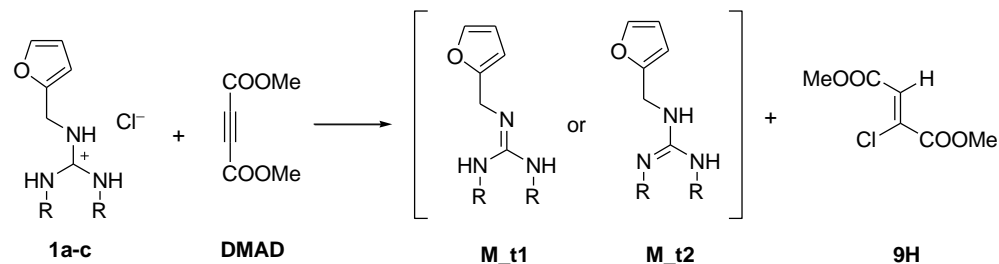


# A DFT Investigation of the Reactivity of Guanidinium Salts in Tandem aza-Michael Addition/Intramolecular Cyclization

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## S1. Formation of the guanidine tautomers



**Scheme S1.** Reaction Scheme for the formation of 2-chlorofumarate (**9H**) by chloride addition to **DMAD** with concomitant deprotonation of the guanidine.

**Table S1.** Calculated electronic energies ( $E_{\text{scf}}$ ), corrections to the Gibbs energies ( $G_{\text{corr}}$ ) and Gibbs energies ( $G_{\text{tot}}$ ) of the relevant structures associated with the reaction given in Scheme S1, and calculated using B3LYP, M06-2X and G3 approaches.<sup>1,2</sup>

Structure	$E_{\text{scf}}(\text{B3LYP})$	$G_{\text{corr}}$	$G_{\text{tot}}(\text{B3LYP})$	$E_{\text{scf}}(\text{M06})$	$G_{\text{tot}}(\text{M06})$	$G_{\text{tot}}(\text{G3})$
<b>1a_t1</b>	-551.12745	0.15260	-550.97485	-550.91208	-550.75948	-550.58275
<b>1a_t2</b>	-551.12689	0.15210	-550.97479	-550.91027	-550.75817	-550.58246
<b>1aH<sup>+</sup></b>	-551.60587	0.16645	-551.43943	-551.38441	-551.21796	-551.04515
<b>1b_t1</b>	-590.45549	0.18059	-590.27490	-590.22084	-590.04025	-589.85684
<b>1b_t2</b>	-590.45523	0.18021	-590.27501	-590.22058	-590.04037	-589.85762
<b>1bH<sup>+</sup></b>	-590.93913	0.19332	-590.74581	-590.69966	-590.50635	-590.32688
<b>1c_t1</b>	-709.64338	0.27518	-709.36820	-709.34168	-709.06650	
<b>1c_t2</b>	-709.64199	0.27572	-709.36627	-709.33991	-709.06420	
<b>1cH<sup>+</sup></b>	-710.12810	0.29144	-709.83666	-709.82090	-709.52947	-709.34213
<b>DMAD</b>	-533.28148	0.07614	-533.20534	-533.07424	-532.99809	-532.80517
<b>Cl<sup>-</sup></b>	-460.40868	-0.01502	-460.42370	-460.37370	-460.38872	-460.24342
<b>9H</b>	-994.16659	0.08874	-994.07785	-993.93546	-993.84672	-993.50921

<sup>1</sup> B3LYP = B3LYP(SMD,ACN)/6-311+G(2df,p)//B3LYP(SMD,ACN)/6-31G(d,p); M06 = M06-2X(SMD,ACN)/6-311++G(3df,2pd) //B3LYP(SMD,ACN)/6-31G(d,p), G3 = G3(SMD,ACN). <sup>2</sup> Energies,  $G_{\text{corr}}$ , and  $G_{\text{tot}}$  were given in a.u.  $\Delta G_{\text{rel}}$  is given in kJ mol<sup>-1</sup>.

## S2. Mechanism of the AMA/CYC reaction

### S2.1. Energies of the investigated structures

**Table S2.** Calculated electronic energies ( $E_{\text{scf}}$ ), corrections to the Gibbs energies ( $G_{\text{corr}}$ ) and Gibbs energies ( $G_{\text{tot}}$ ) of the relevant structures associated with the reaction pathway starting from the guanidine tautomers. <sup>1,2</sup>

Structure	$E_{\text{scf}}(\text{B3LYP})$	$G_{\text{corr}}$	$G_{\text{tot}}(\text{B3LYP})$	$E_{\text{scf}}(\text{M06})$	$G_{\text{tot}}(\text{M06})$	$\Delta G_{\text{rel}}(\text{M06})^3$
NCov(1a_t1)	-1084.40848	0.24775	-1084.16073	-1083.99151	-1083.74376	36
TS1(1a_t1)	-1084.38631	0.25053	-1084.13579	-1083.97220	-1083.72167	94
10a_t1	-1084.41656	0.25665	-1084.15991	-1084.01191	-1083.75526	6
TS2(1a_t1)	-1084.40525	0.25479	-1084.15046	-1083.99846	-1083.74368	37
11a_t1	-1084.41634	0.25566	-1084.16068	-1084.01218	-1083.75653	3
TS3(1a_t1)	-1084.40990	0.25254	-1084.15737	-1084.00555	-1083.75301	12
E-12a_t1	-1084.40990	0.25254	-1084.15737	-1084.04325	-1083.78741	-78
Z-12a_t1	-1084.44936	0.25627	-1084.19309	-1084.04568	-1083.78941	-84
TS4 <sub>sc</sub> (1a_t1)	-1084.42578	0.25757	-1084.16821	-1084.02251	-1083.76494	-19
TS4 <sub>6c</sub> (1a_t1)	-1084.42677	0.25880	-1084.16797	-1084.02770	-1083.76891	-30
13a_t1	-1084.42740	0.25809	-1084.16930	-1084.02493	-1083.76684	-24
E-13a_t1	<b>ring opening</b>					
14a_t1	-1084.42868	0.25873	-1084.16995	-1084.02966	-1083.77093	-35
15a_t1	-1084.43388	0.25938	-1084.17451	-1084.03921	-1083.77984	-58
E-15a_t1	-1084.44658	0.25992	-1084.18666	-1084.05125	-1083.79132	-89
16a_t1	-1084.43354	0.25887	-1084.17467	-1084.04170	-1083.78283	-66
17a_t1	-1084.46626	0.25297	-1084.21329	-1084.05335	-1083.80038	-112
E-17a_t1	-1084.46297	0.25118	-1084.21179	-1084.04959	-1083.79841	-107
18a_t1	-1084.47207	0.25364	-1084.21843	-1084.06322	-1083.80957	-137

<sup>1</sup> B3LYP = B3LYP(SMD,ACN)/6-311+G(2df,p)//B3LYP(SMD,ACN)/6-31G(d,p); M06 = M06-2X(SMD,ACN)/6-311++G(3df,2pd) //B3LYP(SMD,ACN)/6-31G(d,p). <sup>2</sup>  $E_{\text{scf}}$ ,  $G_{\text{corr}}$ , and  $G_{\text{tot}}$  are given in a.u.  $\Delta G_{\text{rel}}$  is given in kJ mol<sup>-1</sup>.

$\Delta G_{\text{rel}}$  is calculated using the equation:  $\Delta G_{\text{rel}}(\text{Structure}) = G_{\text{tot}}(\text{Structure}) - [G_{\text{tot}}(\mathbf{1a\_t1}) + G_{\text{tot}}(\mathbf{DMAD})]$

Table S2. (contd.)

Structure	$E_{\text{scf}}(\text{B3LYP})$	$G_{\text{corr}}$	$G_{\text{tot}}(\text{B3LYP})$	$E_{\text{scf}}(\text{M06})$	$G_{\text{tot}}(\text{M06})$	$\Delta G_{\text{rel}}(\text{M06})^3$
NCov(1a_t2)	-1084.40601	0.24675	-1084.15926	-1083.98737	-1083.74062	45
TS1(1a_t2)	-1084.38402	0.25012	-1084.13390	-1083.96966	-1083.71955	100
10a_t2	-1084.41974	0.25629	-1084.16345	-1084.01203	-1083.75574	5
TS2(1a_t2)	-1084.40853	0.25447	-1084.15406	-1083.99898	-1083.74451	34
11a_t2	-1084.42096	0.25466	-1084.16630	-1084.01342	-1083.75875	-3
TS3(1a_t2)	-1084.41893	0.25176	-1084.16717	-1084.01161	-1083.75985	(-6) <sup>4</sup>
E-12a_t2	-1084.45764	0.25665	-1084.20098	-1084.05259	-1083.79594	-101
Z-12a_t2	-1084.45806	0.25661	-1084.20145	-1084.05182	-1083.79521	-99
TS4 <sub>5c</sub> (1a_t2)	-1084.43855	0.25541	-1084.18315	-1084.03328	-1083.77787	-53
TS4 <sub>6c</sub> (1a_t2)	-1084.43208	0.25710	-1084.17499	-1084.03107	-1083.77397	-43
13a_t2	-1084.43922	0.25533	-1084.18390	-1084.03498	-1083.77966	-58
E-13a_t2	<b>ring opening</b>					
14a_t2	-1084.43295	0.25761	-1084.17534	-1084.03205	-1083.77446	-44
15a_t2	-1084.44078	0.25714	-1084.18365	-1084.04478	-1083.78798	-80
E-15a_t2	-1084.44833	0.25878	-1084.18955	-1084.05165	-1083.79287	-93
16a_t2	-1084.43437	0.25751	-1084.17686	-1084.04121	-1083.78370	-69
17a_t2	-1084.47084	0.25192	-1084.21892	-1084.05733	-1083.80541	-126
E-17a_t2	-1084.46445	0.25017	-1084.21427	-1084.04948	-1083.79930	-110
18a_t2	-1084.47396	0.25299	-1084.22097	-1084.06412	-1083.81113	-141

<sup>1</sup> B3LYP = B3LYP(SMD,ACN)/6-311+G(2df,p)//B3LYP(SMD,ACN)/6-31G(d,p); M06 = M06-2X(SMD,ACN)/6-311++G(3df,2pd) //B3LYP(SMD,ACN)/6-31G(d,p). <sup>2</sup>  $E_{\text{scf}}$ ,  $G_{\text{corr}}$ , and  $G_{\text{tot}}$  are given in a.u.  $\Delta G_{\text{rel}}$  is given in kJ mol<sup>-1</sup>.  $\Delta G_{\text{rel}}$  is calculated using the equation:  $\Delta G_{\text{rel}}(\text{Structure}) = G_{\text{tot}}(\text{Structure}) - [G_{\text{tot}}(\mathbf{1a\_t2}) + G_{\text{tot}}(\mathbf{DMAD})]$ . <sup>4</sup> Interconversion from the fumarate to maleate anion substructure is associated with the barrierless intramolecular proton transfer from the guanidine subunit.

