0.3038710348
C	1.537277806	0.2658341144	-0.403633198
C	-1.7706627917	-0.9896391514	-0.84229175
H	-1.2622981109	-1.9479446506	-0.7184664941
H	-2.7815860198	-1.1888646795	-1.1942007859
H	-1.2523308155	-0.4251601617	-1.6179796369
H	0.1016338794	-0.9064760095	1.2568826698
H	-2.3701922157	-0.7318469954	1.2208955954
C	2.3125109072	1.0318269047	-1.4082305638
H	2.5633283205	2.0184300186	-1.0132478569
H	3.2203868128	0.5045333546	-1.6872973907
H	1.6997435041	1.2095042191	-2.2947465906
H	1.8440383179	-0.6879290518	-0.0056904134

4bE

0 1

C	0.4027656705	0.1196676562	-1.2101546058
C	1.7477789649	-0.2117028427	-0.6086946336
H	0.5168600438	0.8248648766	-2.0292109861
N	-0.4214845726	0.8249902553	-0.207380849

O	-0.0463941529	2.0213092946	0.0123807924
H	2.1584661421	0.6883799524	-0.1400267663
C	-1.4072784886	0.2418157178	0.390652015
C	-1.8155422771	-1.1790534599	0.174630411
H	-1.9183461873	0.8778109426	1.0990672319
H	-2.5706223114	-1.4448969533	0.9102525978
H	-2.253418871	-1.338347849	-0.8136740259
H	-0.9725035267	-1.8592911239	0.2920812524
H	-0.0959535587	-0.7827642648	-1.5530736238
H	2.4308712682	-0.5421521021	-1.4006398621
O	1.562343419	-1.2333878514	0.3407181129
C	2.7451081574	-1.5351122838	1.0391167463
H	2.5099400604	-2.3093113824	1.7652705523
H	3.5213612296	-1.9042296797	0.3598084597
H	3.1280102105	-0.6540478527	1.5637821709

4bZ

0 1

C	-0.2742246654	-0.5963527489	1.0238115663
C	1.1567072337	-0.7240742799	0.5602553617
H	-0.5791186741	-1.4899663164	1.5643757044
N	-1.1650055059	-0.5031615156	-0.1469733971
O	-1.191772875	-1.5368280106	-0.886607635
H	1.219237645	-1.5293497688	-0.1784108719
C	-1.8369897662	0.5731420745	-0.3902284159
C	-2.6934420698	0.6214889825	-1.5981761522
H	-1.718322652	1.3936209732	0.2985735503
H	-3.2039534228	1.5768580294	-1.6792099861
H	-2.0850052592	0.4488591937	-2.4885311934
H	-3.4242336055	-0.1890946591	-1.5698132657
H	-0.3984040879	0.2888140286	1.6437584897
H	1.7950899561	-0.9775286889	1.4158201457
O	1.5420248104	0.505652494	0.0013700006
C	2.8152451472	0.4463987454	-0.5913359239
H	3.0363309791	1.4315615911	-0.9946246903
H	3.5825359108	0.1808528541	0.1445129421
H	2.8379137517	-0.2886216184	-1.4021958491

4cE

0 1

C	0.2511990485	-0.2990958957	-0.780372646
C	1.720686841	-0.266542446	-0.4255246792
H	0.0835173672	0.1388986429	-1.764664947
N	-0.5361453205	0.5005325849	0.2006106838
O	0.1235538263	1.3483690743	0.8770077194
H	2.1273064166	0.7360281413	-0.510518822
C	-1.8088253688	0.3077931881	0.3116647425
C	-2.5698275347	-0.693594178	-0.4915295535
H	-2.2877769668	0.9393424361	1.0449753571
H	-3.6345087182	-0.5556891949	-0.322045432
H	-2.388140782	-0.5934105657	-1.5628157457
H	-2.3196358571	-1.7190558624	-0.2069764299
H	-0.1340507393	-1.3148738473	-0.7765146185
H	2.2619468737	-0.9140860643	-1.1182531275
C	2.0230075431	-0.736509115	0.9756765073
O	3.0283063162	-0.4809840302	1.5731435602
O	1.0500909027	-1.5238652477	1.4648636217
C	1.2432979263	-1.9454386984	2.8139737693
H	2.1633180336	-2.5196869756	2.9041984786
H	1.2999875959	-1.0769387764	3.4674775531

H 0.3823361864 -2.5570772597 3.0635603485

4cZ

0 1

C 0.8130166022 -0.997153504 -0.7630262376
C -0.6378193262 -1.3950581828 -0.5740218272
H 1.3833302524 -1.8551122591 -1.1139589636
N 1.4117769752 -0.6289327153 0.5359015684
O 1.3512193751 -1.5296485061 1.4307465619
H -0.7109827477 -2.1669704815 0.1886328212
C 1.9537469163 0.5303000551 0.7174055617
H 0.9246623833 -0.1672832045 -1.4546332353
H -1.0218242319 -1.8133433876 -1.506218499
C -1.5748271735 -0.2792795212 -0.1791733022
O -2.6532178746 -0.4503398358 0.313889921
O -1.0862412327 0.9378930239 -0.4713453894
C -1.9395795965 2.0282987747 -0.1230225796
H -2.8797613991 1.9605918624 -0.6668211163
H -2.1478170159 2.014957386 0.9448869484
H -1.4013102378 2.9294150545 -0.3980252236
H 1.9252466866 1.219105249 -0.1112607893
C 2.5503260184 0.8408985981 2.0378481583
H 3.321446965 0.1066325704 2.2797371315
H 2.975725248 1.8402819362 2.0506610051
H 1.7922022036 0.7507243977 2.8186684056

4dE

0 1

C -1.6076944731 1.3552761493 -0.1581026957
C -2.8523162741 1.1747009611 -1.0052835954
H -1.0076057929 2.1851504545 -0.5183555557
N -0.7850075045 0.1188147221 -0.2059874434
O -1.4538089155 -0.9561168157 -0.2564958385
H -2.6023849427 0.8468094504 -2.0113027231
C 0.5149853358 0.1413983945 -0.2324811728
H -1.879025907 1.5228800085 0.8825769616
H -3.3485935125 2.1450174473 -1.0790658273
C -3.8611606474 0.1970157777 -0.4536303597
O -4.5568375193 -0.5088416687 -1.1254799571
O -3.9522979942 0.2770511889 0.8820982801
C -4.8353205942 -0.6699321846 1.4786882999
H -5.8542574538 -0.514097412 1.1291068894
H -4.520037661 -1.6798417432 1.2231718844
H -4.7690166965 -0.507414786 2.5496580188
C 1.3912181499 1.3069998581 -0.1186259303
C 1.1642228988 2.3716337116 0.7572276294
C 2.5646964263 1.3104173884 -0.8785960647
C 2.0614764048 3.4248719502 0.8354633907
H 0.2983093537 2.3624122802 1.4041922897
C 3.4599260242 2.3629651701 -0.7988303248
H 2.7636518604 0.4793922292 -1.5432266567
C 3.2079551276 3.4289791249 0.0541158528
H 1.8708966506 4.2384741767 1.522062005
H 4.356755259 2.3517409911 -1.4030024683
H 3.9076795548 4.2505739125 0.1204168113
H 0.951869133 -0.8396827869 -0.3600091997

4dZ

0 1

C -1.4071589344 1.2012732293 0.2128281987

C	-2.466075022	1.2486091449	-0.8760774385
H	-0.648950687	1.9636694966	0.0556272494
N	-0.7574727342	-0.1270296843	0.2244501963
O	-1.5650399331	-1.0952925194	0.3585463045
H	-2.0442541056	0.9937944904	-1.8459573093
C	0.5337309417	-0.2177540474	0.0989874272
H	-1.8639824912	1.3264239057	1.1926525757
H	-2.8512198255	2.2689599375	-0.9250931661
C	-3.6422089505	0.3327782475	-0.63121764
O	-4.1285948929	-0.3851423381	-1.4568119494
O	-4.1280121897	0.4861984682	0.6079805232
C	-5.163834282	-0.4283174524	0.9599206053
H	-6.0069326358	-0.3294008106	0.2792309228
H	-4.7811860106	-1.4464346602	0.9125217005
H	-5.4558755044	-0.1759890059	1.9740862898
C	1.3164725953	-1.4395645237	0.094014595
C	2.7054227646	-1.2890456464	-0.0157703009
C	0.7822228885	-2.730649524	0.1849080179
C	3.5413565393	-2.3886038052	-0.0318719593
H	3.1260968395	-0.2935063165	-0.0881019263
C	1.6303339291	-3.827934751	0.1662096963
H	-0.2841986114	-2.8558859808	0.2658347353
C	3.0035697902	-3.6667038897	0.0597526138
H	4.6107294193	-2.2518580569	-0.1160582608
H	1.2086501231	-4.8215638703	0.2349261807
H	3.6539390648	-4.5307836569	0.0462136757
H	1.0535202647	0.7223101698	-0.0039624174

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C	0.378697441	0.4038800426	-0.9615560315
C	-0.7365360866	-0.6231462307	-0.9121148218
H	1.1604391755	0.0912993365	-1.6444572949
N	0.9576426993	0.5836522532	0.3989363738
O	0.0868938377	0.5476404618	1.3244990644
H	-0.3976642902	-1.5556127819	-0.4668715157
C	2.2415290446	0.755073133	0.589517854
H	-0.010352981	1.3716675901	-1.2734573353
H	-1.0397131813	-0.829376394	-1.9412785131
C	-1.9709859616	-0.1894503662	-0.1611901724
O	-2.6412167564	-0.9132634692	0.5182075409
O	-2.2851153377	1.0889426481	-0.4193321862
C	-3.3897146773	1.5935035358	0.3267039788
H	-4.2907272957	1.0236566929	0.107762209
H	-3.1738814049	1.5268357202	1.3916110531
H	-3.5082224316	2.6292610565	0.0248485251
C	2.8211714836	0.8536067983	1.9414276936
C	4.042196309	1.5217180561	2.0924524561
C	2.2339434124	0.2744227023	3.0729517823
C	4.6537692594	1.6186641903	3.3303913131
H	4.5138247721	1.9767840975	1.2323077619
C	2.8642631129	0.3571090184	4.3044505996
H	1.2865015423	-0.2292523744	2.9815078789
C	4.0683187252	1.0318314842	4.442922736
H	5.5905383774	2.1509713365	3.4236139314
H	2.4013941659	-0.1047684248	5.1661036082
H	4.5461576036	1.100893873	5.4108322895
C	3.1519845013	0.882475365	-0.5778247585
C	3.0479988862	1.954372041	-1.4608010503
C	4.1698159554	-0.0508649943	-0.7633911007

C	3.9291835782	2.0774198373	-2.5254657976
H	2.2770119891	2.6984174779	-1.3048730843
C	5.0483998073	0.0699479343	-1.8284949286
H	4.2692920094	-0.8696547676	-0.0624027399
C	4.9286767727	1.1337554489	-2.7128584088
H	3.8390625233	2.9148125274	-3.20381424
H	5.8297681612	-0.6647461505	-1.9666291132
H	5.6169744084	1.2301582547	-3.541323007

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C	0	-1.434121	1.256096	-0.205189
C	0	-2.635162	1.049622	-1.10843
H	0	-0.769205	2.00833	-0.614103
N	0	-0.691732	-0.026311	-0.054434
O	0	-1.452878	-1.041606	0.023025
H	0	-2.344957	0.611103	-2.060297
C	0	0.616123	-0.070236	-0.013751
H	0	-1.75547	1.557948	0.790238
H	0	-3.070636	2.031862	-1.306403
C	0	-3.727748	0.184956	-0.53011
O	0	-4.387838	-0.588337	-1.163354
O	0	-3.937558	0.452513	0.767578
C	0	-4.895142	-0.390699	1.402652
H	0	-5.868037	-0.291128	0.925111
H	0	-4.569677	-1.427576	1.339297
H	0	-4.941031	-0.06706	2.437595
C	0	1.4273034	1.23879934	-0.01016706
C	0	0.50376085	2.41600103	-0.37467403
H	0	0.0200673	2.2142663	-1.30754254
H	0	-0.23414794	2.54048688	0.39010953
H	0	1.08368132	3.31117545	-0.45985031
C	0	2.02396354	1.46913143	1.39074115
H	0	1.55811099	0.80676443	2.09013472
H	0	3.07657921	1.27866084	1.36581721
H	0	1.85176279	2.48200492	1.68962941
C	0	2.56536591	1.14030032	-1.0429844
H	0	3.48716558	0.93593529	-0.53957571
H	0	2.35324992	0.35069593	-1.73322473
H	0	2.64641364	2.06583219	-1.57375933
C	0	1.38275269	-1.40386887	0.05906581
C	0	2.88202545	-1.12320569	0.2712199
H	0	3.29880535	-0.71466108	-0.62559994
H	0	3.00419763	-0.42412214	1.07200461
H	0	3.38477546	-2.03582773	0.51466074
C	0	0.8458281	-2.24108645	1.23481183
H	0	0.06201135	-2.88157376	0.88795839
H	0	1.63799176	-2.83467185	1.64105449
H	0	0.46442334	-1.58871659	1.99233673
C	0	1.18703394	-2.18094675	-1.25601751
H	0	2.06649502	-2.75286684	-1.46662527
H	0	0.34838496	-2.83852423	-1.16031098
H	0	1.0102355	-1.49136666	-2.05484265

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C	2.1865211407	0.623533178	-0.0912773616
H	1.9683937669	1.412393786	-0.8118875662
N	2.0890212092	-0.6450260759	-0.8262231452
O	0.7098016451	-0.9375650965	-0.8160731395

H	0.456105152	1.4699710812	0.9529117197
C	1.0577498306	0.5613997787	0.957872209
C	0.237382646	-0.6552766273	0.5042484238
C	3.5818412079	0.8111534755	0.4675560662
H	3.805916618	0.0383383043	1.2064688022
H	4.3260057661	0.7582323241	-0.3265481595
H	3.6718581791	1.7792489418	0.9581107585
H	1.4534528974	0.4227177705	1.9642541465
H	0.472928985	-1.5183113164	1.1399786123
H	2.5270577189	-1.3710311409	-0.2535496566
C	-1.25711915	-0.4504740138	0.4372865751
H	-1.6615585299	-0.264176165	1.4318760862
H	-1.48286891	0.4052581941	-0.1991299757
H	-1.745474293	-1.3310200484	0.0226198946

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C	1.8816768018	0.4534504916	0.0473906165
H	1.2250240859	1.0978432569	-0.5396209427
N	1.7513165214	-0.9070486118	-0.4834974268
O	0.5969814384	-1.466712782	0.1663686145
H	0.9798420248	1.2718355806	1.8912741938
C	1.3212390861	0.3338896174	1.4623228045
C	0.165449334	-0.6099790846	1.2098271482
C	3.315743555	0.9262571579	-0.0569052864
H	3.9712256197	0.3080367517	0.5605196224
H	3.6628362335	0.8763224857	-1.0882137774
H	3.4025644916	1.9564655614	0.2847214556
H	2.0577506059	-0.1297536793	2.121552359
H	-0.1100032492	-1.2564290534	2.0499549864
H	2.5197524378	-1.4535336855	-0.0930858151
O	-0.9366944209	0.1512767758	0.8179733266
C	-2.0655412149	-0.6340664274	0.4951740988
H	-2.8678924173	0.0508900276	0.2342195142
H	-1.8563965076	-1.2933665529	-0.3480226843
H	-2.3741963562	-1.2392265797	1.3546919621

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C	2.1006798646	0.4999077834	-0.0236070218
H	1.6433523555	1.2244847678	-0.699891138
N	1.9898047317	-0.811341489	-0.6599562379
O	0.6329222475	-1.1920635525	-0.4688920978
H	0.8395013762	1.3101683498	1.5852310612
C	1.2247714236	0.3603823132	1.2235961151
C	0.1152644684	-0.5433173234	0.7117594516
C	3.5493761605	0.8509594867	0.2361652733
H	4.00552189	0.1267632698	0.9149128043
H	4.1163355447	0.858601568	-0.693330278
H	3.6250575845	1.8355136688	0.694733167
H	1.7875512708	-0.1316980602	2.0184117019
C	-1.0993719015	0.2398923045	0.2363962528
O	-1.1226582648	1.425321846	0.0451341146
H	-0.1996793297	-1.3061595388	1.4247364078
O	-2.1315767839	-0.5718799734	0.0130306887
C	-3.2869545625	0.0499909441	-0.5501517577
H	-3.0351674909	0.5148561609	-1.5012969559
H	-4.0133714532	-0.7429768221	-0.6911840002
H	-3.67295762	0.8110736092	0.1254502769
H	2.5263744283	-1.4713661028	-0.0934674778

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C	-0.5888077337	-0.7070844123	0.3107704114
N	-0.3894944177	-1.5489669283	1.4927415014
O	0.9089074999	-2.0861357058	1.3159807187
H	0.3966958166	-0.9249288898	-1.649512635
C	0.0374622354	-1.5300451996	-0.8191621079
C	1.1757990504	-2.2484795044	-0.0785315798
H	-0.6818566987	-2.2545866984	-1.2009924974
C	2.5265939236	-1.6443763247	-0.4125991323
O	3.3652499647	-2.2019012545	-1.064792444
H	1.2324598246	-3.3070381197	-0.3313261471
O	2.6462405045	-0.3996287456	0.0536284955
C	3.8859221859	0.2430296136	-0.2435607527
H	4.0183332424	0.3308030132	-1.3204380808
H	3.8322718998	1.2227335636	0.2190398434
H	4.7134283501	-0.3309813674	0.1683043422
H	-1.0299899502	-2.3423512073	1.4156584642
C	-2.0397988908	-0.3375246285	0.1516129573
C	-2.7968163233	-0.0247599591	1.2801146821
C	-2.6423994339	-0.2747805848	-1.1003741961
C	-4.1302991292	0.3322557435	1.1555585026
H	-2.3302298415	-0.0647836283	2.2555153527
C	-3.9756373579	0.0911092691	-1.2255250321
H	-2.0694808017	-0.5081046867	-1.9883460747
C	-4.723801756	0.3923564548	-0.0979741534
H	-4.7073651368	0.5672741321	2.0397044275
H	-4.429246519	0.1366292116	-2.2064048272
H	-5.7635324218	0.6734099903	-0.1947948856
H	0.0129276244	0.1910545132	0.469037467

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C	2.2024353474	-0.1015028803	0.4479230803
N	1.9287838704	-1.3997842738	-0.1881615659
O	0.5159467731	-1.5787774399	-0.1003209707
H	0.9492012465	0.883677636	1.9994815648
C	1.1911081989	-0.1002206399	1.6065957007
C	-0.0105024996	-0.7361947527	0.9217444262
H	1.5540094373	-0.7403975976	2.4104945961
C	-0.9560811283	0.321565099	0.3571902206
O	-1.2490741188	1.3171209483	0.9642472697
H	-0.6026289286	-1.3437258863	1.6103102831
O	-1.4529797944	-0.0056623509	-0.8288778579
C	-2.3018447241	0.980334281	-1.4168038383
H	-1.7442544109	1.9047797032	-1.561809589
H	-2.6167347964	0.5687606215	-2.3699109285
H	-3.159414753	1.1749968124	-0.7756137062
H	2.3218027871	-2.1163378059	0.4215666564
C	1.8892588548	1.0343174394	-0.5259947936
C	2.0346326231	2.3525820791	-0.1006104561
C	1.4417286909	0.7845885899	-1.8168371328
C	1.7346332608	3.4053373121	-0.9475086819
H	2.3908000718	2.5551363568	0.9027999544
C	1.1423867506	1.8421956151	-2.6681161969
H	1.3152780549	-0.237296047	-2.1445256713
C	1.285649582	3.151851821	-2.2379500737
H	1.8499478457	4.4238068071	-0.6025229399
H	0.7936609433	1.6358105907	-3.6714231583

H	1.0515948152	3.9725257899	-2.9025720199
C	3.6586226125	-0.0636239351	0.8594179756
C	4.628999205	-0.4510771633	-0.0637357485
C	4.0590142164	0.3728389352	2.11648102
C	5.97175826	-0.4200271028	0.2746942284
H	4.3192224374	-0.7723359116	-1.0499196885
C	5.4068131693	0.4149583362	2.4514296398
H	3.3213724154	0.6880847939	2.8429577547
C	6.3648405106	0.0141987226	1.5342792834
H	6.714527285	-0.7279310151	-0.4487431655
H	5.7042124588	0.7597401012	3.4324882084
H	7.4136826098	0.043326931	1.7961240809

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C	-0.5038878929	0.0818946387	0.1208871208
N	-0.0554729599	-0.1215566221	1.5287462183
O	1.2610512697	-0.6406618331	1.4785145094
H	1.1912853177	-0.1407265228	-1.2661248559
C	0.5040115027	-0.768366752	-0.7110930235
C	1.3025234369	-1.5059438251	0.3465156358
H	0.0271684171	-1.4378808942	-1.4200014449
C	2.7759320048	-1.6690891357	0.0083785723
O	3.4015549266	-0.9329065543	-0.7023794003
H	0.8803695903	-2.4818709499	0.6045184205
O	3.2988146519	-2.72638457	0.630940384
C	4.7002950986	-2.9157485517	0.4307052621
H	5.2493539883	-2.0447213468	0.782668015
H	4.9677457399	-3.7969586885	1.0036578786
H	4.9117842197	-3.0635271794	-0.6266358503
H	-0.6006565268	-0.8729057457	1.9395931226
C	-1.9709027125	-0.5048411381	0.0233486333
C	-2.9039622891	-0.015456741	1.1484912177
C	-2.6404074052	-0.1821919177	-1.314396559
C	-1.9502724017	-2.044536561	0.1449627625
H	-2.4901732768	-0.1741496352	2.1444342673
H	-3.157681509	1.0342214411	1.0615727202
H	-3.8358779328	-0.5802381242	1.0918746927
H	-1.9932149688	-0.4128167473	-2.1618792146
H	-3.5481485411	-0.7797196957	-1.4135458245
H	-2.9333456204	0.863328655	-1.3783130628
H	-2.9786625326	-2.4049598874	0.1313942711
H	-1.431777058	-2.5303511746	-0.679222068
H	-1.5072816051	-2.3978992173	1.0768224279
C	-0.2724807405	1.6118479209	-0.2197048446
C	1.1375930991	2.012142683	0.2595027658
C	-0.3449085759	1.9371676074	-1.7207256762
C	-1.2471433217	2.5395443268	0.5107348621
H	1.2265346496	1.9091597389	1.3384913468
H	1.931183554	1.4245391	-0.2001479733
H	1.3054396804	3.0572876638	-0.0027378031
H	-1.3509637819	1.8801099847	-2.1250548792
H	-0.002400959	2.9633153911	-1.8631640453
H	0.299296347	1.3010885902	-2.3264327329
H	-0.8871770608	3.5661724731	0.4267578284
H	-2.2464913171	2.51687111	0.0784288071
H	-1.3050268346	2.2896272163	1.5699344262

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C	2.2172155598	0.1745215805	0.0743055797
H	3.1761231884	0.0965632526	0.587184574
N	1.9306428018	-1.1310077164	-0.5483409605
O	0.5190870996	-1.1943414326	-0.563994377
H	0.5826611403	1.3779770506	0.8796497473
C	1.0480102164	0.4078160561	1.0579941128
C	0.0823951125	-0.734226578	0.7150380695
C	2.2845139155	1.2422895482	-1.0037003149
H	1.3452210281	1.2561941672	-1.5579234202
H	2.4410008813	2.2277239168	-0.5637228219
H	3.0921560976	1.0328991138	-1.7027568925
H	1.3621595074	0.3693236975	2.0993556578
H	0.2096894998	-1.5551882472	1.4333489519
H	2.2217442314	-1.8649272275	0.0986632533
C	-1.3740743473	-0.3499838329	0.6116146577
H	-1.9737024141	-1.200022708	0.2901116475
H	-1.7464138582	-0.006213133	1.5761924792
H	-1.4900207102	0.4539326325	-0.1155590135

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C	2.0949240264	0.1450227717	0.0634111326
H	3.1764614167	0.2325501789	0.1714750243
N	1.8103888441	-1.2164479655	-0.4051023227
O	0.4976693318	-1.5167090931	0.0847125315
H	1.0987748824	1.2017825345	1.7329803473
C	1.3839173753	0.200992772	1.4192778183
C	0.152691869	-0.6488177826	1.156790432
C	1.5825195401	1.1684011663	-0.9364580372
H	0.5123053903	1.0402304153	-1.0880386944
H	1.7594856591	2.1807669401	-0.5728195514
H	2.0901419855	1.0420703004	-1.8908929343
H	1.9995935713	-0.2587132048	2.1918631736
H	-0.1503895493	-1.2794123633	2.0011498958
H	2.4086609909	-1.8568292352	0.1139652369
O	-0.9112806168	0.1777285276	0.7987052184
C	-2.0975817176	-0.5396028293	0.5246606196
H	-2.8700224352	0.1923696222	0.30414615
H	-1.9662534293	-1.2043272371	-0.3301179545
H	-2.3999359946	-1.1309404781	1.3959033243

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C	2.2538154089	0.1390818546	0.1428175647
H	3.2530539143	0.0558271653	0.5707942779
N	1.9681949712	-1.113052527	-0.5653697105
O	0.5522586421	-1.1625145624	-0.6137321095
H	0.8473215165	1.2155702771	1.4415587063
C	1.1701594017	0.1980115208	1.2345276791
C	0.0417903815	-0.6324240077	0.6219142607
C	2.1828272246	1.3106272968	-0.8206464202
H	1.1847405216	1.3860724935	-1.2503481415
H	2.397588756	2.2440797949	-0.3008840155
H	2.9034830502	1.1771682107	-1.625316902
H	1.5186659655	-0.2597789309	2.1582560366
C	-1.1779871377	0.1835203778	0.2246389514
O	-1.1912132744	1.3733612897	0.0667204801
H	-0.2723677754	-1.4574590196	1.2648890965
O	-2.2340523667	-0.6057829255	0.0317848623
C	-3.4092533442	0.0526226136	-0.4426298865

H	-3.2089745886	0.5313067702	-1.3991048466
H	-4.1612778788	-0.7213784674	-0.5505649911
H	-3.7322208441	0.8078096706	0.2715429293
H	2.2396164659	-1.891591895	0.0358991686

6d

0 1

C	-0.5812159826	-0.5601055267	0.1396009909
N	-0.3601909571	-1.2486571792	1.4083737313
O	0.8837603859	-1.9436342455	1.2468802048
H	0.2383887526	-1.1166270646	-1.8470399976
C	-0.0313002008	-1.5571742878	-0.8917461251
C	1.1952772314	-2.056264279	-0.1382036049
H	-0.74258009	-2.3676072672	-1.0467725464
C	2.4372970503	-1.2483061905	-0.5110287112
O	2.6793477088	-0.9132657209	-1.6396406555
H	1.4245135436	-3.1007805525	-0.3619560121
O	3.2324597177	-1.0137340616	0.5259838569
C	4.3780454468	-0.2129419049	0.2361548174
H	4.0598584432	0.7671527686	-0.1178364099
H	4.9220241683	-0.125591206	1.1708104838
H	4.992192157	-0.6882125943	-0.5261992339
H	-1.0505068431	-1.9931426606	1.480505813
C	0.1474055845	0.766654289	0.0819246526
C	-0.0192684965	1.5797947502	-1.0358723704
C	1.0065732973	1.174087729	1.0943926261
C	0.6600194314	2.7814564722	-1.144143254
H	-0.686053847	1.2664522654	-1.8311058823
C	1.6939842243	2.3771101334	0.9827021217
H	1.1384691205	0.5417761468	1.9613261551
C	1.5245949049	3.1817665189	-0.1334265376
H	0.5185611217	3.4046412949	-2.0166280361
H	2.3633523099	2.6850414847	1.7751629152
H	2.060043695	4.1178360461	-0.2166287861
H	-1.6538326379	-0.4018690378	0.0221301442

TS1aE

0 1

C	-0.5920241269	-0.9631061966	0.4283373666
C	-1.7807136865	-0.2326618905	0.5158406076
H	-0.1104858897	-1.3362849319	1.3232929057
N	0.6887066766	0.470660582	0.0769327284
O	-0.0248243484	1.5401206457	0.1295292175
H	-1.0635537037	0.9665294472	0.3741970547
C	1.9340903422	0.4611185412	-0.161952821
C	-2.7571034661	-0.2348792429	-0.6432451408
H	-3.4077528515	-1.1120482112	-0.6418314659
H	-3.3972575859	0.6471605842	-0.6278767376
H	-2.218089904	-0.2237427453	-1.5925900199
C	2.7039037112	-0.8162371109	-0.2080981699
H	2.4365517431	1.4090726175	-0.3339050135
H	3.5150342079	-0.8004458359	0.5210031468
H	2.0627231281	-1.6681292861	0.0054339305
H	3.1559116027	-0.9569810613	-1.1909762349
H	-0.3634323517	-1.5306471133	-0.4671552177
H	-2.2080554976	-0.1324227916	1.5077548634

TS1aZ

0 1

C	0.5867025296	-0.961317031	-0.4253894267
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C	1.7849281718	-0.2511290493	-0.5205455673
H	0.0919432684	-1.3249749875	-1.316823012
N	-0.6729442735	0.4849262159	-0.0711899151
O	0.0487042763	1.5518240152	-0.138635614
H	1.070513292	0.9724093827	-0.382683414
C	-1.9165193106	0.509432795	0.1762641759
C	2.7635113778	-0.2509303396	0.6361622423
H	3.422508638	-1.1219086956	0.6283268464
H	3.3965051669	0.6365753094	0.6257525765
H	2.2267305421	-0.2512633811	1.5868599355
H	0.3481967661	-1.5205572384	0.4725586461
H	2.2087955593	-0.1547210965	-1.5142068562
C	-2.6691489916	1.7763329946	0.4154431138
H	-2.2726670804	2.2839898149	1.2961140298
H	-2.5341842757	2.4544423277	-0.42791213
H	-3.7288489588	1.5841071142	0.5597944839
H	-2.3984950278	-0.4606138905	0.2062145449

TS1bE

0 1

C	-0.2423186892	-0.6324658166	0.6424311775
C	-1.3007789148	0.2788516733	0.6093857433
H	0.2114745596	-0.8934842093	1.5894135467
N	1.2086968795	0.4858348704	0.0209211886
O	0.696904163	1.6645895258	-0.0472550119
H	-0.3954694837	1.3399985298	0.2969107379
C	2.4147511323	0.2194653695	-0.2641378065
C	2.9493396761	-1.1696129682	-0.1632964467
H	3.0605774082	1.0307278893	-0.5881785301
H	3.7967812059	-1.2031465111	0.5224978714
H	2.1887197168	-1.8606255986	0.1914585016
H	3.3067259119	-1.5132359173	-1.1348915555
H	-0.1620568876	-1.3844000185	-0.1333689938
H	-1.7708800398	0.5755714263	1.5445517258
O	-2.1595100037	0.2396954854	-0.496458206
C	-3.2077544764	-0.6858563301	-0.3388395156
H	-3.8259787179	-0.643467309	-1.2337101468
H	-2.8215211372	-1.7037751574	-0.2134855337
H	-3.822208303	-0.4406029335	0.5343072536

TS1bZ

0 1

C	-0.2420957704	-0.6135437858	0.651012249
C	-1.3119368984	0.2811746695	0.6223792129
H	0.2193343846	-0.8612873356	1.5976396388
N	1.1905422666	0.508966807	0.0163410214
O	0.6782689681	1.6915907368	-0.0417679236
H	-0.3983762526	1.3679746377	0.3047555348
C	2.3960213786	0.2624731181	-0.2876679005
H	-0.1480781138	-1.366781228	-0.1220999393
H	-1.7821174587	0.5768125155	1.5575165314
O	-2.1691183224	0.2439307826	-0.4843235813
C	-3.2068688896	-0.6955317526	-0.3372623199
H	-3.8308194404	-0.642824211	-1.2277270011
H	-2.8096084873	-1.7114785632	-0.2321155429
H	-3.8185261745	-0.4722324117	0.543902658
C	3.3467976485	1.3181976891	-0.7442309753
H	2.9785856967	1.7779413228	-1.6624907343
H	3.4088282439	2.1101581687	0.0030257034
H	4.3375077765	0.9079799479	-0.9197508399

H 2.6887632245 -0.7767836277 -0.1951650117

TS1cE

0 1

C	-0.2196040807	-0.5711998912	0.6978321691
C	-1.3354789672	0.2416939014	0.9917668712
H	0.2447751407	-1.1175201183	1.5112355228
N	1.1177979163	0.5159790033	0.2905058628
O	0.7089426668	1.7605844933	0.4308124404
H	-0.2785003784	1.5756284428	0.7140504133
C	2.2905118745	0.2558788207	-0.1049513412
C	-2.2660595733	0.4761129886	-0.0850333577
C	2.7701431334	-1.1429516939	-0.2750402536
H	2.9465315913	1.0925241418	-0.3259829758
H	3.6442329207	-1.315708117	0.3534431706
H	2.0020143499	-1.8666848801	-0.0195635168
H	3.0761702462	-1.3044293442	-1.3089545136
H	-0.26143932	-1.1181445996	-0.2387056321
H	-1.6546840261	0.4059105266	2.0083622567
O	-2.0716256734	0.2238519428	-1.2586271787
O	-3.4195066995	1.0499509762	0.3376026611
C	-4.3575406398	1.3350829408	-0.6897088535
H	-4.6376673821	0.4269753155	-1.2215139543
H	-5.2233024331	1.7656140239	-0.1948894419
H	-3.9421368859	2.0412842168	-1.4078365489

TS1cZ

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C	0.7055553099	-0.5970955957	0.8615140169
C	-0.5286350384	0.041883097	1.0690503238
H	1.3671454466	-0.7366423706	1.708357642
N	1.7299020588	0.5408444963	-0.0804206691
O	1.0694431619	1.6690382846	-0.246273989
H	0.1852375445	1.409855243	0.2313338988
C	2.8766693367	0.3588926744	-0.5796367202
C	-1.5800013613	-0.2429361864	0.1210130788
H	0.7188394907	-1.4089696096	0.1419849898
H	-0.7830014624	0.4795447382	2.0210222112
O	-1.4410233162	-0.8174883557	-0.9409194044
O	-2.7858968548	0.2279408643	0.5232051003
C	-3.8502057076	0.0033179447	-0.3900340661
H	-4.0061720661	-1.0629411867	-0.548439371
H	-4.7317388756	0.4504902216	0.0601097827
H	-3.6378333382	0.4676981936	-1.3520883607
C	3.6178996702	1.3592192543	-1.3953457874
H	4.1631590873	0.8609568383	-2.1945062932
H	2.9330628677	2.0921343665	-1.8125367631
H	4.3456346733	1.8812162143	-0.7711057704
H	3.301787963	-0.6152320963	-0.3620146196

TS1dE

0 1

C	-1.759348562	0.9761000352	-1.1019546702
C	-2.9313129759	0.1887334142	-1.2313413777
H	-1.3533277235	1.3848322707	-2.0197114639
N	-0.4743304726	-0.1092756075	-0.6375531502
O	-0.9164043651	-1.3470692499	-0.7528269615
H	-1.9172141223	-1.1332468398	-1.0069522774
C	0.670787794	0.0886875187	-0.1208637328
C	-3.7599049713	0.0725856906	-0.0576566341

H	-1.7001797264	1.651660118	-0.2531748693
H	-3.3580797241	-0.00790851	-2.2015274135
O	-3.4342751998	0.3903516064	1.0702296775
O	-4.9731074358	-0.4723082844	-0.3214011002
C	-5.8097988885	-0.6447784695	0.8130173268
H	-6.0362397354	0.3146219821	1.2764647672
H	-6.7199836802	-1.1112059974	0.4472431419
H	-5.3289414652	-1.2804960137	1.5552150224
C	1.3045522138	1.3888557225	0.0982644164
C	2.2903274799	1.4380312938	1.0855185306
C	1.0031163435	2.5499621557	-0.6150068672
C	2.9369378514	2.6256684628	1.380607457
H	2.5395077739	0.5368592536	1.6310672329
C	1.6567729763	3.7351194208	-0.322185952
H	0.2767548909	2.5283405746	-1.4115005025
C	2.6181362013	3.7789330184	0.6785008445
H	3.6916214429	2.649979039	2.1542068874
H	1.4180689688	4.6283145334	-0.8826574496
H	3.1242264221	4.7078515654	0.9022359687
H	1.2012451595	-0.7953613239	0.220548119

TS1dZ

0 1

C	-1.7114604928	0.9518305629	-0.7778623395
C	-2.9708534119	0.3702707494	-0.9782494735
H	-1.2206821079	1.4414447778	-1.6104708881
N	-0.5354101431	-0.4208840739	-0.5814597765
O	-1.201502174	-1.5487633966	-0.6887891411
H	-2.1552145	-1.1571189756	-0.8467468624
C	0.7139165887	-0.3572874041	-0.3686639865
C	-3.8322016314	0.2330197966	0.1764767499
H	-1.5337247488	1.4124440759	0.1879503984
H	-3.4072686334	0.3008924473	-1.9621500163
O	-3.5009284833	0.3856874366	1.3341308922
O	-5.095350286	-0.1188630488	-0.1644616437
C	-5.9859728143	-0.288270429	0.9292322137
H	-6.0861812899	0.6386034714	1.492198352
H	-6.9409148801	-0.5731329964	0.4973455853
H	-5.6276524071	-1.0649138828	1.6035663803
C	1.6903225382	-1.4312013755	-0.2001521767
C	1.3663110725	-2.790682881	-0.1846534877
C	3.0246347201	-1.0455123361	-0.0466737177
C	2.3684471885	-3.7331288146	-0.0210577709
H	0.3406478241	-3.1018496546	-0.2958550742
C	4.0202770516	-1.9921455021	0.1127534841
H	3.2769111138	0.0075451383	-0.054342677
C	3.6918558843	-3.3408974023	0.125416575
H	2.1124217939	-4.7835431955	-0.0076014216
H	5.04901069	-1.6801254101	0.2277756934
H	4.4663414462	-4.0851600219	0.2516321434
H	1.079506352	0.6640110048	-0.3135503141

TS1e

0 1

C	-1.6552099931	1.1741932391	-0.7025634873
C	-2.895139522	0.5601301552	-0.9884062015
H	-1.2557419711	1.8653261331	-1.4325054346
N	-0.4298669989	-0.1091891231	-0.7569074741
O	-1.0239480835	-1.2295392105	-1.1196552352
H	-1.9986531549	-0.858116788	-1.2363438395

C	0.7816509189	-0.0794804651	-0.3535861627
C	-3.6630523048	0.089154322	0.1374140636
H	-1.4749214749	1.4780492713	0.3241641987
H	-3.3909130656	0.7218036119	-1.9321029752
O	-3.2444447251	-0.0540515869	1.2703878383
O	-4.9402125769	-0.2252443316	-0.1937592841
C	-5.7289439714	-0.7309698843	0.8728605214
H	-5.8031581414	-0.0022175328	1.678959094
H	-6.7106629837	-0.9289061054	0.4520217141
H	-5.2971561435	-1.6469739819	1.2745088918
C	1.3446288196	1.2606369671	-0.0393383531
C	1.848038877	1.5105686	1.2345369992
C	1.3990272199	2.256703594	-1.0082811418
C	2.3714118659	2.7557918133	1.5424846822
H	1.818497191	0.7279188088	1.9817127772
C	1.9341730533	3.4990435087	-0.7013641922
H	1.0345291738	2.049191484	-2.0060036343
C	2.4146352868	3.7512115107	0.5752187113
H	2.7475087838	2.9489402313	2.5376211032
H	1.9795139462	4.2677675447	-1.4605021428
H	2.8283608779	4.7211281106	0.8150653427
C	1.6355553466	-1.2742908498	-0.1722759657
C	1.1134696522	-2.5017839048	0.2392543146
C	3.0105161206	-1.1486833612	-0.3744067076
C	1.9601394749	-3.5784915849	0.443649245
H	0.0525194802	-2.605128154	0.4055307836
C	3.8486576397	-2.2362583237	-0.1922334676
H	3.4208587058	-0.1950846197	-0.679349745
C	3.3247113985	-3.4526171138	0.2204682367
H	1.5506834508	-4.5223658254	0.7762923652
H	4.9106581846	-2.1310511423	-0.3658597879
H	3.9790706428	-4.3003020168	0.3721343493

TS1f

0 1

C	1.1758241103	-0.8500954768	-0.8959474536
C	2.3283106034	-0.0624740158	-1.080751279
H	0.620056269	-1.1477769583	-1.7759425452
N	-0.0993926657	0.1276391161	-0.1513849524
O	0.4408217537	1.331354943	0.0528598765
H	1.4148920725	1.1630199309	-0.2822903716
C	-1.3775921167	0.0179178427	-0.036674255
C	3.3858901758	-0.2123520346	-0.1120206093
H	1.2931522876	-1.6236454472	-0.1541504632
H	2.5410563099	0.4243552954	-2.0192888582
O	3.3096014928	-0.8077695679	0.9454705519
O	4.5298577161	0.4103280501	-0.4941294199
C	5.6020813285	0.3114382526	0.4311874363
H	5.8535475101	-0.7305923233	0.6231911133
H	6.4423462319	0.8253337332	-0.0267993797
H	5.3409727924	0.7826361846	1.3783148837
C	-2.2234840428	1.3139837533	0.1208984155
C	-2.0054543894	-1.3865726212	0.058872738
C	-0.9945366695	-2.5411555239	0.0899331163
H	-1.5478019054	-3.4490754072	0.3295070994
H	-0.5097793841	-2.7054741312	-0.8671555469
H	-0.2414856171	-2.4021194389	0.8624582008
C	-2.9588072085	-1.6816593834	-1.1126026968
H	-3.2122162626	-2.7422495139	-1.0936212384
H	-3.8871753483	-1.1250413515	-1.0760913578

H	-2.4692587822	-1.4762379969	-2.0661850786
C	-2.7286573453	-1.4942493017	1.4191828575
H	-3.212452591	-2.4700886621	1.4745666741
H	-2.0013285294	-1.4340434215	2.2300854147
H	-3.485227539	-0.7399199916	1.594144136
C	-3.7234791472	1.1533018491	-0.1911624779
H	-3.8861821396	0.9791002149	-1.254297721
H	-4.2414247551	0.3841931087	0.3687103316
H	-4.1999959289	2.1020646982	0.0552986815
C	-2.0716291012	1.8325098056	1.5611395143
H	-2.5762089951	2.7965285863	1.6438433051
H	-2.523986232	1.1526258701	2.2822245772
H	-1.0238411878	1.9698058746	1.8178981011
C	-1.7626864733	2.4084863196	-0.8754953316
H	-0.9109083729	2.9732950983	-0.5207853887
H	-1.5085999026	1.9758776822	-1.8447258795
H	-2.5901680215	3.1004483599	-1.0301307204

TS1g

01

C	-1.7126801248	0.4492519621	-1.1286985281
C	-2.8239655332	-0.4298093804	-1.0228270201
N	-0.3260578044	-0.5188501556	-0.5622331641
O	-0.6718315623	-1.7887433434	-0.6562316836
H	-1.7119122188	-1.6437047349	-0.8097668063
C	0.8437925448	-0.1500335552	-0.2033582152
C	-3.5114037491	-0.4251639739	0.2416476356
H	-1.6701922801	1.2313581848	-0.3829026945
H	-3.3338827727	-0.7789898106	-1.9081753432
O	-3.0889628117	0.0738333638	1.2707718243
O	-4.6994869755	-1.0760914454	0.2068460027
C	-5.3873798331	-1.1383250613	1.4473057627
H	-5.6071058052	-0.1384687656	1.8193561489
H	-6.3087666468	-1.6795634158	1.2526375857
H	-4.7916202328	-1.6611920175	2.1945688515
C	1.0487572776	1.3101399562	-0.0014050742
C	0.2782644916	1.9961878929	0.9330842646
C	2.0445210803	1.9813428301	-0.7060582422
C	0.4934300093	3.3506694709	1.1448671042
H	-0.4876035012	1.464917534	1.4866018553
C	2.24860427	3.3362167433	-0.4991912675
H	2.6558993801	1.4370270905	-1.4149024216
C	1.4733719353	4.0214437502	0.4273828833
H	-0.1055872995	3.8797388132	1.8730076743
H	3.015939694	3.8563646733	-1.0558662438
H	1.6381067275	5.0772837869	0.5937900469
C	1.97166518	-1.071733473	0.0605012036
C	2.0987332535	-2.3044969035	-0.5837952371
C	2.9574627988	-0.6750007559	0.9667662326
C	3.1928435156	-3.1134875128	-0.3247239705
H	1.3438258469	-2.6254562439	-1.2837228652
C	4.0377878379	-1.4978459665	1.237196464
H	2.8704659876	0.2795667692	1.4673362073
C	4.1600571824	-2.7180907379	0.5886768577
H	3.2860252555	-4.0623370999	-0.8349256488
H	4.7855162355	-1.1829795265	1.951973882
H	5.0060254444	-3.3596466684	0.7950526985
C	-1.2609557299	0.8702454584	-2.5044060278
H	-0.3021790512	1.3862765455	-2.4768969073
H	-1.1839736459	0.0065811623	-3.1650120698

H -2.0039393705 1.5513935606 -2.9190327548

TS1h

0 1

C	1.1557414878	-0.5758866018	-1.0716806475
C	2.2931601094	0.2943569448	-0.9565837566
N	-0.1327360427	0.2998208431	-0.2268639353
O	0.3173227487	1.5333415022	-0.1487995679
H	1.4111614173	1.3039445587	-0.4392775237
C	-1.3707941397	0.0410955778	0.0267012957
C	3.2156097942	-0.0263804549	0.1165604237
H	1.2470497392	-1.4738878878	-0.488779782
H	2.6958788836	0.752443031	-1.8496722155
O	2.9686740562	-0.7466489988	1.062729572
O	4.4062357237	0.6009288197	-0.0109441063
C	5.3238241722	0.369859473	1.0493871647
H	5.5568137649	-0.6905428441	1.1341791582
H	6.2170596096	0.9354204742	0.8014157137
H	4.9100609087	0.7104396889	1.9975363003
C	-2.3342634857	1.2514454777	0.1852718887
C	-1.8209721996	-1.4068710543	0.3038614666
C	-0.6987785032	-2.4538952571	0.2854577422
H	-1.1159241823	-3.3803710243	0.6803839706
H	-0.3425978352	-2.6720302656	-0.7185968112
H	0.136133444	-2.1692024575	0.9237111358
C	-2.8956915282	-1.905835647	-0.6796108063
H	-2.997493468	-2.9853948863	-0.5622426734
H	-3.8740637379	-1.4699364932	-0.5170716442
H	-2.6010640259	-1.712226954	-1.7122996292
C	-2.3392658144	-1.4523092529	1.7590842425
H	-2.7085184123	-2.4583899582	1.9620879851
H	-1.5204163975	-1.247042869	2.4499182985
H	-3.1404920231	-0.7560748798	1.9729159537
C	-3.8324209561	0.9135642756	0.0779937265
H	-4.0960127393	0.6037143925	-0.9327718009
H	-4.1930034427	0.1667381541	0.7753981764
H	-4.3792003214	1.8333948908	0.2856384952
C	-2.0821719733	1.9313934236	1.5416878508
H	-2.6630743599	2.8543568498	1.5861218876
H	-2.395231887	1.2982415801	2.3713673125
H	-1.0310743829	2.179564912	1.665001627
C	-2.1099663126	2.2718498301	-0.9569988754
H	-1.2399969748	2.8958328163	-0.8035330947
H	-2.0066043707	1.7613662374	-1.9169247743
H	-2.9884390758	2.9141639823	-1.0177319914
C	0.5582059403	-0.7459477338	-2.4463000561
H	-0.3954893662	-1.2709904895	-2.4199865802
H	0.4048457306	0.2273336111	-2.9139856936
H	1.2510824281	-1.316939337	-3.0647134224

TS2aE

0 1

C	1.2648026021	-0.1009782529	0.7293151425
N	0.5088768208	-1.160211817	0.4949956865
O	-0.1265921092	-1.229830241	-0.6205380666
H	0.3477838138	2.0838849039	-0.1927538746
C	-0.3090857588	1.3611856098	0.2713127149
C	-1.1508525717	0.5936192522	-0.4983275388
H	-0.5644367701	1.5554177105	1.3070465155
H	-1.1061445476	0.6782019932	-1.5749459259

C	-2.3896149401	-0.0162681644	0.0858701692
H	-3.1918534851	0.7214986734	0.1633537901
H	-2.7434171945	-0.8540589938	-0.5099154725
H	-2.1861658475	-0.3754148147	1.0986186025
H	0.0612860535	-1.6017214194	1.2986173479
C	1.8412571619	0.120955669	2.0889717641
H	2.8320778473	-0.3264445988	2.1820158678
H	1.939656457	1.1887119852	2.2774112885
H	1.1956992812	-0.2975308697	2.8617746934
H	1.7990854273	0.2577766543	-0.1371695545

TS2aZ

0 1

C	-0.3135060286	-0.8961934083	-0.4368147803
H	0.0018346288	-1.3659998784	-1.3617334138
N	0.6870448603	-0.5497807785	0.3622580967
O	0.4397312726	0.2275774586	1.3568036268
H	-1.9469699758	0.9670654842	-0.957577689
C	-0.8933043448	1.1834163907	-0.8580728505
C	-0.4219056281	1.8077339912	0.2750515204
C	-1.6127536212	-1.3307194251	0.1671279733
H	-1.8769868254	-0.6832803819	0.9981050385
H	-2.4052466594	-1.312613386	-0.5771659686
H	-1.5164140399	-2.3541257122	0.5387120174
H	-0.3480090477	1.2955596966	-1.7880176465
H	-1.1051018729	1.9972957809	1.0916034372
C	0.8416428739	2.6148307056	0.2514075525
H	0.662622125	3.6063895539	-0.1714262325
H	1.2615383492	2.7317320867	1.247404099
H	1.5881555089	2.1267062169	-0.380807293
H	1.603814005	-0.4403722649	-0.0672973475

TS2bE

0 1

C	-1.5566754915	-0.1730616949	-0.7408926395
N	-0.6374932906	-1.1084431052	-0.570040508
O	-0.0516919317	-1.1801014515	0.5826833315
H	-0.9996835284	1.9932646647	0.6210496422
C	-0.3326538241	1.4924245069	-0.0636257364
C	0.738900988	0.8066491112	0.4491830921
H	-0.2376219987	1.9079377566	-1.0572326723
H	0.9573357567	0.7248695991	1.5051731406
O	1.7342245038	0.4932627523	-0.4113729674
C	2.7485116592	-0.3304341353	0.1368663496
H	3.4899385045	-0.4835170891	-0.6425195513
H	3.2212111819	0.1623262139	0.9902204133
H	2.3199468935	-1.2812330305	0.45412664
H	-0.0632296307	-1.3521856927	-1.3768162963
H	-2.1913171487	-0.0223848328	0.119620823
C	-2.1041504905	0.090030402	-2.106413221
H	-2.9479347989	-0.5646306658	-2.3301066057
H	-2.4548681571	1.1181460171	-2.1725574587
H	-1.3377571064	-0.0538811162	-2.8683855356

TS2bZ

0 1

C	1.3495877093	0.7292775415	-0.0484044568
H	2.2745733414	0.5936077476	0.5015446579
N	0.964858129	-0.344139682	-0.7274280185
O	-0.2453162423	-0.3677206183	-1.1916622998

H	-0.5897467515	1.7049619911	1.402099197
C	-0.2840572617	0.6707554272	1.3849196452
C	-1.1103820706	-0.2417038387	0.7767824104
C	1.0633832256	2.0893791009	-0.607348224
H	0.0661404506	2.1147093415	-1.0366557178
H	1.1493317053	2.8478468412	0.167374761
H	1.7890104191	2.3181098993	-1.3919110881
H	0.3278103707	0.3235413985	2.2057495055
H	-2.0406186994	0.0154595575	0.2888221405
O	-0.9136709603	-1.5442610362	1.0790014019
C	-1.7014023746	-2.4512340072	0.3275117691
H	-1.4672397553	-3.449010533	0.6883035423
H	-2.7647842993	-2.2535268252	0.483789759
H	-1.4622183239	-2.3578379554	-0.7317907737
H	1.3248920277	-1.2420169403	-0.410191861

TS2cE

0 1

C	2.1300415439	-0.2582725106	0.6440528943
N	1.1582907267	-1.1415254459	0.4225123317
O	0.5613225974	-1.1175086107	-0.7035843509
H	1.7715654039	2.0647148109	-0.2026326214
C	1.0026990853	1.444466134	0.2375420978
C	-0.0079052534	0.9577875386	-0.5618794643
H	0.7799210465	1.6207769654	1.2819116157
H	-0.0397841644	1.0981281562	-1.6300144814
C	-1.1911579929	0.4036243449	0.0984255004
O	-1.213358548	0.0796703837	1.2692732889
O	-2.2376100757	0.2570620002	-0.7209455803
C	-3.3730462693	-0.3805971262	-0.1453735929
H	-4.1274556743	-0.4080910502	-0.9248866662
H	-3.1171484701	-1.3901809112	0.1726797738
H	-3.7316065161	0.1807833487	0.7156747746
H	0.57305965	-1.4013832673	1.2209228627
C	2.7121597722	-0.1512901991	2.0172351172
H	3.4918559763	-0.8959617138	2.1810335904
H	3.1560964905	0.8331073305	2.1529928868
H	1.936192796	-0.2772408037	2.7727408228
H	2.7641997756	-0.0906975542	-0.2150551795

TS2cZ

0 1

C	-1.3289149667	-0.2876128312	0.6282910814
H	-1.6061946973	-0.1123574832	1.6614395891
N	-0.8066815129	0.7870054748	0.0282934291
O	-0.2725588258	0.6309992312	-1.1187456753
H	0.0061600751	-2.3740136279	0.6137870339
C	0.4303719714	-1.381138692	0.6649065996
C	1.1137209444	-0.8893451468	-0.4285663878
C	-2.19209531	-1.2088642281	-0.1824319534
H	-1.7195839168	-1.4299419058	-1.1355078038
H	-2.3705472306	-2.1344498716	0.3598126782
H	-3.1556063626	-0.7324824424	-0.3746008583
H	0.7456230863	-1.0420614998	1.6426741283
H	1.166029491	-1.4019235733	-1.3754645823
C	1.9802380126	0.2739977762	-0.225382023
O	1.9172529905	0.9921573583	0.7519879267
O	2.8292840965	0.48491823	-1.2365104202
C	3.6121637948	1.6697908739	-1.1323097589
H	4.2524488713	1.6828984032	-2.0084818057

H	2.9665956874	2.5466278146	-1.1191437006
H	4.2079784249	1.6557030728	-0.221422609
H	-0.3442226433	1.4755266572	0.625933132

TS2dE

0 1

C	-0.3380434377	0.0265567835	0.3928142135
N	0.4421541101	-0.4016758434	-0.6087377054
O	1.3174186707	-1.2899693861	-0.3494641371
H	0.7329813256	0.1846646394	2.6486333024
C	1.1925389945	0.4862575191	1.7176091884
C	2.2520125744	-0.2504708388	1.2247886647
H	1.1587000531	1.5430342925	1.490246027
H	2.6194998566	-1.1482455325	1.6944834607
C	3.0674133874	0.3546078908	0.1695055114
O	2.6909107014	1.2857773174	-0.5154516167
O	4.2517235062	-0.2414870682	0.0031318471
C	5.0306768015	0.246622142	-1.0846968394
H	5.9562429172	-0.3193123185	-1.066677115
H	4.5049660372	0.0877743366	-2.0249079589
H	5.2282102572	1.3104184039	-0.9661521666
H	0.6961700605	0.2776859285	-1.3293293952
C	-1.1825942288	1.2130865941	0.1659829906
C	-2.5164841156	1.2128576103	0.5641065484
C	-0.6461646429	2.3531372177	-0.434239892
C	-3.3129496049	2.3259857015	0.344238604
H	-2.931178143	0.3326392256	1.0390011904
C	-1.4481947053	3.4599019203	-0.6622183612
H	0.4080194698	2.3780606502	-0.6896798051
C	-2.7820170541	3.4480454783	-0.27602747
H	-4.3488829671	2.3166657126	0.6545409035
H	-1.0269469143	4.3399347152	-1.128634865
H	-3.4041927159	4.3153375583	-0.449984019
H	-0.718052084	-0.7662732405	1.0219819643

TS2dZ

0 1

C	-0.2975518845	-0.063520532	-0.0450739013
N	0.632199001	0.1800486282	-0.9812436199
O	1.5162703167	-0.717613494	-1.2040950745
H	0.4834952837	-1.1984951897	2.0321541304
C	1.0548778543	-0.4630946504	1.4853990124
C	2.1766524823	-0.8691757542	0.7860439002
H	1.0515242191	0.5450430575	1.8781682278
H	2.4764527924	-1.9017803662	0.7055125799
C	3.141386444	0.162222632	0.3854136764
O	2.8690067838	1.3432227309	0.3260136729
O	4.3387409505	-0.3324890375	0.0585397992
C	5.27585553	0.6213071228	-0.4331476893
H	6.1920332057	0.0704789395	-0.6191284074
H	4.9068608105	1.0707536426	-1.3537518398
H	5.4421285489	1.4065764455	0.3019394603
H	0.9862959804	1.1375274004	-1.0247634612
C	-1.1078365786	-1.2996927135	-0.0260546435
C	-2.314429908	-1.2597744992	0.6737929891
C	-0.7348378712	-2.4834287546	-0.664792614
C	-3.1346798187	-2.373719792	0.7394753928
H	-2.61279675	-0.3428058659	1.1676685664
C	-1.5665636717	-3.591229141	-0.6058913461
H	0.1989118066	-2.5256524926	-1.2036940489

C	-2.7626293926	-3.5455950393	0.096591823
H	-4.0665865725	-2.3243955351	1.2860278879
H	-1.2731623945	-4.5012788722	-1.1116416802
H	-3.4013434454	-4.417066248	0.1411328467
H	-0.8287594321	0.8319997978	0.2579082207

TS2e

0 1

C	-0.4127405119	-0.0456527291	-0.2180233581
N	0.5562095512	0.0093808253	-1.163725702
O	1.4353625635	-0.9162161263	-1.1957377522
H	0.3717304315	-0.8394626974	2.0320869347
C	0.9415955906	-0.204451635	1.3687185119
C	2.0729166306	-0.7215942309	0.7581183629
H	0.9378631655	0.8550543787	1.5863230908
H	2.387696819	-1.7467260418	0.8757845078
C	3.0495336777	0.2291478248	0.2096227828
O	2.7824791586	1.3815920737	-0.055808036
O	4.2504515186	-0.3161502091	-0.0073009723
C	5.1966738352	0.5361935843	-0.6461428617
H	6.1126894205	-0.0401832156	-0.7242914097
H	4.8391929633	0.8198542358	-1.6347011477
H	5.3591136181	1.436964039	-0.0571067345
H	0.9289150652	0.9447570072	-1.3490853795
C	-1.1880003835	-1.322026662	-0.0594235111
C	-2.5807862519	-1.2635172551	0.0097148858
C	-0.5757039188	-2.5778863315	-0.0140178036
C	-3.3396592547	-2.4201780355	0.1200451237
H	-3.0841418026	-0.3084369042	-0.0350526755
C	-1.3373751554	-3.7295336895	0.0917830508
H	0.4972717221	-2.6523824527	-0.0710060562
C	-2.7217719244	-3.658740972	0.1620158326
H	-4.4175283241	-2.3461268301	0.1685588683
H	-0.8420065723	-4.6905615873	0.1231589933
H	-3.3112650035	-4.5613741796	0.248365377
C	-1.1576262052	1.2388195879	-0.0574688416
C	-1.6456887712	1.6126582356	1.1933863467
C	-1.389930842	2.0747028361	-1.14644639
C	-2.3317362984	2.8044030382	1.3543853795
H	-1.4881401369	0.9598473449	2.0421099021
C	-2.0711757881	3.273522424	-0.9827027656
H	-1.0581170833	1.7771408437	-2.1325929775
C	-2.5410520082	3.6430402903	0.266957889
H	-2.6999117037	3.0827348736	2.3324056655
H	-2.2402171238	3.9128414994	-1.8383613128
H	-3.0721576672	4.5761808421	0.3951671825

TS2f

0 1

C	-0.422710658	-0.0550020036	0.1209343504
N	0.5447143188	-0.1823645117	1.0595034459
O	1.3551009418	0.7962793944	1.2494699923
H	0.3415709842	0.9598258841	-2.0475871893
C	0.9567679379	0.354569964	-1.3977770551
C	2.0078507816	0.9381690174	-0.7039093933
H	1.1081124834	-0.6663729953	-1.7158454532
H	2.189074318	2.0011241978	-0.6930763341
C	3.0945427928	0.0628706288	-0.2479242322
O	2.9969767013	-1.1436145125	-0.157246973
O	4.1990932829	0.7337133768	0.0956016306

C	5.2414799259	-0.0605387214	0.6528918943
H	6.0515048009	0.6256805498	0.8778576475
H	4.8953259347	-0.5532347977	1.5599458688
H	5.5669002661	-0.8181263222	-0.0577981655
H	0.9998304662	-1.089175671	1.1310118006
C	-1.2506626866	1.2756517883	0.2363540772
C	-2.4296942061	1.346545026	-0.7410784394
H	-3.1633990069	0.5578143175	-0.6037288232
H	-2.9422038899	2.2948220361	-0.5776388433
H	-2.0913595196	1.334818156	-1.7779165423
C	-0.4690411584	2.5860801403	0.005943632
H	-0.1051819784	2.6801931603	-1.0154800014
H	-1.1664741607	3.4086538356	0.170835589
H	0.3597773909	2.6977523922	0.6941840202
C	-1.7858970601	1.3595170451	1.6798522162
H	-2.422220212	0.5185709395	1.941870113
H	-0.9572352025	1.4030951915	2.3855133795
H	-2.3745124834	2.2714918928	1.7874735181
C	-1.0971816299	-1.420540966	-0.2210718076
C	-1.5726162539	-1.5116467691	-1.6810638331
H	-2.0259382147	-2.4931138204	-1.8264025975
H	-2.3164847029	-0.770943331	-1.9470689096
H	-0.7432744421	-1.4298785667	-2.3805338929
C	-2.2867439028	-1.7229235319	0.7071245379
H	-3.1226891225	-1.0414651081	0.5749198723
H	-2.6474912035	-2.7301398211	0.4919019742
H	-1.9785729908	-1.6927699555	1.7525053954
C	-0.1072400659	-2.5878565425	-0.0292957152
H	-0.5561726022	-3.489037687	-0.4452378918
H	0.8478338703	-2.4212873691	-0.5274130195
H	0.0838047363	-2.7973750207	1.0250615171

TS2g

0 1

C	-0.4019938449	0.0518895758	-0.3591140564
N	0.6385141845	0.0727304017	-1.2293875886
O	1.45929549	-0.9158594026	-1.2303410613
C	0.8518480523	-0.363556718	1.3450943385
C	1.9651809739	-0.8951794606	0.7001420297
H	0.9300160692	0.6895920267	1.5877924065
H	2.2123340805	-1.9445411926	0.7730396833
C	3.0408735169	0.0227389835	0.2977042699
O	2.876511341	1.2084764193	0.1076858518
O	4.2158103901	-0.592217539	0.1251045536
C	5.2691477343	0.23803134	-0.3560221462
H	6.1466961303	-0.3975426482	-0.4150046889
H	5.0178748748	0.6344083978	-1.3384719392
H	5.4415081414	1.0683009068	0.3262936976
H	1.0921547193	0.9845298296	-1.3276793256
C	-1.3011112453	-1.1375650849	-0.3135158376
C	-2.576799167	-1.007884682	0.2410898938
C	-0.924536976	-2.3896724564	-0.8130604408
C	-3.4424845774	-2.0889988815	0.3090597413
H	-2.9078483144	-0.0499216073	0.6153835631
C	-1.8005342051	-3.4616408926	-0.7569240351
H	0.0534088936	-2.5200527862	-1.2463931085
C	-3.0591886117	-3.3236146293	-0.1888177477
H	-4.4230677909	-1.9582951405	0.7466048012
H	-1.489251168	-4.4172325988	-1.1571981912
H	-3.7334856587	-4.1676246689	-0.1392683595

C	-1.0296460427	1.4041412924	-0.2080345345
C	-1.3550371713	1.9347417949	1.0378861934
C	-1.304908292	2.1562104298	-1.3489005813
C	-1.9315388002	3.1913420756	1.1399954879
H	-1.1568998489	1.3641820777	1.9347924412
C	-1.8729339981	3.4177827538	-1.2452782227
H	-1.0846608549	1.7409201569	-2.3238110391
C	-2.1879849754	3.9391840218	-0.0004202274
H	-2.1743108639	3.5894956332	2.1158031624
H	-2.0771463058	3.9876211205	-2.1414888374
H	-2.6333214247	4.9210568707	0.0827174791
C	0.0545739144	-1.2198349667	2.2941941162
H	-0.9474841685	-0.8259303684	2.4639700681
H	-0.0582392719	-2.2333561893	1.9083204254
H	0.5555510712	-1.2776191947	3.2622727652

TS2h

0 1

C	-0.8927632655	0.0958015582	-0.242466575
N	0.1279220142	0.1866177706	-1.1284645866
O	0.9680404266	-0.7879883923	-1.1918294942
C	0.4534722309	-0.1458224435	1.3916873835
C	1.5385157748	-0.7441775742	0.7471760858
H	0.5678442216	0.924056034	1.5026956012
H	1.7764178176	-1.7879407126	0.8959846247
C	2.6120096168	0.1137493623	0.2302733116
O	2.49062143	1.303463776	0.0201118802
O	3.7441908199	-0.557014275	-0.0088650642
C	4.7859106547	0.2057294578	-0.609994787
H	5.6246498349	-0.4733834457	-0.7238136909
H	4.4647783259	0.581419506	-1.5801049417
H	5.0576238339	1.0487630888	0.0227344801
H	0.5777694154	1.0942444191	-1.2269460596
C	-1.7117075449	-1.2441850334	-0.3871487309
C	-3.0290196787	-1.2837442333	0.4012426187
H	-3.711026613	-0.4743947378	0.1628277771
H	-3.5347022089	-2.2157684955	0.1457739811
H	-2.8693146215	-1.2953030523	1.4770147994
C	-0.9633863126	-2.5321187088	0.0047443444
H	-0.7736949692	-2.5892735214	1.0713858436
H	-1.6100775095	-3.3738094131	-0.2492107385
H	-0.0313158284	-2.6423008033	-0.5360122755
C	-2.0522046562	-1.4006352222	-1.8854162622
H	-2.6276157216	-0.5633320152	-2.271875994
H	-1.1424975917	-1.5003397607	-2.4747534464
H	-2.6457717403	-2.3062352327	-2.0175836458
C	-1.6048930296	1.4677496398	-0.0332200278
C	-2.1960765664	1.6092704075	1.3781151871
H	-2.7244781328	2.5620702057	1.4335954959
H	-2.9046402578	0.8291545585	1.6345039582
H	-1.4144795528	1.6247389792	2.1363147831
C	-2.7133868496	1.7162749451	-1.0747912208
H	-3.5570602324	1.0374992769	-0.9939805987
H	-3.0943354208	2.7296614549	-0.9368297025
H	-2.311858985	1.6456936941	-2.0858758088
C	-0.6242337635	2.6469090614	-0.2067540805
H	-1.1174811593	3.5540891175	0.1415118958
H	0.3025138677	2.5291341201	0.3523425619
H	-0.3700964659	2.8166073285	-1.25495909
C	-0.1784729305	-0.8039607656	2.6023427564

H	-1.2654364948	-0.7931795842	2.5888115762
H	0.1493890175	-1.8348646256	2.7202607138
H	0.1313448006	-0.2645047134	3.4993621619

TS3aE

0 1

C	1.1975608001	-0.1499419581	0.7153262608
N	0.3672238987	-1.173195632	0.6085089486
O	-0.3653095796	-1.2686620645	-0.4437448098
H	0.3827708018	2.0808144671	-0.0586930789
C	-0.3284999821	1.3641634539	0.3343646657
C	-1.1442931379	0.6753454151	-0.5320432917
H	-0.6298103678	1.52090131	1.3621506816
H	-0.0308618449	-1.5417779831	1.471413788
C	1.8993851536	0.1107715437	2.00748878
H	2.8758766092	-0.3748757567	2.0386429874
H	2.0548847216	1.1810559063	2.1332617511
H	1.3074639368	-0.2426836379	2.8523110578
H	1.676891578	0.1277456849	-0.2120761848
H	-2.0807037451	0.2772490056	-0.1648283345
C	-1.0163683706	0.8010690913	-2.0173913328
H	-1.2615499319	-0.1386722374	-2.508723637
H	-1.6852339002	1.5746724081	-2.4014514616
H	0.0042320902	1.0732785538	-2.2903999599

TS3aZ

0 1

C	1.4489331854	0.132804119	0.3395334302
H	2.2250158636	0.1959062516	1.0944169678
N	1.0845668708	-1.1084762639	0.0433448003
O	0.0077416552	-1.2923359488	-0.6358366639
H	-0.4144204658	1.6763224511	1.0891403285
C	-0.4751742536	0.6124148307	1.278985893
C	-1.3224392519	-0.1602536168	0.5152505492
C	1.4285210558	1.1784500968	-0.7316008595
H	0.5603250599	1.0438341546	-1.3699885688
H	1.4116354767	2.175597906	-0.298161524
H	2.3287949996	1.0893008079	-1.3449968969
H	-0.2184815729	0.302221753	2.2827627261
C	-2.1189109688	0.3947387693	-0.6250274606
H	-3.1514425773	0.576715097	-0.3185794892
H	-1.7041419566	1.3433649071	-0.9669556096
H	-2.1328602788	-0.3005540299	-1.4634381087
H	-1.6841679896	-1.0936477215	0.9259908039
H	1.3012001484	-1.8281095631	0.7288936821

TS3bE

0 1

C	-1.7846743431	0.0220839313	-0.1126399658
N	-1.3517654928	-1.1852509802	-0.4309806953
O	-0.1110575746	-1.4773790136	-0.2003286774
H	-0.4592874667	2.0354925136	-0.6237178635
C	-0.2884227794	1.1238138847	-1.1790121524
C	0.8104383622	0.3642969944	-0.8623363747
H	-0.66379743	1.0898186666	-2.1914430517
H	1.3151438273	-0.2719111062	-1.5775268227
O	1.4796263119	0.6431158759	0.2721202196
C	2.4709131486	-0.3114127347	0.6111906975
H	3.2465775362	-0.3435091919	-0.1588526258
H	2.9115411721	0.0105837788	1.5505678591

H	2.0181337881	-1.2954004073	0.7235397583
H	-1.7780901311	-1.6375355199	-1.237373108
C	-3.150097357	0.4562254312	-0.5379113966
H	-3.8962672036	0.21869883	0.2216725933
H	-3.1657008206	1.5332724209	-0.6954258164
H	-3.439724832	-0.0247708405	-1.4726807354
H	-1.3720921555	0.4049970868	0.8114753079

TS3bZ

0 1

C	0.9139068339	0.9364336334	0.3060358895
H	1.646028053	1.2791834191	1.0295071512
N	1.2663946426	-0.1703860836	-0.332730622
O	0.3662770505	-0.7979420501	-1.0230932971
H	-1.2312957534	0.944673928	1.6199408993
C	-0.7089616893	0.0229572255	1.4081137239
C	-1.2177559798	-0.804746266	0.4345922596
C	0.0998130933	1.9686412659	-0.4123218718
H	-0.7398855482	1.5064807512	-0.9229587598
H	-0.2690630019	2.7142410284	0.2884155541
H	0.7282165061	2.4716903709	-1.1512965873
H	-0.1675357216	-0.4298260728	2.2249891091
H	-1.0633615934	-1.876260628	0.4437160677
O	-2.2176491847	-0.3584948218	-0.3537447683
C	-2.5133281872	-1.2056828646	-1.4508191942
H	-2.8230210819	-2.1931905617	-1.0975486483
H	-3.334577047	-0.7453440949	-1.9929825032
H	-1.6394076306	-1.3021320313	-2.0939688658
H	1.9679089794	-0.7568947175	0.1105121736

TS3cE

0 1

C	2.2286156556	-0.0582872006	-0.0193910033
N	1.8588643461	-1.2771409698	-0.4083586672
O	0.6162012391	-1.5052658988	-0.6037009704
H	1.0229955785	1.115849894	1.6323547038
C	1.0159074817	0.0338970741	1.6504029303
C	-0.110916441	-0.612734511	1.1935630723
H	1.6315835602	-0.4362596001	2.4063987036
C	-1.0717331661	0.1630528611	0.3914638198
O	-0.8575247951	1.2673664387	-0.0482712716
H	-0.4241436256	-1.5823235546	1.5441411432
O	-2.2069549978	-0.508786538	0.1688418609
C	-3.1414070233	0.1509339559	-0.6797272789
H	-2.695030117	0.3408741489	-1.654091932
H	-3.988026282	-0.5216044088	-0.7721054925
H	-3.4506545275	1.0988710931	-0.2424600601
H	2.4137627898	-2.0630741033	-0.0689496927
H	1.6597917786	0.7332878406	-0.4920956244
C	3.6559188796	0.1858498232	0.3530175579
H	3.7154875569	0.9938588555	1.079968774
H	4.1031832558	-0.7027440388	0.8000771746
H	4.2476648335	0.4754937686	-0.5159501174

TS3cZ

0 1

C	-2.2837396054	0.0868570293	0.1820164373
H	-2.7422967869	0.7675986859	0.8916572231
N	-1.4116305065	0.688724885	-0.6303943757
O	-0.6307347115	-0.0289010538	-1.3440748283

H	-1.4648493933	-1.869231429	1.4182238697
C	-0.8180840124	-1.0275881375	1.2106903132
C	0.1496788428	-1.186024099	0.2406334234
C	-3.1263635634	-1.0340825964	-0.3456872615
H	-2.5259342663	-1.7513258919	-0.8967590943
H	-3.6223976181	-1.5480470943	0.4746152728
H	-3.8932701194	-0.6222064452	-1.0056104003
H	-0.6325619865	-0.3502330379	2.0325285566
C	0.1644923944	-2.4006862362	-0.5949682282
O	-0.7109691842	-3.2302212728	-0.637969325
H	1.0524363875	-0.5954551776	0.2279997068
O	1.2812296129	-2.4789487702	-1.33045427
C	1.3471745146	-3.5970379366	-2.2100499401
H	0.5224037155	-3.5673602059	-2.9197725167
H	2.2979524402	-3.5159259696	-2.7266680137
H	1.2937405193	-4.5277926597	-1.647734922
H	-1.022756103	1.5741361435	-0.3117027671

TS3dE

0 1

C	-0.6195693499	-0.3958406246	0.1939601223
N	-0.1215651228	-0.5094604612	1.4309726797
O	1.1403461697	-0.6767521582	1.5534910862
H	0.155040496	-1.7591830066	-1.571973144
C	0.1867026446	-2.1323816821	-0.5571587824
C	1.4061761654	-2.1543577133	0.0889904642
H	-0.5696841066	-2.8608745971	-0.2966510689
C	2.50494681	-1.3617279109	-0.490765095
O	2.3646015066	-0.5419345267	-1.3658763884
H	1.6613550968	-2.8749611536	0.8488884343
O	3.6808414688	-1.6220720066	0.0913309603
C	4.767947996	-0.8207191854	-0.3619384544
H	4.5587230199	0.232285276	-0.1827765512
H	5.6342078741	-1.1414116908	0.2076631334
H	4.9330149371	-0.971331023	-1.4274559176
H	-0.7099507072	-0.9410949152	2.1421844437
C	-2.0795939422	-0.3851008161	-0.0044622859
C	-2.6402593633	0.4981573171	-0.9234001201
C	-2.9159498424	-1.2601347964	0.6888245455
C	-4.0110242558	0.5246027322	-1.1283053456
H	-1.9941189844	1.1695221804	-1.4743797569
C	-4.2867581946	-1.2248754792	0.4936635194
H	-2.493367742	-1.9931321124	1.3659570611
C	-4.8378752352	-0.3312053502	-0.4151170914
H	-4.4335510179	1.2161745935	-1.8442305304
H	-4.9252793934	-1.9057478578	1.0397278605
H	-5.9072246291	-0.3105102062	-0.5739580432
H	-0.0072726279	0.2102586744	-0.463255605

TS3dZ

0 1

C	-0.5916988271	-0.2983740958	0.2766529185
N	-0.1946100369	-1.166877225	1.2159361995
O	1.0598190801	-1.3883760729	1.3761505324
H	0.7254343905	-0.3155953012	-1.8235196034
C	0.5044334431	-1.2281459891	-1.2880412482
C	1.5301170805	-1.8293875992	-0.5850035166
H	-0.2935650363	-1.8412864643	-1.6834229642
C	2.8417365154	-1.155460526	-0.4812715645
O	3.0757908727	-0.0256721065	-0.8244573317

H	1.5263553849	-2.8850376528	-0.3607251544
O	3.7606448363	-1.9623629202	0.0690827572
C	5.0426514872	-1.372574789	0.2592670783
H	4.9674397821	-0.5127687808	0.9229048969
H	5.6638093438	-2.1435169104	0.7036169351
H	5.4576995913	-1.0459046137	-0.6926918925
H	-0.7937346524	-1.9779974157	1.3527311152
C	-0.0783806084	1.0809510628	0.1835448239
C	-0.7792669475	1.9701256393	-0.6322364118
C	1.0378341159	1.5346883879	0.8830370001
C	-0.3738947174	3.2875012607	-0.7543208043
H	-1.6508617593	1.6220158398	-1.1742178627
C	1.4305324256	2.8591016764	0.7689948797
H	1.5953915394	0.8484461635	1.5007931498
C	0.7349351405	3.7365098138	-0.0495122532
H	-0.9259475081	3.9642517481	-1.3921471113
H	2.2976777837	3.2034682468	1.3156593615
H	1.0554287927	4.7654707511	-0.1395085311
H	-1.6402022321	-0.4094410476	0.0208610616