Table S2. (contd.)

Structure	$E_{\text{scf}}(\text{B3LYP})$	$G_{\text{corr}}$	$G_{\text{tot}}(\text{B3LYP})$	$E_{\text{scf}}(\text{M06})$	$G_{\text{tot}}(\text{M06})$	$\Delta G_{\text{rel}}(\text{M06})^3$
NCov(1b_t1)	-1123.73579	0.27347	-1123.46232	-1123.30238	-1123.02974	23
TS1(1b_t1)	-1123.71342	0.27838	-1123.43504	-1123.28164	-1123.00326	92
10b_t1	-1123.74695	0.28566	-1123.46129	-1123.32499	-1123.03933	-3
TS2(1b_t1)	-1123.73506	0.28263	-1123.45243	-1123.31061	-1123.02798	27
11b_t1	-1123.74643	0.28375	-1123.46268	-1123.32406	-1123.04031	-5
TS3(1b_t1)	-1123.74007	0.27989	-1123.46019	-1123.31735	-1123.03746	2
E-12b_t1	-1123.77562	0.28086	-1123.49476	-1123.35280	-1123.07194	-88
Z-12b_t1	-1123.78028	0.28468	-1123.49560	-1123.35847	-1123.07379	-93
TS4 <sub>5c</sub> (1b_t1)	-1123.76549	0.28474	-1123.48075	-1123.34339	-1123.05865	-53
TS4 <sub>6c</sub> (1b_t1)	-1123.75496	0.28514	-1123.46982	-1123.33817	-1123.05303	-39
13b_t1	-1123.76803	0.28565	-1123.48238	-1123.34720	-1123.06155	-61
E-13b_t1	<b>ring opening</b>					
14b_t1	-1123.75382	0.28552	-1123.46830	-1123.33732	-1123.05181	-35
15b_t1	-1123.77238	0.28691	-1123.48546	-1123.35957	-1123.07266	-90
E-15b_t1	-1123.78446	0.28744	-1123.49703	-1123.37118	-1123.08375	-119
16b_t1	-1123.75699	0.28722	-1123.46977	-1123.34765	-1123.05999	-57
17b_t1	-1123.80535	0.28171	-1123.52365	-1123.37546	-1123.09375	-145
E-17b_t1	-1123.80239	0.27881	-1123.52359	-1123.37212	-1123.09332	-144
18b_t1	-1123.79752	0.28241	-1123.51511	-1123.37199	-1123.08958	-134

<sup>1</sup> B3LYP = B3LYP(SMD,ACN)/6-311+G(2df,p)//B3LYP(SMD,ACN)/6-31G(d,p); M06 = M06-2X(SMD,ACN)/6-

311++G(3df,2pd) //B3LYP(SMD,ACN)/6-31G(d,p). <sup>2</sup>  $E_{\text{scf}}$ ,  $G_{\text{corr}}$ , and  $G_{\text{tot}}$  are given in a.u.  $\Delta G_{\text{rel}}$  is given in kJ mol<sup>-1</sup>.

$\Delta G_{\text{rel}}$  is calculated using the equation:  $\Delta G_{\text{rel}}(\text{Structure}) = G_{\text{tot}}(\text{Structure}) - [G_{\text{tot}}(\mathbf{1b\_t1}) + G_{\text{tot}}(\mathbf{DMAD})]$ .

Table S2. (contd.)

Structure	$E_{\text{scf}}(\text{B3LYP})$	$G_{\text{corr}}$	$G_{\text{tot}}(\text{B3LYP})$	$E_{\text{scf}}(\text{M06})$	$G_{\text{tot}}(\text{M06})$	$\Delta G_{\text{rel}}(\text{M06})^3$
NCov(1b_t2)	-1123.73168	0.27424	-1123.45744	-1123.29457	-1123.02033	47
TS1(1b_t2)	-1123.71135	0.27763	-1123.43372	-1123.27658	-1122.99896	103
10b_t2	-1123.74825	0.28251	-1123.46574	-1123.32337	-1123.04087	-7
TS2(1b_t2)	-1123.73591	0.28194	-1123.45397	-1123.30963	-1123.02769	28
11b_t2	-1123.74797	0.28155	-1123.46643	-1123.32281	-1123.04127	-8
TS3(1b_t2)	-1123.74341	0.27793	-1123.46548	-1123.31853	-1123.04060	-6
E-12b_t2	-1123.77978	0.28293	-1123.49685	-1123.35683	-1123.07390	-93
Z-12b_t2	-1123.78161	0.28416	-1123.49746	-1123.35837	-1123.07431	-94
TS4 <sub>5c</sub> (1b_t2)	-1123.76908	0.28465	-1123.48444	-1123.34549	-1123.06084	-59
TS4 <sub>6c</sub> (1b_t2)	-1123.75413	0.28758	-1123.46655	-1123.33802	-1123.05045	-32
13b_t2	-1123.77072	0.28467	-1123.48605	-1123.34874	-1123.06407	-68
E-13b_t2	<b>ring opening</b>					
14b_t2	-1123.75511	0.28576	-1123.46935	-1123.33925	-1123.05349	-40
15b_t2	-1123.77029	0.28685	-1123.48344	-1123.35657	-1123.06972	-82
E-15b_t2	-1123.78201	0.28909	-1123.49292	-1123.36947	-1123.08038	-110
16b_t2	-1123.77341	0.28716	-1123.48625	-1123.34868	-1123.06070	-59
17b_t2	-1123.80600	0.28003	-1123.52597	-1123.37515	-1123.09512	-149
E-17b_t2	-1123.80312	0.27947	-1123.52365	-1123.37220	-1123.09273	-143
18b_t2	-1123.79875	0.28183	-1123.51692	-1123.37245	-1123.09062	-137

<sup>1</sup> B3LYP = B3LYP(SMD,ACN)/6-311+G(2df,p)//B3LYP(SMD,ACN)/6-31G(d,p); M06 = M06-2X(SMD,ACN)/6-311++G(3df,2pd) //B3LYP(SMD,ACN)/6-31G(d,p). <sup>2</sup>  $E_{\text{scf}}$ ,  $G_{\text{corr}}$ , and  $G_{\text{tot}}$  are given in a.u.  $\Delta G_{\text{rel}}$  is given in kJ mol<sup>-1</sup>.  $\Delta G_{\text{rel}}$  is calculated using the equation:  $\Delta G_{\text{rel}}(\text{Structure}) = G_{\text{tot}}(\text{Structure}) - [G_{\text{tot}}(\mathbf{1b\_t2}) + G_{\text{tot}}(\mathbf{DMAD})]$ .

Table S2. (contd.)

Structure	$E_{\text{scf}}(\text{B3LYP})$	$G_{\text{corr}}$	$G_{\text{tot}}(\text{B3LYP})$	$E_{\text{scf}}(\text{M06})$	$G_{\text{tot}}(\text{M06})$	$\Delta G_{\text{rel}}(\text{M06})^3$
NCov(1c_t1)	-1242.92411	0.36801	-1242.55610	-1242.42116	-1242.05315	30
TS1(1c_t1)	-1242.89782	0.37442	-1242.52340	-1242.40141	-1242.02700	99
10c_t1	-1242.92199	0.37979	-1242.54220	-1242.43725	-1242.05746	19
TS2(1c_t1)	-1242.91392	0.38058	-1242.53334	-1242.42491	-1242.04433	53
11c_t1	-1242.92932	0.38010	-1242.54923	-1242.44159	-1242.06149	8
TS3(1c_t1)	-1242.92108	0.37694	-1242.54415	-1242.43350	-1242.05657	21
E-12c_t1	-1242.96302	0.37984	-1242.58318	-1242.47682	-1242.09698	-85
Z-12c_t1	-1242.95167	0.38134	-1242.57033	-1242.47037	-1242.08903	-64
TS4 <sub>sc</sub> (1c_t1)	-1242.93757	0.38311	-1242.55447	-1242.45502	-1242.07192	-19
TS4 <sub>6c</sub> (1c_t1)	<b>ring opening</b>					
13c_t1	-1242.93968	0.38327	-1242.55641	-1242.45808	-1242.07481	-27
E-13c_t1	<b>ring opening</b>					
14c_t1 <sup>4</sup>	-1242.92886	0.38357	-1242.54529	-1242.44173	-1242.05877	15
15c_t1	-1242.94126	0.38305	-1242.55821	-1242.46473	-1242.08168	-45
E-15c_t1	-1242.95457	0.38457	-1242.57000	-1242.47803	-1242.09347	-76
16c_t1	-1242.92606	0.38447	-1242.54159	-1242.45422	-1242.06975	-14
17c_t1	-1242.98168	0.37785	-1242.60384	-1242.48582	-1242.10798	-114
E-17c_t1	-1242.97869	0.37785	-1242.60084	-1242.48509	-1242.10724	-112
18c_t1	-1242.96046	0.37813	-1242.58233	-1242.47065	-1242.09252	-73

<sup>1</sup> B3LYP = B3LYP(SMD,ACN)/6-311+G(2df,p)//B3LYP(SMD,ACN)/6-31G(d,p); M06 = M06-2X(SMD,ACN)/6-311++G(3df,2pd) //B3LYP(SMD,ACN)/6-31G(d,p). <sup>2</sup>  $E_{\text{scf}}$ ,  $G_{\text{corr}}$ , and  $G_{\text{tot}}$  are given in a.u.  $\Delta G_{\text{rel}}$  is given in kJ mol<sup>-1</sup>.  $\Delta G_{\text{rel}}$  is calculated using the equation:  $\Delta G_{\text{rel}}(\text{Structure}) = G_{\text{tot}}(\text{Structure}) - [G_{\text{tot}}(\mathbf{1c\_t1}) + G_{\text{tot}}(\mathbf{DMAD})]$ . <sup>4</sup> Partially-optimized point taken from the Scan calculations at the inflection point. Optimization of the TS structure did not converge.