TS3e

0 1

C	-0.6894149556	-0.3425977173	0.3261300879
N	-0.2393419889	-1.2014870736	1.2602833033
O	1.0196113949	-1.4309206898	1.3610726701
H	0.4549559038	-0.4912012993	-1.8752915503
C	0.3367286898	-1.3738377324	-1.2617709268
C	1.4446372342	-1.8515583465	-0.5930351073
H	-0.4459521899	-2.0666029765	-1.5384701221
C	2.6839057756	-1.0423421009	-0.5905067827
O	2.7876727734	0.0701377956	-1.0376876557
H	1.5571271762	-2.8934366365	-0.3373414399
O	3.6962165879	-1.6997238613	-0.0069792486
C	4.9115454464	-0.9649627439	0.0928202839
H	4.76140147	-0.0675188247	0.6910472111
H	5.6244211341	-1.6285031985	0.5717344284
H	5.2630486348	-0.6722442494	-0.8951049356
H	-0.8456223832	-2.001619712	1.4373869609
C	-0.0485372224	1.0016326637	0.2110588898
C	-0.4293797866	1.8629612838	-0.816210874
C	0.8832135584	1.4424048875	1.1477208764
C	0.1236615346	3.1270160847	-0.9210820634
H	-1.1646896822	1.5448371714	-1.5429325106
C	1.4238703009	2.715043984	1.0479569716
H	1.1957968609	0.7845106551	1.944219908
C	1.0554860368	3.5585986529	0.011883834
H	-0.1767448783	3.776994403	-1.7314563163
H	2.1468478021	3.0434891482	1.7824035808
H	1.4906382325	4.5452502891	-0.0699433277
C	-2.169748867	-0.4175005961	0.1150123957
C	-2.7376690174	-0.5281299712	-1.1520929737
C	-3.0104180389	-0.3601938602	1.2264818332
C	-4.1149973499	-0.5862805126	-1.3016680116
H	-2.1021625577	-0.5746090937	-2.0254580278
C	-4.3872107107	-0.4301927126	1.0755134045
H	-2.578210322	-0.241758354	2.2119638615
C	-4.9436269389	-0.5422027005	-0.1896295134
H	-4.5409467426	-0.6738783693	-2.2919146342
H	-5.0243853493	-0.3876606684	1.9483442833
H	-6.0170725658	-0.591664018	-0.3100357627

TS3f

0 1

C	-1.0690791563	-0.0731567718	0.1538440314
N	-0.3465581193	-0.6237949832	1.1466430602
O	0.9137156859	-0.4263915933	1.3096033695
H	0.6917118989	0.3802188858	-1.844185713
C	0.5391089137	-0.5648160659	-1.3444483998
C	1.5522512079	-0.9899470854	-0.5125784581
H	-0.0751609055	-1.2866083162	-1.8545757915
C	2.8010656068	-0.2046199788	-0.3828104577
O	3.0009164359	0.8852760172	-0.8555639031
H	1.6412137528	-2.0273214337	-0.2212790546
O	3.7171691883	-0.8655765219	0.3384730239
C	4.9407421329	-0.1666474682	0.5434929893
H	4.7549050567	0.7811162498	1.045397741
H	5.5547584277	-0.8127483231	1.1625651495
H	5.4305854139	0.0303461196	-0.4088782847
H	-0.6343313009	-1.5585406233	1.4213597299
C	-1.097254862	1.4771430366	0.0451891477
C	-2.3446161576	-0.9461157145	-0.0960364583
C	-3.1509156044	-1.1081879626	1.2115465181
H	-4.072283115	-1.6497823557	0.9920651655
H	-2.6087464274	-1.687012204	1.9604257317
H	-3.4160789666	-0.1541269224	1.6567733055
C	-3.2875322507	-0.3920915063	-1.1658378034
H	-2.763793031	-0.2023119823	-2.1016455412
H	-4.0566762376	-1.1417610525	-1.3583266646
H	-3.7922651121	0.5186330707	-0.853441879
C	-1.9706302935	-2.3670403854	-0.5694293972
H	-2.8262884876	-3.0259293719	-0.4167456607
H	-1.7366594753	-2.3854026772	-1.6317506938
H	-1.1242539334	-2.8007127926	-0.0356113634
C	-2.1598027334	2.0103938975	1.0290875807
H	-2.118801782	3.1004329308	1.0215023391
H	-3.1732465249	1.7223096678	0.7573866352
H	-1.9542646434	1.6712355662	2.0450647238
C	0.2300043599	2.1204227462	0.4726539265
H	1.0588423232	1.8388824488	-0.1703740741
H	0.1042803038	3.202545288	0.4113526056
H	0.4927309782	1.8648358277	1.4953667847
C	-1.4466491367	2.0205636725	-1.3526459875
H	-1.1540237365	3.070055003	-1.3890699869
H	-0.9182261069	1.5070219087	-2.1514775145
H	-2.5095635864	1.9805617552	-1.5690604719

TS3g

0 1

C	-0.6893452939	-0.1930272801	0.4228457442
N	-0.3365954785	-0.9878223677	1.4527316707
O	0.8996263411	-1.3207210134	1.5810280949
H	0.268813691	-0.8492876024	-1.7796227561
C	0.185044622	-1.6018864184	-1.005576103
C	1.3385196915	-1.8934662885	-0.2968858698
C	2.5444746799	-1.0519232461	-0.4835649413
O	2.6388429463	-0.1257454194	-1.2470605647
H	1.51768999	-2.88541962	0.0924352144
O	3.5466525387	-1.4511491672	0.3111079938
C	4.724685251	-0.655721924	0.2308972985
H	4.4943479724	0.3816176263	0.4692070012

H	5.4178821435	-1.071907697	0.9547443068
H	5.1463011168	-0.6989080369	-0.7722824913
H	-1.0138808254	-1.711358124	1.6919687699
C	0.1399946295	1.0280597716	0.1789016081
C	0.0365077303	1.7456984247	-1.0089896652
C	0.9937217468	1.501942575	1.173734789
C	0.7831781103	2.8934190534	-1.2114152402
H	-0.6193100429	1.4059725697	-1.7969725358
C	1.732332026	2.6576905637	0.9734011592
H	1.0895206268	0.9571433049	2.1009695093
C	1.6380183227	3.3540046068	-0.2216026837
H	0.6992591044	3.4257886323	-2.1488584516
H	2.3888946817	3.0108483608	1.7573699826
H	2.2242778676	4.2486218013	-0.3811336144
C	-2.1642357767	-0.0761971726	0.2209674467
C	-2.7377230397	-0.0071355341	-1.0478385295
C	-3.0023064354	-0.0090693897	1.3343902064
C	-4.1087015885	0.1216494541	-1.1977043872
H	-2.1122685783	-0.0781258725	-1.9264167933
C	-4.3762586444	0.1094846144	1.1834430621
H	-2.570001381	-0.0187819651	2.3266008671
C	-4.9342702738	0.1775557361	-0.083046194
H	-4.5342917929	0.1723197779	-2.1906582762
H	-5.0074923111	0.1616811285	2.060068139
H	-6.0042645879	0.2769557026	-0.2034060665
C	-0.8445059914	-2.6910441472	-1.1537865507
H	-1.0349351962	-3.1736518516	-0.191468917
H	-1.7951622163	-2.3317544814	-1.5392329697
H	-0.4847613759	-3.4685970849	-1.8310862629

TS3h

0 1

C	1.1022240177	-0.0555223596	-0.3060393288
N	0.4377876096	-0.4542046445	-1.4145537891
O	-0.8126731255	-0.1575447737	-1.5489460524
C	-0.4063905972	-1.007423942	0.9749179539
C	-1.4812044831	-1.0412606527	0.0754513078
H	0.1612361224	-1.9279123534	0.9658333326
C	-2.7517697936	-0.2960198814	0.2368603294
O	-2.9881845032	0.6028295896	1.0039181135
H	-1.6141876515	-1.9291121003	-0.525733351
O	-3.6711063329	-0.7642524798	-0.6246921171
C	-4.9270838558	-0.095316033	-0.5890109767
H	-4.7983590662	0.9640664367	-0.803926461
H	-5.5389708519	-0.5679537017	-1.3504918065
H	-5.3874671122	-0.2002108994	0.3922116898
H	0.666431991	-1.3726683592	-1.7750119385
C	1.0436219631	1.497063579	-0.0692106493
C	2.421199104	-0.8596910135	-0.0888299889
C	3.6213399011	-0.231582296	-0.8227990975
H	4.4823921199	-0.892867896	-0.7100865753
H	3.4130033225	-0.1306348744	-1.8881227303
H	3.9041982306	0.742579203	-0.4361912117
C	2.7692180879	-1.0140449931	1.4012387675
H	2.0275106188	-1.6144178541	1.9252029023
H	3.7272929687	-1.5305130181	1.4781828756
H	2.8654847399	-0.0684890967	1.921943989
C	2.3163914527	-2.2930724861	-0.6494902702
H	3.1813516569	-2.8599228144	-0.3066521657
H	1.4251054615	-2.8207851294	-0.3100661081

H	2.3464397687	-2.3181882935	-1.7406644219
C	1.4891790777	2.1713146652	-1.3858165116
H	1.453602156	3.2529879415	-1.2497520952
H	2.5013694738	1.9061913319	-1.6807784813
H	0.8093657511	1.9092025751	-2.1948940111
C	-0.3540181776	2.0610386896	0.2296585104
H	-0.7649336859	1.6937515367	1.1619531935
H	-0.2565839379	3.1447146906	0.3189528483
H	-1.0594212808	1.846716853	-0.5639883505
C	1.9462946075	2.0160235938	1.0594342957
H	1.8630470542	3.1032664379	1.0675520471
H	1.6226124653	1.6659061807	2.0370180872
H	2.9984538274	1.7788022202	0.9344321757
C	-0.4642128651	-0.4072404525	2.3657036273
H	0.4597407918	0.099061241	2.6367300476
H	-1.2910049776	0.2834303889	2.4868315662
H	-0.6003560438	-1.215890756	3.0878258293

Intramolecular reactions

6aE

0 1

C	0.3375104755	-0.8465860824	1.6802533341
C	0.4177966673	-1.8499960606	2.5426316113
H	1.029031243	-0.0121691146	1.7842519958
N	-2.5891545186	-0.1485151662	-1.360977579
O	-3.5772000875	0.2109352788	-2.2711382482
H	-3.5041101847	-0.460823125	-2.9530152343
C	-2.5440069764	0.6550137276	-0.3871223259
C	-1.55692551	0.4691063233	0.718848614
H	-3.234600905	1.4973609225	-0.3496296034
H	-2.1022826729	0.4065534832	1.6650583765
H	-0.9499884	1.3773473357	0.7916171346
C	-0.6532065567	-0.7513171548	0.5616787162
H	-1.2630873961	-1.6543620728	0.518941708
H	-0.1365536387	-0.6804282375	-0.3982465538
C	1.4024893305	-1.9385197445	3.6655834007
H	0.8934961919	-2.0168473028	4.6280880367
H	2.0313790436	-2.82519527	3.5662551796
H	2.0486416882	-1.0618918331	3.6903635072
H	-0.2744025437	-2.6817082969	2.4363640198

6aZ

0 1

C	6.7005695982	-2.0971200577	1.983306567
C	7.2592888314	-3.2988927385	2.0113540979
H	6.8255040768	-1.4382318565	2.8401385529
N	3.6079200285	0.4834805584	-0.2041023708
O	4.4590387336	1.2680454942	0.5713479344
H	4.3467010717	2.1435373774	0.1945130331
C	3.608960949	-0.7250295679	0.1776844186
C	4.4219756181	-1.2967810993	1.2961089009
H	2.963691432	-1.3667712871	-0.4119476435
H	3.9717762944	-2.2281567739	1.6381576018
H	4.4252519656	-0.5939567548	2.130005089
C	5.8733680887	-1.5627568784	0.8564959589
H	5.883193743	-2.2687198525	0.0239592444
H	6.2905606458	-0.6214073078	0.493274667
H	7.1271358462	-3.9520787284	1.1522052633
C	8.0760110417	-3.8398827131	3.1419314339

H	9.0889073289	-4.0795950659	2.8130025173
H	8.1424347948	-3.1211317361	3.9575987567
H	7.6429707516	-4.762772202	3.532124617

6bE

0 1

C	-1.7351219382	0.0533640182	0.5296227978
C	-2.6722817453	-0.6153061607	-0.1252973729
H	-2.041718321	0.8682793449	1.1771926849
N	2.4946456211	-0.4102065643	0.0748431913
O	3.8721219666	-0.4112165824	-0.1181904092
H	4.1332415909	-1.2915212545	0.1613770414
C	1.982794609	0.6967423732	-0.2552186682
C	0.5118387732	0.929840889	-0.1374745939
H	2.6204319524	1.4945732007	-0.6358771475
H	0.1236897846	1.2049438524	-1.1226116791
H	0.3525036618	1.8099220753	0.4935248881
C	-0.2755714022	-0.2562266869	0.4142723231
H	-0.1219603114	-1.1233615663	-0.2299293827
H	0.1381045934	-0.5255797107	1.3886992684
H	-2.428204422	-1.4409408337	-0.7907449304
O	-3.9952535703	-0.3381382192	0.0026123301
C	-4.830178608	-1.0096796247	-0.9161580279
H	-5.852013121	-0.7184339304	-0.6901141976
H	-4.5943036995	-0.7243182892	-1.9445280081
H	-4.734781794	-2.0939623008	-0.8136957278

6bZ

0 1

C	6.3600385121	-2.2183874946	2.499368985
C	7.4623621412	-2.7906537735	2.0391934743
H	5.900272443	-2.6273482119	3.3928492338
N	3.8454048936	0.2607311625	-0.4505904214
O	4.7726467721	-0.5176730909	-1.1407063665
H	4.8148268236	-0.0907429412	-1.9993094597
C	3.6367455592	-0.1856198214	0.7171697099
C	4.2942959723	-1.37928333	1.3352795857
H	2.9279112591	0.4062891995	1.2858019865
H	4.36355246	-2.177296239	0.5962356517
H	3.6877402277	-1.7378150007	2.1672883195
C	5.7115012226	-1.0453024773	1.8362386978
H	6.3088384	-0.7106240445	0.987352854
H	5.6479883224	-0.2060869603	2.5344251475
H	7.965756183	-2.4298104764	1.1445340675
O	8.0522525028	-3.8446400992	2.658197401
C	9.0882176806	-4.4578888211	1.9208918761
H	9.4793376468	-5.2654231604	2.5331272225
H	8.7123892106	-4.8687568946	0.9806357271
H	9.8917494771	-3.7478447448	1.7074286377

6cE

0 1

C	-1.750387448	0.0862978609	0.4281093212
C	-2.7191038896	-0.4668211956	-0.291993063
H	-2.0169153933	0.8491787026	1.1533911641
N	2.4606482766	-0.4322884531	0.0802533654
O	3.8423954477	-0.4562873836	-0.0517600281
H	4.0704141913	-1.3642776851	0.161007319
C	1.9896633423	0.711144646	-0.1768360816
C	0.5200361797	0.9691193117	-0.0950960635

H	2.6580528049	1.5229597496	-0.4616137654
H	0.178183648	1.3480644351	-1.0624418357
H	0.3521693302	1.7837838678	0.6160656388
C	-0.3026698024	-0.2545863368	0.3046723224
H	-0.1555395464	-1.054124281	-0.4208865769
H	0.0697943917	-0.6256673185	1.2625000937
H	-2.5173059403	-1.2310579737	-1.0315996566
C	-4.1494469153	-0.1169212715	-0.1671559416
O	-5.0188623299	-0.6257430709	-0.8249515823
O	-4.3899447381	0.8294762926	0.7557583886
C	-5.7610399977	1.1882764949	0.9038053415
H	-6.3499380316	0.3229509149	1.2027800335
H	-5.7882610475	1.9533203164	1.672975779
H	-6.1566471219	1.5732986774	-0.0343627426

6cZ

0 1

C	6.6241376884	-2.2229040999	1.9779153594
C	7.2581165636	-3.3833533953	1.8596071464
H	6.6153797652	-1.7307051344	2.9454021663
N	3.6597131956	0.5750486924	-0.0627730295
O	4.4196919994	1.2320689608	0.9008708129
H	4.3102792384	2.1571770697	0.6688765767
C	3.6616800192	-0.6795807981	0.1154890816
C	4.3907298055	-1.4102802176	1.1996277199
H	3.0864479618	-1.2264695025	-0.6227692824
H	3.9562077637	-2.4004851488	1.331146118
H	4.2792912119	-0.8613393193	2.1354253348
C	5.8896403644	-1.5443044723	0.8707166595
H	6.0207860172	-2.0951442604	-0.0614805957
H	6.2903227826	-0.5390939976	0.7251305611
H	7.2967551895	-3.921007845	0.9208331509
C	7.9687343135	-4.0584810308	2.9657292611
O	8.5293091658	-5.1168142304	2.8485542311
O	7.9297508637	-3.3753871496	4.1212621771
C	8.6080004369	-3.9971522909	5.2095690703
H	9.6575377089	-4.1490897744	4.9646990106
H	8.5045182303	-3.3205147876	6.0515959846
H	8.1578459145	-4.9621794278	5.4360032854

6dE

0 1

C	0.2561024031	-1.8423668901	1.5589473946
C	0.3744122029	-1.645537003	2.8647645392
H	1.1072997988	-1.619616119	0.9173975964
N	-2.5734870245	0.6982160619	-1.749138026
O	-3.1091314594	1.7655815678	-2.4635798887
H	-3.0975906918	1.450936618	-3.3702504473
C	-2.5221215087	0.9502992574	-0.512091772
C	-1.9772943306	-0.0485048766	0.4556853228
H	-2.8781014068	1.9123154526	-0.1433582809
H	-2.748116881	-0.254164988	1.2066957398
H	-1.1568685766	0.4194146667	1.0080987256
C	-0.9751560849	-2.3390624742	0.8649792515
H	-1.7498230055	-2.5533981509	1.6058446327
H	-0.7487519511	-3.2823174851	0.3609084307
C	-1.5089285698	-1.3508377391	-0.1755609183
H	-2.334384437	-1.8023498285	-0.7267330777
H	-0.7336061727	-1.1346974786	-0.9137001048
C	1.6068577312	-1.1447720955	3.5496410231

H	1.4047485981	-0.221543304	4.0960537974
H	1.9724452141	-1.8702424014	4.2788973937
H	2.4029232908	-0.950463257	2.8319184912
H	-0.4793959885	-1.8656442333	3.5012668372

6dZ

0 1

C	5.038415926	-2.3220688884	4.3475979831
C	4.3219286527	-2.0034600181	5.4164861874
H	5.993444622	-1.8242392026	4.1881805012
N	4.2160537526	-0.1118492034	-0.0162862669
O	5.1833690216	0.2591470124	0.9162106899
H	5.6892676907	0.9259954835	0.4468574579
C	3.4233833223	-0.9823675194	0.4532690719
C	3.4848336725	-1.5869965895	1.8201050664
H	2.663062568	-1.2998072704	-0.2519568706
H	2.5100804143	-2.0056861403	2.0756767987
H	3.716372981	-0.8084364906	2.5472267596
C	4.6317551209	-3.3101988428	3.2979839348
H	3.6661434966	-3.7488834601	3.5627541849
H	5.3564427588	-4.128452668	3.2691949334
C	4.5525349948	-2.6837794031	1.9030704137
H	4.337430589	-3.4607170693	1.1669725531
H	5.5176301677	-2.2487795342	1.6373015014
H	3.3644755413	-2.4972419425	5.5651766622
C	4.7278874758	-1.0060355884	6.4550859738
H	4.7885896629	-1.4688137791	7.4418464201
H	5.6978680609	-0.5692716933	6.2210567347
H	3.9973448678	-0.1981034924	6.5279359293

6eE

0 1

C	-2.1259773207	0.6553742071	-0.4954266911
C	-3.0388590266	0.007538908	0.2129115228
H	-2.0981543728	0.4923417747	-1.5680157792
N	2.8626329566	-0.0803300841	-0.2295625517
O	4.0900939058	-0.7361188746	-0.2471866147
H	4.6373684007	-0.1633537634	-0.7889025611
C	2.008754314	-0.7186641988	0.4487194246
C	0.6130537377	-0.2111447459	0.6073590764
H	2.2923007657	-1.6576337824	0.924114497
H	0.4068564925	-0.105651811	1.6786207587
H	-0.0762226918	-0.9850439738	0.2568617313
C	-1.1098854657	1.5768666185	0.1050852535
H	-1.3051652096	1.6880938489	1.1755225651
H	-1.2141242085	2.5709274664	-0.3367049096
C	0.3310593441	1.1014703763	-0.1057413276
H	1.0271619585	1.8629331068	0.2479352836
H	0.5285691364	0.9814927823	-1.1729272545
H	-3.1221727666	0.1275924262	1.2917673471
O	-3.915128183	-0.8674948607	-0.3454840829
C	-5.0188259854	-1.1965720033	0.4705847399
H	-5.6029299389	-1.9387231886	-0.0661747362
H	-4.6897373142	-1.6201410193	1.4235985215
H	-5.6412324484	-0.3194513693	0.664177987

6eZ

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C	5.4489140038	-2.2457134641	4.5747966832
C	4.5173892107	-2.4724200032	5.4892925966

H	6.2474233183	-1.5511021924	4.8152275404
N	3.5271561119	-0.4954983585	-0.2409423578
O	3.253966723	-1.8566021291	-0.3697861823
H	2.9967293923	-1.9370638688	-1.2908191033
C	3.858180636	-0.1948060271	0.9451401049
C	3.9798070746	-1.1400525872	2.0977936076
H	4.0892436596	0.8567903673	1.0754996056
H	3.172370357	-1.8724541672	2.0457683235
H	3.8774591687	-0.5894009411	3.0324421694
C	5.4490451743	-2.8866756912	3.2219250841
H	4.6282602055	-3.6062245288	3.1575739626
H	6.3740372403	-3.452481169	3.0843219761
C	5.3225971657	-1.8783867358	2.0761957255
H	5.4212299134	-2.3950043078	1.1210695172
H	6.1388121179	-1.1537163391	2.1364812612
H	3.689862799	-3.1551346703	5.3065990202
O	4.5318286613	-1.8848294582	6.7131621051
C	3.4338763261	-2.2110992634	7.5382471371
H	3.5828792569	-1.698931446	8.4844525262
H	2.4935337514	-1.8767883605	7.092643135
H	3.3832892824	-3.2882279987	7.7176686922

6fE

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C	-2.1177776379	0.4595434154	-0.4187123498
C	-3.0349647055	-0.1914164219	0.2877104125
H	-2.0494677994	0.2638473785	-1.4848622359
N	2.8975023807	0.0158911753	-0.2794633549
O	4.1675684718	-0.54830774	-0.3109537273
H	4.6650906714	0.0575810565	-0.8646781474
C	2.1030036836	-0.6737793126	0.4202245062
C	0.6785380488	-0.2595658038	0.597193951
H	2.4583648703	-1.5840931627	0.902149647
H	0.4786437323	-0.1693418789	1.6703881364
H	0.038394916	-1.0779287635	0.253441711
C	-1.1453046061	1.44156834	0.1468257602
H	-1.3193988455	1.560857163	1.2183902636
H	-1.3212925998	2.4143478869	-0.3198157251
C	0.3095362198	1.0360318306	-0.1098564315
H	0.9728799337	1.8332891652	0.2251602823
H	0.4815799053	0.9271089708	-1.1823128081
H	-3.1465738873	-0.0423686505	1.3541390246
C	-3.9870956541	-1.1664775561	-0.2833950165
O	-4.8094504077	-1.7537684407	0.3697622083
O	-3.8469949968	-1.3376448364	-1.6083392025
C	-4.752061226	-2.2708499285	-2.1921776264
H	-5.780628422	-1.9553646141	-2.0272516455
H	-4.52249722	-2.2868217993	-3.2526912748
H	-4.6141576659	-3.2579998234	-1.7547238975

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C	5.2728265379	-2.0538873729	4.4893844322
C	4.3359790815	-2.2009027929	5.4189353843
H	6.0570394838	-1.3205284423	4.6543242347
N	3.6022119046	-0.6953042431	-0.4927878652
O	3.3085076912	-2.0567758192	-0.4731160157
H	3.0664268	-2.238843226	-1.3839099659
C	3.9078317078	-0.2669857494	0.6602936494
C	3.9764126858	-1.0850554822	1.9116121579

H	4.1537928699	0.7887705615	0.6808341988
H	3.1308537418	-1.7749940856	1.9305863333
H	3.8944941786	-0.4303180528	2.7790268643
C	5.3218827237	-2.8133976996	3.2047045021
H	4.4934348677	-3.5229517199	3.1600137597
H	6.2494334166	-3.3912365075	3.1726509942
C	5.2787756238	-1.8902601835	1.9826631914
H	5.3712993209	-2.4876079277	1.076118688
H	6.1317507774	-1.2076434683	2.0093365834
H	3.5286715673	-2.9134550283	5.3074778052
C	4.2884770719	-1.435634747	6.6821012478
O	3.4418974411	-1.5912601186	7.5229713172
O	5.2837955088	-0.5413088359	6.8041801686
C	5.2673029134	0.210690877	8.0148886123
H	5.3418402322	-0.4536852129	8.8737707085
H	6.125966827	0.8726085424	7.9676355998
H	4.3446333052	0.7829084246	8.0935298034

6gE

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C	2.5895674421	-0.5902931835	-0.5449989914
C	3.446262204	0.3823053638	-0.2739651548
H	2.4599830382	-0.9086973617	-1.5767046353
N	-2.4403334269	-0.5226309965	-0.2309724078
O	-3.757335281	-0.1200191655	-0.4285702691
H	-4.2128677517	-0.9430763161	-0.6190920853
C	-1.6924622011	0.460525729	0.0349320264
C	-0.2321693158	0.2719800406	0.2853753041
H	-2.1171347201	1.4632229452	0.0815391902
C	1.7442394172	-1.302705601	0.4654674178
H	1.9706759226	-0.9214818	1.4644053112
H	2.0037894711	-2.3645566291	0.4617886479
C	0.2460714894	-1.1681543727	0.1798770201
H	-0.3200438381	-1.7890764517	0.8745529178
H	0.0231352274	-1.550172984	-0.8186720336
H	3.5989969013	0.7277886614	0.7420313581
H	4.0276856226	0.8612615991	-1.0500352504
H	-0.001195771	0.6698746171	1.279871928
H	0.3222404497	0.9070469756	-0.4120491639

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C	-4.6984912609	3.7745224334	0.8625746318
C	-4.0680313368	4.8786789988	1.2314302602
H	-5.1710948959	3.1544871414	1.6205209985
N	-2.3253955792	-0.5378676208	0.2808624805
O	-3.0221311728	-0.1322492197	1.4177072518
H	-3.0186365849	-0.921100151	1.9642164487
C	-2.2024126594	0.4076918779	-0.5541497228
C	-2.737102339	1.7963889152	-0.3987979348
H	-1.6720188602	0.1221724214	-1.4559413461
C	-4.8028935752	3.2727510885	-0.544666796
H	-4.2842062131	3.9604296507	-1.2175140989
H	-5.8540477637	3.2612893733	-0.8453499595
C	-4.237729316	1.8590275018	-0.7034917331
H	-4.4199750407	1.5088757834	-1.7211931511
H	-4.7579127749	1.1747797131	-0.0309379333
H	-3.578945057	5.5150480712	0.5029434333
H	-4.0217179062	5.1880940563	2.2666431048
H	-2.199442619	2.469260969	-1.0686802527

H	-2.5641056451	2.1334739564	0.6236330587
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C	2.6246692147	0.1001199519	0.5435225203
C	3.4217800305	-0.9230472651	0.2490182574
H	2.5017405303	0.4040857622	1.5800995105
N	-2.391733916	0.3733317176	0.1523820662
O	-3.7353671649	0.0511860514	0.315409046
H	-4.1408189902	0.8960477781	0.5228107042
C	-1.7041786399	-0.6479202938	-0.1321362638
C	-0.230122382	-0.5480505605	-0.3507847586
H	-2.1914822921	-1.6190172939	-0.2178908759
C	1.8485320948	0.8959642652	-0.4580433449
H	2.0632534593	0.5294468287	-1.4648790852
H	2.1771782319	1.9380126058	-0.4201348961
C	0.3391070949	0.8546239719	-0.199133803
H	-0.1718877627	1.5297895975	-0.8858820232
H	0.1257940714	1.2247391591	0.8058587853
H	3.5504060191	-1.1899967202	-0.7968718016
H	-0.0057142325	-0.9356814957	-1.3507091755
H	0.2676199904	-1.2348373924	0.3404690643
C	4.1928197315	-1.7362819238	1.2017057857
C	5.2249290264	-2.5445213213	0.7252681701
C	3.9323952791	-1.7403036013	2.5739124635
C	5.9878746037	-3.3165076707	1.5884832772
H	5.4335731872	-2.5594511693	-0.3374619956
C	4.6918493321	-2.5103000672	3.4374511321
H	3.1173463919	-1.1479557829	2.9677367103
C	5.7257599875	-3.3005127403	2.949733073
H	6.7866815228	-3.931707791	1.1967011023
H	4.4713133677	-2.501971421	4.4964815852
H	6.315464493	-3.9041076492	3.6259406597

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C	2.1399694624	-0.5515674618	0.4277375694
C	2.9415996188	-0.9913650001	-0.5381201477
H	1.7367316461	-1.25120651	1.1552592958
N	-2.7002532619	-0.225059657	-0.1822994678
O	-1.9782782403	-1.2775832668	0.3773260763
H	-2.6667392536	-1.8573328331	0.7102142579
C	-1.9358518525	0.6315695962	-0.7195923779
C	-0.4413608603	0.5730904528	-0.7559529928
H	-2.4659872306	1.470092903	-1.1573296798
C	1.6966974567	0.8683038996	0.5891256363
H	2.1330040577	1.4830404086	-0.2021165852
H	2.0727575366	1.2565645617	1.5400431651
C	0.1712267299	1.0035925157	0.5814231732
H	-0.104037777	2.0377347017	0.7960112148
H	-0.2556860396	0.3863900013	1.3738270158
H	3.3025734416	-0.2741087307	-1.2708762543
H	-0.0699925251	1.2167717561	-1.5547338786
H	-0.1310955668	-0.4488874519	-0.9766931623
C	3.3943040511	-2.3752260973	-0.7438852283
C	4.0620208923	-2.702780912	-1.9238552888
C	3.1840152589	-3.3873473312	0.1957956579
C	4.4939601612	-3.9979389818	-2.1685115438
H	4.2395557047	-1.9282494653	-2.6599572229
C	3.6129855441	-4.680058143	-0.0459636849

H	2.6886317278	-3.1601982262	1.1298828496
C	4.2687968354	-4.9934421562	-1.2306521494
H	5.007975213	-4.2283179701	-3.0919583324
H	3.4404831691	-5.4487799144	0.6953546926
H	4.6050848204	-6.0044105779	-1.4157907575

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C	-2.1027343299	0.4926767956	-0.4142695035
C	-2.9998608241	-0.1781185953	0.2884904871
H	-2.0437321206	0.3196127334	-1.4849468486
N	2.8944956466	0.0014533491	-0.2816148369
O	4.1568553857	-0.5775924572	-0.3228481859
H	4.6529673733	0.0119602582	-0.8952036582
C	2.1027098776	-0.6673873007	0.4407519519
C	0.6855999113	-0.2340496292	0.6294047043
H	2.4533475065	-1.5743403139	0.9322523017
H	0.4999261825	-0.125214941	1.7035242508
H	0.0319646538	-1.0500927542	0.3058799784
C	-1.1291138234	1.4711988954	0.158269528
H	-1.3074121457	1.5885047614	1.2293215128
H	-1.3002544746	2.4448017344	-0.3070475512
C	0.323552596	1.0553817017	-0.0927351148
H	0.9914534155	1.8527261363	0.2329824843
H	0.4966809065	0.9334212392	-1.1636741315
C	-3.941355466	-1.1619918241	-0.3180289511
H	-3.1093125025	-0.0585795542	1.3594319467
F	-3.8098081539	-1.2624796879	-1.64437384
F	-3.7571031043	-2.3902953273	0.1923402154
F	-5.2178830701	-0.8356555197	-0.0680569497

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C	1.7549802558	-0.3083906686	-0.5376526131
C	2.6546281543	0.0788221338	0.3504609311
H	1.5531180232	0.332467557	-1.3909736366
N	-2.9912807453	0.7145368235	0.064612364
O	-2.045839218	1.4307348519	-0.6647976418
H	-2.5724481228	2.1051200283	-1.0999859991
C	-2.4516874969	-0.2008639819	0.7553332695
C	-0.989119952	-0.515907359	0.7984494574
H	-3.1590332456	-0.7866731833	1.3312636751
H	-0.7670786642	-1.0920557007	1.6978546995
H	-0.430121927	0.4193924757	0.8527312077
C	0.9609033661	-1.5714090983	-0.4471591103
H	1.2485449685	-2.1275453737	0.4477684424
H	1.2016043979	-2.1979019662	-1.3097195382
C	-0.5461463163	-1.300509894	-0.4412915405
H	-1.0809556385	-2.2504322396	-0.485439663
H	-0.8219012436	-0.7343507694	-1.3323261343
H	2.8965348777	-0.5071543675	1.2286766722
C	3.4212045636	1.3518846774	0.2336618764
F	3.199909203	2.1525394477	1.2877542434
F	3.1135809046	2.0506822319	-0.8632665967
F	4.7432704357	1.1235311048	0.2014863848

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C	-0.3700543614	-0.1554987936	-0.3713329816
C	-1.2194935478	0.7987987282	-0.0091088888

N	3.8784096311	0.2345060052	-0.2480921786
O	5.2592420757	0.2813232203	-0.0896822447
H	5.5465292797	0.8310748768	-0.8222204269
C	3.3350530228	-0.4836655338	0.6376581943
C	1.8544955731	-0.6790076286	0.6695541149
H	3.9512349583	-0.9702533335	1.3931734577
H	1.4821004838	-0.3309670534	1.6381408667
H	1.6456258163	-1.7504821592	0.6279522857
C	1.1159105949	0.0362560666	-0.4602734456
H	1.3461415644	1.1004247067	-0.43098202
H	1.4804501441	-0.3491167888	-1.4128947705
C	-0.8622962078	-1.5217950327	-0.7202523099
O	-0.1369122464	-2.421311144	-1.0601660965
O	-2.1911444758	-1.6581974306	-0.6263955414
C	-2.6899626404	-2.9503320008	-0.9650345203
H	-2.4148870446	-3.2063158339	-1.9864942803
H	-2.2816091608	-3.7023320054	-0.2921776134
H	-3.7683225756	-2.889037238	-0.8620453
H	-2.282353274	0.6158970036	0.0497797841
H	-0.8612607297	1.7910440887	0.2339177853

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C	5.743415425	-1.8450858901	2.7394435646
C	6.2130037989	-3.0703380997	2.5369863407
N	2.9627574408	-0.2833452641	-0.5687260087
O	3.3402660866	-1.5993067932	-0.831969336
H	3.1492012916	-1.6937046084	-1.7677252476
C	3.1170233734	0.0124076048	0.6538429087
C	3.6505027207	-0.8918998116	1.7198718629
H	2.8457835197	1.0346101314	0.8925604383
H	3.2402706817	-1.8922949195	1.5815815336
H	3.3502769247	-0.5177462695	2.6969619921
C	5.1869267256	-0.9713207891	1.6543734558
H	5.4775680265	-1.3656026227	0.6820433385
H	5.5968497537	0.0342623225	1.755968558
C	5.7230540011	-1.2478548381	4.1078045161
O	5.318087067	-0.1369791963	4.3391058101
O	6.2026585556	-2.0585056383	5.0591122408
C	6.2101170712	-1.5079634552	6.3743869704
H	6.8153516661	-0.603801738	6.4021639611
H	5.1972752221	-1.2630546535	6.6890736426
H	6.6353761199	-2.2730208366	7.0154214024
H	6.5874963791	-3.6713867316	3.3526429852
H	6.2298420189	-3.495813243	1.5417273702

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C	-0.8095119023	0.8254920656	-0.6089244481
C	-1.6018446405	0.767688864	0.4555498454
N	4.0665260246	-0.448930627	-0.0820162994
O	5.2018233026	-1.1715578881	0.2692171066
H	5.7484158131	-1.1183496012	-0.5180838289
C	3.2251402722	-0.4245870881	0.8598734494
C	1.9217705274	0.2905892847	0.7114072727
H	3.4483535296	-0.9354472599	1.7964859748
H	1.8473888012	1.0340813323	1.5132546464
H	1.1184449863	-0.4259591396	0.9079145373
C	0.3913070986	1.7195686237	-0.7223596457
H	0.3462633115	2.4678265319	0.0713180783

H	0.348704514	2.241677138	-1.6786357164
C	1.7195146499	0.9580022301	-0.6405092492
H	2.5398490995	1.6520740772	-0.8245116155
H	1.7665368562	0.213031054	-1.4347192728
H	-1.415969378	1.3987601232	1.3157353477
C	-1.0821433164	-0.0263423769	-1.8062302002
O	-0.4627930487	0.0577972208	-2.8348943334
O	-2.0901904962	-0.8915479034	-1.6326123343
C	-2.390105636	-1.7043558446	-2.7650281561
H	-2.6654993509	-1.0831074075	-3.6152340712
H	-1.5267241458	-2.3090794034	-3.0364953096
H	-3.2210838869	-2.3350076285	-2.4668055763
H	-2.4503232649	0.1000698527	0.4911810485

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C	-6.1227688052	1.2140751701	-3.69888026
C	-5.3747965965	1.9527551788	-4.5105970407
N	-2.8846446054	-0.9831153802	0.1208544373
O	-2.7013289532	-1.8995679801	-0.9130316036
H	-2.2315110315	-2.6172110406	-0.4826745756
C	-3.4911202738	0.0560536583	-0.2771545515
C	-3.9901453405	0.3109780945	-1.6644907599
H	-3.6601306109	0.7863262217	0.5063867667
H	-3.2503754624	-0.0527854008	-2.3801023345
H	-4.1035670327	1.3847912498	-1.8128898168
C	-5.8284356945	-0.2162951911	-3.3502640646
H	-5.0813301871	-0.6003765235	-4.0468353104
H	-6.739603033	-0.8023525999	-3.4754215473
C	-5.3252531661	-0.3997181372	-1.9141191466
H	-5.1910535283	-1.4642845077	-1.7225880776
H	-6.0815150586	-0.0371068209	-1.2166420608
H	-4.4937306349	1.532582574	-4.9790949446
C	-7.3483177663	1.7833408216	-3.0623108218
O	-8.0957661486	1.1406980921	-2.3706628301
O	-7.5468162197	3.0795168385	-3.336652304
C	-8.7222939363	3.643949111	-2.7601104411
H	-9.6057744461	3.1067552575	-3.0998533188
H	-8.6744623248	3.591231208	-1.6738990002
H	-8.7508317988	4.6764915701	-3.0920864018
H	-5.6224841348	2.981561016	-4.7276082016

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C	-2.2710899828	0.5704125112	-0.2450858245
C	-3.2917577986	0.2563031964	0.5384633132
H	-2.2494859263	0.1906798509	-1.2640244175
N	2.9316842684	0.1936921226	-0.2301356555
O	4.2573049621	-0.230114059	-0.2107581769
H	4.7089121875	0.4362770592	-0.7337159395
C	2.1886162039	-0.5871863681	0.4269171468
C	0.7020278186	-0.3822664521	0.5634546293
H	2.6226468325	-1.4639532766	0.9127691777
C	-1.122219925	1.4465772278	0.149716896
H	-1.2035900269	1.6981046106	1.2088825129
H	-1.2186561198	2.3906242361	-0.3953420562
C	0.2729445752	0.8992790526	-0.1690875838
H	0.9967486229	1.6794421206	0.0693687448
H	0.362649406	0.7308084793	-1.2454530774
H	-3.3448173211	0.6143772217	1.5604183694