Table S2. (contd.)

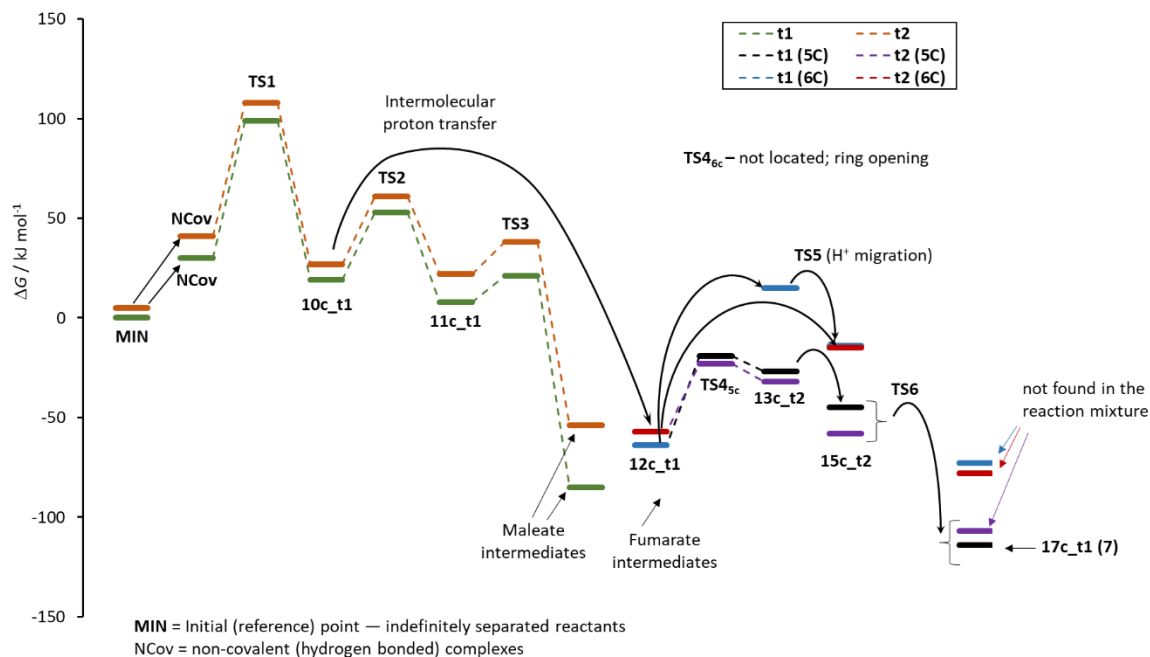
Structure	$E_{\text{scf}}(\text{B3LYP})$	$G_{\text{corr}}$	$G_{\text{tot}}(\text{B3LYP})$	$E_{\text{scf}}(\text{M06})$	$G_{\text{tot}}(\text{M06})$	$\Delta G_{\text{rel}}(\text{M06})^3$
NCov(1c_t2)	-1242.92146	0.36859	-1242.55287	-1242.41772	-1242.04913	41
TS1(1c_t2)	-1242.89318	0.37533	-1242.51785	-1242.39876	-1242.02343	108
10c_t2	-1242.92400	0.38114	-1242.54286	-1242.43538	-1242.05424	27
TS2(1c_t2)	-1242.91212	0.37855	-1242.53357	-1242.41989	-1242.04133	61
11c_t2	-1242.92485	0.37923	-1242.54561	-1242.43537	-1242.05614	22
TS3(1c_t2)	-1242.91580	0.37622	-1242.53958	-1242.42618	-1242.04996	38
E-12c_t2	-1242.95221	0.37937	-1242.57284	-1242.46448	-1242.08512	-54
Z-12c_t2	-1242.95012	0.37936	-1242.57076	-1242.46582	-1242.08646	-57
TS4 <sub>sc</sub> (1c_t2)	-1242.94073	0.38303	-1242.55771	-1242.45631	-1242.07328	-23
TS4 <sub>6c</sub> (1c_t2)	ring opening					
13c_t2	-1242.94293	0.38300	-1242.55993	-1242.45960	-1242.07660	-32
E-13c_t2	ring opening					
14c_t2	ring opening					
15c_t2	-1242.94526	0.38208	-1242.56318	-1242.46893	-1242.08685	-58
E-15c_t2	-1242.95590	0.38296	-1242.57294	-1242.47842	-1242.09546	-81
16c_t2	-1242.92394	0.38368	-1242.54025	-1242.45352	-1242.06983	-14
17c_t2	-1242.97853	0.37646	-1242.60207	-1242.48200	-1242.10554	-107
E-17c_t2	-1242.97582	0.37731	-1242.59850	-1242.47947	-1242.10216	-99
18c_t2	-1242.96251	0.37897	-1242.58354	-1242.47340	-1242.09443	-78

<sup>1</sup> B3LYP = B3LYP(SMD,ACN)/6-311+G(2df,p)//B3LYP(SMD,ACN)/6-31G(d,p); M06 = M06-2X(SMD,ACN)/6-311++G(3df,2pd) //B3LYP(SMD,ACN)/6-31G(d,p). <sup>2</sup>  $E_{\text{scf}}$ ,  $G_{\text{corr}}$ , and  $G_{\text{tot}}$  are given in a.u.  $\Delta G_{\text{rel}}$  is given in kJ mol<sup>-1</sup>.  $\Delta G_{\text{rel}}$  is calculated using the equation:  $\Delta G_{\text{rel}}(\text{Structure}) = G_{\text{tot}}(\text{Structure}) - [G_{\text{tot}}(\mathbf{1c\_t2}) + G_{\text{tot}}(\mathbf{DMAD})]$ .

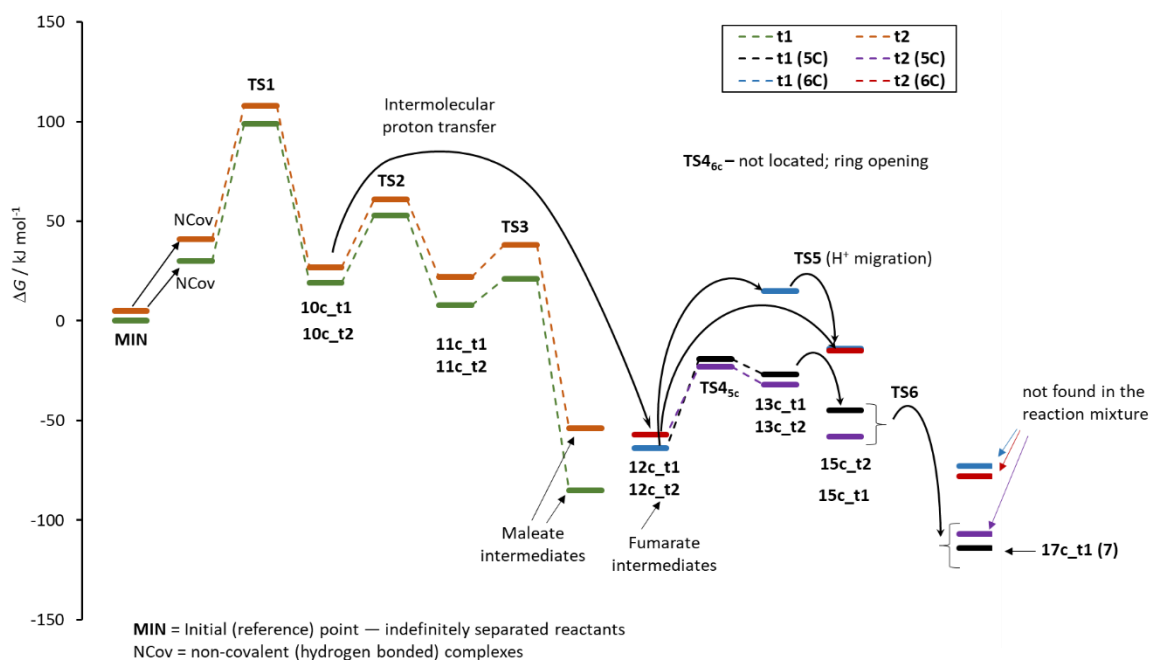


### S3. The reaction energy profiles calculated for **1a** and **1c**

Calculation method: M06-2X(SMD=ACN)/6-311++G(3df,2pd)//B3LYP(SMD=ACN)/6-31G(d,p)