H	-4.1079005984	-0.3617065806	0.1894566572
C	0.0404039655	-1.6397445997	-0.0219067468
H	-1.0339976441	-1.628690328	0.1479185526
H	0.226400634	-1.7100893153	-1.0944229596
H	0.4458540628	-2.5362560183	0.4518230853
C	0.3821439731	-0.3009156826	2.0610850084
H	0.8039020702	-1.156121802	2.5917553325
H	0.7927659664	0.6094403185	2.5007011195
H	-0.6968701763	-0.3109025954	2.2186569519

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C	-4.6730336183	4.0960180922	0.720067531
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H	-5.0127262834	3.644275599	1.6491198477
N	-2.3332175741	-0.7139314365	0.0313507773
O	-3.3158792266	-0.6587335106	1.0170378398
H	-3.4214698368	-1.5804538286	1.2633155533
C	-2.0267147202	0.4237197596	-0.4335628039
C	-2.551526393	1.8015627057	-0.0760869674
H	-1.2590051115	0.3590367421	-1.2003082994
C	-4.7234085454	3.2150535446	-0.4901222387
H	-4.2952833485	3.7426798336	-1.3441769944
H	-5.775651538	3.0398390218	-0.7349228789
C	-4.0810846694	1.8336794827	-0.3179526501
H	-4.2917113604	1.2601989926	-1.2243816269
H	-4.5732126183	1.3051359953	0.4978886369
H	-3.9227747808	5.8405526727	-0.1799391782
H	-4.2799887017	5.9530860945	1.629477568
C	-2.1833342891	2.1076347958	1.3843566875
H	-2.450108999	3.1333304934	1.6334485407
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H	-1.1074088492	1.9959621809	1.5298001169
C	-1.8386184611	2.804065648	-0.9880375505
H	-0.7566202835	2.6947285638	-0.8985133642
H	-2.1100408977	2.6506208848	-2.0348780375
H	-2.0948881367	3.8256848129	-0.7094230994

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N	2.1674961955	-2.1109430938	0.6120813424
O	3.427885528	-2.5200355125	0.1961538147
C	1.9375566954	-0.9166217787	0.2456498441
H	2.6998829863	-0.3822252347	-0.3174621356
C	0.6895008903	-0.2652317687	0.589034202
C	-0.332600359	-0.7004182143	1.40698782
N	0.3470572713	0.9844483468	0.1186976752
C	-1.3110494036	0.3110184782	1.4390019273
H	-0.3451602593	-1.6497652764	1.9136498949
C	-0.8625373413	1.3361388173	0.640795566
H	-2.2417682877	0.2972218431	1.9788638004
H	-1.3052732543	2.2858538597	0.3962137729
C	1.1602636884	1.8519021851	-0.723618969
H	1.7916548455	2.4947143324	-0.1058748823
H	1.8126406745	1.2183422556	-1.3235837697
C	0.3187566417	2.684955213	-1.6412829265
H	-0.3613951374	2.1379747207	-2.2857165872
C	0.38741853	4.0042539963	-1.7004871612
H	1.0540605626	4.561517066	-1.0531946999
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H 0.9517285042 0.1228685096 -0.1017599177
C 1.2286697854 -2.0256555224 -0.3334677769
C 1.8725837173 -3.2514325421 -0.2887260611
N -0.0917577836 -2.2680341446 -0.6762141473
C 0.9246084242 -4.2434306795 -0.5969675419
H 2.9104559713 -3.3908512134 -0.0553448904
C -0.2725501019 -3.6077312607 -0.824268142
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H -1.2393593103 -4.0037023314 -1.0817631834
C -1.1477111399 -1.2683944218 -0.7858781035
H -1.5116941532 -0.9942495528 0.2069649778
H -0.7191138051 -0.3766111273 -1.2446408709
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H -2.0310276115 -2.0202821843 -2.6555099772
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N 1.918736737 -1.2506116086 0.4778870105
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H 1.9143502987 0.0072533379 -1.1473491955
C 0.4165581686 0.5980466183 0.4236466717
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C -1.8945158534 -1.4230186146 0.4698553981
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H -3.4257570402 -2.2410746301 1.6537510498
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N 2.8121120275 -1.2138917862 -0.4589039535
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C 1.6905063277 -0.7329021668 -0.7914433892
H 1.4685931101 -0.7463883708 -1.8522638348
C 0.6970695821 -0.1457966381 0.1647767943
C 1.1410925067 1.2082982151 0.7469747416
N -0.532869762 0.2463085087 -0.4890418958

H	1.8362486199	1.7157063434	0.076835082
C	-1.0269920234	1.4014035312	0.0771077648
C	-1.4862490314	-0.7381184465	-0.9881256191
H	-2.2742590203	-0.1769795219	-1.4863834086
H	-0.979383904	-1.3533451036	-1.7332055448
C	-2.0699409922	-1.590384081	0.1065532202
H	-1.4635433878	-2.4108418305	0.4769334148
C	-3.2607593021	-1.357994511	0.6353625122
H	-3.8739712466	-0.5358532601	0.2860513472
H	-3.6531250743	-1.9691736461	1.4370915409
O	-0.0594598655	1.9702563334	0.8377046847
O	-2.1214772474	1.862818961	-0.0598903493
H	1.5815056067	1.1140257807	1.7335705922
H	0.5178521971	-0.8615054824	0.9749769359
H	3.86109151	-1.5290889251	1.0511640855

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N	3.0436423938	0.0682313256	-1.1384428915
O	3.9905665695	0.8593928782	-0.5102910904
C	1.9628122292	0.0212466074	-0.4853665988
H	1.8401356608	0.5714925563	0.4461908607
C	0.8163104086	-0.7742515292	-1.0292659686
N	-0.3024385776	0.0882366017	-1.371444733
C	-1.3753423689	0.2924985498	-0.5641777783
C	-0.2786212539	0.7733195627	-2.6601994262
H	-0.7879061443	1.7282383599	-2.5505161042
H	0.7688679927	0.9644536597	-2.9035944266
C	-0.9393234525	-0.0402329304	-3.7356185781
H	-0.4625949557	-0.9807927482	-3.9951709065
C	-2.0598202011	0.3257758824	-4.3347249193
H	-2.552550918	1.250962883	-4.0661520938
H	-2.52417004	-0.2851546148	-5.0969952906
O	-1.2561524525	-0.3658360302	0.6100656786
O	-2.3243241305	0.9868540208	-0.8430057793
H	1.1489756269	-1.3002637648	-1.9244765464
H	4.7492621767	0.8101847395	-1.0971702606
H	0.486822377	-1.508428268	-0.2992106342
C	-2.3640228768	-0.1969755166	1.4905434375
H	-2.1368652375	-0.792777181	2.3690482721
H	-2.4805583746	0.8511624617	1.7585160982
H	-3.2807749377	-0.5442078157	1.0187596592

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N	3.2267237485	0.1161071099	-0.3998824294
O	3.4297954417	-0.7417643659	0.6786225399
C	1.9946974151	0.3480711908	-0.5626977026
H	1.7430278035	1.0144245731	-1.3790902866
C	0.8924946478	-0.2235035358	0.2842705867
N	-0.4251750448	0.0729540834	-0.2450037735
C	-1.0111409744	1.2873688886	-0.0741148769
C	-1.2377843928	-0.9974172928	-0.813428029
H	-1.9402680424	-0.5488164335	-1.5116906218
H	-0.5691993954	-1.6556791835	-1.3714650463
C	-1.9849855569	-1.7619635378	0.2420026416
H	-1.3863544861	-2.3369854617	0.9423688462
C	-3.3016783477	-1.7318546975	0.3618954059
H	-3.9078429485	-1.1433543078	-0.3162369851
H	-3.8136079362	-2.2789026358	1.1420804905

O	-0.1619163057	2.1579014019	0.5124647244
O	-2.135329073	1.5738876488	-0.4122269413
H	1.0105948469	-1.3063323371	0.3369550004
H	4.3831550251	-0.8514901596	0.6968212702
H	1.0005199514	0.1479572855	1.3041568729
C	-0.6975482621	3.4639659818	0.7078610249
H	0.0793991014	4.0287854758	1.213092865
H	-0.9422383379	3.9213648747	-0.2489506657
H	-1.5975098173	3.4180635045	1.3172517696

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N	2.8266644279	-0.5193664531	-0.2136569271
O	3.4609728078	-1.743246042	-0.3336962555
C	1.56524821	-0.647778625	-0.2469733928
H	1.1393331429	-1.6422556493	-0.3531670859
C	-1.3098291195	-1.0243065074	0.1465932426
H	-1.2577766565	-1.5395355287	-0.8167223615
H	-0.7039689883	-1.6094505483	0.8436447156
C	-2.7247704346	-1.0402723849	0.6371082751
H	-2.8906342499	-0.6165693176	1.6233499806
C	-3.7485922155	-1.5395165543	-0.0362886921
H	-3.6187231162	-1.964004005	-1.0248823855
H	-4.7484694646	-1.5451073957	0.3757623443
C	0.6818797822	0.5246418136	-0.1588253252
C	-0.7002897547	0.3602976036	0.0180596339
C	1.2199870164	1.8066706735	-0.2704672696
C	-1.5034931805	1.495910818	0.0632813359
C	0.4079813401	2.9236733764	-0.2094029045
H	2.286854268	1.9087661822	-0.4116467418
C	-0.9607825546	2.7667581087	-0.0464113758
H	-2.5725432914	1.3809385867	0.1801909581
H	0.8386216728	3.9115501775	-0.2983182691
H	-1.6080598298	3.6325443127	-0.0078208322
H	4.3929483382	-1.5172358215	-0.2863488274

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N	2.7224343901	-0.8553454078	-0.1846259704
O	3.3091691165	0.1778558342	0.526829077
C	1.5180186324	-0.6263089875	-0.5192955403
H	1.0769738947	-1.4593778216	-1.0559085519
C	-1.2874353462	-1.0106261533	0.0320741332
H	-1.3507309526	-1.4488575367	-0.9687968334
H	-0.5996620364	-1.6413840126	0.6013982129
C	-2.635188544	-1.0729386904	0.682020615
H	-2.6844971297	-0.7163247754	1.7067820516
C	-3.7312323252	-1.5313606237	0.0992205547
H	-3.7163667915	-1.8865515182	-0.9245180372
H	-4.6769969671	-1.5720853644	0.6221121487
C	0.6745292905	0.5637322287	-0.2928714066
C	-0.6990850908	0.3846578684	-0.0606355544
C	1.2004681008	1.8515949233	-0.379747011
C	-1.5055767881	1.5074513442	0.0774850539

C	0.3799084517	2.9594889418	-0.2430424858
H	2.2566494586	1.9769861186	-0.5611124647
C	-0.97503476	2.786533218	-0.0127379048
H	-2.5656176082	1.3790049813	0.2513175508
H	0.7998328768	3.9532171729	-0.3167556361
H	-1.6235435007	3.6455185991	0.0965035268
H	4.1794587786	-0.1720970389	0.7317115919

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N	0	-2.884192	-0.665085	-0.076643
O	0	-3.547178	-1.876105	0.015653
C	0	-1.632687	-0.81155	0.068453
H	0	-1.234447	-1.809475	0.233426
C	0	1.25878	-1.240412	-0.066576
H	0	1.115276	-1.731634	0.899992
H	0	0.7053	-1.832904	-0.800029
C	0	2.710208	-1.289295	-0.432482
H	0	2.967503	-0.891816	-1.409987
C	0	3.663652	-1.787588	0.337952
H	0	3.441998	-2.186334	1.320929
H	0	4.69504	-1.818005	0.014091
C	0	-0.725219	0.345061	0.030605
C	0	0.664053	0.155846	-0.022415
C	0	-1.249079	1.637311	0.066425
C	0	1.487345	1.277892	-0.023608
C	0	-0.415972	2.740243	0.050633
H	0	-2.322249	1.758725	0.112535
C	0	0.958877	2.558986	0.010125
H	0	2.560381	1.144153	-0.045066
H	0	-0.835821	3.736304	0.079729
H	0	-4.467647	-1.637352	-0.117143
N	0	1.85963235	3.7206798	0.00742197
O	0	1.3757002	4.81765283	0.03706473
O	0	3.04248817	3.5250948	-0.02431717

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N	0	-2.424611	-1.852068	0.138349
O	0	-3.205767	-1.015943	-0.641793
C	0	-1.324792	-1.330558	0.503732
H	0	-0.724364	-2.013756	1.094669
C	0	1.514144	-1.057286	0.07009
H	0	1.633604	-1.429436	1.092357
H	0	1.021313	-1.854743	-0.492224
C	0	2.866588	-0.821958	-0.528466
H	0	2.876783	-0.50315	-1.566733
C	0	4.012253	-0.98399	0.113652
H	0	4.0352	-1.293263	1.152038
H	0	4.963633	-0.818483	-0.373203
C	0	-0.776726	0.016441	0.25044
C	0	0.609422	0.160507	0.075345
C	0	-1.595241	1.144597	0.257192
C	0	1.133443	1.436802	-0.087883
C	0	-1.054111	2.409832	0.096582
H	0	-2.658282	1.021992	0.395204
C	0	0.312381	2.555469	-0.077532
H	0	2.20061	1.557646	-0.218094
H	0	-1.69968	3.277228	0.107965
H	0	-3.958605	-1.570393	-0.860122

N	0	0.89890507	3.89223759	-0.25056166
O	0	2.08585642	3.97942013	-0.39876605
O	0	0.16705056	4.84229194	-0.23661656

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N	0	-2.884192	-0.665085	-0.076643
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H	0	-1.234447	-1.809475	0.233426
C	0	1.25878	-1.240412	-0.066576
H	0	1.115276	-1.731634	0.899992
H	0	0.7053	-1.832904	-0.800029
C	0	2.710208	-1.289295	-0.432482
H	0	2.967503	-0.891816	-1.409987
C	0	3.663652	-1.787588	0.337952
H	0	3.441998	-2.186334	1.320929
H	0	4.69504	-1.818005	0.014091
C	0	-0.725219	0.345061	0.030605
C	0	0.664053	0.155846	-0.022415
C	0	-1.249079	1.637311	0.066425
C	0	1.487345	1.277892	-0.023608
C	0	-0.415972	2.740243	0.050633
H	0	-2.322249	1.758725	0.112535
C	0	0.958877	2.558986	0.010125
H	0	2.560381	1.144153	-0.045066
H	0	-0.835821	3.736304	0.079729
H	0	-4.467647	-1.637352	-0.117143
O	0	1.835122	3.68906909	0.00749552
C	0	1.27587804	4.72483475	-0.80449936
H	0	0.46946483	5.19315887	-0.27983731
H	0	2.02926346	5.45243098	-1.02339229
H	0	0.9104507	4.3039275	-1.71784483

6tZ

0 1

N	0	-2.424611	-1.852068	0.138349
O	0	-3.205767	-1.015943	-0.641793
C	0	-1.324792	-1.330558	0.503732
H	0	-0.724364	-2.013756	1.094669
C	0	1.514144	-1.057286	0.07009
H	0	1.633604	-1.429436	1.092357
H	0	1.021313	-1.854743	-0.492224
C	0	2.866588	-0.821958	-0.528466
H	0	2.876783	-0.50315	-1.566733
C	0	4.012253	-0.98399	0.113652
H	0	4.0352	-1.293263	1.152038
H	0	4.963633	-0.818483	-0.373203
C	0	-0.776726	0.016441	0.25044
C	0	0.609422	0.160507	0.075345
C	0	-1.595241	1.144597	0.257192
C	0	1.133443	1.436802	-0.087883
C	0	-1.054111	2.409832	0.096582
H	0	-2.658282	1.021992	0.395204
C	0	0.312381	2.555469	-0.077532
H	0	2.20061	1.557646	-0.218094
H	0	-1.69968	3.277228	0.107965
H	0	-3.958605	-1.570393	-0.860122
O	0	0.89890507	3.89223759	-0.25056166
C	0	2.18676214	3.98683174	-0.41136528

H	0	2.68397553	3.57237767	0.44063629
H	0	2.47691112	3.44950669	-1.28999795
H	0	2.45834581	5.01639134	-0.51695565

6uE

0 1

C	0.8375223794	0.516969573	-0.3151693233
C	-0.3741834918	0.2445534516	0.3007280151
C	1.1187008273	1.8081803341	-0.7306008853
C	-1.273584303	1.2740385516	0.5089312286
C	0.2230901532	2.8560955951	-0.5280469359
H	2.0579068814	2.0123559435	-1.2288616074
C	-0.9892802735	2.5885966456	0.1298346518
H	-2.2211976966	1.0694052272	0.9918556746
C	-2.0068763137	3.6042898299	0.4612341647
C	-1.7963712856	4.8570104703	0.8484649159
H	-3.0301235483	3.2422244335	0.4347925334
H	-2.6254569318	5.500618981	1.1085667641
H	-0.8033920881	5.2726543116	0.9496739014
H	-0.618102551	-0.7612226194	0.6142218504
H	1.5565006259	-0.2729536048	-0.4839553167
C	0.5781737876	4.2325913486	-1.0534684341
H	-0.3400909347	4.7804244572	-1.271065971
H	1.1263926125	4.8092038224	-0.305861157
C	1.4068574665	4.1787178424	-2.2948230606
H	1.0179153944	3.6756246702	-3.1800087688
O	3.1578750032	4.5623993669	-3.5592204641
N	2.5535621292	4.7093170102	-2.3162770116
H	4.0037812274	5.0022008484	-3.4475969341

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0 1

C	0.8418619706	0.5624110586	-0.2749193349
C	-0.3685134739	0.2643886572	0.3320544577
C	1.0887422697	1.8544712356	-0.7083655433
C	-1.2998977253	1.2701497307	0.5125473108
C	0.1601831534	2.8793397193	-0.5349745655
H	2.028407574	2.0785086485	-1.1985084947
C	-1.0504444164	2.5864156156	0.1149898623
H	-2.2456501707	1.0450757298	0.9899135147
C	-2.1018641239	3.5751190137	0.4212495892
C	-1.9374524084	4.842086716	0.7840266946
H	-3.1118828344	3.1772157914	0.3990265179
H	-2.7911557375	5.4597104844	1.0268070023
H	-0.9613360196	5.2967052456	0.8803480311
H	-0.5849013637	-0.7424057096	0.6620142465
H	1.5867365017	-0.2077493026	-0.4215968026
C	0.4856675458	4.2545416088	-1.07146446
H	-0.4393288002	4.7913135464	-1.2928140507
H	1.0179374727	4.8496842634	-0.3297403194
C	1.2991264541	4.2045192709	-2.3287470438
H	1.0497463536	3.4635438593	-3.0814142558
O	2.5570890476	5.898223919	-1.669155987
N	2.2679781125	4.9540621471	-2.649351481
H	3.3164787184	6.358449781	-2.0331244385

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C	0	-1.061311	-2.366634	0.228462
C	0	-2.361568	-1.965406	-0.036338

C	0	-0.05068	-1.4207	0.280467
C	0	-2.630041	-0.621833	-0.223004
C	0	-0.305044	-0.063483	0.094635
H	0	0.966361	-1.740904	0.467969
C	0	-1.628319	0.348557	-0.136392
H	0	-3.643897	-0.300477	-0.427671
C	0	-2.055152	1.751802	-0.296623
C	0	-1.58273	2.81429	0.344865
H	0	-2.889714	1.894045	-0.976402
H	0	-2.006751	3.794482	0.175461
H	0	-0.788722	2.743889	1.075349
H	0	-3.159583	-2.692423	-0.099412
C	0	0.858267	0.907654	0.116861
H	0	0.613269	1.773732	-0.500037
H	0	1.043556	1.275821	1.127832
C	0	2.124082	0.301291	-0.393647
H	0	2.159942	-0.094821	-1.408409
O	0	4.219441	-0.342471	-0.309897
N	0	3.145201	0.244079	0.348627
H	0	4.919124	-0.323367	0.347006
N	0	-0.74763335	-3.78765209	0.4363416
O	0	0.38970566	-4.09340249	0.66304734
O	0	-1.64158482	-4.58450944	0.37093593

6vZ

0 1

C	0	-1.619948	-2.186082	0.264671
C	0	-2.782693	-1.444815	0.120472
C	0	-0.391476	-1.550422	0.193691
C	0	-2.693826	-0.078387	-0.070801
C	0	-0.284599	-0.174253	0.000357
H	0	0.514629	-2.136399	0.288612
C	0	-1.463247	0.582833	-0.106814
H	0	-3.598355	0.507212	-0.17982
C	0	-1.510464	2.050007	-0.255091
C	0	-0.70325	2.94419	0.304093
H	0	-2.346784	2.414625	-0.843803
H	0	-0.867123	4.00245	0.154283
H	0	0.119922	2.662487	0.945802
H	0	-3.750016	-1.926783	0.15687
C	0	1.092092	0.440704	-0.106842
H	0	1.040218	1.357715	-0.697721
H	0	1.47209	0.726481	0.873767
C	0	2.081375	-0.472953	-0.76375
H	0	1.765215	-1.048199	-1.627971
O	0	3.668866	0.099956	0.66377
N	0	3.291688	-0.65748	-0.440692
H	0	4.579971	-0.16653	0.804575
N	0	-1.68295597	-3.63943979	0.47605008
O	0	-0.65378564	-4.24345161	0.59603747
O	0	-2.76101948	-4.163128	0.52007849

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0 1

C	0	-1.061311	-2.366634	0.228462
C	0	-2.361568	-1.965406	-0.036338
C	0	-0.05068	-1.4207	0.280467
C	0	-2.630041	-0.621833	-0.223004
C	0	-0.305044	-0.063483	0.094635
H	0	0.966361	-1.740904	0.467969

C	0	-1.628319	0.348557	-0.136392
H	0	-3.643897	-0.300477	-0.427671
C	0	-2.055152	1.751802	-0.296623
C	0	-1.58273	2.81429	0.344865
H	0	-2.889714	1.894045	-0.976402
H	0	-2.006751	3.794482	0.175461
H	0	-0.788722	2.743889	1.075349
H	0	-3.159583	-2.692423	-0.099412
C	0	0.858267	0.907654	0.116861
H	0	0.613269	1.773732	-0.500037
H	0	1.043556	1.275821	1.127832
C	0	2.124082	0.301291	-0.393647
H	0	2.159942	-0.094821	-1.408409
O	0	4.219441	-0.342471	-0.309897
N	0	3.145201	0.244079	0.348627
H	0	4.919124	-0.323367	0.347006
O	0	-0.7561688	-3.74898493	0.43068501
C	0	-1.91794718	-4.42857077	0.91373166
H	0	-2.63587028	-4.51253823	0.12478559
H	0	-1.64436986	-5.40595012	1.2525311
H	0	-2.34290376	-3.87572501	1.72531867

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0 1

C	0	-1.619948	-2.186082	0.264671
C	0	-2.782693	-1.444815	0.120472
C	0	-0.391476	-1.550422	0.193691
C	0	-2.693826	-0.078387	-0.070801
C	0	-0.284599	-0.174253	0.000357
H	0	0.514629	-2.136399	0.288612
C	0	-1.463247	0.582833	-0.106814
H	0	-3.598355	0.507212	-0.17982
C	0	-1.510464	2.050007	-0.255091
C	0	-0.70325	2.94419	0.304093
H	0	-2.346784	2.414625	-0.843803
H	0	-0.867123	4.00245	0.154283
H	0	0.119922	2.662487	0.945802
H	0	-3.750016	-1.926783	0.15687
C	0	1.092092	0.440704	-0.106842
H	0	1.040218	1.357715	-0.697721
H	0	1.47209	0.726481	0.873767
C	0	2.081375	-0.472953	-0.76375
H	0	1.765215	-1.048199	-1.627971
O	0	3.668866	0.099956	0.66377
N	0	3.291688	-0.65748	-0.440692
H	0	4.579971	-0.16653	0.804575
O	0	-1.68124147	-3.59989264	0.47029827
C	0	-2.98120881	-3.95697681	0.94724251
H	0	-3.69879792	-3.81623731	0.16611623
H	0	-2.98049474	-4.98317356	1.25026019
H	0	-3.2370362	-3.33870827	1.78222536

7a

0 1

C	-0.096969034	0.245776168	0.7573365895
C	-1.5902686723	0.38524716	0.5524112758
H	0.1882099784	0.7004802581	1.7103832837
N	0.6508140213	1.0250849209	-0.2830951113
O	0.2676475215	2.1868856009	-0.5699454839
H	-1.8368288225	1.4456142771	0.5486225072

C	1.6731735878	0.3715993384	-0.7343735873
H	2.3178319662	0.8489812494	-1.4547072033
C	1.8355595894	-0.961542613	-0.0858201434
H	2.0589768534	-1.7517699029	-0.801489815
H	2.6551030918	-0.9445612843	0.6383456047
C	0.4714608313	-1.1620289204	0.6020339538
H	-0.1872749521	-1.7397314292	-0.0483285693
H	0.5503850254	-1.6855693382	1.551477661
H	-1.8424885865	-0.0055044167	-0.4368757146
C	-2.3675088616	-0.3554251592	1.6326954433
H	-3.4400280123	-0.2291824965	1.4958308947
H	-2.1541457954	-1.4253690839	1.6177517639
H	-2.1110787898	0.0220313417	2.6239407004

7b

0 1

C	0.0431397309	-0.1513416339	0.7601624233
C	-1.2441081889	0.590525739	0.4364886213
H	0.0407389542	-0.3963023268	1.8238009626
N	1.2461326572	0.7139251347	0.5432183006
O	1.2171019613	1.9174412538	0.9095113742
H	-1.0672649201	1.2576436135	-0.413764683
C	2.2203112001	0.0550933113	0.0030118782
H	3.1610004932	0.5562063911	-0.1598375793
C	1.8702602381	-1.3723061069	-0.2551799275
H	2.2062075177	-1.7166291632	-1.2321649889
H	2.3265147414	-2.0279329983	0.4921789668
C	0.3367548816	-1.3532777698	-0.1285969446
H	-0.1085911728	-1.1863904445	-1.1113643721
H	-0.0726496624	-2.2754939737	0.2757453212
O	-1.7445130655	1.2855588098	1.5457664634
C	-1.8082784843	2.6891056945	1.3909168279
H	-2.1784726878	3.0912760792	2.3310711597
H	-0.8212736583	3.099588126	1.177522503
H	-2.5060519558	2.9619113873	0.5921781375
H	-1.9856837797	-0.1555121632	0.1318279558

7c

0 1

C	0.4559556475	0.4650290243	0.8121461948
C	-0.8041320463	1.2754870426	0.5778452119
H	0.9204905672	0.7700697458	1.7505027391
N	1.4545441853	0.7899907103	-0.2555916052
O	1.6319076435	1.9922269488	-0.5765525582
H	-0.541186697	2.3338337402	0.5834526852
C	2.0581329572	-0.2705381925	-0.6860272773
H	2.8384093804	-0.1607507491	-1.4219281016
C	1.6001631951	-1.5129812502	0.0014303271
H	1.4235165457	-2.3335274918	-0.6924877016
H	2.3487282945	-1.856412942	0.7207736988
C	0.3071327359	-1.0483697657	0.6996818914
H	-0.5552364053	-1.279249294	0.0731907486
H	0.1550602765	-1.5177956109	1.6684750274
H	-1.2433130563	1.0318591895	-0.3878247479
C	-1.8395382764	1.0111946817	1.6372081704
O	-2.9835161233	0.7155740969	1.4306828216
O	-1.3275651528	1.148930688	2.8714201968
C	-2.2529157264	0.9477898777	3.9395747131
H	-2.6673231007	-0.0576910423	3.8975477408
H	-1.6882411303	1.0922882717	4.8546932172

H	-3.0667379441	1.6671118312	3.8732939177
7d			
0 1			
C	0.3425732549	0.1793649114	-0.863462061
C	1.8232978463	0.3783614102	-0.5618645174
H	0.165694443	0.3777431506	-1.9240399496
N	-0.4271266788	1.2643861297	-0.1698817476
O	0.0414383061	2.4316295736	-0.3458877641
H	2.084928198	1.3996031881	-0.8237792359
C	-1.4871012537	1.0226706638	0.5325382361
C	-2.1293629524	-0.3182994309	0.6743111247
H	-1.9140633603	1.9052372908	0.9877887148
H	-3.2116801793	-0.1829563818	0.6475402793
H	-1.8997122563	-0.7411058595	1.6584735477
C	-0.1514593318	-1.2127838171	-0.4966872051
H	0.2758676635	-1.5007111082	0.4695261118
H	0.230733289	-1.9156577116	-1.2364344318
C	-1.667000135	-1.2701852092	-0.4178361723
H	-2.0082181206	-2.2838288515	-0.2113319795
H	-2.0973211356	-0.9668432548	-1.3751877101
H	1.9718785602	0.2745671276	0.5164943249
C	2.7007348324	-0.6136170184	-1.3148514879
H	3.7531608043	-0.3760815374	-1.1681306383
H	2.5454931003	-1.6394308539	-0.9802254462
H	2.4996426058	-0.5762043016	-2.3873783325
7e			
0 1			
C	0.0425590282	0.0157846348	0.8796532845
C	-1.4665024016	0.0799603731	0.6943167131
H	0.2728428222	0.174059143	1.9353027275
N	0.6340228688	1.1903587035	0.1758195554
O	0.0121512334	2.2843016721	0.3667478542
H	-1.8640278639	0.9967165961	1.1305505902
C	1.6979650321	1.0895427706	-0.5530135646
C	2.4892314098	-0.1635304709	-0.7439745207
H	1.9962775786	2.0215540778	-1.0123682647
H	3.5496228102	0.090294831	-0.6988805142
H	2.3136887944	-0.5519814166	-1.7531057852
C	0.6176496805	-1.3040023328	0.3969990594
H	0.1879740667	-1.5440558769	-0.5806703952
H	0.2948260545	-2.0819684157	1.0852300258
C	2.1308239674	-1.2236622283	0.2877004866
H	2.5550006806	-2.1862492474	0.0055286754
H	2.5544964007	-0.9516807761	1.257495145
O	-2.0017955233	-1.0609022842	1.3199871172
C	-3.4052184539	-1.0873690226	1.2552763509
H	-3.7517753013	-1.1063130285	0.2162156569
H	-3.7411211681	-1.99005823	1.7597842822
H	-3.8407023977	-0.2133937458	1.7507347151
H	-1.7020477881	0.0812588538	-0.3795704949
7f			
0 1			
C	-0.8363475091	1.0233690397	-0.6883781174
C	0.6250848616	1.4528290079	-0.7499437239
H	-1.4490394247	1.7735514088	-1.1897164478
N	-1.2664321102	1.0901581105	0.744169223
O	-0.9129689114	2.1506590625	1.3481310578

H	0.7174453409	2.4450869519	-0.3119715008
C	-1.9617150643	0.1487754051	1.2959473606
C	-2.4647119162	-1.0689963106	0.5917258293
H	-2.1885341337	0.3323997631	2.3367423796
H	-3.4818289718	-1.2656929824	0.9342677451
H	-1.8699981239	-1.9380125101	0.8928637849
C	-1.0577912985	-0.3488805341	-1.3034392165
H	-0.2708739844	-1.0284326705	-0.962837663
H	-0.9550263437	-0.2548634588	-2.3853824883
C	-2.417575117	-0.906895288	-0.9205810626
H	-2.6001455216	-1.8616271931	-1.4114237182
H	-3.2009500276	-0.2166724817	-1.2419584647
H	1.2503702288	0.7631300303	-0.1858886852
C	1.1339492637	1.483370541	-2.1647152532
O	2.1347533555	0.9498875663	-2.5561178005
O	0.325469318	2.2004938955	-2.9643586521
C	0.7537690216	2.3060896878	-4.3216395568
H	0.8241152823	1.318665701	-4.774417682
H	0.004795595	2.9077111043	-4.8258147694
H	1.7292630205	2.7857096034	-4.3719727979

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C	1.4836146481	-0.4356735756	-0.4194146795
C	2.7535664996	-0.6287127308	0.3885770176
H	1.7328260948	-0.3589794401	-1.4800506912
N	0.909540093	0.9108311388	-0.0950134844
O	1.7597401951	1.8534304909	-0.0910952119
H	3.4641295705	0.1647426044	0.1836914264
C	-0.3526991956	1.0852498523	0.1348804234
C	-1.3940042661	0.0161747794	0.0492734468
H	-0.612616525	2.1083643642	0.3674055757
C	0.4848382152	-1.5597633111	-0.1926842388
H	0.4215565396	-1.7703659232	0.8792160901
H	0.875128426	-2.4583200412	-0.6714949526
C	-0.8919523324	-1.1964362836	-0.7202165982
H	-1.586190384	-2.0288489956	-0.6130392423
H	-0.8272808219	-0.9563654561	-1.7840406134
H	2.5224079802	-0.6247130857	1.4546296363
H	3.1929930102	-1.5930959127	0.1340832567
H	-1.6980837853	-0.2839739722	1.0579903509
H	-2.2824280619	0.4411169177	-0.4206124715

7h
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C	0.6112229895	-0.7167804049	-0.3283896344
C	1.8884940512	-1.1819062671	0.3739148442
H	0.7171746929	-0.8942605536	-1.4014540357
N	0.5281801246	0.7765552999	-0.2212848435
O	1.6065053065	1.385581921	-0.5058941182
H	2.7077314418	-0.5618510253	0.01841518
C	-0.5667269531	1.3835328996	0.1070284552
C	-1.8794084335	0.7106390192	0.3441236786
H	-0.4668054116	2.4588157493	0.1560135681
C	-0.6316514198	-1.4117082901	0.204394716
H	-0.586720331	-1.4345089325	1.2981308886
H	-0.6119244995	-2.4469368745	-0.1354420542
C	-1.8978951037	-0.6968396003	-0.2335561
H	-2.7847804591	-1.2341262197	0.0995050588
H	-1.9346783311	-0.6468269412	-1.3243371431

H	1.7803937658	-1.0111038407	1.4471769654
H	-2.0877724449	0.6751537839	1.4189153622
H	-2.6640038601	1.3287611767	-0.0951604525
C	2.1573355792	-2.6358597126	0.094695739
C	1.8717011044	-3.6264195371	1.028676271
C	2.6796561996	-3.0166985028	-1.1397200867
C	2.0996516799	-4.9650733497	0.7387057411
H	1.4713707385	-3.3450878956	1.995502487
C	2.907368142	-4.351636361	-1.434874588
H	2.9188676706	-2.2520667527	-1.869877734
C	2.6164417955	-5.331564198	-0.495003148
H	1.8756371457	-5.7218935232	1.4785892497
H	3.3192762842	-4.6278877467	-2.3962402726
H	2.7971960954	-6.3733532706	-0.7215793539

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C	0.5292546241	-0.027889224	-0.3440539458
C	1.8377308925	0.3281529912	0.3539080641
H	0.679463504	0.0375203592	-1.4232264022
N	-0.4328277236	1.0826824878	-0.0438092321
O	0.0620206137	2.2485875477	-0.1542816608
H	2.1652598473	1.3064324363	0.0141088868
C	-1.6663669933	0.8554719037	0.2724243752
C	-2.3010601952	-0.4949851099	0.326771217
H	-2.2338321224	1.754763057	0.4669706717
H	-3.3031102406	-0.4189913717	-0.0978223832
H	-2.4358914957	-0.7950007149	1.3715524764
C	-0.0214178063	-1.3960705895	0.0295533256
H	0.0521674046	-1.5361834126	1.1117884932
H	0.6077661449	-2.1554808838	-0.4323546578
C	-1.4690508536	-1.5333149609	-0.409059324
H	-1.8414134082	-2.5357587611	-0.2042704509
H	-1.5442552157	-1.369711747	-1.4866165227
H	1.6982875617	0.372130058	1.4347898591
C	2.9371949466	-0.659650795	0.0750230639
F	2.7728480252	-1.8211173996	0.7307793395
F	4.1256152449	-0.1758070178	0.4470741843
F	3.0207687052	-0.9642832631	-1.2300910075

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C	0.5566943485	-0.0391284774	-0.251316675
C	-0.2071051957	-1.0375220471	0.5875494125
N	1.9720442029	-0.5082358044	-0.4328232528
O	2.1609890838	-1.695399367	-0.7993853065
H	-0.2068796652	-2.0081994726	0.0994029578
C	2.8334114003	0.4319532998	-0.2200500453
H	3.8798050245	0.2126683353	-0.3594171609
C	2.1993243832	1.742003744	0.0944931889
H	2.6644448331	2.2406911351	0.9439034223
H	2.2727822941	2.4148284625	-0.7630858536
C	0.7381702004	1.3478662739	0.383114904
H	0.5786494774	1.2583216942	1.4565931117
H	0.02371737	2.0716062364	-0.0029153768
H	0.2630765432	-1.1260183039	1.5662684683
C	-0.0646255431	0.0681595115	-1.6426801201
O	-1.1511172044	-0.3442338159	-1.9305758632
O	0.7282531242	0.7383909676	-2.4834328107
C	0.2202316365	0.8829304116	-3.8110603555

H	0.9831967823	1.4190013722	-4.365152537
H	0.0425915581	-0.0966818592	-4.2494692762
H	-0.7132243267	1.4423869982	-3.7976320751
H	-1.2345931674	-0.6995431449	0.7055654831

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C	-0.2490389729	0.2708591678	-0.1404868494
C	0.7268550692	0.7454514098	0.9259336113
N	-1.4543624374	1.1549054398	-0.088480899
O	-1.1739040358	2.3919246737	-0.1730804023
H	1.0191691263	1.7738950899	0.7434931535
C	-2.655062042	0.6909445509	0.0250991455
C	-3.0146048731	-0.7585754039	0.0284434326
H	-3.4109763852	1.4616076212	0.0809821828
H	-3.9477001562	-0.8777827306	-0.523813669
H	-3.2239762381	-1.0854159937	1.0530340249
C	-0.5905680353	-1.2113210151	0.0675791813
H	-0.6451097059	-1.3923508501	1.1441098206
H	0.2453092249	-1.8017733697	-0.3101292473
C	-1.9078699836	-1.6111591773	-0.5744016704
H	-2.1056362899	-2.6683396652	-0.4019192819
H	-1.8663341422	-1.4516322382	-1.6516987362
H	0.2526819701	0.6717802137	1.9041829615
C	0.3794907961	0.4707198087	-1.520982309
O	1.5629925547	0.4904663223	-1.7089116962
O	-0.5305025935	0.5424707015	-2.4926858288
C	-0.0036124211	0.7664461541	-3.8012845598
H	0.6871339173	-0.0290362551	-4.0731289606
H	-0.8594308646	0.7801090554	-4.46760732
H	0.5196871296	1.7199713789	-3.8293604331
H	1.6083393387	0.1080930713	0.9018753991

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C	0.5304343698	0.0197730303	-0.3694104754
C	1.8681268458	0.3581573502	0.2617642147
H	0.6112806028	0.0791870616	-1.4571678856
N	-0.4497190554	1.1016272877	-0.0283295099
O	0.0063155091	2.2805470749	-0.1492103248
H	2.2238755556	1.3242009776	-0.0792675079
C	-1.6655789819	0.8413793307	0.3315842364
C	-2.3038671638	-0.5150753477	0.4119045506
H	-2.2495116981	1.726148721	0.5543880914
C	0.031109738	-1.3533523182	0.0482037509
H	0.1791057911	-1.4750430365	1.1237987048
H	0.6550798654	-2.102521925	-0.4400903182
C	-1.4318760844	-1.5431713156	-0.3105014473
H	-1.7729354281	-2.5491238026	-0.0591070141
H	-1.555729696	-1.4193830074	-1.3901082774
H	1.7718263093	0.3855426873	1.3479523789
H	2.589251053	-0.4153539814	-0.0020576482
C	-3.6768114893	-0.4374474722	-0.2642621918
H	-4.1587279023	-1.4164063193	-0.241024407
H	-4.3267508404	0.2723708008	0.2496353575
H	-3.5825915035	-0.1240064331	-1.3041339295
C	-2.5072442089	-0.8996234849	1.8848464635
H	-3.0811677193	-0.1313093006	2.4042595559
H	-3.0570211547	-1.8401079687	1.9544562463
H	-1.5572931438	-1.0126543988	2.4060338162