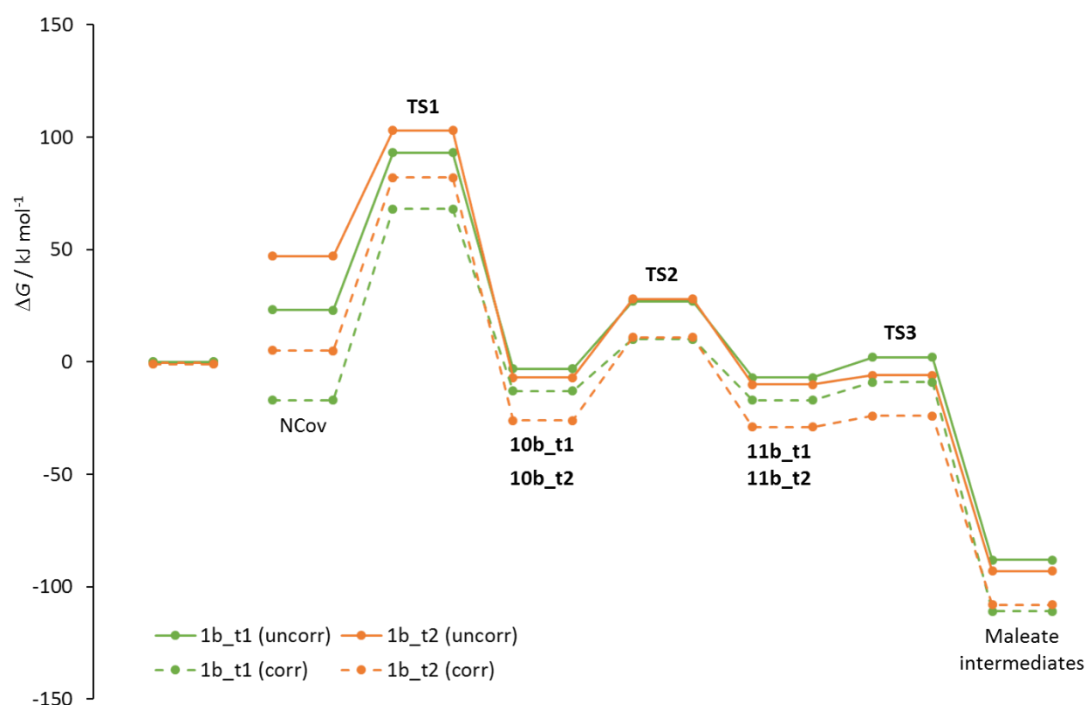
**Figure S1.** Energy profile for the AMA/CYC reaction of the tautomers of furfurylguanidine **1a**. Only the lowest energy points are labeled.



**Figure S2.** Energy profile for the AMA/CYC reaction of the tautomers of furfurylguanidine **1c**. Only the lowest energy points are labeled.

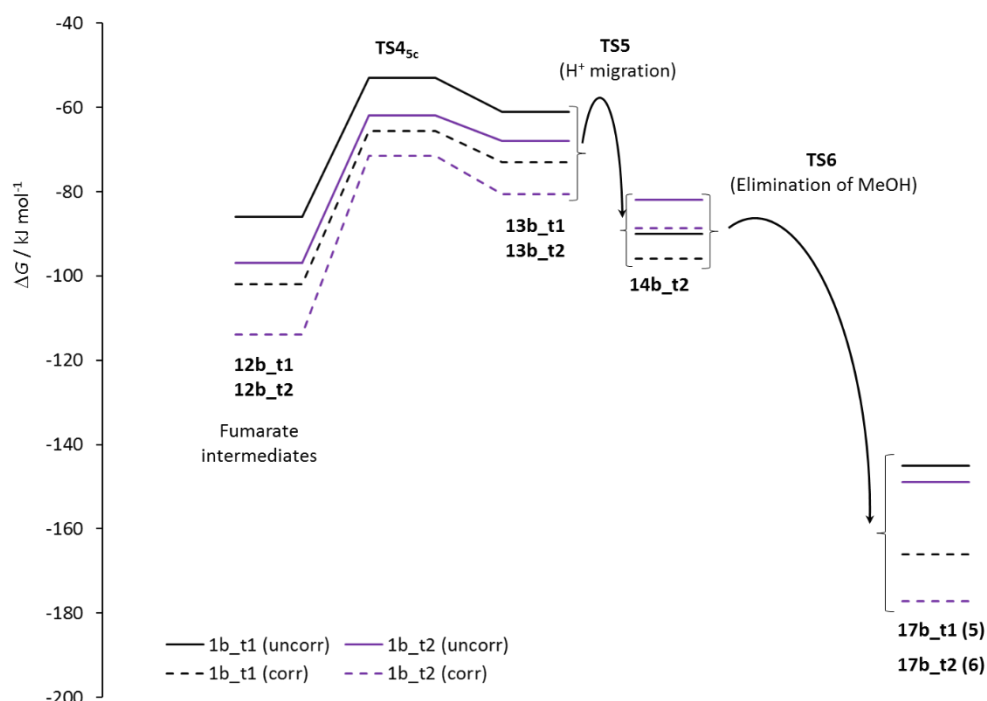
## S4. The Entropy correction approach

- Gibbs energies of the stationary points along the reaction paths starting from **1b\_t1** and **1b\_t2** were corrected for the entropy contributions of the low-energy vibrations.
- The correction approach proposed by Cramer and Truhlar [1] was applied in which all vibrations below 100 cm<sup>-1</sup> were shifted to 100 cm<sup>-1</sup> and the vibrational entropy was recalculated.
- The uncorrected and corrected energy profiles were compared in Figures S3 and S4.
- The color coding was taken from the Figure 3 in the main text.



**Figure S3.** The first part of the uncorrected (solid lines) and corrected (dashed lines) reaction profiles starting from **1b\_t1** (green) and **1b\_t2** (yellow) tautomers.

Correction for the entropy contributions lowered the relative energies of covalently bonded structures by approximately 20-30 kJ mol<sup>-1</sup> giving no change in the qualitative interpretation. The main difference is visible in the energetics of the non-covalent intermediates (**NCov**, Fig. S3) where the stabilization amounts more than 40 kJ mol<sup>-1</sup>. This confirms an entropy as the main source of the unusually high energy of the **NCov** type of the intermediates. The barrier for the intramolecular cyclization step was reduced from -53 to -66 kJ mol<sup>-1</sup> (33 and 36 kJ mol<sup>-1</sup> above intermediates **12b\_t1** for the uncorrected and corrected approach, respectively) and they are not considered as the reaction rate determining step. However, they do discriminate between the intramolecular cyclization to the smaller and larger ring. Both approaches predict the formation of the imidazolidinone system as the more favorable process.



**Figure S4.** The second part of the uncorrected (solid lines) and corrected (dashed lines) reaction profiles starting from **1b\_t1** (black) and **1b\_t2** (purple) tautomers

The second important point is the difference in the relative energies of the products **17b\_t1** and **17b\_t2**. These structures correspond to the isolated products **5** and **6**, respectively, and their energy difference is compared with their relative abundance obtained experimentally (Figure 1, the main text). Entropy corrected approach predicts significantly larger difference in their relative energies ( $11 \text{ kJ mol}^{-1}$ ) with respect to the uncorrected approach ( $4 \text{ kJ mol}^{-1}$ ). Although both approaches favor the same isomer, the large difference obtained by entropy corrected approach would imply the absence of the NMR detectable amount of the other isomer. In this respect, the uncorrected data led to better agreement with the experiment. The described feature is consequence of the molecule of methanol hydrogen bonded to the product that remained for the sake of consistency with other structures along the considered paths. Therefore, we decided to present the uncorrected results since they provide trends in relative energies consistent with the entropy corrected ones and better agreement with the experimental results.

## S5. Comparison of selected density functionals

Relative energies of all possible products (Scheme 1 in the main text) were calculated by five selected DFT methods. Besides B3LYP and M06-2X approach used for the reaction path calculations, The M08-HX in conjunction with the Jensen's polarization consistent basis sets as well as M11 and wB97xD functionals with Dunning's augmented correlation consistent basis sets were employed. These three methods were recommended by Molteni and Ponti [2] and by Yepes et al. [3] as the very good methods for the kinetics and thermodynamics of the reactions.

B3LYP: B3LYP(SMD)/6-311+G(2df,p)//B3LYP(SMD)/6-31G(d,p)

M06-2X: M06-2X(SMD)/6-311++G(3df,2pd)//B3LYP(SMD)/6-31G(d,p)

M08-HX: M08-HX(SMD)/pcseg-3//M08-HX/pcseg-2

M11: M11(SMD)/aug-cc-pvtz//M11(SMD)/6-31+G(d,p)

wB97xD: wB97xD(SMD)/aug-cc-pvtz//wB97xD(SMD)/6-31+G(d,p)

In all cases the solvent of choice was acetonitrile and it was approximated as the dielectric continuum with the dielectric constant of 35.688 as implemented in Gaussian16.

The relative amount of the isomer  $i$  ( $\gamma_i$ ) were calculated using the equation (S1):

$$\gamma_i = e^{-\frac{\Delta G_{\text{rel}}}{RT}} \quad (\text{S1})$$

where  $\Delta G_{\text{rel}}$  is the Gibbs energy of the product  $i$  relative to the most stable product.

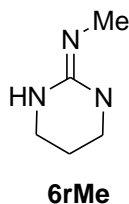
This is a variant of the approach used by Molteni and Ponti [2] except that the relative Gibbs energies of the final products instead of the relative enthalpies of the key TS structures were used.

**Table S3.** The product abundances ( $\Upsilon$ ) relative to the most stable one calculated by different DFT approaches using the equation (S1).