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C	0.4654949718	-0.0273818867	-0.2793427177
C	1.8760416137	0.3440679115	0.1221003878
H	0.3868387547	-0.1284716432	-1.3647029815
N	-0.4810929451	1.088278661	0.066858928
O	0.0139462973	2.2527549443	0.1168483419
H	2.1864644677	1.2568921533	-0.3737986612
C	-1.7468197789	0.8217564007	0.2151412522
C	-2.2551276753	-0.5185576973	0.1209730068
H	-2.3905732073	1.6695990192	0.387694481
C	0.0261438368	-1.3271324034	0.3781197209
H	0.1994756577	-1.2665439081	1.4573230663
H	0.6170667352	-2.1508371847	-0.0189471887
H	1.9338890336	0.50622401	1.1979208741
H	2.5494001174	-0.4683049798	-0.1514661948
N	-1.3732398109	-1.5644244873	0.1141541339
C	-3.5309189316	-1.0369587574	0.0466113063
C	-2.061184046	-2.7410495045	0.0595224422
C	-3.4017981626	-2.445856152	0.0052088265
H	-4.4415513486	-0.4642994201	0.0086718969
H	-4.1993925602	-3.1640317979	-0.0713475875
H	-1.5421724894	-3.6840732479	0.0547393969

7n

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C	1.4268840976	-0.5636669377	-0.3955040495
C	2.7310716582	-1.2264814926	-0.021719091
H	1.4229968375	-0.3008177805	-1.456476303
N	1.2667812234	0.7458042887	0.3319687012
O	2.240956439	1.1709780233	1.0003865919
H	3.5746861663	-0.592181145	-0.2747075456
C	0.1252838392	1.3486628185	0.1970100236
C	-0.9364798123	0.6904585846	-0.6289867939
H	0.0084652421	2.2970216527	0.7000310837
C	0.2258088464	-1.4597173847	-0.1009669653
H	0.2682988355	-1.8184434288	0.9295855444
H	0.274680391	-2.3272265974	-0.75958134
H	2.7646139184	-1.4230442527	1.0476860678
H	2.8110036838	-2.1689531493	-0.5628572548
N	-1.0171180026	-0.7288820889	-0.301313654
C	-2.365921071	1.1284931737	-0.2918586284
C	-2.03669421	-0.9345670326	0.6080849059
H	-3.0003234739	1.1079890038	-1.1769052414
O	-2.8369029246	0.1595559425	0.6370888134
O	-2.2089321926	-1.9051182739	1.2812532762
H	-2.412161539	2.1108370483	0.1719708626
H	-0.7431543461	0.8225820279	-1.6972187136

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C	1.3096012376	-0.6776478485	-0.4162000137
C	2.6059398534	-1.3294679211	0.0202930287
H	1.1252943669	-0.8642959836	-1.4750788839
N	1.4420316342	0.8111592804	-0.3090457209
O	2.5621894909	1.2826603514	-0.6646659976
H	3.4320589816	-0.9759762975	-0.5865269315
C	0.4537851673	1.5396109855	0.0976276619
C	-0.913865425	1.0393908802	0.4310315089

H	0.6635017192	2.5978942005	0.146787311
C	0.1351796368	-1.1640002745	0.4106014381
H	0.393275705	-1.1034657742	1.4749519921
H	-0.0859552081	-2.2001459049	0.1703129027
H	2.8172680681	-1.091746148	1.0631725767
H	2.5107986069	-2.4103238751	-0.0800770396
N	-1.0409136943	-0.3704134308	0.1378496364
C	-2.2442529946	-0.9864414423	-0.0345746008
O	-3.2499728002	-0.0930755181	-0.0779695203
O	-2.401237698	-2.1781368038	-0.1466285745
H	-1.643245275	1.5960773381	-0.1548670923
H	-1.1331882668	1.2466683827	1.4874511734
C	-4.5380479817	-0.6643925216	-0.3007001248
H	-5.2351541252	0.1671216462	-0.2864297528
H	-4.56708043	-1.171652708	-1.2628290956
H	-4.7762061891	-1.379194683	0.4838796884

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7r
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C	1.3384346882	-0.6069120044	-0.3792769691
C	2.6998339829	-1.2214304995	-0.1361242869
H	1.0976340653	-0.6274068802	-1.4461087879
N	1.3709194928	0.8596766771	-0.0379538617
O	2.4905661999	1.4315901609	-0.111184966
H	3.4650778687	-0.7280219161	-0.7252252385
C	0.2555413004	1.4773847597	0.2292959727
H	0.3484492175	2.5422327522	0.3841587773
C	0.2417866956	-1.3018972009	0.4111014355
H	0.545185599	-1.3331104991	1.4641092258
H	0.1608982287	-2.3338610893	0.0701644098
H	2.9697856229	-1.1347730524	0.9161038997
H	2.6585729487	-2.2773969998	-0.4025152745
C	-1.0739538155	-0.5917453061	0.2967251535
C	-1.0289523132	0.8054098221	0.2431446319
C	-2.2982717975	-1.2379717571	0.3016290141
H	-2.3283862955	-2.3198824954	0.3421507851
C	-3.4805403316	-0.5092852988	0.2628135873
C	-2.2172688291	1.5339378276	0.2146784123
H	-2.1781505743	2.6151540431	0.1784020694
C	-3.4371304792	0.8776142755	0.224285349
H	-4.3554542579	1.4479120946	0.198183681
H	-4.4322277367	-1.0224380736	0.26624705

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C	-1.706534	0.617921	-0.386335
C	-3.071517	1.180791	-0.054428
H	-1.544711	0.627342	-1.46812
N	-1.652158	-0.841793	-0.019292
O	-2.748976	-1.460428	-0.000907
H	-3.855861	0.644986	-0.577694
C	-0.49523	-1.407921	0.175821
H	-0.531559	-2.47244	0.354693
C	-0.585901	1.37262	0.310049

H	-0.81329	1.412018	1.381773
H	-0.573634	2.400148	-0.052948
H	-3.260647	1.103795	1.016024
H	-3.094354	2.232135	-0.340587
C	0.746955	0.714869	0.111482
C	0.757322	-0.683738	0.084499
C	1.939984	1.41069	0.016071
H	1.92717	2.493512	0.036345
C	3.146095	0.730436	-0.097074
C	1.970202	-1.363383	-0.018771
H	1.974322	-2.445797	-0.034164
C	3.158704	-0.657566	-0.109333
H	4.096021	-1.19016	-0.193111
N	4.40625299	1.48049023	-0.19866377
O	5.43058707	0.86417848	-0.29519541
O	4.35970831	2.67879274	-0.18095932

7t
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C	-1.706534	0.617921	-0.386335
C	-3.071517	1.180791	-0.054428
H	-1.544711	0.627342	-1.46812
N	-1.652158	-0.841793	-0.019292
O	-2.748976	-1.460428	-0.000907
H	-3.855861	0.644986	-0.577694
C	-0.49523	-1.407921	0.175821
H	-0.531559	-2.47244	0.354693
C	-0.585901	1.37262	0.310049
H	-0.81329	1.412018	1.381773
H	-0.573634	2.400148	-0.052948
H	-3.260647	1.103795	1.016024
H	-3.094354	2.232135	-0.340587
C	0.746955	0.714869	0.111482
C	0.757322	-0.683738	0.084499
C	1.939984	1.41069	0.016071
H	1.92717	2.493512	0.036345
C	3.146095	0.730436	-0.097074
C	1.970202	-1.363383	-0.018771
H	1.974322	-2.445797	-0.034164
C	3.158704	-0.657566	-0.109333
H	4.096021	-1.19016	-0.193111
O	4.37196298	1.46008059	-0.19589942
C	5.26513244	1.0348663	0.83673852
H	5.68403008	0.08508613	0.5772344
H	6.0506389	1.75301189	0.94694973
H	4.72904363	0.94833367	1.7587043

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C	1.5057320142	-0.7885501706	-0.3076916844
C	2.6241777836	-0.6925033256	0.7261166975
H	1.8734307833	-1.3037489803	-1.1932400711
N	1.2357868316	0.5887158495	-0.8016441027
O	2.0967731405	1.0136658742	-1.6305847129
H	3.4627372341	-0.1454307473	0.3004776072
C	0.2391221234	1.2785031778	-0.3562653054
H	0.1746569908	2.2820362474	-0.7505339368
H	2.267183856	-0.1786426903	1.6194536585
H	2.9483671513	-1.6918718814	1.0118661321
C	-0.7390666139	0.7682640758	0.6471892638

H	-0.4995980079	1.1755418912	1.6374103858
H	-1.7276770417	1.1598093641	0.4003362515
C	0.2799970486	-1.4723335801	0.2269037254
C	0.235580694	-2.8627311938	0.2697743935
C	-0.7889539696	-0.7328393812	0.7135472866
C	-0.8620039874	-3.5147162932	0.8040183454
H	1.0680810727	-3.4340011003	-0.1236852426
C	-1.8930784239	-1.3927501479	1.2438936485
C	-1.9314439795	-2.7755470374	1.2950616306
H	-0.8884992483	-4.5952945644	0.8328049299
H	-2.7294047203	-0.812165867	1.6141641791
H	-2.7954965216	-3.2777787994	1.7080910503

7v
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C	0	1.020236	0.920058	0.097548
C	0	1.418555	1.556457	-1.231077
H	0	1.212937	1.620919	0.907787
N	0	1.97878	-0.185419	0.367429
O	0	3.110275	0.207948	0.784566
H	0	2.475707	1.812258	-1.20588
C	0	1.669317	-1.415996	0.1278
H	0	2.463135	-2.124131	0.315098
H	0	1.228863	0.863449	-2.051628
H	0	0.829679	2.456663	-1.399433
C	0	0.342736	-1.849426	-0.397976
H	0	0.419415	-2.051998	-1.473543
H	0	0.080554	-2.803931	0.062214
C	0	-0.413606	0.473504	0.119082
C	0	-1.416989	1.405047	0.369015
C	0	-0.74895	-0.846914	-0.14619
C	0	-2.748243	1.027742	0.344572
H	0	-1.147429	2.431471	0.588122
C	0	-2.088387	-1.223013	-0.163398
C	0	-3.085695	-0.293199	0.075429
H	0	-3.52138	1.757842	0.540519
H	0	-2.345606	-2.256536	-0.361615
N	0	-4.4962732	-0.70646019	0.0558244
O	0	-5.33654231	0.12297091	0.26656286
O	0	-4.7505096	-1.8565551	-0.1701276

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C	0	1.544287	0.660931	0.774864
H	0	1.824025	0.951131	1.785171
N	0	2.775716	0.455622	0.001002
O	0	2.320953	-0.370177	-1.085785
C	0	0.882918	-0.745517	0.72531
C	0	1.698393	-1.43077	-0.392224
H	0	0.979258	-1.291735	1.662203
H	0	1.079198	-1.971657	-1.104635
H	0	3.049644	1.314451	-0.467914
H	0	2.457747	-2.092213	0.033345
C	0	0.518696	1.647053	0.162758
C	0	-0.551975	-0.475758	0.37146
C	0	-1.597341	-1.385268	0.314079
C	0	-0.760303	0.861347	0.056219
C	0	-2.859262	-0.942321	-0.05878
H	0	-1.43381	-2.42747	0.560248
C	0	-2.020154	1.304976	-0.31658

C	0	-3.068909	0.396469	-0.371347
H	0	-3.684574	-1.639929	-0.103425
H	0	-2.187468	2.346478	-0.560993
H	0	0.853202	1.95844	-0.830244
H	0	0.40355	2.546043	0.768928
N	0	-4.41114785	0.85204147	-0.76089623
O	0	-4.56537341	2.01161242	-1.02552526
O	0	-5.29840335	0.04595825	-0.79852984

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0 1

C	0.8076550258	0.1315693635	0.8788363856
H	1.0063779881	0.1496504556	1.9474401903
N	0.2011951878	-1.1444166361	0.5138883051
O	-0.3905245576	-0.8584200051	-0.7717431112
C	-0.1722462378	1.1953281627	0.3130915215
C	-1.1214128631	0.3409701331	-0.5310530066
H	-0.7047893537	1.8267505767	1.0199907813
H	-1.2889796139	0.7775926608	-1.5164447762
C	-2.4409504358	0.0544419867	0.1634890405
H	-3.0068393791	0.9766269317	0.2990094083
H	-3.0343785833	-0.6359989406	-0.4339389058
H	-2.2631532839	-0.3960777728	1.139099737
H	0.9171372618	-1.8252459535	0.2747909445
C	0.9961279109	1.8467962443	-0.4587104351
H	1.2908771579	2.8106725386	-0.0499949328
H	0.835800549	1.9543792342	-1.5306697822
C	1.9281343785	0.6902760842	-0.032113749
H	2.1721023558	0.0076958874	-0.8448684634
H	2.8425337327	0.9830171085	0.4788142685

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C	0.6773816165	0.0692978705	0.7829987998
H	0.7632873075	-0.1017410257	1.8524807984
N	-0.0316407069	-1.0511085493	0.1685634163
O	-0.5122837045	-0.4838000992	-1.0760306387
C	-0.1060139982	1.326776514	0.3209779817
C	-1.0825380698	0.7418226146	-0.6858340014
H	-0.6225611837	1.9217545405	1.0669401917
H	-1.184502613	1.3153126888	-1.6142266703
H	0.6323127549	-1.7462820308	-0.1624609393
C	1.1870243478	1.9027190942	-0.2929498298
H	1.5542244353	2.7832156151	0.228244497
H	1.1262518825	2.1255282592	-1.3574350464
C	1.9432668273	0.6034607648	0.0680925788
H	2.2227779693	0.0006788457	-0.7950825901
H	2.8125494144	0.7324092323	0.7087720549
O	-2.314641495	0.5938031075	-0.0571441125
C	-3.2619908379	-0.1025916703	-0.8382541594
H	-4.2041098162	-0.069367989	-0.2974347855
H	-3.3898085561	0.3753864229	-1.8159264698
H	-2.9608275043	-1.139809916	-0.9879612454

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C	0.596380164	-0.0403624888	0.7272654967
H	0.6847411805	-0.3207803218	1.7732229248
N	-0.2524860441	-1.0077282405	0.0354936418
O	-0.6388844248	-0.2986056589	-1.1626894886

C	-0.0621062885	1.3286390871	0.4027969888
C	-1.1038493131	0.9194293088	-0.6334054893
H	-0.4973844987	1.9035681686	1.2127008629
H	-1.181513969	1.6226780716	-1.4644276028
H	0.2944324787	-1.7808224816	-0.3335660249
C	1.2759556019	1.8218367449	-0.1897865026
H	1.7439647029	2.5991936314	0.4091814576
H	1.2239617392	2.1592056579	-1.2240883605
C	1.8939256582	0.4203322259	0.0207092423
H	2.0765713318	-0.1217317716	-0.9059748662
H	2.7898388391	0.3903629702	0.636270675
C	-2.4915059582	0.7843054551	-0.0057704217
O	-2.8850734267	1.475972855	0.8952368142
O	-3.2299834241	-0.1384297744	-0.6133843071
C	-4.5456176248	-0.3007794853	-0.0867216042
H	-5.1081987885	0.6264614189	-0.1804026711
H	-5.0050864121	-1.0904376	-0.6715437055
H	-4.4971674737	-0.5794452325	0.9642108405

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C	0.9623261946	0.4468118305	0.789122465
H	1.112799921	0.3730934925	1.8656044122
N	0.7653207468	-0.9120253076	0.263338208
O	-0.0223302743	-0.688918187	-0.9241320162
C	-0.3697250093	1.1685837306	0.4334667972
C	-1.0831156108	0.1284815185	-0.4441206147
H	-0.9544639605	1.3916177758	1.3245726273
H	-1.5193893126	0.5871245615	-1.3320487651
C	-2.1244522676	-0.6898617171	0.2983148553
H	-2.9444364034	-0.0501350546	0.6262597767
H	-2.5243441796	-1.4660065361	-0.3525432597
H	-1.6787723601	-1.1655924789	1.1706923158
H	1.6363954076	-1.2703146265	-0.1178126004
C	0.0463801169	2.4586785503	-0.2949703507
H	0.0239465822	2.2847066922	-1.3737839002
H	-0.617141001	3.295056978	-0.0810153273
C	1.4946714858	2.7015050311	0.1335776714
H	1.5257375949	3.1160709426	1.1442057114
H	2.0286701741	3.3861245564	-0.5238939119
C	2.066283724	1.2858075526	0.1325625556
H	2.1887571012	0.9489231307	-0.9005931125
H	3.0248243504	1.1943403747	0.6417540326

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C	0.8168743616	0.4197991765	0.6894547647
H	0.9551148719	0.2149492879	1.7496904629
N	0.4429175948	-0.8445528765	0.0317821189
O	-0.3756999408	-0.4079346539	-1.0798630756
C	-0.4036075404	1.3481027123	0.4354264098
C	-1.269315057	0.4996559961	-0.488031381
H	-0.950952555	1.5676868318	1.3481090963
H	-1.7161813836	1.0478909986	-1.3248830989
H	1.2506653732	-1.2359469255	-0.444950116
C	0.1689950578	2.6174072441	-0.2140081098
H	0.1237009117	2.5212326852	-1.302114031
H	-0.3818790378	3.5145350215	0.0624503901
C	1.6361855612	2.6391752158	0.2173301419
H	1.7183092145	2.9675106763	1.2561915576

H	2.253803439	3.2984028345	-0.3908146255
C	2.0239577412	1.1666863575	0.1021368623
H	2.1153021487	0.9031095933	-0.9555484708
H	2.9593993165	0.9151677759	0.5998410542
O	-2.2550307961	-0.1229430137	0.2728030897
C	-3.0056706669	-1.0715157089	-0.4538645559
H	-3.7977851979	-1.4209426466	0.2031735064
H	-3.4512699628	-0.6177886778	-1.3463633493
H	-2.3831149239	-1.9132127847	-0.7585355611

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C	0.7778476532	0.3871157645	0.6881417053
H	0.9564770589	0.1576244981	1.737191131
N	0.2254729726	-0.8215826881	0.0514066245
O	-0.5512027117	-0.2890068688	-1.0429119823
C	-0.361385888	1.4319959225	0.5066201762
C	-1.3450784611	0.6558416928	-0.3694664369
H	-0.8225303281	1.7070232162	1.4506614476
H	-1.826434976	1.2754917942	-1.1275945572
H	0.9552012494	-1.3431441151	-0.4258084425
C	0.292442449	2.6368502211	-0.188294799
H	0.1728019666	2.54316073	-1.2709034177
H	-0.1495103186	3.5839188443	0.1158782362
C	1.777956041	2.51535553	0.1546219051
H	1.9523970651	2.8351608376	1.1846617902
H	2.4197918942	3.1112651373	-0.4924464904
C	2.0143519325	1.01138941	0.027051193
H	2.0175969291	0.7383097129	-1.0318887719
H	2.9480305564	0.6711268816	0.4724360703
C	-2.4434625132	-0.0151730439	0.4564682074
O	-2.8493045163	0.4075803499	1.5059016542
O	-2.9396991544	-1.0860019285	-0.1559182542
C	-3.9753703204	-1.7623640892	0.5539027949
H	-4.2619812622	-2.6036888793	-0.0680258884
H	-3.605574425	-2.1063329146	1.5180821866
H	-4.8218079629	-1.0975839756	0.7170797379

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C	0.0847181565	-0.3316501925	-0.8677556684
H	-0.1965225023	-0.4360120292	-1.9146300573
N	0.9385479553	-1.4783024804	-0.512191113
O	1.7461827107	-0.9626572273	0.5636622949
C	1.0143173149	0.8936742517	-0.6278091864
C	2.2454804707	0.2291088306	-0.0079246287
H	1.2599027571	1.4002127245	-1.5591389263
H	2.6981763126	0.8113704682	0.7925150809
H	0.3858884108	-2.1951275289	-0.0498128164
C	0.2345985504	1.8194254916	0.3203621895
H	0.5227171077	1.6003922398	1.3519361537
H	0.4353755016	2.8736021873	0.1358596104
C	-1.2315484377	1.4307521414	0.1235447015
H	-1.6099603038	1.8486386669	-0.8125997108
H	-1.8808956861	1.7738332295	0.9278385177
C	-1.1453062716	-0.090815686	0.0187143188
H	2.9936295197	-0.0119444503	-0.7683111621
H	-0.9442208943	-0.5072846665	1.0096705436
H	-2.0465150422	-0.5587905304	-0.3752860316

8h

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C	-0.0826047933	-0.9195874587	0.435108328
H	-0.0079808101	-1.5263105221	1.336273235
N	-1.4262254888	-1.1157097495	-0.1293682764
O	-1.6864712516	0.1281474356	-0.8165397568
C	-0.0371558961	0.6007747791	0.7568773224
C	-1.362625822	1.1044001534	0.1539706748
H	-0.0023396607	0.7814542342	1.8286873109
H	-1.2084871366	2.0310356166	-0.4021498356
H	-1.3882675909	-1.7797638861	-0.8979413745
C	1.2292373015	1.1282063392	0.0610968433
H	0.9647355505	1.5102151832	-0.928305034
H	1.7033910649	1.937916913	0.6137439381
C	2.1185864023	-0.1039009933	-0.1081324772
H	2.5851256894	-0.3671472752	0.8442610517
H	2.9126567581	0.0346058172	-0.840409502
C	1.1034173224	-1.1732294321	-0.5059677659
H	0.7764227018	-0.9916297333	-1.533758232
H	1.4836824161	-2.191604513	-0.4402024728
C	-2.4613742666	1.320245617	1.1739322981
C	-3.6558212594	0.6149076976	1.123662957
C	-2.2812558709	2.277271059	2.1682656485
C	-4.6501857852	0.8581159487	2.0615497683
H	-3.7925368236	-0.1303370257	0.3538606856
C	-3.2748039819	2.5245010149	3.1024555648
H	-1.354895459	2.8399676366	2.2089293422
C	-4.4646026182	1.810634357	3.0525165827
H	-5.5746594382	0.2978276174	2.0169402651
H	-3.1221959634	3.2743979684	3.8671325966
H	-5.2418149406	1.997381281	3.781159894

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C	-0.4468677853	0.7802893408	0.6683805587
H	-0.5420517085	1.0139073632	1.727637228
N	0.6694214426	1.5767921504	0.1363649692
O	1.1793419632	0.7662310262	-0.9505520788
C	0.0013549776	-0.6922472149	0.4458899335
C	1.2681433141	-0.5166211705	-0.3949840019
H	0.2166217587	-1.194982717	1.3863615596
H	1.3327348037	-1.222643033	-1.2229833177
C	2.5421477582	-0.7066479641	0.4193888265
H	0.3149497153	2.3905746157	-0.3585603558
C	-1.1609454747	-1.3718813177	-0.2983705016
H	-0.9747770659	-1.3325912488	-1.3745512785
H	-1.2793043303	-2.4170737255	-0.0195489166
C	-2.378765471	-0.504611385	0.0224659859
H	-2.7303269024	-0.7090166831	1.0364251339
H	-3.2126404637	-0.6677829871	-0.658170001
C	-1.795080127	0.9043736497	-0.0544514575
H	-1.6075389492	1.1602788349	-1.1011847938
H	-2.433693116	1.6726023595	0.3784613421
F	2.5505957449	-0.0362057262	1.5724685398
F	2.6705212933	-2.011439095	0.7224030279
F	3.6226078023	-0.3464177224	-0.2700392219

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0 1

C	1.5390206951	-0.3953426308	0.9137179748
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H	1.5590149429	-0.3555135338	1.9989596743
N	0.4930068873	-1.302482473	0.4497923961
O	0.2999440013	-0.892368807	-0.9200511088
C	1.2057732775	0.9345403298	0.1919398025
C	0.1144975007	0.50183854	-0.7876613258
H	0.2115373621	0.9460863015	-1.7757146403
H	0.8551955892	-2.2470603408	0.3497972849
C	2.6455028299	0.9506485921	-0.3995569098
H	3.2652252716	1.73319909	0.0322903744
H	2.6762819539	1.0196921757	-1.4852247874
C	2.9107031102	-0.446046078	0.2012428362
H	2.9612972103	-1.2360738594	-0.5460338008
H	3.7710310612	-0.5124290233	0.8619297138
C	0.8831751486	2.1251502686	1.0402327844
O	1.2731072047	2.2960915794	2.1636986565
O	0.1431227856	3.0228091267	0.3732272487
C	-0.1615015816	4.2178303325	1.0929048281
H	0.7543150024	4.7435660855	1.3562869343
H	-0.771277797	4.8195019293	0.4272552196
H	-0.7064175938	3.979769466	2.0042015682
H	-0.8748282621	0.7158054692	-0.3746872439

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C	-1.2519788073	0.60114786	0.8004732815
H	-1.1823272479	0.5845652545	1.8860383737
N	-0.1586576507	1.4328432607	0.2675328507
O	0.0787352074	0.8653908855	-1.0362425353
C	-0.9390391839	-0.7998357833	0.2019044672
C	0.2515909809	-0.4962086595	-0.7176825898
H	0.2394816514	-1.0656035563	-1.6440646115
H	-0.502188027	2.3635101663	0.0474594178
C	-2.227331019	-1.202973079	-0.558482233
H	-2.1321438037	-0.8622737021	-1.5919102278
H	-2.3841913669	-2.2811948141	-0.5726312756
C	-3.3348260626	-0.4158293171	0.1370522966
H	-3.5615835922	-0.8666475294	1.105179414
H	-4.2553383857	-0.372091215	-0.4432097189
C	-2.6743585594	0.9459693338	0.3357885046
H	-2.6148502904	1.4619946544	-0.6266485693
H	-3.1973002223	1.5901773339	1.0405710731
C	-0.6599494486	-1.8415239606	1.2518318845
O	-1.0968952676	-1.8411754239	2.3713550615
O	0.0996795991	-2.832900434	0.7622788964
C	0.3597680306	-3.9071236515	1.6658879998
H	-0.5718925941	-4.3905517579	1.9542379529
H	1.0008991864	-4.5991707503	1.1301623956
H	0.856228901	-3.5363890993	2.5603169897
H	1.2008558026	-0.6437740357	-0.1959095384

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C	-0.3948083277	0.7667805643	0.5918515733
H	-0.4782746624	1.067903234	1.6365659491
N	0.7787484919	1.4611569651	0.0346360734
O	1.2756718886	0.5601549568	-0.9746102373
C	-0.0099285253	-0.7340890117	0.4587286491
C	1.333444376	-0.6587970296	-0.2641776113
H	0.0885733683	-1.2042559401	1.4356482961
H	1.4823796497	-1.4540164903	-0.9926072929

H	0.4994464728	2.2726970578	-0.5081097471
C	-1.1500846572	-1.3777290378	-0.3419991277
H	-0.911957193	-1.3511133946	-1.4075476692
H	-1.3146391232	-2.4189568906	-0.0689397072
C	-2.349621025	-0.4814471902	-0.0511715708
H	-2.7188801436	-0.6824518194	0.9589843855
H	-3.1833899953	-0.6215180854	-0.7408068567
C	-1.7784336741	0.9454360775	-0.1043559785
H	2.1672638497	-0.635652604	0.4436912012
C	-1.6491112201	1.4094205856	-1.5571251719
H	-2.6287996146	1.3806347719	-2.036576142
H	-1.2990874927	2.4422022664	-1.6132513086
H	-0.9584030134	0.7955900012	-2.13218842
C	-2.6565896525	1.9341433413	0.6554689467
H	-3.6433224804	2.0083386637	0.1945095705
H	-2.7908994438	1.6229159904	1.692900651
H	-2.2136039231	2.9325318275	0.6576368052

8m

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C	0.1509492933	0.4200868656	0.8943114942
H	0.7840237642	0.3674277027	1.7772295066
N	0.8546575292	1.2756398589	-0.1048494391
O	0.5618968389	0.6639888115	-1.375787206
C	0.0108026763	-0.9511575401	0.1666461921
C	0.8066346983	-0.6951918904	-1.108152096
H	0.4154103311	-1.767977361	0.7578921698
H	0.4640284553	-1.2693934785	-1.9666370073
H	0.365161462	2.1636821684	-0.1741346716
C	-1.4996467486	-1.1511616719	-0.1030678204
H	-1.7252981327	-1.0390230702	-1.1649088886
H	-1.8551294385	-2.1255442088	0.2302139017
C	-1.2566942523	0.7978128581	1.2105462126
H	1.8753385049	-0.8643368017	-0.9448339014
N	-2.1270584122	-0.0872012453	0.654894987
C	-3.4096504634	0.2831182778	0.9195684173
C	-1.9838259471	1.7669203714	1.8600342755
C	-3.3520303651	1.4359302101	1.6699786139
H	-4.2497208706	-0.2883147643	0.5654773659
H	-4.2019590383	1.9765994236	2.0504157426
H	-1.5921462446	2.6034801043	2.4129047913

8n

0 1

C	0.6433186825	0.6228986553	1.1046722685
H	0.8980507562	0.9428115149	2.1126093869
N	1.2709421092	1.5316011032	0.1536775976
O	1.1341404717	0.8050470494	-1.0760106743
C	1.2758675546	-0.7370098055	0.7082073214
C	1.7262755386	-0.440198289	-0.7410053032
H	2.120733566	-1.0009590238	1.3384776795
H	1.3605884734	-1.1683682955	-1.4626723741
H	0.7204581568	2.3706721081	-0.0019545202
C	0.1353208199	-1.7522173947	0.7967237704
H	0.2330987262	-2.5873063078	0.1066359041
H	0.0247690119	-2.141151601	1.8096970226
C	-0.8983946424	0.3785864411	0.9683544061
H	2.813333241	-0.3590060577	-0.7981938258
N	-1.0415532394	-0.9724394044	0.4467709899
C	-1.4315577447	-0.9254132714	-0.8816865076

C	-1.7136964678	1.1808428224	-0.0582049882
H	-2.6772956024	1.4805714346	0.3497588692
O	-1.3614710853	-1.8085723744	-1.684475974
H	-1.1982559334	2.0616350512	-0.4371405982
H	-1.3496388828	0.4541545335	1.957743314
O	-1.9383745096	0.2972490516	-1.1504503045

8o

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C	0.7181699028	0.7041066168	0.8535786254
H	0.5282452696	0.9633328348	1.8923403273
N	1.9049580344	1.4410955526	0.3994918669
O	2.4044757281	0.6191471209	-0.6703234178
C	1.1356826255	-0.7823408891	0.6803023642
C	2.4813725491	-0.6412722476	-0.0363990419
H	1.2383072041	-1.2862258405	1.6376712457
H	2.6451092446	-1.3883840062	-0.810317901
H	1.6360978184	2.297062593	-0.0782773318
C	0.0298059743	-1.4271766071	-0.168607284
H	0.3693814241	-1.5561217721	-1.2022240685
H	-0.304907625	-2.3924457517	0.201380964
C	-0.5468020665	0.8763772585	-0.0031198926
H	3.3102182362	-0.6473084922	0.6759931309
N	-1.0627859708	-0.4727821394	-0.1126817837
C	-2.3219767892	-0.8295555506	-0.4565027249
O	-2.6798718649	-1.9612612185	-0.6869317049
H	-1.2838744156	1.5362995238	0.4449891061
O	-3.1457870674	0.2395640055	-0.4925883228
H	-0.2665993969	1.2700445173	-0.9877627302
C	-4.5010150724	-0.0749798823	-0.7990440373
H	-4.9250845902	-0.7223819181	-0.0336220231
H	-5.0263564999	0.8744224829	-0.8272970009
H	-4.5671725826	-0.5782234709	-1.761354455

8p

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8r

0 1

C	0.6735978116	0.7821959267	0.7825263055
H	0.9901181789	1.8232824422	0.7289040157
N	1.7148844168	-0.0335129659	0.1146779435
O	1.5779189873	-1.3198032737	0.7391330309
C	0.6432747266	0.2117117554	2.2317414476
C	1.607716393	-0.9745583411	2.1056438692
H	1.0107406368	0.9300411534	2.9599203166
H	1.2985023942	-1.8506424572	2.6713930943
H	1.4347444033	-0.2225079047	-0.8445081783
C	-0.8216358022	-0.1863450453	2.5251717402
H	-0.8962792544	-1.2181275349	2.8732147248
H	-1.2528299734	0.4417274925	3.3065833567
H	2.6224372923	-0.6814957177	2.3913635129
C	-0.7273300485	0.5818125937	0.2666983923
C	-1.5521798878	0.0118888092	1.2246045742
C	-1.2087239059	0.8760030863	-1.0007765123
C	-2.8738492588	-0.2834170734	0.9227029231
C	-2.5306901892	0.5826240871	-1.3046192265

H	-0.5645160015	1.3294200833	-1.7453376387
C	-3.3571627822	0.003747758	-0.3464717174
H	-3.5220184954	-0.7328578405	1.6646604838
H	-2.921606622	0.8041019795	-2.288385941
H	-4.3856745296	-0.2226149732	-0.5932405774

8s

0 1

C	0	-0.935976	-0.645376	0.835857
H	0	-1.022083	-1.068766	1.835981
N	0	-1.73049	-1.499482	-0.077887
O	0	-2.081672	-0.604387	-1.144996
C	0	-1.602047	0.755252	0.690302
C	0	-2.613369	0.489493	-0.432144
H	0	-2.11027	1.061114	1.601033
H	0	-2.717074	1.316437	-1.131155
H	0	-1.116176	-2.16485	-0.540639
C	0	-0.478191	1.748014	0.313627
H	0	-0.728437	2.317812	-0.583027
H	0	-0.308372	2.47366	1.110878
H	0	-3.59043	0.222126	-0.018566
C	0	0.497343	-0.428025	0.426973
C	0	0.745298	0.897429	0.103761
C	0	1.500241	-1.381877	0.331363
C	0	2.003511	1.286956	-0.332506
C	0	2.759844	-0.994341	-0.103613
H	0	1.306518	-2.415855	0.592749
C	0	3.007646	0.334076	-0.435429
H	0	2.202524	2.319521	-0.591011
H	0	3.552572	-1.725487	-0.185306
N	0	4.34572905	0.7310195	-0.89680695
O	0	4.53432646	1.88186967	-1.17679578
O	0	5.1953885	-0.1118344	-0.97481262

8t

0 1

C	0	-0.935976	-0.645376	0.835857
H	0	-1.022083	-1.068766	1.835981
N	0	-1.73049	-1.499482	-0.077887
O	0	-2.081672	-0.604387	-1.144996
C	0	-1.602047	0.755252	0.690302
C	0	-2.613369	0.489493	-0.432144
H	0	-2.11027	1.061114	1.601033
H	0	-2.717074	1.316437	-1.131155
H	0	-1.116176	-2.16485	-0.540639
C	0	-0.478191	1.748014	0.313627
H	0	-0.728437	2.317812	-0.583027
H	0	-0.308372	2.47366	1.110878
H	0	-3.59043	0.222126	-0.018566
C	0	0.497343	-0.428025	0.426973
C	0	0.745298	0.897429	0.103761
C	0	1.500241	-1.381877	0.331363
C	0	2.003511	1.286956	-0.332506
C	0	2.759844	-0.994341	-0.103613
H	0	1.306518	-2.415855	0.592749
C	0	3.007646	0.334076	-0.435429
H	0	2.202524	2.319521	-0.591011
H	0	3.552572	-1.725487	-0.185306
O	0	4.34572905	0.7310195	-0.89680695
C	0	5.26762342	-0.18349074	-0.98144437

H	0	6.17985191	0.26010236	-1.32197975
H	0	5.42276535	-0.62372229	-0.01862188
H	0	4.95828459	-0.9388123	-1.67332502

8u

0 1

C	0.4967557385	0.7699459002	0.9517846859
H	0.5454061642	1.8498573715	1.0726737046
N	1.6370970492	0.3508085717	0.1263293531
O	1.7513653714	-1.0468034156	0.4480158555
C	0.7565373849	0.0133450548	2.2852123729
C	1.8343081482	-1.0056699198	1.8568781802
H	1.1327558848	0.6627835485	3.0739416328
H	1.6452665715	-2.0108751553	2.2274423578
H	1.3794524759	0.3354883479	-0.8564680041
H	2.8286294962	-0.6673421626	2.1603481429
C	-0.8985213873	0.3148979034	0.456726725
C	-0.5702810823	-0.5966077065	2.6379266508
C	-0.9091676525	-1.2798822372	3.7961943817
C	-1.4991347941	-0.4301668627	1.6180461643
C	-2.1924173266	-1.7934352339	3.9273605486
H	-0.1842382231	-1.4088918388	4.590775384
C	-2.7810739937	-0.9428352898	1.7477119976
C	-3.1233563878	-1.6243627882	2.9081571688
H	-2.471638505	-2.3246055733	4.8271850189
H	-3.5087391097	-0.8135870619	0.9563473554
H	-4.1211958594	-2.0260069807	3.0215960003
H	-0.7861039697	-0.3527687947	-0.4014640971
H	-1.5151682335	1.156879893	0.1409765402

8v

0 1

C	0	1.020236	0.920058	0.097548
C	0	1.418555	1.556457	-1.231077
H	0	1.212937	1.620919	0.907787
N	0	1.97878	-0.185419	0.367429
O	0	3.110275	0.207948	0.784566
H	0	2.475707	1.812258	-1.20588
C	0	1.669317	-1.415996	0.1278
H	0	2.463135	-2.124131	0.315098
H	0	1.228863	0.863449	-2.051628
H	0	0.829679	2.456663	-1.399433
C	0	0.342736	-1.849426	-0.397976
H	0	0.419415	-2.051998	-1.473543
H	0	0.080554	-2.803931	0.062214
C	0	-0.413606	0.473504	0.119082
C	0	-1.416989	1.405047	0.369015
C	0	-0.74895	-0.846914	-0.14619
C	0	-2.748243	1.027742	0.344572
H	0	-1.147429	2.431471	0.588122
C	0	-2.088387	-1.223013	-0.163398
C	0	-3.085695	-0.293199	0.075429
H	0	-3.52138	1.757842	0.540519
H	0	-2.345606	-2.256536	-0.361615
O	0	-4.45789012	-0.69521499	0.05635786
C	0	-5.05076634	-0.42994213	1.33033906
H	0	-5.23093517	0.62023344	1.42816781
H	0	-5.97702641	-0.95966624	1.40992951
H	0	-4.38795788	-0.7519028	2.10617814

8w

0 1

C	0	1.544287	0.660931	0.774864
H	0	1.824025	0.951131	1.785171
N	0	2.775716	0.455622	0.001002
O	0	2.320953	-0.370177	-1.085785
C	0	0.882918	-0.745517	0.72531
C	0	1.698393	-1.43077	-0.392224
H	0	0.979258	-1.291735	1.662203
H	0	1.079198	-1.971657	-1.104635
H	0	3.049644	1.314451	-0.467914
H	0	2.457747	-2.092213	0.033345
C	0	0.518696	1.647053	0.162758
C	0	-0.551975	-0.475758	0.37146
C	0	-1.597341	-1.385268	0.314079
C	0	-0.760303	0.861347	0.056219
C	0	-2.859262	-0.942321	-0.05878
H	0	-1.43381	-2.42747	0.560248
C	0	-2.020154	1.304976	-0.31658
C	0	-3.068909	0.396469	-0.371347
H	0	-3.684574	-1.639929	-0.103425
H	0	-2.187468	2.346478	-0.560993
H	0	0.853202	1.95844	-0.830244
H	0	0.40355	2.546043	0.768928
O	0	-4.37462434	0.83964494	-0.75029625
C	0	-5.2604699	0.72480856	0.36639092
H	0	-6.15654892	1.27520374	0.16888767
H	0	-5.50233291	-0.30530833	0.52532953
H	0	-4.78536306	1.11860379	1.24051837

9aZ

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C	6.0795217969	-2.5173397906	2.6232890624
C	6.9738325394	-3.3920103154	2.1853875828
H	5.6623791794	-2.6466719709	3.6203339504
N	3.8404359856	-0.255189232	-0.5107364878
O	4.5392644431	-1.0566975468	-1.1925386435
C	3.5416180901	-0.351209925	0.7437393604
C	4.0592155156	-1.4965414563	1.5349360192
H	2.9365531684	0.4464510502	1.1478229838
H	3.9118266213	-2.4094259042	0.953635737
H	3.4984401998	-1.583970838	2.4652896967
C	5.565315661	-1.356570585	1.8306338134
H	6.0945183019	-1.2818519666	0.8806068306
H	5.729217285	-0.4260836262	2.3808513624
H	7.3801532605	-3.2595950413	1.1860726939
H	3.4667908605	0.5571160003	-1.0112211759
C	7.4787794562	-4.5638665906	2.9657320921
H	8.5600162416	-4.5053787212	3.1040322654
H	7.0099757069	-4.6137135855	3.9477699688
H	7.277470457	-5.499421225	2.440628618

9bE

0 1

C	-1.6965863971	0.0378951268	0.5419245203
C	-2.6297064139	-0.6419297994	-0.1082291682
H	-2.0041851098	0.846450197	1.1955599569
N	2.625516297	-0.3110769086	0.0298738503
O	3.8597547049	-0.5637925125	-0.0561240895
C	2.0032020817	0.7703605259	-0.300501344

C	0.5277752774	0.9464735517	-0.1574689861
H	2.6309006554	1.5538316273	-0.7023323618
H	0.1061367765	1.1973676709	-1.1348432083
H	0.3387357156	1.8200894091	0.4740603374
C	-0.2339916648	-0.2521522905	0.4119798161
H	-0.0949297478	-1.1242401379	-0.2333195065
H	0.176200386	-0.5082149283	1.3946006841
H	-2.3803186944	-1.4602711765	-0.7813901235
H	2.0466199307	-1.0653960279	0.414134371
O	-3.9513674811	-0.3899608054	0.0407707879
C	-4.7851220603	-0.998893986	-0.9246519155
H	-5.8101888638	-0.773870486	-0.6453356058
H	-4.5862717546	-0.6000789337	-1.9220776549
H	-4.6446806976	-2.0828371062	-0.9344519798

9bZ

0 1

C	6.0150603118	-2.5542992863	2.7032929205
C	7.0076371321	-3.3094865317	2.255694351
H	5.5533031389	-2.8137767023	3.6499367939
N	3.9948315151	-0.2463688936	-0.5279735502
O	4.8611124098	-0.9236714197	-1.1510552048
C	3.5333921241	-0.4696839438	0.659239513
C	4.048676799	-1.622338368	1.4411101082
H	2.7986602956	0.2344449904	1.0199063255
H	4.0620952506	-2.5008968583	0.7920957031
H	3.3857863193	-1.8253467829	2.2816080969
C	5.4868186464	-1.3808163448	1.9419052041
H	6.1159069506	-1.1766814547	1.0748817861
H	5.4937601952	-0.4868771021	2.5708398862
H	7.5006657646	-3.1019242062	1.3083522546
H	3.6155075306	0.5664906405	-1.0233484995
O	7.4798162286	-4.3791413184	2.9432667816
C	8.4722319155	-5.1243835414	2.2695326942
H	8.7517020194	-5.9452495665	2.9237552947
H	8.0899905865	-5.5281316908	1.3289006033
H	9.3537479264	-4.5110005394	2.0658730776

9cE

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C	-1.7202916719	0.0827440594	0.4450632778
C	-2.6778648996	-0.475231669	-0.2838795211
H	-1.9917849653	0.8434499634	1.1698951525
N	2.5948144649	-0.3501673186	0.0143757717
O	3.823313648	-0.6247130433	-0.0574847537
C	2.0141590647	0.7852397096	-0.1878851871
C	0.53965835	0.9887221261	-0.0755151214
H	2.6758864489	1.5970687484	-0.4556819677
H	0.1605177941	1.3620542862	-1.0311155775
H	0.3516376993	1.7879030113	0.6477224706
C	-0.2676891161	-0.2482621647	0.3266534954
H	-0.1342574637	-1.0488163752	-0.4041421064
H	0.0880354956	-0.6145986629	1.2953729635
H	-2.4672135173	-1.2378450262	-1.0227621509
H	1.9829028002	-1.1338789547	0.2662711793
C	-4.1125981789	-0.1301625066	-0.1712263011
O	-4.971330123	-0.6485293623	-0.8341478289
O	-4.3609600218	0.8197883353	0.7428142134
C	-5.7348295464	1.1785593613	0.8786477401
H	-6.3233895743	0.3148685015	1.1822863732

H	-5.767398428	1.9508379142	1.6400071778
H	-6.1233231095	1.5536005368	-0.0662580296

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C	6.17343832	-2.6465625775	2.2722301763
C	6.8493969457	-3.7716857306	2.0719253989
H	5.9732805645	-2.3324355927	3.2917556344
N	3.7314600735	0.5416147666	0.4536386278
O	4.2971203195	1.0830917825	1.4443824045
C	3.5723285639	-0.7249671898	0.2477203316
C	4.1036219247	-1.6926067906	1.2413439108
H	3.066150128	-1.0017831853	-0.6643006922
H	3.6694856072	-2.6766559734	1.0732011326
H	3.8127138419	-1.3485539687	2.2372513571
C	5.6426180534	-1.7751418804	1.1847922301
H	5.9608120773	-2.1489202768	0.2110311054
H	6.0284294251	-0.7607644015	1.3077283573
H	7.076513125	-4.1335166807	1.0772411315
H	3.3575645727	1.1769088322	-0.2583152788
C	7.3640868664	-4.635678959	3.1547576327
O	7.9690375473	-5.6576908127	2.9597253599
O	7.0917655273	-4.1700147316	4.3841667861
C	7.5816679817	-4.9742113746	5.4537066469
H	8.6635003787	-5.0741926249	5.3871954167
H	7.2995308446	-4.4604462075	6.3668766493
H	7.1355452214	-5.9666023731	5.4182013208

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C	0.2654445994	-1.8305907302	1.545411951
C	0.3941490031	-1.6381768653	2.8507865216
H	1.1075468528	-1.5987529147	0.8954431998
N	-2.6826308021	0.7887451174	-1.7080677006
O	-3.1466923378	1.5835083468	-2.5734061904
C	-2.5706785426	0.965733587	-0.4344926187
C	-1.9971214909	-0.0558521665	0.4899978701
H	-2.9239279103	1.9224038377	-0.0749561391
H	-2.7436090376	-0.2921658629	1.2561718395
H	-1.1604305477	0.3934094074	1.0325623917
C	-0.968701396	-2.3408502787	0.8666389684
H	-1.7329089893	-2.5649788756	1.6144845693
H	-0.7399656535	-3.2782082652	0.3535673372
C	-1.5305684379	-1.352466025	-0.1610865961
H	-2.36228177	-1.8277976347	-0.687568186
H	-0.7561556219	-1.1386407475	-0.9045871061
C	1.6277198723	-1.1286532514	3.5258253725
H	1.4194218272	-0.2119841131	4.080474877
H	2.006953869	-1.855406752	4.2464891297
H	2.4147435531	-0.9207351015	2.8022281477
H	-0.4512141428	-1.8699131629	3.4943414673
H	-2.3523716263	-0.1129500888	-2.0682193659

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C	4.5367812527	-2.0258224518	4.8690042504
C	3.500295696	-2.0461425658	5.6956037721
H	5.3702942912	-1.361520772	5.0929441181
N	3.5135843002	-0.9771457929	-0.2925429869
O	3.2929752909	-2.2086693768	-0.4719289921

C	3.6385318533	-0.3626436012	0.8383323788
C	3.5402282478	-1.1301891219	2.1053856003
H	3.8334943687	0.6976926396	0.7805412792
H	2.6838541608	-1.8057886816	2.0241389587
H	3.3624332184	-0.4516788018	2.9385026315
C	4.6625271147	-2.8384205658	3.6169668056
H	3.7957825925	-3.49575384	3.5151946467
H	5.5440372694	-3.4808797342	3.6884028145
C	4.7961404578	-1.9738864118	2.3610727771
H	4.9640861424	-2.6095137574	1.4915398587
H	5.6625504214	-1.3146581159	2.4612643603
H	2.6689695861	-2.7086923048	5.4672537208
H	3.5969896767	-0.4053081586	-1.1384365889
C	3.3792873763	-1.2266203363	6.9415850982
H	3.2757853741	-1.864222131	7.8215382556
H	4.2537765055	-0.592011158	7.0809213457
H	2.4938811831	-0.5890123799	6.9075700856

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C	-2.0908177883	0.670157281	-0.4904173596
C	-3.0194243818	0.0343201107	0.2094449096
H	-2.0658627263	0.5242847882	-1.5653494307
N	2.946838409	-0.2366760938	-0.1607653913
O	4.1408084595	-0.6150394134	-0.3256500396
C	1.9953866025	-0.8359307141	0.4728037386
C	0.6142619314	-0.28421827	0.595766725
H	2.2688326909	-1.7846096017	0.9138317139
H	0.3676299473	-0.1958302833	1.659843573
H	-0.09249052	-1.016655064	0.1957360356
C	-1.0601678394	1.5612173719	0.1292503986
H	-1.2541195399	1.656486719	1.2008259312
H	-1.1381813854	2.5651100244	-0.2946039959
C	0.3741157338	1.0597852218	-0.0796308846
H	1.0654103649	1.8083598254	0.3169127579
H	0.5657118921	0.9774025301	-1.1540255787
H	-3.0996527226	0.1440798361	1.289743191
H	2.7055014707	0.6636373873	-0.5885982035
O	-3.9143999954	-0.8096687415	-0.3591045949
C	-5.0186186298	-1.1409535359	0.4579944993
H	-5.6083647608	-1.8733573513	-0.0854285801
H	-4.6882843943	-1.5768804029	1.4045629975
H	-5.633828398	-0.2614515042	0.6618746078

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C	4.7431402109	-2.0877332398	4.8759592774
C	3.7209986202	-2.1573693182	5.7157303933
H	5.5630319795	-1.4198553334	5.120592846
N	3.3014511798	-0.9679871497	-0.1660442182
O	3.0773864779	-2.2018749624	-0.325636215
C	3.5269367952	-0.3538537679	0.9492229628
C	3.554082709	-1.1244138144	2.2178025802
H	3.7045333322	0.7085699246	0.8762649307
H	2.7008611722	-1.8093632209	2.2131466894
H	3.4477023568	-0.4495839703	3.0656752253
C	4.8113201756	-2.8547817139	3.5921841441
H	3.956847771	-3.532852665	3.5227727451
H	5.7090555313	-3.4778569807	3.5845535283
C	4.8366403766	-1.9552497083	2.3535456751

H	4.944551504	-2.5685342877	1.4586024822
H	5.6995067029	-1.2862704544	2.4042101494
H	2.8695706097	-2.8106526651	5.5319614434
H	3.2984247451	-0.3944550608	-1.0149391896
O	3.6451970377	-1.4043586618	6.8438381649
C	2.7348803597	-1.8857159062	7.8097520331
H	2.7138523592	-1.1604053758	8.6182676293
H	1.7305844666	-1.981999603	7.3878788568
H	3.0529128271	-2.8546941049	8.2022211358

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C	-2.0863407186	0.4782055338	-0.4070374268
C	-3.0159359082	-0.1698466289	0.2842934538
H	-2.0181497996	0.3036087936	-1.4768396744
N	2.9887310254	-0.1247699382	-0.2346265583
O	4.197428931	-0.4301142693	-0.4306404165
C	2.0961847333	-0.7743496236	0.4351111743
C	0.6867620668	-0.3098292007	0.5935200126
H	2.4417911189	-1.6964993959	0.8811781987
H	0.4627038457	-0.2350430966	1.6629990626
H	0.0187434781	-1.0885399848	0.2132045517
C	-1.1037006754	1.4355737682	0.1844830696
H	-1.2752724797	1.5292731995	1.2584457718
H	-1.2644231026	2.4222154332	-0.2569821658
C	0.3477679402	1.0168831703	-0.0757777153
H	1.0053565922	1.8048662193	0.2986855318
H	0.5073421189	0.9453266081	-1.1557932648
H	-3.1288324146	-0.0390232946	1.3530088505
H	2.6808109879	0.7534277063	-0.6661288447
C	-3.9825618028	-1.1195421551	-0.3087422653
O	-4.8160927594	-1.7026222267	0.3328084114
O	-3.8375439188	-1.2694284629	-1.6343903445
C	-4.7525398508	-2.1805481858	-2.2399001961
H	-5.7774080642	-1.8556436412	-2.0712940876
H	-4.5193578283	-2.1783207095	-3.2996040331
H	-4.6267399153	-3.1772636786	-1.8211518453

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C	4.4470974049	-2.1463100388	4.7090629682
C	3.5887099895	-2.0346037842	5.7160662249
H	5.2797841394	-1.4513720081	4.651435676
N	4.146245678	0.1026022907	0.6077677964
O	4.944913804	0.5081731593	1.4993640435
C	3.2761917639	-0.8478191306	0.7170436778
C	3.1679467866	-1.5850250464	2.0017736502
H	2.6812879677	-1.0513994829	-0.1602665843
H	2.2381638745	-2.1535883205	2.026992271
H	3.1399445668	-0.8474231304	2.8086514646
C	4.342659684	-3.1596422349	3.6156852251
H	3.4353093271	-3.7538954002	3.7457351902
H	5.1915450081	-3.844628895	3.6939335703
C	4.3678974567	-2.5139365664	2.2283611229
H	4.3763434286	-3.2941203934	1.4658657711
H	5.2813275154	-1.9283772392	2.1133111722
H	2.7323329545	-2.689825211	5.8123649997
H	4.1936460618	0.5841207221	-0.2953960717
C	3.6946996585	-1.0273387435	6.7920486885
O	2.8910927694	-0.9185286841	7.6820509101

O	4.775948499	-0.2409504265	6.6816692336
C	4.9035279196	0.7533306007	7.6937279305
H	4.9658415082	0.2890347268	8.6763668424
H	5.81626605	1.2946226535	7.4673322915
H	4.0461965739	1.4239638831	7.6767395153

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C	2.5562138088	-0.6507653994	-0.5035579166
C	3.4315260063	0.3208277948	-0.2981460873
H	2.4261949353	-1.0437768734	-1.508956542
N	-2.5405317635	-0.37630254	-0.2355248633
O	-3.7766996304	-0.2844778677	-0.4773519713
C	-1.6906739166	0.5729668692	-0.0287814645
C	-0.2432327447	0.3350212255	0.2460545991
H	-2.1032702446	1.5715522406	-0.0709114856
C	1.6947848767	-1.2683111182	0.5548915247
H	1.922192675	-0.8167771518	1.5231465569
H	1.929986979	-2.3325174975	0.6334757409
C	0.1988753392	-1.1234017291	0.2550450907
H	-0.3638033473	-1.6819459619	1.0073509677
H	-0.0124970334	-1.5834822677	-0.7154336629
H	3.5860835328	0.7371687391	0.69053847
H	-2.1674459887	-1.3309158305	-0.2007367442
H	4.0275871813	0.7280159597	-1.1033289755
H	0.0083672442	0.7886091736	1.2110479527
H	0.3480126604	0.8844547046	-0.4920535295

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C	-4.3553115591	4.0689266466	0.9552417982
C	-3.705780434	5.1539159916	1.3472971196
H	-4.8699957487	3.459964686	1.6940953238
N	-2.3934061372	-0.2140533942	0.7210652226
O	-3.1232343492	0.0831566425	1.7095783358
C	-2.0060389158	0.574335563	-0.2277866324
C	-2.4464691151	1.9924617945	-0.2229622635
H	-1.3854143228	0.1272037921	-0.9895656082
C	-4.4246567594	3.5721050237	-0.4562076273
H	-3.8438566377	4.2316300927	-1.1064526161
H	-5.4613009259	3.6133897165	-0.8012980039
C	-3.9302295359	2.1297734673	-0.5874344058
H	-4.089251413	1.7797135975	-1.6088412272
H	-4.50564803	1.482698811	0.0767757141
H	-3.171754519	5.7758046725	0.6379509311
H	-2.0734805738	-1.1860902858	0.6715820286
H	-3.6866365575	5.4601803071	2.3842982082
H	-1.8333894856	2.5741115328	-0.9118890391
H	-2.2979942605	2.3894000327	0.7846147515

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C	2.5925850417	-0.1202961452	-0.5387451105
C	3.4019181865	0.8994220369	-0.2674440989
H	2.4702032927	-0.4510757259	-1.5669322101
N	-2.4980510132	-0.2704557225	-0.1630193212
O	-3.742754006	-0.2603660791	-0.3768796644
C	-1.7232400495	0.723394362	0.1163815184
C	-0.25488874727	0.5807569378	0.3434061208
H	-2.2150060818	1.6847162365	0.1719845216

C	1.8102335809	-0.8820147401	0.4845782727
H	2.0230854201	-0.4888853924	1.4811247473
H	2.1280476465	-1.9277552502	0.4774816392
C	0.2998127404	-0.8341680007	0.2251753563
H	-0.199051766	-1.4939971449	0.939551233
H	0.1024302005	-1.2312448775	-0.7755264179
H	3.5317594389	1.1901338506	0.771890378
H	-2.0472407367	-1.1898145339	-0.2211235819
H	-0.0156689692	0.9737326507	1.3375156034
H	0.2725210654	1.2333473531	-0.3584133575
C	4.1856868264	1.6767915017	-1.2392739988
C	5.2416238543	2.466114732	-0.7842342324
C	3.9135191517	1.6623234929	-2.6088404969
C	6.0179893703	3.2009675022	-1.6676170523
H	5.4592593428	2.4949481645	0.2763983893
C	4.6860658374	2.3959047435	-3.4921928103
H	3.0795459611	1.0851981859	-2.9853855747
C	5.7445870965	3.1663122839	-3.0262717732
H	6.8353293774	3.8027103447	-1.2937137018
H	4.4562282499	2.3751298099	-4.5489950026
H	6.3447091539	3.7413831037	-3.7179217345

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C	2.202276678	-0.3345436677	0.2618994577
C	2.930866652	-0.8311541236	-0.7324348819
H	1.8011179017	-1.01106231	1.0118828818
N	-1.8722646011	-0.980289405	0.1973256409
O	-0.9040704393	-1.6994808805	0.588196801
C	-1.7941489168	0.1483348835	-0.4281625154
C	-0.451248683	0.7014032987	-0.7330722083
H	-2.7327402336	0.6190806651	-0.6790354523
C	1.7942542708	1.0970943663	0.4089226872
H	2.1500153997	1.6817508477	-0.4430883554
H	2.2428776235	1.5257080288	1.3090995401
C	0.2693540252	1.1958476505	0.5362925048
H	-0.0294830237	2.2214312026	0.7551969611
H	-0.0395758901	0.575599272	1.3789522467
H	3.3523050254	-0.1540009169	-1.4713002984
H	-2.8099911337	-1.3361514952	0.4027758139
H	-0.5320492178	1.5009808828	-1.4675085005
H	0.1397630655	-0.1086243249	-1.170285986
C	3.2226788158	-2.2615075423	-0.9167497747
C	4.3870008057	-2.6594843504	-1.5726603501
C	2.3389749183	-3.2442772076	-0.4638364295
C	4.6840599498	-4.0030372011	-1.7426688734
H	5.0690108459	-1.9037734833	-1.9432209671
C	2.63739665	-4.5866686814	-0.6338096327
H	1.4003787775	-2.9489484015	-0.009223805
C	3.8116884965	-4.9718916988	-1.2680213147
H	5.5952772738	-4.2937395485	-2.2482610813
H	1.9420581658	-5.3370949553	-0.2819161137
H	4.0383921782	-6.0207849639	-1.4037909846

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C	-2.0721745844	0.5067561885	-0.4037150678
C	-2.9797210153	-0.158033037	0.2904313347
H	-2.018211052	0.350988428	-1.4772314265
N	2.9963214536	-0.1333831605	-0.2199700664

O	4.2030355342	-0.4480545002	-0.4107013821
C	2.0989580939	-0.7697010445	0.4559494446
C	0.6924708002	-0.2941985264	0.6081614444
H	2.4363096839	-1.6901912585	0.9115179008
H	0.4675500539	-0.2100531171	1.6768831795
H	0.019904494	-1.0714350906	0.232792522
C	-1.0847821499	1.4614726485	0.1863780689
H	-1.2562162188	1.5584634127	1.2599914553
H	-1.2411782077	2.4470343715	-0.2577644915
C	0.363471514	1.03047886	-0.0711625416
H	1.0262312973	1.8167315564	0.2979616868
H	0.5242719733	0.9504010128	-1.1504635862
C	-3.9389876248	-1.1167887781	-0.3312657189
H	-3.0857383479	-0.0533517733	1.3632651266
H	2.6938932078	0.741716779	-0.6616152045
F	-3.8108254925	-1.19321702	-1.6590930154
F	-3.7690907916	-2.3549453453	0.1569496116
F	-5.207866091	-0.7740632258	-0.0708452244

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C	-2.0360068522	0.5543439801	-0.3757743628
C	-2.7998654529	-0.0345233184	0.5289525181
H	-2.2654080436	0.405407166	-1.4270606247
N	3.1739988195	-0.4865982462	0.028870161
O	3.2236060076	0.4689183159	0.8543060041
C	2.1112622983	-1.0513122695	-0.4440409924
C	0.7766957593	-0.5592148381	-0.01609116
H	2.2720653953	-1.855599091	-1.1456917974
H	0.7951705995	-0.4455640281	1.0720586338
H	0.0130356841	-1.2935748902	-0.2685200444
C	-0.8436062359	1.3986818975	-0.0632703394
H	-0.7429618296	1.5203721601	1.0167635282
H	-0.9930051953	2.3927997955	-0.4908524284
C	0.4469746341	0.8053827383	-0.6354821759
H	1.2742989011	1.4844731275	-0.431807286
H	0.3573828819	0.7043052461	-1.7196919922
H	-2.6256317609	0.0669360682	1.5931241074
H	4.0749303476	-0.8530002305	-0.2936957639
C	-3.9635631587	-0.8971343786	0.177153717
F	-5.0977449181	-0.4405142276	0.7277765587
F	-4.1707253214	-0.9854424299	-1.1409780099
F	-3.7951882898	-2.1479912772	0.6345908092

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C	-0.3650026031	-0.1488223872	-0.3405483892
C	-1.2166311724	0.7680171558	0.1014861011
N	3.9868713865	0.1589221879	-0.2104410506
O	5.2311574847	0.3559157164	-0.2983347667
C	3.3465046977	-0.5445649479	0.6617587596
C	1.8624379292	-0.7024191702	0.66958312
H	3.9668507323	-1.0263548894	1.4047744078
H	1.4828416289	-0.3772219119	1.6428276689
H	1.62171077	-1.7648008009	0.5855022059
C	1.1196755249	0.0606931227	-0.4300336671
H	1.3247225934	1.1299628897	-0.3504713922
H	1.4619010032	-0.2876008082	-1.4073853378
H	-0.867368406	1.7440614869	0.4134927661
H	3.4172158167	0.6180235227	-0.9292518281

C	-0.8408362904	-1.4926715978	-0.7869615131
O	-0.1031682574	-2.3410266504	-1.2193202549
O	-2.1604109215	-1.663448112	-0.6669092505
C	-2.6478219215	-2.9355308543	-1.0940334729
H	-2.3986413934	-3.1028402563	-2.1399579889
H	-2.2061366782	-3.7290160678	-0.4941870815
H	-3.7232101505	-2.9027969769	-0.9554981017
H	-2.2763464129	0.567909879	0.1602697958

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C	5.286192919	-1.7484111072	3.2677323919
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O	3.2028910272	-2.0571050748	-0.4550920289
C	2.951596881	-0.108753071	0.7199629655
C	3.3633461085	-0.7320944683	2.0029528555
H	2.6859623117	0.9310770985	0.6037414887
H	2.8315863642	-1.6814454463	2.1043592845
H	3.1024917917	-0.0825806487	2.8354991209
C	4.87662358	-1.0262048866	2.0188011165
H	5.1164214415	-1.6373012956	1.1500553432
H	5.4186967419	-0.0825896363	1.9500464302
H	5.5247202081	-3.6449170881	2.4089293039
H	2.6413938269	-0.3559421996	-1.2185704666
C	5.3315886301	-0.910978669	4.5016478864
O	5.0574728111	0.2627978572	4.5159068172
O	5.7088990834	-1.5808637443	5.5974454233
C	5.7706479713	-0.803025084	6.7904636093
H	6.4814255287	0.0129225162	6.6732891865
H	4.7923900937	-0.3865581941	7.0235682612
H	6.0933498666	-1.481940529	7.5728078337
H	5.8382200395	-3.5332374772	4.2344986377

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C	-0.7898481768	0.8140944007	-0.6057388416
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O	5.2157204674	-1.1773283566	0.0960437691
C	3.2066865419	-0.459692244	0.9503985117
C	1.9227865145	0.2758493652	0.7538201173
H	3.445961933	-0.9406086758	1.8887912697
H	1.8382595653	1.0382697366	1.5361727226
H	1.0952112238	-0.4166831077	0.9344209249
C	0.4174260268	1.7012233236	-0.7104569769
H	0.3696477485	2.4544971752	0.0775246583
H	0.3906801884	2.2172670993	-1.6705479593
C	1.7436042517	0.9369165724	-0.6076175037
H	2.5562670245	1.6458795052	-0.7845606127
H	1.7787735858	0.1935810481	-1.4067261678
H	-1.4439243953	1.4445369533	1.2859742287
H	3.8949049509	-0.1321941875	-0.8670187306
C	-1.0302984673	-0.0701674848	-1.7861267417
O	-0.3456375503	-0.0476049632	-2.7768858273
O	-2.0798155793	-0.8859584127	-1.6431351394
C	-2.3405761128	-1.738158381	-2.7579666759
H	-2.5348792303	-1.1455633	-3.6498246294
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C 2.207965866 -0.6300839595 0.4818890383
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C 0.3072442935 0.9088193723 -0.089219232
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C	-4.3445999602	4.3603400477	0.8638856084
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H	-4.7642047472	3.9133841735	1.7618443586
N	-2.4365713204	-0.5059540765	0.3422467639
O	-3.3662659687	-0.5670225277	1.1979147922
C	-1.9082114546	0.5402237682	-0.2028201374
C	-2.3317855767	1.9456680999	0.1210493872
H	-1.119140109	0.3332698471	-0.913751827
C	-4.382430415	3.5096450206	-0.3680923132
H	-3.8755488347	4.0283663535	-1.1841103803
H	-5.428366235	3.4077700718	-0.6736030938
C	-3.841023142	2.0854512169	-0.2020011967
H	-4.40334846433	1.5561331307	-1.1392231613
H	-4.4038715685	1.5581772023	0.5680102007
H	-3.4360304349	6.068691799	0.0441010955
H	-2.0500378973	-1.406430076	0.0412708513
H	-3.8862228298	6.1717143849	1.8333017464
C	-2.0321576177	2.2069941796	1.6067065334
H	-2.286292702	3.231717777	1.8698692621
H	-2.5981043535	1.5201599681	2.2335710987
H	-0.9681654132	2.0633054894	1.8033777685
C	-1.496556708	2.891704457	-0.743493627
H	-0.4315140112	2.7018813872	-0.5995984029
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H	-1.6906294771	3.9271584499	-0.4653900555

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C	2.0143933753	-0.840202544	0.2906909663
H	2.9380094932	-0.2880773078	0.1906423289
H	1.2241532629	-2.6422439708	0.199997023
C	0.7436549641	-0.2374913074	0.6275131624
C	-0.2817780982	-0.7178566149	1.4188967158
N	0.3668123282	0.9997164707	0.1609642854
C	-1.3047545359	0.2551013272	1.423801587
H	-0.2645096453	-1.6447723337	1.9677267498
C	-0.8718099493	1.3022343222	0.6506290948
H	-2.2446033457	0.2046035416	1.9450582792
H	-1.3401992094	2.2395583977	0.4058981274
C	1.1780148731	1.8748817844	-0.6748561261
H	1.7742363501	2.5455681803	-0.0518996571
H	1.863859824	1.239238006	-1.2370411197
C	0.339335362	2.6673925326	-1.6293499921
H	-0.3000682927	2.0898941461	-2.2886444972
C	0.3619598589	3.9877883405	-1.6998114112
H	0.9884168963	4.5757001179	-1.0395741106
H	-0.2380479504	4.5257190461	-2.4205459773

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N	2.5950160489	-0.7462155157	0.5495744179
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C	1.8085688192	-0.6050836329	-0.4789300509
H	1.4474236521	0.3985657776	-0.637921181
H	2.7864681241	0.1055721303	1.0829985889
C	1.4305458192	-1.6978207473	-1.3195316483
C	1.7264425895	-3.0494447495	-1.2287187745
N	0.6107627091	-1.519812643	-2.4200861714

C	1.0600989033	-3.6949360829	-2.28742855
H	2.3547992911	-3.4785431231	-0.4712526286
C	0.3809595121	-2.7329899164	-2.9955427681
H	1.0763326637	-4.74613655	-2.5161814196
H	-0.2450119756	-2.8113084483	-3.8675260978
C	0.0063714604	-0.266221851	-2.8450627661
H	-0.910556189	-0.0750164855	-2.2817479107
H	0.7112692432	0.53592966	-2.6208700446
C	-0.2799206055	-0.2489031173	-4.3151532437
H	0.5691841734	-0.4331941424	-4.9649179297
C	-1.475812509	-0.0059313746	-4.8244082476
H	-2.3337115273	0.1676584693	-4.1858549682
H	-1.6381502024	0.0333591445	-5.8925713319

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N	2.1372476946	-1.3231380097	0.6050551947
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C	1.7133370377	-0.3371741002	-0.1213432361
H	2.2520058983	-0.1369615099	-1.0369027933
H	1.5975885903	-1.4994375443	1.4650045135
C	0.5282796505	0.4533861117	0.2959169654
C	0.7742883611	1.9674574237	0.3523171889
N	-0.5483101594	0.4304796186	-0.6788293774
H	1.5235124124	2.2635832937	-0.3844754895
C	-1.2318295794	1.6264027726	-0.6509597565
C	-1.2808112508	-0.7918754842	-0.9844205182
H	-2.0105399583	-0.5245459139	-1.7458277547
H	-0.5790158596	-1.5072341528	-1.4143585639
C	-1.9751160311	-1.369316223	0.2213798425
H	-1.3993936421	-2.0302027378	0.8624431474
C	-3.2317635973	-1.0862584202	0.5269235524
H	-3.8208123351	-0.4270988499	-0.0999559316
H	-3.706150686	-1.4941103591	1.4094801105
O	-2.4778873833	2.5458649883	0.0069447193
O	-2.3063265197	1.861574079	-1.1171757524
H	1.0680249307	2.3163934379	1.3378411742
H	0.1743875488	0.0896414122	1.2716299132

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N	2.7223814329	-0.5630481992	0.6112710355
O	2.8947821879	0.2063907676	1.5976942012
C	1.6572411295	-0.6318509434	-0.1125770663
H	1.6450281722	-1.3158776012	-0.9470151133
H	3.5027667959	-1.1813566197	0.367764778
C	0.5176701299	0.257004043	0.2451623755
C	0.8437774418	1.7590154716	0.0979658908
N	-0.587077338	0.1260739983	-0.6765994167
H	1.6846573298	1.9163342751	-0.5779322451
C	-1.1515280776	1.3568330419	-0.9366135153
C	-1.4527588088	-1.0469575523	-0.6872156156
H	-2.1034375828	-0.9448602895	-1.553532082
H	-0.8256293203	-1.9283965575	-0.8333644509
C	-2.2770734501	-1.1731688191	0.5647195975
H	-1.7724781015	-1.5140957327	1.4631757266
C	-3.5615101163	-0.8580197648	0.6070347739
H	-4.0747323059	-0.5017442351	-0.2780701586
H	-4.1343170098	-0.9313820322	1.5216895819
O	-0.3305651793	2.3288555174	-0.475972536

O	-2.1928202754	1.5671355123	-1.4852880039
H	1.0480986256	2.2331268712	1.0509109875
H	0.2246097603	0.0462451082	1.2820362455

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N	2.6270665134	0.4697185009	0.0232140774
O	3.7322205039	0.524791823	-0.5634330344
C	1.7641938769	-0.4942111353	0.0383638633
H	2.0083354733	-1.3667923702	-0.5497985907
H	2.3503269419	1.3070218391	0.5533091426
C	0.4857530093	-0.3404208897	0.7961077832
N	-0.6586925862	-0.014290828	-0.0463097018
C	-0.9011021563	1.2525058737	-0.4733005301
C	-1.6325198138	-1.0465941362	-0.3874464818
H	-2.0825949498	-0.7803808213	-1.3407979849
H	-1.08677508	-1.9834995624	-0.5169820213
C	-2.6965555225	-1.1869135862	0.6631431291
H	-2.373383614	-1.535845986	1.6397109473
C	-3.9662328575	-0.8817652773	0.4549258212
H	-4.2995423347	-0.5133665718	-0.5077347037
H	-4.7084394688	-0.979153379	1.2355973458
O	0.0672282202	2.1070858026	-0.0645134412
O	-1.8489042387	1.593870741	-1.1376452723
H	0.2495839328	-1.2726956346	1.3087336731
H	0.6019647281	0.4229777176	1.5655837025
C	-0.1186620604	3.4539604575	-0.5017009236
H	0.7387869794	4.0069685763	-0.1309262188
H	-0.1599480673	3.495774729	-1.5875071042
H	-1.0417854491	3.8595456873	-0.0937408168

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N	2.9046038602	-0.3778805153	0.274815098
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C	1.7977710143	0.0383971158	-0.2385589773
H	1.8221020949	0.4836297826	-1.220552071
H	3.7525040513	-0.2757008084	-0.2916899566
C	0.5510697516	-0.1013976976	0.5659392004
N	-0.646023116	0.1470790732	-0.2143968437
C	-1.0720317972	1.4074339356	-0.4944212344
C	-1.5577770683	-0.9560091483	-0.5034919572
H	-2.1368948313	-0.6873881022	-1.3836214946
H	-0.9485256112	-1.8295002643	-0.7430133868
C	-2.4794653845	-1.2439436606	0.6471814108
H	-2.0204314342	-1.6207560764	1.5563528857
C	-3.7835253739	-1.0295999961	0.5996046815
H	-4.2490198902	-0.6331301294	-0.2946650461
H	-4.4233808544	-1.2297893618	1.4483995266
O	-0.1579071694	2.3257063532	-0.1127458198
O	-2.1160028999	1.6877352881	-1.033621224
H	0.5129942642	-1.1162293633	0.9678117985
H	0.6078120717	0.5597980145	1.4340088585
C	-0.5341153172	3.6751792012	-0.375797524
H	0.2806562299	4.2872831387	-0.0023764658
H	-0.6723064624	3.8302773022	-1.4440620727
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N	2.7477643938	-0.6786817432	-0.127804927
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C	1.5028332998	-0.6669571637	-0.4955973675
H	1.1459786796	-1.5846056734	-0.9397615667
H	3.0772707382	0.1703394052	0.3486537766
C	-1.3136219092	-1.0280069348	0.047566121
H	-1.3552227162	-1.477587729	-0.9492608048
H	-0.6392433571	-1.6546714611	0.638501799
C	-2.6760493737	-1.0748954741	0.6671955425
H	-2.7456992179	-0.7150045584	1.6895590287
C	-3.7624391512	-1.5249156286	0.0604657912
H	-3.7275698531	-1.8856671477	-0.9606549915
H	-4.7200078073	-1.5545465492	0.5618989784
C	0.6614233502	0.5127681755	-0.3092726653
C	-0.7115562597	0.3591676565	-0.04731517
C	1.2020464843	1.7961805645	-0.4087828027
C	-1.4899613649	1.4967625355	0.1173805783
C	0.4143734203	2.9190504077	-0.2159977826
H	2.2428072005	1.920440102	-0.6815311792
C	-0.9372540913	2.7685135627	0.0450781076
H	-2.5495060499	1.3856645116	0.3057075863
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H	-1.5666458064	3.6376053199	0.178763233

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N	2.8068272842	-0.6811857253	-0.4373349453
O	3.6346249677	0.2654878239	-0.4880594495
C	1.5132728296	-0.6566698981	-0.2863247314
H	1.0709247919	-1.6395133073	-0.2866819527
H	3.2084647107	-1.6194698542	-0.5285668136
C	-1.3160318685	-1.0263194454	0.1473701293
H	-1.2449496318	-1.5299822791	-0.8211969155
H	-0.7257800805	-1.6203232186	0.8515589604
C	-2.740184974	-1.051282341	0.6105738059
H	-2.9237757224	-0.6516117002	1.6035274462
C	-3.7516125622	-1.5305861354	-0.0950054354
H	-3.6032637459	-1.9293095633	-1.0916859217
H	-4.7598604024	-1.5424300796	0.2959524359
C	0.6850933859	0.5267295568	-0.1481634256
C	-0.7044104781	0.3593118072	0.0479502119
C	1.2202829699	1.8182888374	-0.2270395775
C	-1.5055571567	1.4867602553	0.1337566754
C	0.395332934	2.9275637707	-0.1258896508
H	2.281838362	1.9322986464	-0.3703005761
C	-0.9669225655	2.7651006094	0.0486636211
H	-2.5727141754	1.3679787976	0.2614946078
H	0.8244855602	3.9181561856	-0.1883116941
H	-1.6166540128	3.6270375674	0.1193135852

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N	0	-2.771922	-0.959717	-0.195791
O	0	-3.602763	-1.896629	-0.11987

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H	0	-1.234043	-1.808059	0.784481
H	0	-3.074663	-0.128629	-0.719303
C	0	1.294806	-1.205532	0.025444
H	0	1.251309	-1.635279	1.0309
H	0	0.695819	-1.860543	-0.613989
C	0	2.71123	-1.228146	-0.459922
H	0	2.870066	-0.885596	-1.478269
C	0	3.744886	-1.638157	0.257244
H	0	3.620799	-1.980677	1.277699
H	0	4.746664	-1.651953	-0.149576
C	0	-0.742315	0.28924	0.159321
C	0	0.65282	0.166887	0.033158
C	0	-1.32108	1.559649	0.179697
C	0	1.41553	1.321264	-0.080189
C	0	-0.546089	2.69903	0.039591
H	0	-2.385957	1.661595	0.348987
C	0	0.82764	2.579195	-0.087801
H	0	2.490662	1.234533	-0.163944
H	0	-1.012649	3.674183	0.057846
N	0	1.66773449	3.77911364	-0.21164162
O	0	1.13229593	4.85229158	-0.21531514
O	0	2.85502845	3.63698363	-0.3040585