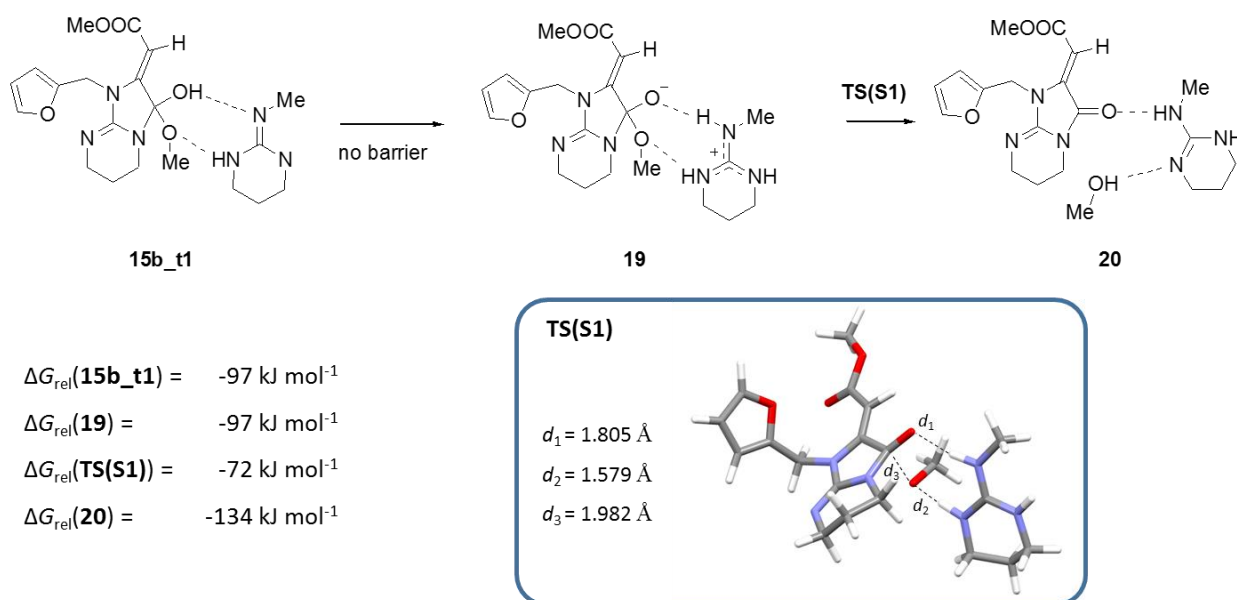
Ratios	Exp.	M08-HX		M06-2X		M11		B3LYP		wB97xD	
	$\Upsilon$	$\Delta G_{\text{rel}}$	$\Upsilon$	$\Delta G_{\text{rel}}$	$\Upsilon$	$\Delta G_{\text{rel}}$	$\Upsilon$	$\Delta G_{\text{rel}}$	$\Upsilon$	$\Delta G_{\text{rel}}$	$\Upsilon$
17a_t1	-	21.7	0.00	31.2	0.00	26.8	0.00	22.1	0.00	21.3	0.00
E-17a_t1	-	33.3	0.00	41.9	0.00	35.1	0.00	29.6	0.00	28.3	0.00
17a_t2	1.00	4.3	<b>0.18</b>	14.0	0.00	15.9	0.00	2.0	0.45	12.8	0.01
E-17a_t2	-	25.9	0.00	32.3	0.00	38.1	0.00	17.5	0.00	30.2	0.00
18a_t1	0.33	0.9	<b>0.69</b>	8.8	0.03	4.0	0.20	11.1	0.01	0.0	1.00
18a_t2	0.39	0.0	<b>1.00</b>	0.0	1.00	0.0	1.00	0.0	1.00	4.6	0.16
17b_t1	0.50	2.1	<b>0.44</b>	4.7	0.15	0.0	1.00	10.5	0.01	0.1	0.96
E-17b_t1	-	10.2	0.02	11.5	0.01	8.8	0.03	15.1	0.00	8.4	0.03
17b_t2	1.00	0.0	<b>1.00</b>	0.0	1.00	0.5	0.83	0.0	1.00	0.0	1.00
E-17b_t2	-	8.5	0.03	12.7	0.01	9.1	0.03	14.0	0.00	7.6	0.05
18b_t1	-	14.6	0.00	15.2	0.00	11.7	0.01	31.3	0.00	17.9	0.00
18b_t2	-	18.1	0.00	18.9	0.00	14.8	0.00	36.6	0.00	22.2	0.00
17c_t1	1.00	0.0	<b>1.00</b>	0.0	1.00	0.1	0.94	0.0	1.00	0.3	0.90
E-17c_t1	0.23	2.7	<b>0.34</b>	1.7	0.51	0.0	1.00	4.9	0.14	0.0	1.00
17c_t2	-	9.0	0.03	12.2	0.01	8.2	0.04	8.1	0.04	4.8	0.15
E-17c_t2	-	11.6	0.01	12.1	0.01	14.2	0.00	11.1	0.01	9.0	0.03
18c_t1	-	48.3	0.00	45.7	0.00	45.3	0.00	62.3	0.00	52.3	0.00
18c_t2	-	43.5	0.00	40.9	0.00	38.0	0.00	59.3	0.00	43.4	0.00

## S6. The methanol elimination catalyzed with guanidine

The steps within the suggested mechanism that are assumed to occur due to intermolecular interactions are modeled using guanidine **6rMe** as the catalyst and / or a supporting molecule for the proton shift.



**Figure S5.** Structure of the guanidine catalyst **6rMe** representing the simplified **1b\_t1** structure.



**Figure S6.** Calculated relative Gibbs energies ( $\Delta G_{\text{rel}}$ ) for the methanol elimination step catalyzed with guanidine. The values are calculated relative to the sum of the Gibbs energies of the guanidine **1b\_t1**, **DMAD**, and guanidine catalyst **6rMe**.

## S7. Cartesian coordinates

### S7.1. G3 Optimized geometries

#### **1aH<sup>+</sup>**

C 0.240948 0.079294 0.095551  
N 0.539287 -0.775482 1.069933  
C 1.691474 -0.301009 1.835088  
C 2.319614 0.693091 0.850583  
N 1.179241 1.008427 -0.010802  
H -0.161131 -1.363768 1.471251  
H 2.352255 -1.117766 2.07947  
H 1.366003 0.185402 2.745633  
H 3.11297 0.239966 0.270598  
H 2.689517 1.583472 1.333902  
H 1.267658 1.597262 -0.811101  
N -0.838966 -0.01549 -0.649608  
C -1.237514 0.934633 -1.689527  
C -2.204148 0.298663 -2.626612  
H -1.698941 1.806636 -1.246366  
H -0.357954 1.2472 -2.235631  
C -3.502415 0.521682 -2.875804  
C -3.874539 -0.411296 -3.909713  
C -2.764774 -1.109928 -4.182114  
O -1.739833 -0.693228 -3.415159  
H -2.551639 -1.903444 -4.866162  
H -4.834959 -0.528763 -4.368235  
H -4.125434 1.249555 -2.397122  
H -1.515373 -0.696529 -0.368689

#### **1a\_t1**

C 0.2608827016 0.0087151 0.0148626769  
N 0.5238908068 -0.6899281043 1.1692605503  
C 1.4359817557 0.0697103675 2.0110698943  
C 2.1905759698 0.8838675528 0.9613506762  
N 1.166188066 1.0357365116 -0.0635825119  
H -0.2563416204 -1.1433421307 1.5956724637  
H 2.0845170285 -0.5817886694 2.579576002  
H 0.9022510115 0.7201418547 2.6979636241  
H 3.0497022119 0.3372464552 0.5852134001  
H 2.5206611301 1.8438440751 1.3322867752  
H 1.4437221827 1.3502698813 -0.9690395245  
N -0.6784904255 -0.2912129713 -0.7837502927  
C -0.829134663 0.5223865551 -1.9671088979  
C -2.0571060985 0.1122591541 -2.7174887201  
H -0.9135182195 1.5841731777 -1.7331912756  
H 0.0226587475 0.4322208459 -2.6427888167  
C -3.0136544992 -0.807847801 -2.5173689761  
C -3.9265134073 -0.682779829 -3.6301538681

C -3.4367646474 0.2983968533 -4.3957838966  
O -2.3014302085 0.7928299764 -3.8564402763  
H -3.7589271619 0.7448048055 -5.3123338391  
H -4.8144806869 -1.253676568 -3.8128216976  
H -3.0781739736 -1.4910590923 -1.6969584697

#### 1a\_t2

C 0.2690074093 0.1504381254 0.1251336102  
N 0.170758332 -0.0568173271 1.4882380095  
C 1.3106969397 0.6424850221 2.0771228312  
C 2.2505316742 0.7407672217 0.8608623302  
N 1.3877685517 0.5726152523 -0.3074641278  
H -0.7257621672 0.1199024082 1.8943315949  
H 1.7344514167 0.084901831 2.9015531002  
H 1.0197640639 1.624917576 2.4367425044  
H 3.0013067564 -0.0454962608 0.8845738311  
H 2.7774852921 1.6873682268 0.8270036437  
N -0.8281684481 -0.108655506 -0.6366423696  
C -0.7063911893 -0.1904765877 -2.0824176756  
C -2.0508113953 -0.2333042369 -2.7274166965  
H -0.1647086725 0.6804614911 -2.4245496205  
H -0.1505997792 -1.0688688172 -2.393542841  
H -1.4736527537 -0.7536825011 -0.2298903168  
C -2.6777032638 -1.1719952786 -3.4530881484  
C -3.9550953421 -0.6106397278 -3.81802307  
C -3.9783314911 0.6134511234 -3.2759864398  
O -2.8327904211 0.8608279017 -2.6123369135  
H -4.7063027782 1.3965537219 -3.2718321418  
H -4.72910089 -1.0690378587 -4.3991257775  
H -2.2950048444 -2.1404287996 -3.7046023165

#### 1bH<sup>+</sup>

C -0.0635268286 1.063706493 -0.1261343825  
N -0.2143293604 2.0040809079 0.7891350673  
N 1.0862015624 0.9176435085 -0.7793203841  
C -1.4498963231 2.2169829854 1.5456090675  
H 0.5125778103 2.6755156092 0.9054254478  
C -2.2283321298 0.9150411338 1.6327857116  
H -1.1690190909 2.5714781079 2.5264599259  
H -2.0389621431 2.9851368307 1.0592085987  
C -2.3740645773 0.3142481978 0.2444284089  
H -1.7083132742 0.2175452924 2.2805324251  
H -3.2067100032 1.105984745 2.0554008911  
N -1.0568130872 0.2264892128 -0.382391871  
H -2.7752614784 -0.6872991932 0.2911123176  
H -3.0319676902 0.9185472038 -0.3692179186  
H -0.9036108109 -0.4780494903 -1.0726384457  
C 2.2667867589 1.7661728268 -0.6278839173  
H 2.1047382698 2.7371381643 -1.0779637805  
H 2.4723411757 1.9030919659 0.42616609



C 3.4419765691 1.1251657261 -1.2805370359  
C 4.1746551863 1.4548100797 -2.3537716488  
C 5.1902688884 0.4383015276 -2.4693052613  
C 4.9700164267 -0.4092458915 -1.4559686215  
O 3.9145686735 -0.0090954749 -0.7220972473  
H 5.4557014092 -1.3063347321 -1.1360224989  
H 5.9617158205 0.3672810169 -3.208426889  
H 4.0253773776 2.3044986085 -2.988448748  
H 1.0833588684 0.2773496376 -1.5456703009

#### 1b\_t1

C 0.0563616708 0.8727678337 0.0289373934  
N -0.1367422221 1.9118033237 0.8910014106  
N 1.1292724993 0.6390238666 -0.6271904361  
C -1.4485282871 2.3376443382 1.3654210562  
H 0.5424235338 2.6381478312 0.8416492765  
C -2.3536530837 1.1313083454 1.5465590509  
H -1.3074254372 2.8610020958 2.3022964083  
H -1.900292424 3.0338968733 0.663078398  
C -2.3436890775 0.310967941 0.2680828253  
H -1.9983584321 0.5226506391 2.3722339115  
H -3.3609260623 1.4597578707 1.7762100921  
N -0.9697730282 -0.0323959111 -0.0575844754  
H -2.894954435 -0.6118201195 0.3949831713  
H -2.818219786 0.8712187113 -0.5357519927  
H -0.8437082656 -0.6783713955 -0.8070202215  
C 2.25079033 1.5390534399 -0.4590356269  
H 2.031587097 2.5515623578 -0.7955560577  
H 2.5584311339 1.6193540051 0.5845387965  
C 3.4281571885 1.0683680449 -1.2508916529  
C 4.096369515 1.5936816158 -2.2903517963  
C 5.1585206472 0.6662274981 -2.5984116504  
C 5.0327948643 -0.3308729649 -1.7145788702  
O 3.9918186668 -0.1026947049 -0.8886831012  
H 5.5797788127 -1.2346670154 -1.5493068703  
H 5.8967056827 0.7487630124 -3.3702484604  
H 3.8743638989 2.5171804675 -2.786102579

#### 1b\_t2

C -0.8959972992 -0.0052116743 -0.3674442102  
N -1.4962866005 0.1609243595 0.7389442035  
C -1.1229426469 1.2954887945 1.5703086698  
N 0.0175642726 0.8524938874 -0.9309884048  
H 0.6400717452 0.4309949632 -1.5879765324  
N -1.1405077178 -1.116425785 -1.1463735282  
C -2.2655895335 -1.9806085937 -0.8365210313  
C -2.2597868209 -3.1866483043 -1.7160129156  
H -2.1887211697 -2.2857227382 0.1973479426  
H -3.2180734847 -1.4746019729 -0.9585800454  
O -1.2515322933 -4.0702219739 -1.5568446371

C -1.4503954214 -5.0770143705 -2.4292635115  
C -2.5617063544 -4.8675580191 -3.1459885592  
C -3.0970474417 -3.6141274416 -2.6739282407  
H -3.9836275137 -3.1157823482 -3.0103305291  
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H -2.0130415435 1.6403767195 2.0872804189  
H -0.4326842102 0.9624886153 2.3441175115  
C -0.4944122184 2.4507458764 0.7959007001  
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H -1.2502392069 2.9447339731 0.1912463784  
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H 1.4245223606 1.5301778291 0.4828444351

### 1cH<sup>+</sup>

C 0.1455778506 0.4814245667 0.9232843496  
N 0.6426521833 0.260374922 2.130692018  
N 0.9560799872 0.8401061104 -0.0705857116  
N -1.1559456002 0.364581104 0.6976572543  
H 0.0402463456 -0.1840098514 2.7896549604  
C 2.0081060785 0.5353641224 2.6065278875  
H -1.4408731894 0.307495424 -0.2564837146  
C -2.2243555324 0.1553613286 1.6867810245  
H -1.8948215934 0.5933166476 2.6183716436  
C -3.4582348021 0.914080073 1.2107900074  
C -2.5096558617 -1.3313218703 1.8861623506  
C 1.916333676 1.0081682567 4.0530932537  
C 2.8977127333 -0.6965223951 2.4628465641  
H 2.4056127033 1.3444198576 2.0098274386  
C 0.5666053933 1.3875336902 -1.3657966962  
C 0.463405125 0.3598251154 -2.4440168704  
H 1.3222167692 2.1056052374 -1.6467318118  
H -0.3658772844 1.9245737487 -1.256813879  
O -0.5164619034 -0.5622059715 -2.32045398  
C -0.4431956698 -1.3788038791 -3.3926323392  
C 0.5542515473 -1.001383225 -4.2009723303  
C 1.1558828956 0.1493131599 -3.5718143753  
H 1.9865939486 0.7258580949 -3.9249829601  
H 0.8414791469 -1.4654808721 -5.122224255  
H -1.1603986256 -2.1701924043 -3.4343004313  
H 1.9347065414 0.7187658041 0.0722582052  
H -3.2911574273 -1.4638519705 2.6271281975  
H -2.8401115199 -1.7825383483 0.9554280455  
H -1.6264944921 -1.8619155813 2.2267041912  
H -4.2632514282 0.7957016103 1.9274406949  
H -3.244559927 1.9721162917 1.1045924947  
H -3.8004395261 0.5330778922 0.2526450101  
H 2.9072820441 1.2363807404 4.4293104796

H	1.3047557981	1.9005541914	4.1305701845
H	1.4844238651	0.2373362633	4.6851300789
H	3.9007344525	-0.4734978698	2.8115894151
H	2.5053946297	-1.5196634488	3.0523765427
H	2.9627806684	-1.0188395653	1.4285342335

#### 1c\_t1

C	1.3002778968	0.2686462433	0.9113701204
N	2.5838195682	0.660842059	0.5645107507
N	1.0793000687	-0.9641170965	1.2599466662
N	0.3397381908	1.2655317393	0.8437319688
C	0.6350424441	2.7033146078	0.9146308623
H	-0.5087573427	1.0345657373	1.3550774655
H	2.6207358044	1.4256365991	-0.1055488322
C	3.6169327516	-0.3471940288	0.3208844017
C	-0.2736144635	-1.2821155915	1.7060950472
C	1.2064920759	3.1143812553	2.2662119709
C	-0.6547471467	3.4469266364	0.6025316666
H	1.3579834602	2.9432121294	0.1283821428
H	3.5592706908	-1.0528184081	1.1537052467
C	3.3974028367	-1.1035148249	-0.984098094
C	4.9666154525	0.3536831669	0.3434885284
H	-1.0202011071	-1.0720544321	0.9223607866
H	-0.5781648896	-0.7027610973	2.5931137603
C	-0.3598315473	-2.717533343	2.076026415
H	4.1797190828	-1.8555121627	-1.1319275111
H	2.4295176674	-1.6093093941	-0.9721280247
H	3.425517964	-0.4088945271	-1.8309079977
H	5.7757811923	-0.3682862955	0.1988129434
H	5.0257572918	1.0945954794	-0.4618265565
H	5.1222271865	0.8668579785	1.2965555933
H	-0.4817484149	4.5266897375	0.6080950593
H	-1.0417764191	3.158720166	-0.3785234356
H	-1.4156972742	3.2200359215	1.357573388
H	1.4174550348	4.1886696203	2.2831713882
H	0.4842918314	2.8913642457	3.0587642597
H	2.1345079603	2.5769079524	2.474260861
C	-0.5064014601	-3.3856175978	3.2615447257
C	-0.4970934886	-4.779644484	2.954713501
C	-0.3434073131	-4.8693868051	1.6012392065
O	-0.2597707004	-3.6219364881	1.0495326762
H	-0.2798355812	-5.6962878285	0.9077441728
H	-0.5908891385	-5.6085596162	3.6440372356
H	-0.6074261648	-2.9272122537	4.237075641

#### 1c\_t2

C	-0.8493651505	0.0296617036	-0.4755077332
N	-1.4173967759	0.1445053501	0.683188617
C	-1.0363311814	1.2496630486	1.5594842097
N	0.0103004258	0.93708443	-1.0826912611

C 1.1037968169 0.5128860623 -1.97242643  
N -1.1098861766 -1.0978468529 -1.2506358295  
C -2.1616635138 -2.0019589569 -0.7931612411  
C -2.2390548129 -3.1787782593 -1.6927555032  
H -1.921634921 -2.3145786924 0.226482149  
H -3.1492770002 -1.5210948853 -0.7579431415  
O -1.1914508824 -4.063193456 -1.649021462  
C -1.4630007933 -5.0518508669 -2.5521779707  
C -2.6584702993 -4.8171079094 -3.1683161674  
C -3.1600644506 -3.6023568518 -2.613406689  
H -4.0868028915 -3.0990755228 -2.8580129047  
H -3.1203515266 -5.4379097872 -3.9247138497  
H -0.7199983373 -5.8330243847 -2.631777513  
C -1.2687612065 0.8071174347 2.9972071212  
H 0.0336540308 1.4989604749 1.4580400551  
C -1.8568696797 2.4935114047 1.2290477537  
H 0.3197941094 1.6645873303 -0.4415991357  
C 1.715013975 1.7689793055 -2.5736219071  
C 2.1466321546 -0.3287254073 -1.2476094115  
H 0.6675070875 -0.0775600204 -2.7831637291  
H 2.9449662135 -0.6283205543 -1.9346896807  
H 2.5927410873 0.2494480587 -0.4312511009  
H 1.6943835995 -1.2329842802 -0.8323886528  
H -0.9905365755 1.5975847482 3.702028208  
H -2.3256394434 0.5634624581 3.145505605  
H -0.6768967296 -0.0843765532 3.2250353453  
H -1.6202168444 3.3149634772 1.9136422398  
H -1.6650567667 2.8327046917 0.2066858003  
H -2.9230448103 2.2620358699 1.3193841095  
H -1.1750645107 -0.900667765 -2.2473790402  
H 2.5135262922 1.5071914121 -3.2735631465  
H 0.9589477426 2.3518584634 -3.1066437916  
H 2.1458787451 2.3965292823 -1.7854429217