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N	0	-2.584269	-1.646773	0.022289
O	0	-3.598436	-0.901719	0.002991
C	0	-1.318332	-1.340118	0.014874
H	0	-0.675748	-2.204996	0.041779
H	0	-2.780002	-2.652284	0.047785
C	0	1.552968	-1.077761	-0.113583
H	0	1.494008	-1.628626	0.829774
H	0	1.180919	-1.751228	-0.891491
C	0	2.988398	-0.777309	-0.417986
H	0	3.181637	-0.30283	-1.37555
C	0	4.001995	-1.061569	0.383499
H	0	3.842382	-1.527778	1.348659
H	0	5.023417	-0.840298	0.105494
C	0	-0.756872	-0.002293	-0.004904
C	0	0.648465	0.139565	-0.050901
C	0	-1.564666	1.140461	0.04365
C	0	1.190455	1.414634	-0.022879
C	0	-0.994053	2.403569	0.058633
H	0	-2.634631	1.018823	0.071955
C	0	0.381548	2.543469	0.031177
H	0	2.265304	1.532101	-0.03525
H	0	-1.631938	3.275961	0.095735
N	0	0.99449142	3.87929252	0.05903183
O	0	2.19095352	3.95842056	0.03381175
O	0	0.27362578	4.83666821	0.10586426

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N	0	-2.771922	-0.959717	-0.195791
O	0	-3.602763	-1.896629	-0.11987
C	0	-1.568773	-0.908498	0.289052
H	0	-1.234043	-1.808059	0.784481
H	0	-3.074663	-0.128629	-0.719303
C	0	1.294806	-1.205532	0.025444

H	0	1.251309	-1.635279	1.0309
H	0	0.695819	-1.860543	-0.613989
C	0	2.71123	-1.228146	-0.459922
H	0	2.870066	-0.885596	-1.478269
C	0	3.744886	-1.638157	0.257244
H	0	3.620799	-1.980677	1.277699
H	0	4.746664	-1.651953	-0.149576
C	0	-0.742315	0.28924	0.159321
C	0	0.65282	0.166887	0.033158
C	0	-1.32108	1.559649	0.179697
C	0	1.41553	1.321264	-0.080189
C	0	-0.546089	2.69903	0.039591
H	0	-2.385957	1.661595	0.348987
C	0	0.82764	2.579195	-0.087801
H	0	2.490662	1.234533	-0.163944
H	0	-1.012649	3.674183	0.057846
O	0	1.64487478	3.74646279	-0.20827181
C	0	1.18005259	4.75021633	0.6979948
H	0	1.93164421	5.50317038	0.81231994
H	0	0.28659547	5.19395983	0.31105025
H	0	0.97411421	4.30457877	1.64872954

9tz

01

N	0	-2.584269	-1.646773	0.022289
O	0	-3.598436	-0.901719	0.002991
C	0	-1.318332	-1.340118	0.014874
H	0	-0.675748	-2.204996	0.041779
H	0	-2.780002	-2.652284	0.047785
C	0	1.552968	-1.077761	-0.113583
H	0	1.494008	-1.628626	0.829774
H	0	1.180919	-1.751228	-0.891491
C	0	2.988398	-0.777309	-0.417986
H	0	3.181637	-0.30283	-1.37555
C	0	4.001995	-1.061569	0.383499
H	0	3.842382	-1.527778	1.348659
H	0	5.023417	-0.840298	0.105494
C	0	-0.756872	-0.002293	-0.004904
C	0	0.648465	0.139565	-0.050901
C	0	-1.564666	1.140461	0.04365
C	0	1.190455	1.414634	-0.022879
C	0	-0.994053	2.403569	0.058633
H	0	-2.634631	1.018823	0.071955
C	0	0.381548	2.543469	0.031177
H	0	2.265304	1.532101	-0.03525
H	0	-1.631938	3.275961	0.095735
O	0	0.97781269	3.84294358	0.05827388
C	0	0.27982155	4.70728196	-0.84207469
H	0	-0.64906592	5.00522387	-0.40241722
H	0	0.87572589	5.57401748	-1.03846091
H	0	0.0905318	4.18934692	-1.75903308

9uE

01

C	0.8058689587	0.5235261358	-0.2999828658
C	-0.4010285022	0.2641739994	0.3300754717
C	1.082434683	1.8051653293	-0.7476768982
C	-1.3027787915	1.2960426707	0.5154882143
C	0.1870440799	2.8553011691	-0.5622928948
H	2.0147136548	1.9932163738	-1.2646847266

C	-1.0243798905	2.6015811518	0.1032285612
H	-2.2488274629	1.1008240683	1.0049976024
C	-2.0521281398	3.6167003504	0.4029280226
C	-1.8672790578	4.8878969998	0.7399928361
H	-3.0693092395	3.2370811843	0.3962157536
H	-2.7107855623	5.5210809337	0.9781009443
H	-0.8861839508	5.3332262648	0.8250889677
H	-0.6407561764	-0.7338112578	0.6701315343
H	1.524510351	-0.269095112	-0.4569043416
C	0.5322588245	4.2273959223	-1.1146906226
H	-0.3922110541	4.7433544615	-1.380189074
H	1.0040311272	4.8376584902	-0.3374212095
C	1.4301441684	4.1833819097	-2.3019096889
H	1.1464467357	3.7045707246	-3.2287214031
H	2.8799035907	5.1460595392	-1.3872059998
O	3.4788769759	4.7380655653	-3.1887269125
N	2.613444218	4.7017938254	-2.2760822008

9uZ

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C	0.7484760109	0.4392004802	-0.2193527865
C	-0.5224491979	0.2113402638	0.2866388599
C	1.108765759	1.7187055913	-0.6063424778
C	-1.3974065692	1.2733069274	0.4187870047
C	0.2369419851	2.7998392402	-0.4848045225
H	2.0989655169	1.8883695951	-1.0114005721
C	-1.0340063286	2.5770208891	0.0691093073
H	-2.3894614145	1.1051419279	0.8193708902
C	-2.0329452341	3.6332040528	0.323667518
C	-1.7960482454	4.8616873083	0.7682163471
H	-3.0647076358	3.3253390079	0.1845885586
H	-2.6102852663	5.5459101935	0.9625771381
H	-0.7962587995	5.2178703928	0.9771442383
H	-0.8283713234	-0.7841916834	0.5771711255
H	1.4524420502	-0.3753908457	-0.3213378072
C	0.6866733698	4.1566207792	-0.9710511754
H	-0.1747738115	4.7980582992	-1.17116201
H	1.2638931757	4.688896148	-0.2081299498
C	1.5280557864	4.0971960518	-2.1953383718
H	1.5061795943	3.2774000895	-2.8976599355
H	2.8704707173	4.9929623604	-3.3342610881
O	2.482238476	6.1421338841	-1.8118789772
N	2.3168249945	5.0816811165	-2.4764336338

9vE

0 1

C	0	-1.09914	-2.364016	0.188766
C	0	-2.403534	-1.926157	0.022411
C	0	-0.062422	-1.444974	0.179014
C	0	-2.648474	-0.57422	-0.134296
C	0	-0.294354	-0.08024	0.028725
H	0	0.955883	-1.797945	0.280356
C	0	-1.618533	0.36945	-0.10973
H	0	-3.664783	-0.224577	-0.266975
C	0	-2.021171	1.782591	-0.241892
C	0	-1.479709	2.842219	0.347794
H	0	-2.903775	1.939483	-0.854436
H	0	-1.899632	3.827511	0.199524
H	0	-0.634027	2.77017	1.016927
H	0	-3.223127	-2.631277	0.009887

C	0	0.889475	0.87029	-0.016022
H	0	0.631916	1.724818	-0.644348
H	0	1.081645	1.278473	0.981773
C	0	2.139281	0.242186	-0.526996
H	0	2.220967	-0.162176	-1.526267
H	0	3.102966	0.506258	1.16617
O	0	4.307857	-0.377208	-0.074166
N	0	3.192234	0.128718	0.213296
N	0	-0.80807632	-3.7952973	0.35494595
O	0	-0.74753608	-4.23957562	1.46731751
O	0	-0.64277313	-4.46159012	-0.62848553

9vZ

0 1

C	0	-1.859764	-2.087897	0.28199
C	0	-2.935139	-1.247725	0.035255
C	0	-0.57617	-1.569168	0.284992
C	0	-2.705584	0.098637	-0.177821
C	0	-0.32657	-0.215008	0.066705
H	0	0.260635	-2.232453	0.467101
C	0	-1.41879	0.643277	-0.138675
H	0	-3.540414	0.762809	-0.364514
C	0	-1.313492	2.105179	-0.311753
C	0	-0.489199	2.924841	0.329815
H	0	-2.040195	2.535103	-0.994194
H	0	-0.52497	3.991532	0.157159
H	0	0.224978	2.570498	1.060903
H	0	-3.943341	-1.637613	0.010814
C	0	1.103975	0.267048	0.039979
H	0	1.180009	1.215151	-0.497512
H	0	1.477221	0.482295	1.046411
C	0	2.044231	-0.704862	-0.577796
H	0	1.741891	-1.46601	-1.28139
H	0	3.909871	-1.328776	-0.755943
O	0	3.874853	0.179923	0.473515
N	0	3.30459	-0.639328	-0.299261
N	0	-2.07434553	-3.52148403	0.52629105
O	0	-1.11764835	-4.21380021	0.73568931
O	0	-3.197546	-3.94152682	0.50645338

9wE

0 1

C	0	-1.09914	-2.364016	0.188766
C	0	-2.403534	-1.926157	0.022411
C	0	-0.062422	-1.444974	0.179014
C	0	-2.648474	-0.57422	-0.134296
C	0	-0.294354	-0.08024	0.028725
H	0	0.955883	-1.797945	0.280356
C	0	-1.618533	0.36945	-0.10973
H	0	-3.664783	-0.224577	-0.266975
C	0	-2.021171	1.782591	-0.241892
C	0	-1.479709	2.842219	0.347794
H	0	-2.903775	1.939483	-0.854436
H	0	-1.899632	3.827511	0.199524
H	0	-0.634027	2.77017	1.016927
H	0	-3.223127	-2.631277	0.009887
C	0	0.889475	0.87029	-0.016022
H	0	0.631916	1.724818	-0.644348
H	0	1.081645	1.278473	0.981773
C	0	2.139281	0.242186	-0.526996

H	0	2.220967	-0.162176	-1.526267
H	0	3.102966	0.506258	1.16617
O	0	4.307857	-0.377208	-0.074166
N	0	3.192234	0.128718	0.213296
O	0	-0.81599642	-3.75635087	0.35042405
C	0	-1.99978698	-4.43828788	0.77291879
H	0	-2.70909327	-4.45117136	-0.0280922
H	0	-1.7539146	-5.44272404	1.04779107
H	0	-2.42212607	-3.93122855	1.61518985

9wZ

0 1

C	0	-1.859764	-2.087897	0.28199
C	0	-2.935139	-1.247725	0.035255
C	0	-0.57617	-1.569168	0.284992
C	0	-2.705584	0.098637	-0.177821
C	0	-0.32657	-0.215008	0.066705
H	0	0.260635	-2.232453	0.467101
C	0	-1.41879	0.643277	-0.138675
H	0	-3.540414	0.762809	-0.364514
C	0	-1.313492	2.105179	-0.311753
C	0	-0.489199	2.924841	0.329815
H	0	-2.040195	2.535103	-0.994194
H	0	-0.52497	3.991532	0.157159
H	0	0.224978	2.570498	1.060903
H	0	-3.943341	-1.637613	0.010814
C	0	1.103975	0.267048	0.039979
H	0	1.180009	1.215151	-0.497512
H	0	1.477221	0.482295	1.046411
C	0	2.044231	-0.704862	-0.577796
H	0	1.741891	-1.46601	-1.28139
H	0	3.909871	-1.328776	-0.755943
O	0	3.874853	0.179923	0.473515
N	0	3.30459	-0.639328	-0.299261
O	0	-2.06850658	-3.48247486	0.5196434
C	0	-3.37134938	-3.68243053	1.0741868
H	0	-4.11006252	-3.5173712	0.31790754
H	0	-3.45327063	-4.68457429	1.44010591
H	0	-3.52556896	-2.99496319	1.87948487

TS4a

0 1

C	-0.3189943884	-0.4782907945	0.8010536725
C	-1.6464996469	-0.1089728797	0.6200604161
H	0.0502507526	-0.3520062612	1.8212744211
N	0.6458254795	0.9367056768	0.0260855552
O	-0.1075124799	1.9809075963	-0.0436936079
H	-1.0268333514	1.4576707428	0.2263317046
C	1.7924180879	0.6044755636	-0.3570523512
H	2.5204883033	1.2636429361	-0.8199704249
C	1.9655663098	-0.8877613071	-0.133072425
H	2.4992681362	-1.3400006305	-0.9678723184
H	2.5597003304	-1.0740159209	0.7656119258
C	0.5345940514	-1.4536609561	0.0083298475
H	0.0972896174	-1.5849517803	-0.9832649037
H	0.5498560234	-2.4266618626	0.499250959
H	-2.1280928476	-0.4345747271	-0.2985344128
C	-2.5572667273	0.1599225245	1.7980604212
H	-3.3086641966	0.9183118955	1.5729023931
H	-3.0968147933	-0.7328073319	2.1281590975

H	-1.9820077304	0.5230831863	2.6525340603
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TS4b

0 1

C	-0.0477879788	-0.1581634601	0.7934857999
C	-1.1496237034	0.6552327797	0.571735285
H	0.3077196932	-0.1045288282	1.8224756792
N	1.3723653474	0.7645530202	-0.0303501268
O	1.057915602	2.0042598203	-0.187439129
H	0.0059886088	1.8768032634	0.0711279538
C	2.3195623932	0.0114311189	-0.357157077
H	3.2430339658	0.3282151709	-0.8318659791
C	1.931109006	-1.4241595405	-0.0490135387
H	2.2707130248	-2.0901761289	-0.8409151506
H	2.4044208226	-1.7588239617	0.8777245835
C	0.391400328	-1.4188782439	0.0750480868
H	-0.0529491811	-1.4406527797	-0.9217707224
H	0.0417608706	-2.2976649601	0.6161936275
O	-1.7922152323	1.1674532422	1.7103147809
C	-2.244847354	2.4845429622	1.5431771905
H	-2.7823237688	2.7668961373	2.4470269528
H	-1.4090478816	3.1775894756	1.3887676594
H	-2.923808798	2.5686684023	0.6871006457
H	-1.8121109744	0.4704914403	-0.2731741112

TS4c

0 1

C	-0.1049044114	-0.3019327303	0.8281437355
C	-1.3329582275	0.3512724036	0.6505304204
H	0.2196540979	-0.3515888513	1.8661274197
N	1.1995302711	0.7219485018	0.2321800228
O	1.0013602833	2.0231043676	0.300406196
H	0.0237245173	2.0413251665	0.5099281386
C	2.1830727095	0.0890618968	-0.2267802285
H	3.0761313719	0.5609320168	-0.6206944459
C	1.8982931724	-1.3912228644	-0.1611978112
H	2.259137796	-1.8940986465	-1.0564393069
H	2.4247086536	-1.828812858	0.6906817105
C	0.367488142	-1.4869656466	-0.000447221
H	-0.1081860704	-1.445895503	-0.9812758356
H	0.073162024	-2.4176558291	0.4795538258
H	-1.8728836888	0.2647325027	-0.2814224946
C	-2.0496939504	0.9675381783	1.7307289608
O	-3.171823177	1.4231508172	1.6844864958
O	-1.3222842735	1.0238841629	2.8980605583
C	-2.0104630345	1.604396387	3.9941539671
H	-2.9169944203	1.0462426288	4.224054939
H	-1.3226481042	1.5701089498	4.834960136
H	-2.2890878909	2.6345444495	3.7757681175

TS4d

0 1

C	0.590818389	-0.5615405602	-0.7475326797
C	1.9285477624	-0.2100449001	-0.5532834963
H	0.2482996343	-0.5045962512	-1.7805544788
N	-0.2929167785	1.062715571	-0.1518718839
O	0.6418077598	1.955772494	-0.1315028756
H	1.5075765311	1.178028491	-0.3121883595
C	-1.4725298738	1.2107827523	0.2767320118
C	-2.3538314721	0.0044473241	0.3875187691

H	-1.7994732601	2.1770354633	0.6535282657
H	-3.3260264576	0.2060237858	-0.0670029859
H	-2.5524699427	-0.1427256731	1.4548109393
C	-0.2602150834	-1.4868649385	0.0792703574
H	-0.0367157358	-1.3576220335	1.1413132341
H	0.0064834693	-2.5155351577	-0.1770021438
C	-1.7525333446	-1.2721183613	-0.2085314069
H	-2.3278346591	-2.122320223	0.158342867
H	-1.8856147421	-1.2549581368	-1.2930833202
H	2.3814489908	-0.5340977376	0.3806703237
C	2.8667861661	-0.0802247108	-1.7376157426
H	3.6875120939	0.6060582842	-1.5266783363
H	3.3099343387	-1.0353861202	-2.0303412649
H	2.3333437042	0.3130287282	-2.6053041536

TS4e

0 1

C	-0.14488826	-0.9426029471	0.6978335474
C	-1.5307118187	-0.897416182	0.5553417696
H	0.1754795016	-0.8466893683	1.732841771
N	0.3364678462	0.8588538415	0.132560962
O	-0.7786772023	1.513588821	0.1159642815
H	-1.4408963796	0.561653301	0.2757900408
C	1.4486972684	1.2763806127	-0.2975359603
C	2.5795556407	0.3038953671	-0.4332924136
H	1.5435991095	2.2960382646	-0.663769543
H	3.4799376009	0.7026044388	0.0385951434
H	2.8098013754	0.2436424857	-1.5026119073
C	0.8678745975	-1.6263165606	-0.1766826694
H	0.6060751324	-1.5121754996	-1.2315209929
H	0.8394862896	-2.6964608	0.0427576379
C	2.2797546795	-1.0967219824	0.1114462945
H	3.0226119968	-1.7838116776	-0.2938866243
H	2.4199026841	-1.0955209055	1.194870331
O	-2.267523196	-1.017981614	1.7470716996
C	-3.4323090679	-0.2308901685	1.7553101419
H	-4.0939149793	-0.4901594749	0.9212475394
H	-3.9533819923	-0.4266704817	2.6906396968
H	-3.1934806876	0.8360820365	1.6915158107
H	-1.9975185988	-1.3706569466	-0.3087278668

TS4f

0 1

C	-0.5045844019	0.2469417319	-1.1942230538
C	0.8414335518	0.6885194705	-1.268013402
H	-1.1361826154	0.6751771414	-1.9692332393
N	-1.2121707095	1.0692331199	0.1784061786
O	-0.5149595136	2.1585459469	0.4483299605
H	0.3062324805	1.9653398935	-0.1589439493
C	-2.1730025402	0.6919439289	0.9076228144
C	-2.8556767496	-0.6098406357	0.6455526463
H	-2.4406863954	1.302151263	1.7654928337
H	-3.9356100104	-0.4518918447	0.637028481
H	-2.6553302274	-1.2411574184	1.5175915892
C	-0.8856906062	-1.1792444264	-0.8749742074
H	-0.3147275816	-1.5354465153	-0.0135590422
H	-0.5962188332	-1.7938440566	-1.7274526302
C	-2.390821964	-1.3054986761	-0.6344075569
H	-2.6843567314	-2.3534455614	-0.587821718
H	-2.9126161829	-0.8706370778	-1.4895714125

H	1.6192524899	0.1223539668	-0.7752186962
C	1.2969199469	1.5811433454	-2.3011031892
O	2.4493469091	1.8328102556	-2.5754234967
O	0.2677142677	2.1860533086	-2.9793092809
C	0.678705477	3.0920373139	-3.9909973245
H	1.2773177881	2.5845038756	-4.746136156
H	-0.2329364118	3.4857830444	-4.4324767893
H	1.2737253737	3.9002820661	-3.5678695993

TS4g

0 1

C	1.6425769713	-0.7403937189	-0.4011047999
C	2.9178536403	-0.4689884194	0.1031800028
H	1.5591978925	-0.7209454369	-1.4858020133
N	0.7726646209	0.9362812963	-0.1033746519
O	1.7281880035	1.7902576646	0.0891269128
H	2.5669171513	0.9959947582	0.1463785324
C	-0.4617268225	1.1734801864	0.0274183149
C	-1.4296045175	0.031972171	-0.0243078269
H	-0.7976603818	2.1786575678	0.2700626813
C	0.5687607816	-1.5862133457	0.2305663691
H	0.5472078091	-1.4196015911	1.3106102823
H	0.8301965249	-2.6357108091	0.076477658
C	-0.7986462403	-1.3106053796	-0.4067655278
H	-1.4994942044	-2.1038212729	-0.1465796857
H	-0.6770179927	-1.350071768	-1.4921354808
H	3.1513139071	-0.7740822748	1.1168119066
H	3.745309649	-0.4640279482	-0.5927125918
H	-2.2485468398	0.2685500453	-0.7066204799
H	-1.8845890827	-0.0397612851	0.9694274777

TS4h

0 1

C	-0.8232527584	-0.8424733728	0.2830170737
C	-2.1943479683	-0.7291340679	-0.0462102159
H	-0.6342834387	-1.1124644547	1.3213792643
N	-0.2568417218	0.865884453	0.3769068705
O	-1.3170714937	1.6213439679	0.4677471018
H	-2.0476005692	0.8182294752	0.2255430709
C	0.9244845265	1.3013311349	0.2651501372
C	2.0441285244	0.355116704	-0.0314479979
H	1.094613435	2.3740319362	0.2947077415
C	0.2497029482	-1.3891114767	-0.625778785
H	0.1496976593	-0.9611797055	-1.6264300317
H	0.0979059318	-2.4654728997	-0.719297409
C	1.6393096165	-1.1224103519	-0.0386845732
H	2.3960002439	-1.6840673097	-0.5856727149
H	1.6509443775	-1.5029132671	0.9851440105
H	-2.4558687835	-0.873554589	-1.0895879535
H	2.8632771213	0.5250284889	0.6697944223
H	2.4327707928	0.6427792618	-1.014118009
C	-3.2415731139	-1.0670421019	0.9290895061
C	-4.4626745823	-1.6007769516	0.5005994414
C	-3.0900685596	-0.8427660784	2.3039539147
C	-5.4711720316	-1.9117854402	1.3976654258
H	-4.6114464711	-1.7806328145	-0.5571924371
C	-4.0944873747	-1.1649452767	3.2021669311
H	-2.1814666564	-0.3838531327	2.6757501932
C	-5.2944439824	-1.7038877615	2.7588911364
H	-6.4013886622	-2.3258987045	1.030233051

H	-3.943946001	-0.9769816828	4.2574808217
H	-6.0796829683	-1.9492896723	3.4602254432

TS4i

0 1

C	0.6056685935	-0.584343404	-0.117511229
C	1.8473075041	-0.2921910918	0.4742813085
H	0.643403616	-0.6793232168	-1.2012608057
N	-0.2846367956	1.0028836535	-0.0674223171
O	0.5984775136	1.9583704061	0.1014953461
H	1.4340024213	1.333695492	0.3199627109
C	-1.532199278	1.2027390371	-0.0676805416
C	-2.4708179167	0.040176997	-0.0989871138
H	-1.9029957172	2.2186277838	0.0385155442
H	-3.2233580246	0.199921262	-0.8732351453
H	-3.0156103613	0.0599814586	0.8507072377
C	-0.4676899161	-1.4542827459	0.4851756741
H	-0.5976206273	-1.2143941681	1.5434104185
H	-0.1217288443	-2.4877170494	0.4313379653
C	-1.7827080917	-1.3138375141	-0.2857314708
H	-2.4778403815	-2.0991133122	0.0090334744
H	-1.5730640261	-1.4660315499	-1.3469295265
H	2.0098873658	-0.5306127472	1.5176629584
C	3.0588773903	-0.3753283174	-0.357329672
F	2.8550696776	0.0874737293	-1.6103369437
F	4.0839200036	0.3291421321	0.1583631461
F	3.5464954047	-1.6322465148	-0.519277859

TS4j

0 1

C	-0.3304120384	-0.0283156658	0.8780754272
C	-0.1838022421	1.0015055066	1.8112613548
N	-1.076387905	0.8423114265	-0.5817152201
O	-0.8159306315	2.1000248162	-0.5107082556
H	-0.41386577	2.0707704241	0.5165878492
C	-1.7840916694	0.0874892659	-1.2938943544
H	-2.3149820205	0.4006317575	-2.1868394934
C	-1.8541940213	-1.286402881	-0.6562826154
H	-2.8683729579	-1.6773495854	-0.7265390399
H	-1.1918532884	-1.9881339736	-1.1653324369
C	-1.4251688409	-1.0815874796	0.8144174845
H	-2.2746433129	-0.7262057209	1.3982739421
H	-1.0674778073	-2.0140261434	1.2455233531
H	-0.98757746	1.1772024641	2.5150653121
C	0.9450225015	-0.5263255268	0.2412044676
O	1.1481315973	-1.6781872837	-0.0463804241
O	1.8260530237	0.4501395426	0.0132086528
C	3.0496383882	0.0358658166	-0.591951205
H	2.8535285602	-0.443416857	-1.5493546932
H	3.6340293767	0.9394689836	-0.7285275478
H	3.5723904537	-0.6674121723	0.0536727437
H	0.8088810643	1.2896192858	2.1205016986

TS4k

0 1

C	0.0300311297	0.5307579932	0.6160319661
C	0.1088956685	1.8309092364	1.1146034831
N	-1.5513931923	0.6719086739	-0.4509942135
O	-1.7272858577	1.9405019447	-0.6434813503
H	-0.9201239656	2.2729282549	0.1225004683

C	-2.3427715977	-0.2472789273	-0.8044654879
C	-2.1062012093	-1.6453216549	-0.3217780612
H	-3.2376625542	0.0011215814	-1.3694521601
H	-2.1733044722	-2.34296697	-1.1588455864
H	-2.9482365073	-1.8917497381	0.3344423643
C	-0.394083983	-0.7034534942	1.3680737142
H	-1.2224500361	-0.4271933169	2.0233804212
H	0.4398037655	-1.011390236	1.9984384466
C	-0.7859616243	-1.8483565403	0.4286009274
H	-0.8538915468	-2.77292842	1.0007916392
H	0.0168287714	-1.9941374587	-0.2948475187
H	-0.2692939799	2.0005664425	2.1140068295
O	0.8954413888	0.2725902118	-0.4732253343
C	2.1542617042	-0.1343885073	-0.1949396353
O	2.5600780029	-0.3492528583	0.9104787055
C	2.9467160246	-0.2755579711	-1.461608738
H	3.9259354287	-0.6801654475	-1.2303801281
H	2.4181000306	-0.9237917116	-2.1583575857
H	3.0449483559	0.701728993	-1.932443417
H	0.9715822558	2.4115339206	0.8195512511

TS4l

0 1

C	0.62905698	-0.6520422952	-0.1304998169
C	1.85267503	-0.2946969287	0.442889326
H	0.6316837562	-0.7345268228	-1.2156163471
N	-0.3070722901	1.0114233872	-0.0570667798
O	0.6071211135	1.9124283183	0.1246723576
H	1.4596812326	1.1579022051	0.3194328414
C	-1.5530597022	1.2189828233	-0.0521478619
C	-2.5152817714	0.0606805751	-0.070831866
H	-1.935343591	2.233015402	0.0598406172
C	-0.4718113041	-1.4669447243	0.4936761023
H	-0.5709707128	-1.2117445648	1.5511426849
H	-0.1818380349	-2.5194905552	0.4504350736
C	-1.7902599283	-1.2838806112	-0.2667679
H	-2.4931676635	-2.0746183267	0.004674145
H	-1.579439899	-1.4128041148	-1.3324672234
H	2.0107751177	-0.4964857909	1.4961315615
H	2.7333457678	-0.3274679289	-0.1832893287
C	-3.2552214713	0.0720536298	1.2752373917
H	-3.7245732003	1.0404839447	1.4551000098
H	-4.0378877265	-0.6882356435	1.2750083171
H	-2.5754294705	-0.1308342273	2.1028712478
C	-3.5332329907	0.2613954229	-1.1966088337
H	-4.2439163151	-0.5666760167	-1.2108812031
H	-4.0954897459	1.1860167543	-1.0554536574
H	-3.0377622303	0.3060080382	-2.1668126879

TS4m

0 1

C	-1.437383042	-0.9138293305	0.4339191951
C	-2.7740194542	-1.1650719466	0.1206582217
H	-1.1792020361	-0.8206771645	1.4858221967
N	-1.2657205635	0.9163433766	0.0261999904
O	-2.466093814	1.3797405431	-0.1164536053
H	-2.9815092098	0.3805967204	-0.0577824569
C	-0.1690464123	1.5431685712	-0.0951963375
C	1.0312557685	0.7376698003	-0.0248957802
H	-0.1291070249	2.6124219788	-0.2732217769

C	-0.2761569382	-1.3824386569	-0.4031173107
H	-0.5271741238	-1.2944925208	-1.4631340046
H	-0.0699363181	-2.431277399	-0.1907449511
H	-3.0084305075	-1.6090545744	-0.8396708526
H	-3.4562880523	-1.3856372821	0.9285283474
N	0.9440595092	-0.6332986737	-0.1152747999
C	2.1992232504	-1.1555574999	-0.0279476893
C	2.3581743241	1.075248546	0.1249647062
C	3.0980118115	-0.1275691297	0.1247580287
H	2.3516851831	-2.2200507042	-0.0834672343
H	4.1631732363	-0.2338270291	0.2322494836
H	2.7391264139	2.0760303751	0.2388846294

TS4n

0 1

C	1.6524119197	0.9197893909	0.5809263116
C	2.8916688092	1.351417732	0.1172713279
H	1.5715434198	0.630690509	1.6254171509
N	1.6192280049	-0.8906677765	-0.1032098701
O	2.7792981079	-1.1056137925	-0.6065012397
H	3.1819048625	-0.0421134596	-0.4215559266
C	0.6132000756	-1.6498651926	-0.0628832877
C	-0.5978800735	-1.0009116701	0.5531815977
H	0.617783764	-2.6680024108	-0.4417471356
C	0.3524422964	1.36382118	-0.0307594613
H	0.500852719	1.5534882503	-1.0966552722
H	0.0401162827	2.3056156364	0.4250744914
H	2.9208336481	1.9846847475	-0.7613766693
H	3.6896597398	1.4896914876	0.8328509734
N	-0.7206608412	0.3938111139	0.1591324541
C	-2.0148985682	0.7268373449	-0.1126354884
C	-1.9440072474	-1.537517451	0.0548868889
H	-2.3906505349	-2.2640939974	0.7273824036
O	-2.787359978	-0.3947754882	-0.0142906798
O	-2.4447854936	1.8073377927	-0.3906332506
H	-1.8457855076	-1.9699519904	-0.9439426014
H	-0.5376984052	-1.0870909561	1.6448092833

TS4o

0 1

C	-1.1462587227	-0.9271016613	0.4795818038
C	-2.5216947364	-1.1187402162	0.6191341102
H	-0.5588812052	-0.9444094969	1.3936694862
N	-1.0872019619	0.9696107053	0.1786318354
O	-2.2340637651	1.416246195	0.5719395677
H	-2.7026828706	0.358162708	0.7361854656
C	-0.2097895246	1.6260828843	-0.4486179289
C	0.9757356787	0.8931980976	-1.0085145727
H	-0.3496173848	2.6806779541	-0.6694263362
C	-0.2991893183	-1.2494805435	-0.7234350263
H	-0.8228822392	-0.9955012213	-1.6469745623
H	-0.0642678867	-2.3112783959	-0.7350092179
H	-3.095123709	-1.4243398283	-0.2489490926
H	-2.886395003	-1.4693879717	1.5742561335
N	0.9641683123	-0.5164336129	-0.6671817745
C	2.0202397198	-1.1437549181	-0.0744880728
O	3.1203407469	-0.3662710432	-0.0300852012
O	1.9920903252	-2.2732471019	0.3541126216
H	1.9024885848	1.3360262906	-0.6561311914
H	0.9560800002	1.0222688506	-2.0980593149

C	4.2496090025	-0.9803403342	0.587964408
H	4.5461469624	-1.8707295943	0.0377556406
H	5.0384350461	-0.2353225417	0.5645034081
H	4.0162749886	-1.2590522839	1.6133904211

TS4p
0 1

TS4q
0 1

TS4r
0 1

C	-1.7402440578	-0.9318449249	0.463681486
C	-3.0936864707	-1.1416698399	0.2092956799
H	-1.4486010008	-0.8069088517	1.5043363154
N	-1.5475956342	0.9157327477	-0.0013019686
O	-2.741659979	1.3880042784	-0.1147290408
H	-3.2682654536	0.3911839868	-0.0060066505
C	-0.4512400319	1.5287113085	-0.1609171054
H	-0.4148369488	2.595237872	-0.366215377
C	-0.6096620516	-1.4021061674	-0.4160247769
H	-0.9107455922	-1.2783947625	-1.4613282305
H	-0.4591819776	-2.4713877943	-0.2559318829
H	-3.3812191715	-1.6016694647	-0.7289738462
H	-3.7552500894	-1.3105251285	1.0470266312
C	0.7001576379	-0.6822300167	-0.1730300132
C	0.7695277152	0.7204537737	-0.0738788163
C	1.9992312349	1.3497952872	0.0898492792
H	2.0326616466	2.4303802403	0.1550400857
C	3.1684619182	0.6108891965	0.174833251
H	4.1184369427	1.1105732284	0.3043026633
C	3.1077370684	-0.7710584517	0.0947409381
C	1.8826781752	-1.4028302383	-0.0773236129
H	1.8439886186	-2.4828440838	-0.1474332823
H	4.0124065013	-1.359952195	0.1604502739

TS4s
0 1

C	0	-1.742109	-0.929812	0.459979
C	0	-3.095878	-1.136415	0.204699
H	0	-1.450491	-0.80823	1.501038
N	0	-1.545886	0.918649	0.000028
O	0	-2.739036	1.39346	-0.112415
H	0	-3.267534	0.397338	-0.00651
C	0	-0.448345	1.530001	-0.157666
H	0	-0.409895	2.597008	-0.360078
C	0	-0.612191	-1.399815	-0.420718
H	0	-0.912782	-1.272721	-1.465757
H	0	-0.463752	-2.469805	-0.263473
H	0	-3.384039	-1.593343	-0.734878
H	0	-3.757965	-1.30629	1.04181
C	0	0.698914	-0.683052	-0.175463
C	0	0.770885	0.719227	-0.072511
C	0	2.001724	1.345821	0.093213
H	0	2.037161	2.426162	0.161327
C	0	3.169548	0.6045	0.176488
H	0	4.120425	1.102053	0.307536
C	0	3.106256	-0.777111	0.092653
C	0	1.88006	-1.406121	-0.081413

H	0	1.839366	-2.485867	-0.154446
N	0	4.33443438	-1.58012347	0.1801106
O	0	4.24224613	-2.7734698	0.10365993
O	0	5.37960206	-1.00985362	0.32442131

TS4t

0 1

C	0	-1.742109	-0.929812	0.459979
C	0	-3.095878	-1.136415	0.204699
H	0	-1.450491	-0.80823	1.501038
N	0	-1.545886	0.918649	0.000028
O	0	-2.739036	1.39346	-0.112415
H	0	-3.267534	0.397338	-0.00651
C	0	-0.448345	1.530001	-0.157666
H	0	-0.409895	2.597008	-0.360078
C	0	-0.612191	-1.399815	-0.420718
H	0	-0.912782	-1.272721	-1.465757
H	0	-0.463752	-2.469805	-0.263473
H	0	-3.384039	-1.593343	-0.734878
H	0	-3.757965	-1.30629	1.04181
C	0	0.698914	-0.683052	-0.175463
C	0	0.770885	0.719227	-0.072511
C	0	2.001724	1.345821	0.093213
H	0	2.037161	2.426162	0.161327
C	0	3.169548	0.6045	0.176488
H	0	4.120425	1.102053	0.307536
C	0	3.106256	-0.777111	0.092653
C	0	1.88006	-1.406121	-0.081413
H	0	1.839366	-2.485867	-0.154446
O	0	4.30101456	-1.55827279	0.1777308
C	0	5.2537218	-1.07870972	-0.77477546
H	0	5.69333796	-0.17228755	-0.41416973
H	0	6.01794521	-1.81415551	-0.91613342
H	0	4.76274677	-0.89085234	-1.70673743

TS4u

0 1

C	0.9642734336	0.9352115677	0.6826990823
C	1.6199816683	2.0727929716	0.214451311
H	1.2476367821	0.5834272053	1.6732851713
N	1.9130593088	-0.4654448339	-0.2026369538
O	2.9360483461	0.0838824915	-0.7653194639
H	2.658132967	1.1439300284	-0.5045679559
C	1.5523757671	-1.6703327595	-0.1995354437
H	2.1282833798	-2.4503583423	-0.6877737591
H	1.1662917109	2.6490399786	-0.5819168624
H	2.2651978193	2.6135886877	0.8919325885
C	-0.7708387346	-0.8472379279	0.2504540094
C	-0.4141941783	0.5101731014	0.2951449877
C	-1.3760444755	1.473561633	0.0121576684
H	-1.0934940112	2.5165025366	0.0588576034
C	-2.677589854	1.1142823344	-0.3059948979
C	-3.0304599803	-0.2242684098	-0.3462542849
H	-4.0413860518	-0.5164898966	-0.5956952782
C	-2.0763024503	-1.1938312443	-0.0724758102
H	-2.347701321	-2.2414776508	-0.1183832459
C	0.2463032612	-1.9399993932	0.505800917
H	-0.1553324115	-2.8971623416	0.1783505312
H	0.437222337	-2.0348198727	1.5806055153
H	-3.4119743127	1.8792671365	-0.5182654295

TS4v

0 1

C	0	0.963251	0.937982	0.679755
C	0	1.616979	2.075566	0.208752
H	0	1.247317	0.589018	1.671138
N	0	1.914317	-0.463149	-0.202378
O	0	2.936313	0.086583	-0.766468
H	0	2.656628	1.14677	-0.508188
C	0	1.555678	-1.668636	-0.196393
H	0	2.132855	-2.448834	-0.682853
H	0	1.162228	2.649161	-0.588924
H	0	2.26135	2.619052	0.884884
C	0	-0.768881	-0.848422	0.25191
C	0	-0.414535	0.509694	0.293358
C	0	-1.378048	1.470779	0.008205
H	0	-1.097262	2.514305	0.052412
C	0	-2.679016	1.108543	-0.308955
C	0	-3.02962	-0.230695	-0.346017
C	0	-2.07379	-1.19799	-0.070056
H	0	-2.343417	-2.2462	-0.113461
C	0	0.25014	-1.938851	0.509722
H	0	-0.149907	-2.897464	0.184576
H	0	0.441334	-2.030811	1.584727
H	0	-3.414719	1.871779	-0.522949
N	0	-4.40308821	-0.6310275	-0.68397998
O	0	-4.66725141	-1.80071674	-0.70551426
O	0	-5.20463795	0.22803616	-0.92467981