## 9H

C -0.25033607 0.2469728768 -0.0682378327  
O -0.0879080996 0.0199175077 1.2044321856  
O 0.6098658934 0.6048621792 -0.8107262294  
C 1.219197842 0.2152185245 1.747394019  
C -1.6647266216 0.0124187944 -0.5439916635  
H 1.1342417831 -0.0232833044 2.7949185209  
H 1.9235384055 -0.4466736718 1.2664489254  
H 1.5247945338 1.2426241657 1.6187323895  
C -1.9290223098 0.2168621039 -1.8223593571  
C -3.2351045936 0.0548646446 -2.5233679005  
O -3.089216152 0.3549315967 -3.7958336145  
O -4.2625170858 -0.2891939771 -2.0312043526  
C -4.2397374224 0.2584397588 -4.6309068509  
H -3.9086154327 0.5423232593 -5.6168895336  
H -4.612823385 -0.7552522454 -4.639830199

H -5.0103224164 0.9329402623 -4.2872601588  
Cl -2.8150467336 -0.5056524046 0.636991996  
H -1.1130271351 0.5380469296 -2.4384543437

#### DMAD

C 0.0717134319 0.0295736226 -0.2122909237  
O -0.0404939993 -0.0291039367 1.0862694224  
O 1.0853985399 0.0392649684 -0.831708356  
C 1.1694731379 -0.0873043413 1.8493161106  
C -1.2408324254 0.0838802585 -0.856448544  
H 0.8558111084 -0.1353361902 2.8789255976  
H 1.7320101712 -0.9697625444 1.5844524664  
H 1.7596918847 0.7998659093 1.6758817414  
C -2.2887206424 0.1254068029 -1.4104633133  
C -3.58123962 0.2204931764 -2.089450081  
O -4.0779973878 -0.9619112238 -2.3291137149  
O -4.0787092372 1.2628231649 -2.3676575893  
C -5.3455360024 -1.0210925964 -2.9920514351  
H -5.5704053433 -2.0706344295 -3.0852329064  
H -6.0977408417 -0.5251541914 -2.3974369306  
H -5.2753887745 -0.5624474492 -3.9668505438

#### S7.2. B3LYP Optimized geometries (from 1a tautomers)

##### 1a\_t1

C 0.272352 -0.009719 0.01303  
N 0.550169 -0.717592 1.175585  
C 1.441815 0.071384 2.029531  
C 2.191558 0.907206 0.981699  
N 1.163125 1.053039 -0.054921  
H -0.235466 -1.19078 1.604889  
H 2.11082 -0.56596 2.612493  
H 0.883223 0.719253 2.71941  
H 3.071179 0.368603 0.60484  
H 2.512619 1.877019 1.369083  
H 1.455923 1.359399 -0.974573  
N -0.671349 -0.331952 -0.803207  
C -0.815241 0.499977 -1.986651  
C -2.052696 0.112524 -2.735445  
H -0.873466 1.575697 -1.740786  
H 0.04736 0.408287 -2.671776  
C -3.040568 -0.803237 -2.524573  
C -3.958577 -0.675425 -3.624538  
C -3.46218 0.306994 -4.421993  
O -2.297784 0.799822 -3.894635  
H -3.788266 0.75578 -5.348479  
H -4.864249 -1.242188 -3.792412  
H -3.103805 -1.483163 -1.688126

**1a\_t2**

C 0.276957 0.103401 0.1375  
N 0.212029 -0.117316 1.516392  
C 1.314908 0.6736 2.090454  
C 2.236377 0.836415 0.855237  
N 1.376559 0.609615 -0.321674  
H -0.701115 0.011227 1.940857  
H 1.795264 0.148144 2.920425  
H 0.957082 1.645426 2.456085  
H 3.048299 0.094522 0.872494  
H 2.707721 1.824847 0.8213  
N -0.817424 -0.228571 -0.618672  
C -0.708883 -0.287775 -2.076931  
C -2.047442 -0.262266 -2.731584  
H -0.11138 0.572966 -2.391502  
H -0.181549 -1.189406 -2.416685  
H -1.437205 -0.914183 -0.203796  
C -2.736851 -1.176974 -3.473198  
C -3.977134 -0.556471 -3.844132  
C -3.952104 0.689463 -3.29791  
O -2.784969 0.888636 -2.617733  
H -4.6468 1.516413 -3.297537  
H -4.775179 -0.983347 -4.435451  
H -2.399814 -2.173079 -3.725296

**NCov(1a\_t1)**

C 1.0838098504 0.4074396551 2.0668025817  
N 1.6672426181 0.1903451158 3.3111579633  
C 2.8977242507 0.9825497445 3.4251686561  
C 2.6076086083 2.1302584567 2.4471572431  
N 1.7631833004 1.4548439369 1.4604518119  
H 1.6905155128 -0.761563726 3.6545320878  
H 3.7779795988 0.4081312044 3.1069447265  
H 3.0580245598 1.3318986319 4.4480394388  
H 3.5166356341 2.5334109581 1.9941107381  
H 2.0758370056 2.9487325295 2.9531205817  
H 1.2255350792 2.0127641505 0.8049370388  
N 0.0850021586 -0.198401395 1.5186450046  
C -0.5075165965 -1.2991379669 2.2797812943  
C -1.8801309557 -1.6315046869 1.7923364697  
H 0.0907756554 -2.2193324068 2.1956366747  
H -0.5689055016 -1.0698745676 3.3570927637  
O -2.8746382945 -0.7250519346 2.0629695873  
C -4.0337862729 -1.2207596016 1.533857378  
C -3.8051610426 -2.4221908265 0.9381147977  
C -2.4036803235 -2.6885975337 1.1068388067  
H -1.8547879109 -3.5540335157 0.7615459759  
H -4.5382419049 -3.0431323548 0.4418493956  
H -4.915892626 -0.6132178115 1.6715922013  
C 0.9534576891 0.084766917 -2.7130042903

C 0.1818036055 0.7195379679 -2.0288004378  
C 1.8868620609 -0.742049209 -3.4563753151  
C -0.679741119 1.5510497032 -1.2099387079  
O 2.0263923741 -0.3018182669 -4.7091273214  
O 2.4501096834 -1.7024378721 -2.9699768834  
C 2.941822905 -1.0577672061 -5.5413545786  
O -1.9379189086 1.1229500591 -1.2389817026  
O -0.273369386 2.5284119122 -0.6051382919  
C -2.8702459303 1.8534281486 -0.4012866557  
H -2.5645644959 1.7762671929 0.6431176867  
H -2.9128638639 2.9005797291 -0.7071395841  
H -3.8323969615 1.3688966087 -0.5578100977  
H 2.9231135548 -0.5614895603 -6.5104009147  
H 3.9475513338 -1.031784408 -5.1166755264  
H 2.6033670554 -2.091840772 -5.6333115963

#### NCov(1a\_t2)

C 0.4974175568 -1.125426568 0.810625074  
N 0.7237104639 -2.1295917612 1.7591915778  
C 2.1319801692 -2.5265155677 1.5819140104  
C 2.7063152027 -1.2860433225 0.853486004  
N 1.5481569153 -0.5986744069 0.2588465225  
H 0.0513352141 -2.8899898258 1.7643007541  
H 2.2095073771 -3.4295443147 0.96178645  
H 2.61588833 -2.7258903509 2.54215282  
H 3.4450232299 -1.5625955111 0.0922804775  
H 3.2157921508 -0.61849432 1.5651504295  
N -0.7840771456 -0.743148826 0.5392358239  
H -0.8953921047 0.0551357546 -0.0759442149  
C -1.9467996382 -1.120365202 1.3409671349  
C -2.6614595547 -2.3434292511 0.8571211926  
H -1.6434829986 -1.2579674491 2.3855397029  
H -2.655245858 -0.2894315791 1.3180750479  
O -2.0090939173 -3.5420837449 1.0195555344  
C -2.8186556811 -4.5208234773 0.5093715649  
C -3.9696733748 -3.9753547801 0.0340736116  
C -3.866895159 -2.5600814055 0.2588965863  
H -4.5954036528 -1.8015734856 0.0075933705  
H -4.7917230235 -4.5100161995 -0.421185013  
H -2.4349899521 -5.5286515806 0.5635711881  
C 1.3795906825 2.8043329867 -0.5199838579  
C 0.2080640027 2.8565794395 -0.8207978871  
C 2.7571111516 2.7344316721 -0.0658290029  
C -1.1966786118 2.7577062711 -1.1549893308  
O 3.5838769315 2.4701416517 -1.079185057  
O 3.077936962 2.9058688588 1.0932850427  
C 4.988270233 2.3705544672 -0.733677373  
O -1.6816134633 3.9027093707 -1.624949589  
O -1.8308738269 1.7244031632 -1.011593654  
C -3.0878413125 3.8969141946 -1.9856277959