TS4w

0 1

C	0	0.963251	0.937982	0.679755
C	0	1.616979	2.075566	0.208752
H	0	1.247317	0.589018	1.671138
N	0	1.914317	-0.463149	-0.202378
O	0	2.936313	0.086583	-0.766468
H	0	2.656628	1.14677	-0.508188
C	0	1.555678	-1.668636	-0.196393
H	0	2.132855	-2.448834	-0.682853
H	0	1.162228	2.649161	-0.588924
H	0	2.26135	2.619052	0.884884
C	0	-0.768881	-0.848422	0.25191
C	0	-0.414535	0.509694	0.293358
C	0	-1.378048	1.470779	0.008205
H	0	-1.097262	2.514305	0.052412
C	0	-2.679016	1.108543	-0.308955
C	0	-3.02962	-0.230695	-0.346017
C	0	-2.07379	-1.19799	-0.070056
H	0	-2.343417	-2.2462	-0.113461
C	0	0.25014	-1.938851	0.509722
H	0	-0.149907	-2.897464	0.184576
H	0	0.441334	-2.030811	1.584727
H	0	-3.414719	1.871779	-0.522949
O	0	-4.36571492	-0.6201341	-0.67478371
C	0	-5.26059267	-0.16082971	0.34164794
H	0	-5.40327244	0.89480836	0.2407978
H	0	-6.20191397	-0.65929548	0.2399322
H	0	-4.84618515	-0.37432685	1.30476027

TS5a

0 1			
C	1.0470443591	-0.7109123728	0.6608575227
H	1.4350381778	-0.8779096073	1.6595650706
N	0.1238358306	-1.5863767013	0.2671829659
O	-0.5644642594	-1.2734240073	-0.7877580257
C	-0.0139893587	1.0451482398	0.4461562471
C	-1.0557168322	0.6263279059	-0.3683145583
H	-0.2419204288	1.3339899831	1.4653656459
H	-0.9920483665	0.8214329127	-1.4317873828
C	-2.4301287245	0.4195545001	0.1945685134
H	-2.959371513	1.3689632473	0.3032513912
H	-3.0218570793	-0.2332420811	-0.4431674092
H	-2.3662526784	-0.0344031598	1.1860566973
H	-0.3895382071	-2.0708731531	0.9991951796
C	1.334215237	1.4321953551	-0.1486399791
H	1.9272660261	1.9898030461	0.5750839188
H	1.2664354258	2.0281140014	-1.0592984433
C	1.8951336739	0.0231827945	-0.3610821545
H	1.6315112102	-0.3594807033	-1.3454868459
H	2.9668135074	-0.0993321998	-0.2039293536

TS5b

0 1			
C	-1.3890854932	-0.752804569	-0.6432794525
H	-1.765180656	-0.9701786547	-1.6365435357
N	-0.4252267479	-1.5676959148	-0.2219814904
O	0.2332626043	-1.1836102087	0.8361419955
C	-0.4420007143	1.0593715628	-0.490496514
C	0.7156338114	0.7149303619	0.1789875399
H	-0.3500832705	1.3567796733	-1.5258173654
H	0.8765816447	0.9359173945	1.2277787753
H	0.1274630247	-2.0357388257	-0.9353890499
C	-1.7104354921	1.3591231677	0.2899026862
H	-2.3619021032	2.0317614333	-0.2652446158
H	-1.5224250792	1.808628205	1.2650448732
C	-2.2827956277	-0.0629408381	0.3750564714
H	-2.104851028	-0.5166977624	1.3481312453
H	-3.3404521781	-0.1536065285	0.1292151802
O	1.8161186008	0.4729594913	-0.5682540906
C	2.9295254951	0.008033825	0.1726103226
H	3.7340749548	-0.1624724697	-0.5372176828
H	3.2459958598	0.7572049585	0.9032794586
H	2.6714903945	-0.9178683015	0.6882592489

TS5c

0 1			
C	1.6955480962	0.9656912732	-0.442815666
H	1.8327602335	1.5138070789	-1.3680489096
N	0.8325290189	1.5310029158	0.4099031068
O	0.4293300819	0.801752283	1.3937635264
C	0.8399035725	-0.8091896941	-0.7102618858
C	0.0004455802	-0.894580634	0.3953085823
H	0.3910102711	-0.7164891932	-1.6896481945
H	0.2639192202	-1.492109426	1.2555743029
H	0.1191267133	2.1288143728	-0.0030323119
C	2.2959660937	-1.2417243512	-0.5768428648
H	2.7415078125	-1.4148302307	-1.5547669344
H	2.4437797613	-2.1335756255	0.0308051059
C	2.8080650931	0.0585901221	0.055623488
H	2.7510057765	0.0175383817	1.1416267253

H	3.8042469897	0.3832023289	-0.2416240749
C	-1.4386814674	-0.6041822334	0.2840382644
O	-2.3100176225	-1.0825911009	0.9580981774
O	-1.6812946775	0.3198268635	-0.678143502
C	-3.0558185835	0.6651339825	-0.8313403725
H	-3.0961374874	1.3976546786	-1.6317848173
H	-3.6417107418	-0.2148254723	-1.0900844737
H	-3.4464827345	1.0847316802	0.094016728

TS5d

0 1

C	-0.5044553331	1.0777933738	0.6657974969
H	-0.6971569016	1.3024060874	1.7107007354
N	0.6408737454	1.5800492804	0.2124246473
O	1.1221871082	1.1124206269	-0.889719516
C	0.0567634394	-1.0335806393	0.4006168718
C	1.1954922293	-0.8646876652	-0.3634509994
H	0.1839712466	-1.2035706561	1.4657379554
H	1.1593237272	-1.1249707536	-1.4132589296
C	2.5484296776	-0.8067147912	0.2777427621
H	2.8776240363	-1.7989055896	0.5942362101
H	3.2928397049	-0.3910893437	-0.3970089128
H	2.5123826352	-0.1848783659	1.1770874362
H	1.3303509928	1.8543805532	0.9091961425
C	-1.2422322946	-1.4894797883	-0.2123858935
H	-1.1024098525	-1.5939910194	-1.2909784252
H	-1.5421278092	-2.4664974813	0.1708765164
C	-2.3343208016	-0.4489688387	0.04269343
H	-2.6613078736	-0.4990177363	1.0853458472
H	-3.2128844512	-0.6131038242	-0.5814549535
C	-1.698305534	0.9074542031	-0.2267285288
H	-1.3615167115	0.9690359089	-1.2616655614
H	-2.40134898	1.7223134591	-0.0391963309

TS5e

0 1

C	0.9089942119	1.0540792894	-0.6704807569
H	1.1091090496	1.264930884	-1.7165585103
N	-0.2055631293	1.6151664898	-0.2095344397
O	-0.68330427	1.1666399457	0.9123691954
C	0.2796045658	-1.0089420734	-0.4627511874
C	-0.915114349	-0.8042440716	0.1900244358
H	0.222965721	-1.1667667337	-1.5332089205
H	-1.0887798826	-1.0928917831	1.2191957651
H	-0.902992099	1.8830936779	-0.9002134217
C	1.4843694466	-1.5219466845	0.2740667295
H	1.2608542986	-1.5538366563	1.343314128
H	1.7488404922	-2.5347488886	-0.0344240443
C	2.6504514911	-0.5590988784	0.0403252565
H	3.0206299557	-0.6717696098	-0.9826425348
H	3.4863431025	-0.7535400356	0.7123127781
C	2.0922242952	0.8443152075	0.2325130925
H	1.7544584231	0.9770905189	1.2600486839
H	2.8447603934	1.6047760733	0.0127850423
O	-2.0026736265	-0.5655115621	-0.5767420938
C	-3.1767848319	-0.249885112	0.1510326098
H	-3.9668969276	-0.0879836885	-0.5769457118
H	-3.4554044948	-1.0792687322	0.8058892204
H	-3.011009836	0.6481874232	0.7468806837

TS5f

0 1

C	-1.3416187939	1.145661747	0.4234037105
H	-1.4054952468	1.538610743	1.4337514396
N	-0.3145163109	1.641803262	-0.2695437751
O	0.0464067756	1.0351042592	-1.3423556728
C	-0.6556081593	-0.8569934371	0.4807245614
C	0.2641295493	-0.8382619602	-0.5579829635
H	-0.2713301545	-0.7885501406	1.4907386671
H	0.0469731509	-1.328599341	-1.4952912177
H	0.452154014	2.0279669607	0.2782151323
C	-1.9913814136	-1.5380905916	0.2832112258
H	-2.0307889691	-1.9489741738	-0.7272891138
H	-2.1117916627	-2.3712947807	0.9760628848
C	-3.123146443	-0.5187973716	0.4454206499
H	-3.3034648945	-0.3235296659	1.5060524978
H	-4.059355815	-0.8756182293	0.0176943214
C	-2.6355179226	0.7559391149	-0.2283308657
H	-2.4545972984	0.586909505	-1.2900358598
H	-3.3552816071	1.5701360578	-0.1223305665
C	1.7010994083	-0.6102213125	-0.3356378119
O	2.5936026613	-1.0332666407	-1.0191017692
O	1.9255987448	0.1654130385	0.7564299643
C	3.3023277409	0.4168447304	1.0293392358
H	3.3252047182	1.0289668826	1.925854311
H	3.8314830899	-0.5198377074	1.1939111947
H	3.7667998383	0.9381380515	0.1942258197

TS5g

0 1

C	-0.0666666432	-0.6194702585	-0.9329491688
H	-0.3430412675	-0.668196391	-1.9820279332
N	0.8251354568	-1.5369600994	-0.5747023571
O	1.4671126494	-1.3826979373	0.533783295
C	1.2510920261	1.1094294472	-0.5374447973
C	2.1912398273	0.4689171617	0.2450805317
H	1.4774262938	1.2802255519	-1.5833871426
H	2.2233461144	0.6490543011	1.3106583973
H	1.3548619885	-1.9715826931	-1.3261818923
C	0.1947502032	1.9884648475	0.0879012939
H	0.3602558188	2.0167071347	1.1674334543
H	0.2698361254	3.0149614545	-0.2747749889
C	-1.201955532	1.4205541155	-0.1786500098
H	-1.5027378668	1.6328124918	-1.2086210444
H	-1.9544357817	1.8595764886	0.4764475614
C	-1.0954446011	-0.0858371972	0.016315595
H	3.1109049508	0.1016667261	-0.1888053536
H	-2.0501683596	-0.5814825808	-0.1747374287
H	-0.7805001025	-0.3172752333	1.034107848

TS5h

0 1

C	-0.2497444427	-0.8575798778	0.7747720462
H	-0.1081385663	-1.1257154937	1.8180660055
N	-1.5351810215	-0.7967127578	0.4110296454
O	-1.8193418934	-0.1892887131	-0.6835970788
C	0.2207063664	1.1994188257	0.4543228397
C	-0.9408797936	1.6393217104	-0.1639451417
H	0.3528441404	1.4216693046	1.5070527141
H	-0.9130361393	1.8949841413	-1.214686168

H	-2.2272517454	-0.6947533563	1.1535113729
C	1.487434729	1.0015034323	-0.3391047015
H	1.2622307993	1.1205045427	-1.401290559
H	2.2380414632	1.7491645379	-0.0778127116
C	2.0133915737	-0.4136254795	-0.0983455885
H	2.4478735792	-0.4838246172	0.9028592427
H	2.7886901851	-0.6934193734	-0.8111885871
C	0.7996535109	-1.3263603795	-0.1954012787
H	1.0553201412	-2.3638942441	0.0288844144
H	0.3756950834	-1.282435626	-1.1987499033
C	-2.0992359074	2.1239859236	0.5886647064
C	-3.1059668394	2.8451017189	-0.0610443395
C	-2.2692194854	1.8363570955	1.9458653281
C	-4.2306558096	3.2724308135	0.6188211691
H	-2.9958894569	3.0614865934	-1.1161775697
C	-3.4047705206	2.2568849234	2.6271018464
H	-1.5015514068	1.2959924028	2.4849340467
C	-4.3882704129	2.9769900988	1.9691103157
H	-4.9935950527	3.8333513052	0.0957887012
H	-3.5151085619	2.0240415111	3.6780636414
H	-5.2703067057	3.3070524275	2.5004392816

TS5i

0 1

C	-0.5516151272	1.0878993688	0.6747419634
H	-0.8027464353	1.2941924714	1.7107271927
N	0.6152064191	1.6028797542	0.3021138825
O	1.170600954	1.1652416118	-0.774168766
C	0.072919191	-0.9952506097	0.4297510463
C	1.1693228296	-0.7904802823	-0.3833931251
H	0.2461740234	-1.1620731948	1.4865814028
H	1.1408466559	-1.0482184536	-1.4325679682
C	2.5420563091	-0.8081988133	0.2050652691
H	1.2635402928	1.8512968311	1.0453340786
C	-1.2222080135	-1.5032806222	-0.156742818
H	-1.0769221519	-1.6853869049	-1.2235613144
H	-1.5076804767	-2.4537386513	0.2952954924
C	-2.3295472374	-0.4604236074	0.0182855429
H	-2.6967282706	-0.4734740496	1.0481746691
H	-3.1813749277	-0.6563925437	-0.6320616382
C	-1.6935084234	0.8917795519	-0.2747559124
H	-1.3109238389	0.9251055282	-1.295082175
H	-2.4088969063	1.7066948858	-0.1443470446
F	2.6183691725	-0.0373913848	1.3119753576
F	2.9039103939	-2.0446496711	0.5935249168
F	3.4794965976	-0.3866263045	-0.6410635123

TS5j

0 1

C	1.6114845508	1.0385715372	-0.4759110908
H	1.7164346174	1.6041635913	-1.3945666845
N	0.6388061546	1.4364347807	0.3207884205
O	0.2634993728	0.624784168	1.2711463051
C	0.8401791214	-0.9643549272	-0.7337011456
C	0.0428398285	-0.9973016495	0.4147159489
H	0.4051670102	-1.5489733569	1.2725111781
H	-0.1008078428	2.0016071727	-0.0874731528
C	2.3403881681	-1.1731845243	-0.612787727
H	2.7694165157	-1.2877272808	-1.605681627
H	2.6141388547	-2.0399414906	-0.0112526257

C	2.7423348726	0.1648397328	0.0208734195
H	2.6842324046	0.1241107621	1.1077566114
H	3.7202782811	0.5478117357	-0.2688888437
C	0.2639926054	-0.8296647276	-2.0652026967
O	0.8439881544	-1.0173183415	-3.1104144062
O	-1.0276465103	-0.4080693967	-2.0351832585
C	-1.6435515063	-0.2784275773	-3.310925119
H	-1.1046316218	0.4381546914	-3.9287558937
H	-1.6604515202	-1.236501716	-3.827702301
H	-2.6556920862	0.0666820818	-3.1218569398
H	-1.0304820546	-0.9895232154	0.2940646784

TS5k

0 1

C	1.2350340272	1.1956329568	-0.4978915379
H	1.2543299552	1.5831561526	-1.5116708979
N	0.1451862699	1.498024962	0.1743738841
O	-0.1464671787	0.8351036937	1.2508836738
C	0.6386066387	-1.066035599	-0.4417120855
C	-0.2455333106	-0.9383126534	0.6266045071
H	0.0355931206	-1.3681940717	1.5783790728
H	-0.6546905307	1.8172355556	-0.3669171829
C	2.0433109557	-1.5722901983	-0.2463486455
H	2.1503017408	-1.9176894966	0.7835295039
H	2.2369923089	-2.4174311904	-0.9071765652
C	3.0611823058	-0.4575081606	-0.5115437946
H	3.1550530094	-0.3069314399	-1.5894548705
H	4.0488907545	-0.7097091455	-0.1255716453
C	2.5301960441	0.8183846538	0.1380987892
H	2.3716469688	0.6725211165	1.2066895446
H	3.232580334	1.6441143485	-0.0018639243
C	0.1668940241	-0.9713090175	-1.818998207
O	0.7832418008	-1.3172672845	-2.8012392062
O	-1.0647653463	-0.3959520743	-1.9212883752
C	-1.5750466311	-0.3111551295	-3.2469366857
H	-0.9021901065	0.2619700778	-3.8831770724
H	-1.69365068	-1.3044313436	-3.6765227027
H	-2.5389913098	0.1830261354	-3.1674855466
H	-1.3069448447	-0.904534108	0.4308951497

TS51

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C	-0.4896492035	1.0650246784	0.6066566922
H	-0.75012854	1.288044095	1.6389712083
N	0.6956695197	1.5577744709	0.2669687916
O	1.3217785882	1.1004304272	-0.7623907143
C	0.0919759651	-1.0457483266	0.4285652481
C	1.2274005353	-0.9017413612	-0.3374318165
H	0.2091553081	-1.1771450256	1.4984423561
H	1.2093727145	-1.1521118897	-1.3897355577
H	1.29256887	1.8464407858	1.0388457587
C	-1.2139256471	-1.517713555	-0.1651726463
H	-1.0705768125	-1.7242953157	-1.2267888956
H	-1.5314839518	-2.4540874359	0.2967418543
C	-2.2941422747	-0.4498704384	0.013820321
H	-2.6333414985	-0.4446773665	1.0549865687
H	-3.1709618336	-0.637629782	-0.6100763938
C	-1.6871089094	0.9188317498	-0.310382271
H	2.2069845001	-0.8814580313	0.1180077315
C	-2.6801926135	2.0320710443	0.0500471985

H	-3.5806763244	1.9421939937	-0.559117467
H	-2.9746962356	1.9758444862	1.0996451539
H	-2.2421841072	3.014217974	-0.1326762162
C	-1.3389759414	1.0365647703	-1.7931585056
H	-2.2582666246	0.9490728697	-2.3757726688
H	-0.8818257866	2.002403727	-2.0054634724
H	-0.6383368766	0.2737970058	-2.1196286575

TS5m

0 1

C	-0.6711921036	-0.8846080888	0.9158914317
H	-0.7382663535	-1.1748267598	1.9599238298
N	-1.6356859889	-1.4039103643	0.1674986132
O	-1.8513278901	-0.9386923522	-1.0076828669
C	-1.3342952191	1.2456087986	0.4852054866
C	-2.0924812054	0.9725443046	-0.6362583173
H	-1.8238597242	1.3932815837	1.4372354714
H	-1.7159683548	1.2357988864	-1.6154301819
H	-2.4498763198	-1.7686196295	0.6575012909
C	0.0537090895	1.8066760528	0.3315973301
H	0.1139156354	2.501828399	-0.5070331789
H	0.3617928131	2.3388389563	1.2327649987
C	0.6557193377	-0.5712634471	0.3658154231
H	-3.1677406616	0.8949723704	-0.5601267233
N	0.9866846847	0.7148412974	0.0726985022
C	2.2702781311	0.7680959578	-0.3737707515
C	1.7510621937	-1.364734144	0.1075981704
C	2.7740049833	-0.5118451752	-0.3699448777
H	2.7182942985	1.7042674085	-0.6595182571
H	3.7609818306	-0.8014372897	-0.6872896962
H	1.7942758234	-2.4335907646	0.2276793026

TS5n

0 1

C	-0.5091765009	-0.8233694139	0.6639906018
H	-0.1775047533	-1.0029034462	1.682564908
N	-1.669133334	-1.3775005349	0.3468209873
O	-2.2766048709	-0.9780347194	-0.715000189
C	-1.1991071647	1.2607282428	0.4005899093
C	-2.3257142415	1.0107238891	-0.3547557239
H	-1.3052751766	1.4396686702	1.4629378358
H	-2.3263937367	1.2283883742	-1.414092684
H	-2.266506385	-1.6846424739	1.1107393963
C	0.0594540282	1.7754719129	-0.2578263573
H	-0.1594771278	2.0831558741	-1.2812022017
H	0.4911144362	2.6226097208	0.2725990636
C	0.5620574408	-0.6186370089	-0.3785611477
H	-3.3008144549	0.9548300901	0.1074655658
N	1.0785893807	0.7298622217	-0.2969360324
C	2.1653638857	0.7636699585	0.5463654413
C	1.8477171502	-1.3975929125	-0.0864119523
H	2.3884867339	-1.6127212729	-1.0081506534
O	2.6641610262	1.7164138576	1.0669014764
O	2.6210003268	-0.510631397	0.7171291326
H	1.6823671392	-2.3188295552	0.467171923
H	0.1437430385	-0.8388351471	-1.3598121394

TS5o

0 1

C	-0.8779501699	-0.7742048079	1.1843969827
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H	-1.155885196	-0.7752631264	2.2311984767
N	-1.6864984953	-1.4705694938	0.4000798193
O	-1.5807700265	-1.3311141505	-0.8680266814
C	-1.3620665291	1.1703604753	0.2715883568
C	-1.6945020996	0.7368394731	-0.9892185861
H	-2.1498589008	1.4585111666	0.9552990834
H	-0.9549131431	0.7488916475	-1.7781107023
H	-2.6120531496	-1.6984904599	0.755697659
C	0.0210158522	1.689395794	0.5691848212
H	0.3130986113	2.5139279171	-0.0770235698
H	0.0797201672	2.0418381633	1.603846845
C	0.5873270272	-0.7059105665	0.8245390662
H	-2.7251083548	0.6804838444	-1.3048561928
N	0.9687059028	0.6109761911	0.3418672604
C	2.1832950813	0.8649254274	-0.2011650393
O	2.5712879736	1.9458132474	-0.5811181164
O	2.9275439875	-0.2607192652	-0.2743458133
H	0.7776985427	-1.4492862796	0.052524139
H	1.1714172828	-0.9693818177	1.7098112006
C	4.2070896258	-0.0801370811	-0.8732344208
H	4.1026416149	0.2676419405	-1.8991419761
H	4.790364519	0.6483005029	-0.3135534062
H	4.6853639762	-1.0542622519	-0.8486511055

TS5p
0 1

TS5q
0 1

TS5r
0 1

C	-0.9184365143	-0.82044805	0.9401537497
H	-1.0211075641	-1.030949814	2.0004376211
N	-1.7606189694	-1.5000521221	0.174636516
O	-1.9092390314	-1.1539543954	-1.0502064712
C	-1.7409699439	1.1744439561	0.4125060558
C	-2.3078216778	0.8386744784	-0.796460187
H	-2.3861568747	1.2706842251	1.2758599091
H	-1.7984276453	1.0770871809	-1.7204133609
H	-2.5794658586	-1.8978796312	0.6299170535
C	-0.4011367071	1.8759144414	0.465966133
H	-0.3478894829	2.68559479	-0.2647552801
H	-0.2589603974	2.3359754375	1.4468101244
H	-3.3695847112	0.660171393	-0.8798550054
C	0.4294713385	-0.4429761786	0.4342015827
C	0.7164890594	0.8961312736	0.2111099241
C	1.4023584867	-1.4146050455	0.2229361722
C	2.6631131355	-1.0467441615	-0.2197908642
H	3.4154418498	-1.8028858653	-0.3976355925
C	1.9832541323	1.2602042024	-0.2279752094
C	2.953726304	0.2934643115	-0.4416521745
H	2.2039124463	2.3040874461	-0.4147479307
H	3.9354739162	0.5829360156	-0.7915030189
H	1.1629277093	-2.4568018881	0.3909202534

TS5s
0 1

C	0	-0.934841	-0.792758	0.943749
H	0	-1.046855	-0.987746	2.006052

N	0	-1.780437	-1.472214	0.181872
O	0	-1.916971	-1.140785	-1.048422
C	0	-1.729351	1.204791	0.384181
C	0	-2.29258	0.859796	-0.823881
H	0	-2.378793	1.320491	1.241937
H	0	-1.774407	1.079543	-1.747581
H	0	-2.607009	-1.85385	0.637054
C	0	-0.381344	1.890469	0.437041
H	0	-0.313467	2.689563	-0.304049
H	0	-0.239764	2.361872	1.412572
H	0	-3.355908	0.693195	-0.911829
C	0	0.420813	-0.438628	0.441633
C	0	0.725726	0.893754	0.202585
C	0	1.382981	-1.424835	0.249708
C	0	2.650969	-1.0784	-0.189633
H	0	3.395041	-1.846008	-0.352456
C	0	1.999654	1.236377	-0.233024
C	0	2.959482	0.255056	-0.427441
H	0	2.234344	2.274883	-0.432253
H	0	1.12966	-2.461677	0.430005
N	0	4.30143163	0.62568252	-0.89935961
O	0	4.53692952	1.78519325	-1.09555961
O	0	5.10719067	-0.24625217	-1.06933318

TS5t

0 1

C	0	-0.934841	-0.792758	0.943749
H	0	-1.046855	-0.987746	2.006052
N	0	-1.780437	-1.472214	0.181872
O	0	-1.916971	-1.140785	-1.048422
C	0	-1.729351	1.204791	0.384181
C	0	-2.29258	0.859796	-0.823881
H	0	-2.378793	1.320491	1.241937
H	0	-1.774407	1.079543	-1.747581
H	0	-2.607009	-1.85385	0.637054
C	0	-0.381344	1.890469	0.437041
H	0	-0.313467	2.689563	-0.304049
H	0	-0.239764	2.361872	1.412572
H	0	-3.355908	0.693195	-0.911829
C	0	0.420813	-0.438628	0.441633
C	0	0.725726	0.893754	0.202585
C	0	1.382981	-1.424835	0.249708
C	0	2.650969	-1.0784	-0.189633
H	0	3.395041	-1.846008	-0.352456
C	0	1.999654	1.236377	-0.233024
C	0	2.959482	0.255056	-0.427441
H	0	2.234344	2.274883	-0.432253
H	0	1.12966	-2.461677	0.430005
O	0	4.30143163	0.62568252	-0.89935961
C	0	5.17569334	-0.32038085	-1.08378371
H	0	5.33449637	-0.84352238	-0.16399866
H	0	4.81240809	-1.00240966	-1.82389216
H	0	6.09904107	0.10688482	-1.41510383

TS5u

0 1

C	1.5700706826	-0.8064516215	-0.8087568252
H	1.5107782016	-1.0247067533	-1.8692552056
N	2.7833373102	-0.495397223	-0.3747935308
O	2.8975272981	0.0378460137	0.7917981156

C	0.7136577706	1.1712944941	-0.4216020137
C	1.5223975875	1.5222011707	0.6432359484
H	0.8896393771	1.6556813487	-1.3757567453
H	1.1802785364	1.3612826638	1.6559977786
H	3.4617239119	-0.1919054156	-1.068921794
H	2.2953970272	2.2665861375	0.521592488
C	-0.6449346384	0.6051188852	-0.2089433587
C	-1.8128474419	1.3565705439	-0.2859767384
H	-1.7521904047	2.4137964551	-0.5108182408
C	-0.7294109024	-0.7569251801	0.0779319604
C	-1.9614158047	-1.35593977	0.2970406594
H	-2.0161827016	-2.4158125115	0.5131384425
C	-3.1212993691	-0.5973299874	0.2240182491
H	-4.0832238388	-1.0636947683	0.3887735452
C	-3.0460874848	0.7574251155	-0.0713025636
H	-3.9506212929	1.3474788923	-0.1326904962
C	0.5880917648	-1.4806432982	0.1132740832
H	0.4663515392	-2.5256394463	-0.1792920926
H	1.0153028722	-1.4564357453	1.1170963343

TS5v

0 1

C	0	-1.567787	-0.796545	0.81747
H	0	-1.50753	-1.007199	1.87945
N	0	-2.781378	-0.488226	0.382464
O	0	-2.896537	0.036663	-0.787816
C	0	-0.71113	1.178094	0.41529
C	0	-1.520796	1.521605	-0.651254
H	0	-0.88603	1.669377	1.366112
H	0	-1.179715	1.353308	-1.663166
H	0	-3.458992	-0.179539	1.075053
H	0	-2.293443	2.267093	-0.534208
C	0	0.647077	0.60997	0.205382
C	0	1.8153	1.36158	0.275882
H	0	1.755194	2.420413	0.493185
C	0	0.730845	-0.754126	-0.071786
C	0	1.962448	-1.355095	-0.287785
H	0	2.016671	-2.41651	-0.496319
C	0	3.12264	-0.596353	-0.22134
C	0	3.048142	0.760512	0.064318
H	0	3.952921	1.350701	0.120587
C	0	-0.586919	-1.477656	-0.10065
H	0	-0.465222	-2.520564	0.199295
H	0	-1.0151	-1.460521	-1.104204
N	0	4.42952636	-1.23217812	-0.44196287
O	0	5.4137881	-0.5498671	-0.37793694
O	0	4.4593122	-2.40784667	-0.6771756

TS5w

0 1

C	0	-1.567787	-0.796545	0.81747
H	0	-1.50753	-1.007199	1.87945
N	0	-2.781378	-0.488226	0.382464
O	0	-2.896537	0.036663	-0.787816
C	0	-0.71113	1.178094	0.41529
C	0	-1.520796	1.521605	-0.651254
H	0	-0.88603	1.669377	1.366112
H	0	-1.179715	1.353308	-1.663166
H	0	-3.458992	-0.179539	1.075053
H	0	-2.293443	2.267093	-0.534208

C	0	0.647077	0.60997	0.205382
C	0	1.8153	1.36158	0.275882
H	0	1.755194	2.420413	0.493185
C	0	0.730845	-0.754126	-0.071786
C	0	1.962448	-1.355095	-0.287785
H	0	2.016671	-2.41651	-0.496319
C	0	3.12264	-0.596353	-0.22134
C	0	3.048142	0.760512	0.064318
H	0	3.952921	1.350701	0.120587
C	0	-0.586919	-1.477656	-0.10065
H	0	-0.465222	-2.520564	0.199295
H	0	-1.0151	-1.460521	-1.104204
O	0	4.39396483	-1.21487676	-0.43595953
C	0	5.23645026	-0.97933004	0.69525046
H	0	6.06567829	-1.65505537	0.66924753
H	0	5.59624426	0.02800696	0.66840906
H	0	4.67781913	-1.13469353	1.5945243

TS6d

0 1

C	-0.6040357341	-0.9524550318	0.6693449168
N	-0.0457183468	-1.5399971805	-0.3747381257
O	1.2317496354	-1.4630908629	-0.5248030357
C	0.2691469887	0.998041677	0.3544416297
C	1.4149297753	0.6602144671	-0.3266110598
H	-0.5871865813	-1.573591447	-1.2365718808
H	-0.0809635132	-1.0798483149	1.6049832868
H	0.3905452723	1.1972598494	1.4151528573
C	-0.9830385345	1.5939160776	-0.2714144136
H	-0.7401818085	2.0923879794	-1.2108798289
H	-1.3614218797	2.3688687197	0.3974140077
C	-2.1025523364	0.5627800385	-0.5109267038
C	-2.0341266349	-0.5149691368	0.5802652258
H	-2.3336546281	-0.1004694079	1.5426199684
H	-2.7072852615	-1.3468993176	0.3623939791
H	-1.965245073	0.0893548506	-1.4860556362
H	-3.0833532066	1.038277906	-0.5403697151
C	2.7513390578	0.5717082897	0.3398166793
H	3.3706677646	-0.1896206614	-0.1301952979
H	3.2789993498	1.5271698609	0.286067628
H	2.6321273001	0.3105613487	1.3919640356
H	1.4208973946	0.7492202962	-1.4076825169

TS6e

0 1

C	-0.9194190058	-0.9476589418	0.5972277484
N	-0.4253378843	-1.5004017055	-0.4967151079
O	0.8595153506	-1.4448734403	-0.6886698592
C	-0.1585708479	0.9905298017	0.3552780444
C	1.0760050847	0.7210832888	-0.1810795569
H	-0.9955811987	-1.4689311127	-1.3385228747
H	-0.3445586712	-1.1320514887	1.494349246
H	-0.1596940115	1.2069011463	1.4176657276
C	-1.3240379915	1.5201121479	-0.4532611233
H	-1.0049851325	1.7193875597	-1.4768634147
H	-1.6347516462	2.4812792467	-0.0426385843
C	-2.5376080512	0.5491485437	-0.4633590205
C	-2.3545558406	-0.5172000337	0.6266883457
H	-2.5617771288	-0.096172295	1.6098562481
H	-3.0411847236	-1.3536103593	0.4836122603

H	-2.6145325527	0.0591911095	-1.4357770435
H	-3.4762641048	1.084418901	-0.3248740288
H	1.2917809225	0.8243634121	-1.2385883355
O	2.1342221971	0.6067940364	0.6409400138
C	3.2883800847	0.054124947	0.0317838262
H	4.0710423402	0.052406962	0.78523989
H	3.080024521	-0.9596281161	-0.3065208531
H	3.6042632904	0.6696613904	-0.8150375483

TS6f

0 1

C	-1.2628089681	-0.9436453574	0.5698570272
N	-1.0359473868	-1.4669751391	-0.6331930017
O	0.1498740653	-1.40869625	-1.1133531732
C	-0.5472633568	0.9386043298	0.1916216821
C	0.4229818301	0.6997100892	-0.7614926275
H	-1.788472412	-1.4079654887	-1.3181797609
H	-0.5073025128	-1.1762038188	1.3073393859
H	-0.1863591752	1.0585452664	1.20586724
C	-1.8852485761	1.5977669896	-0.1069420176
H	-1.8658464082	2.0681069903	-1.0899482708
H	-2.0452061238	2.3972255335	0.6171908537
C	-3.0561213226	0.5939107999	-0.0226743029
C	-2.6622513699	-0.5415741051	0.9318295783
H	-2.6614921262	-0.188104257	1.9625294474
H	-3.3620800169	-1.3771718188	0.8762602167
H	-3.2565732183	0.1769855629	-1.012121253
H	-3.9791441542	1.0780386008	0.2942096035
H	0.2683389513	0.9286210162	-1.8060178303
C	1.8276589951	0.4330647218	-0.4124148713
O	2.7494659301	0.4834880683	-1.1823751483
O	1.9782356267	0.0974730817	0.8866616788
C	3.3082886116	-0.2442137145	1.261480408
H	3.9845449918	0.5886739115	1.0769105807
H	3.2718021517	-0.4776138655	2.3212147908
H	3.6498539741	-1.106717147	0.6917447646

TS6g

0 1

C	0.0857053556	-0.9762705993	0.6411958024
N	0.9499382613	-1.1647895176	-0.3428435745
O	2.0861944068	-0.5607013526	-0.3038547033
C	0.1072928259	1.1849740043	0.5666611232
C	1.3274120424	1.3941529973	-0.0285367962
H	0.5638189625	-1.3080994124	-1.2748897813
H	0.5061055991	-0.9901440753	1.63483128
H	0.0678106277	1.3042927426	1.6433032358
C	-1.2365474354	1.2936706775	-0.1410489751
H	-1.1718220197	1.9907121496	-0.9776126824
H	-1.9580540053	1.7186351684	0.5588543281
C	-1.7739388423	-0.0598144174	-0.6378200085
C	-1.3765131457	-1.1515383793	0.3654333261
H	-1.9262512415	-1.0282866315	1.2982393984
H	-1.6065451607	-2.1483508546	-0.0170029828
H	-1.3341102914	-0.2940859901	-1.6104422634
H	-2.8531970597	-0.0300966161	-0.7904078796
H	1.3984976198	1.60068368	-1.0890037663
H	2.1958415006	1.6495804265	0.5583139196

TS6h

0 1			
C	1.9111149962	-0.5552772638	-0.9546875661
N	1.6878193879	-1.6043794798	-0.1716014009
O	0.4789636007	-1.8403758833	0.200120745
C	1.0503335463	0.893475823	0.2523839306
C	0.0280453029	0.1921994753	0.8597612776
H	2.4136287716	-1.8522410437	0.4986109998
H	1.1962597881	-0.4360247826	-1.7566889825
H	0.7746274448	1.5170458837	-0.5913830661
C	2.3339542834	1.3099378616	0.9545773774
H	2.2402858794	1.1495324578	2.028790803
H	2.4694566152	2.3835172993	0.8167626889
C	3.5817389159	0.5690269247	0.4184939201
C	3.2834708797	0.0477106319	-0.9939176602
H	3.2761345978	0.8698403263	-1.7089969148
H	4.0393077307	-0.6650946622	-1.3285540344
H	3.8219233338	-0.2748986244	1.0685676548
H	4.4620578998	1.2108890912	0.4235615253
H	0.1804075795	-0.1939006947	1.8602989109
C	-1.3648333911	0.1968489408	0.3826525417
C	-2.2033466646	-0.8736532548	0.704545364
C	-1.8909933328	1.2434921157	-0.373795721
C	-3.5202613197	-0.8968206874	0.281980109
H	-1.7910668041	-1.7022709002	1.2649464939
C	-3.2101685463	1.2177446193	-0.8047247429
H	-1.2757544278	2.1029195744	-0.6045026735
C	-4.0302702336	0.1490328721	-0.478248447
H	-4.1514806808	-1.7371815722	0.5386370527
H	-3.6003287283	2.0431202928	-1.385350926
H	-5.0598524247	0.1311046594	-0.8093402593

TS6i

0 1			
C	-1.4700064108	-0.8772217902	0.6905348777
N	-1.0724076955	-1.5739559293	-0.362609337
O	0.1825580295	-1.6683484844	-0.6115049356
C	-0.4247764982	0.910145461	0.1820413535
C	0.6047266997	0.3950841634	-0.5644154215
H	-1.6826874431	-1.5813555901	-1.1784457285
H	-0.8840265181	-1.0258332309	1.5854003273
H	-0.1942771549	1.1329295359	1.2174490187
C	-1.6344118935	1.6332235986	-0.386362572
H	-1.4107955506	2.032059742	-1.376088332
H	-1.8479421131	2.4917861383	0.2513979276
C	-2.8884540944	0.7399646437	-0.4558198839
C	-2.8451567299	-0.2814810831	0.6905326641
H	-3.0096345323	0.2111078177	1.6482411123
H	-3.6227138907	-1.0395804191	0.5785565733
H	-2.9068076793	0.2044086228	-1.4080017059
H	-3.8016354873	1.3337679275	-0.4247909346
H	0.6236784448	0.4558615035	-1.6438542715
C	1.9444860563	0.1871487582	0.0585627665
F	2.6892956968	-0.6981688345	-0.601658782
F	1.8497418116	-0.2223143489	1.3323707138
F	2.6541649528	1.3350257978	0.0835905696

TS6l

0 1			
C	0.0262300641	-0.6860958418	0.5800002614
N	0.7940470234	-1.4261869975	-0.2023601533

O	2.0544329423	-1.5045775121	0.0492574917
C	1.1982505842	1.1132847235	0.4189184169
C	2.4272752873	0.5822095157	0.1149381463
H	0.5442877939	-1.468607918	-1.1892167435
H	0.2205089635	-0.7827155574	1.6391630921
H	1.0389219365	1.4042307225	1.4510331899
C	0.2681676011	1.772029821	-0.5911050156
H	0.8381448998	2.1171015748	-1.4547955254
H	-0.1617536265	2.665279245	-0.1356593543
C	-0.8688189333	0.847946519	-1.0665627193
C	-1.2743141264	-0.1309549601	0.0540228367
H	-0.5365608358	0.2679385968	-1.9326186746
H	-1.7370431475	1.4202480076	-1.4019879797
H	2.7874860693	0.5652638865	-0.9055424022
H	3.1744660307	0.4367097214	0.8795269262
C	-1.9810926419	0.6188056312	1.1823964451
H	-2.8989118435	1.0757979476	0.810441337
H	-2.2440277637	-0.0613450123	1.9936229092
H	-1.3494564692	1.4077401791	1.591399433
C	-2.1954829887	-1.2253139508	-0.4919725197
H	-2.4777081626	-1.9249626159	0.294850593
H	-3.1052083695	-0.7795147187	-0.8977139819
H	-1.7168452875	-1.7919700071	-1.291868009