H	5.499573521	2.1653781333	-1.6729346351
H	5.3393352572	3.3103738267	-0.3026601429
H	5.1457362392	1.5544210998	-0.0254296473
H	-3.2934561829	4.9046454396	-2.3426132197
H	-3.2708609688	3.1642647406	-2.7739652073
H	-3.6990231638	3.6662158594	-1.1108682928

#### TS1(1a\_t1)

C	-0.4993518012	0.0086627884	-0.2499200529
N	-0.0479819636	-0.2960267642	1.0210980303
C	0.8948592749	0.7355952549	1.4737008795
C	0.4513349547	1.9397533278	0.6322063156
N	-0.0778656858	1.2811332132	-0.566591274
H	0.1763243596	-1.2616306248	1.224408606
H	1.9305702577	0.4526774186	1.2463778264
H	0.8057610152	0.9155604681	2.5472555527
H	1.2798768219	2.6087220164	0.3889675026
H	-0.3264518193	2.5171862246	1.1498889302
H	-0.6418204334	1.8330774001	-1.2096089065
N	-1.2144237287	-0.7386518315	-1.0356396305
C	-1.5599675005	-2.0911613422	-0.6057575567
C	-2.8057569332	-2.5836054659	-1.2665256732
H	-0.7586341467	-2.7991013928	-0.8499331133
H	-1.708697499	-2.1277258211	0.4844273053
O	-3.9762258338	-1.9460699747	-0.9446297298
C	-4.9795647279	-2.5648110349	-1.6351474429
C	-4.4799187055	-3.5838843491	-2.3851878974
C	-3.0639332588	-3.5954472616	-2.1454590048
H	-2.3317164677	-4.267601385	-2.5709699587
H	-5.0435769733	-4.2439928594	-3.0298515342
H	-5.9722448327	-2.1659960117	-1.4863004259
C	-1.3937933792	-0.1669754848	-3.1482180542
C	-2.0039181803	0.8945535031	-3.367624295
C	-0.6564255603	-1.2929777294	-3.7418566721
C	-2.5873523194	2.1034113337	-2.8779221019
O	-1.0002708644	-1.4068478671	-5.0391158802
O	0.1576670981	-2.0060114048	-3.1919238154
C	-0.3083258981	-2.4398797874	-5.7744951295
O	-3.9005479047	2.1956362935	-3.1449879606
O	-1.9457299623	2.9749721905	-2.2920513495
C	-4.5624167388	3.3776889735	-2.6438139794
H	-4.4830402782	3.4323872349	-1.5554233591
H	-4.1308822573	4.2776982768	-3.087925967
H	-5.6053676919	3.2724801413	-2.9415169266
H	-0.7040338838	-2.3857628423	-6.7883677346
H	0.7685980598	-2.2555768453	-5.7763154919
H	-0.5111366121	-3.4213109792	-5.339397031

#### TS1(1a\_t2)

C	0.0812954888	0.1558044619	-0.6576379496
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N	-0.1349458845	-0.4534805767	0.5666811136
C	1.1878314405	-0.5907194628	1.2020584684
C	2.005692204	0.4779516826	0.4425531785
N	1.2742962238	0.6748126891	-0.8225471645
H	-0.7318029364	-1.274284383	0.5709366175
H	1.5930246088	-1.5973583396	1.0393917846
H	1.1326069084	-0.4057560513	2.2775781775
H	3.0352720206	0.1677358042	0.2588731204
H	2.0393460712	1.4198590826	1.0067163791
N	-0.9113198778	0.2203470146	-1.5737310496
H	-0.7213570937	0.7429456178	-2.4171527112
C	-2.3078753334	-0.1387440935	-1.3195781609
C	-2.6475746754	-1.5582296246	-1.6410507583
H	-2.5485072137	0.0765364523	-0.2723519866
H	-2.9275324352	0.5133951608	-1.9376641962
O	-2.1407654442	-2.5157675333	-0.795338766
C	-2.5536839488	-3.7332927626	-1.2644225927
C	-3.3134326568	-3.5721242955	-2.3804364445
C	-3.3734263472	-2.1581852792	-2.6260742193
H	-3.8893614559	-1.6533321663	-3.4310475553
H	-3.776275592	-4.3591748183	-2.9593889708
H	-2.2289288474	-4.5938962678	-0.6989375144
C	1.4076885549	2.4610853151	-2.0124473201
C	0.3639895724	3.0960153163	-2.2437826287
C	2.8592773297	2.4410895168	-2.2501839298
C	-1.0253506066	3.3978832013	-2.3211154019
O	3.1333609302	3.1213748988	-3.3812636707
O	3.7086689787	1.9306911991	-1.5490772004
C	4.5347491525	3.2315744735	-3.7117060124
O	-1.3850967264	4.385115578	-1.4739770753
O	-1.801340559	2.8443182601	-3.0967255846
C	-2.7782582007	4.7578987623	-1.5063851049
H	4.5684767247	3.8010935674	-4.6402422137
H	5.0762825303	3.7592513988	-2.9229468685
H	4.9746375226	2.2420408572	-3.8571232666
H	-2.8799792664	5.5614397138	-0.7769776387
H	-3.0618300866	5.1126500136	-2.5002517342
H	-3.4129120741	3.9132856164	-1.2266521491

#### 10a\_t1

C	1.296988	0.567029	1.441002
N	1.627521	0.287599	2.724018
C	2.595526	1.283152	3.216177
C	2.380847	2.440835	2.227482
N	1.802361	1.757015	1.056775
H	1.710827	-0.673153	3.031663
H	3.612609	0.881454	3.156079
H	2.381548	1.561874	4.249127
H	3.311128	2.948202	1.967004
H	1.671064	3.178563	2.618272

H	1.267215	2.323688	0.380646
N	0.545860	-0.223768	0.668740
C	0.006750	-1.487321	1.239088
C	-1.231054	-1.942849	0.552429
H	0.757487	-2.277805	1.167987
H	-0.216579	-1.303690	2.294112
O	-2.370675	-1.213063	0.767041
C	-3.374296	-1.821628	0.071863
C	-2.905786	-2.925667	-0.572088
C	-1.508119	-3.004113	-0.259474
H	-0.799253	-3.748085	-0.595060
H	-3.479285	-3.599611	-1.192931
H	-4.346228	-1.355536	0.138544
C	0.479606	0.004223	-0.792061
C	-0.135638	1.020976	-1.396254
C	1.258040	-1.041774	-1.516524
C	-0.763216	2.152626	-0.822238
O	1.101886	-0.987878	-2.853979
O	1.973158	-1.873496	-0.972873
C	1.853464	-1.958883	-3.602846
O	-2.123467	2.141669	-0.898052
O	-0.150247	3.159967	-0.406189
C	-2.785342	3.333559	-0.448164
H	-2.558085	3.545792	0.600597
H	-2.502463	4.198910	-1.054611
H	-3.852769	3.137069	-0.561680
H	1.611980	-1.771785	-4.649686
H	2.927173	-1.835628	-3.437479
H	1.562779	-2.975997	-3.326508

#### 10a\_t2

C	0.3539824618	-0.5419705628	0.8141834355
N	0.4746045944	-1.6342897088	1.5992758593
C	1.7591836386	-2.3064581861	1.3387351929
C	2.5426087647	-1.2447234595	0.540322659
N	1.5018905967	-0.257107076	0.1740116286
H	-0.3463074685	-2.1988363918	1.7878290933
H	1.5911275527	-3.2155033696	0.7536191434
H	2.2549016323	-2.5747717722	2.2736090017
H	3.0069052621	-1.6541638173	-0.3595627166
H	3.3040266793	-0.7555977067	1.149759232
N	-0.7590142901	0.1876294008	0.707356795
H	-0.8697692782	0.7345687614	-0.1591005714
C	-1.9789302363	-0.0657514292	1.4898376865
C	-2.8483047453	-1.1667343283	0.9766063264
H	-1.6917430841	-0.2604146491	2.5279385079
H	-2.5534317826	0.8618205154	1.4783569686
O	-2.4392035796	-2.4520459452	1.2493264176
C	-3.3555786775	-3.2993364085	0.6871815802
C	-4.3365496213	-2.5858803007	0.0731668003

C	-4.0064581505	-1.20110071	0.2595107243
H	-4.5597071735	-0.3416283614	-0.0928903759
H	-5.1930191485	-2.9911480658	-0.4471309022
H	-3.1676489762	-4.3542086825	0.8192388332
C	1.8192656974	1.036149226	-0.4351497455
C	1.2671803547	1.5176105267	-1.5534870922
C	2.7715316943	1.8190891286	0.4074858672
C	0.2112305393	0.9367166612	-2.3017192786
O	3.2996656323	2.8797058129	-0.235575633
O	3.0546413777	1.5498083655	1.5676727979
C	4.1863345974	3.6982134015	0.5470950157
O	0.5980001053	0.3954546608	-3.4916603545
O	-0.9963028947	1.0193528583	-1.9931814699
C	-0.4594989449	-0.0805383484	-4.3383923392
H	4.5175963985	4.4933126189	-0.1216443744
H	3.6666882294	4.1252332687	1.4091511331
H	5.0454121546	3.119742885	0.8973074638
H	0.0337995397	-0.4961021018	-5.2186778089
H	-1.0492112016	-0.8574614813	-3.843429074
H	-1.1253192492	0.7339537711	-4.6382674268

# TS2(1a\_t1)

C	1.2824862565	0.3106807691	1.7458983302
N	1.6618262592	0.0134395102	3.0150022732
C	2.5128192962	1.0939302111	3.5451986461
C	2.1298065362	2.2712548867	2.6348062002
N	1.6240071408	1.5788251931	1.440930926
H	1.8816842505	-0.9414313864	3.2666052363
H	3.5704791928	0.8291205642	3.4405528564
H	2.2931116282	1.2833365342	4.5967475965
H	2.9813870536	2.9072489807	2.3882405575
H	1.3405505961	2.8871296232	3.0802426675
H	1.1632624745	2.0951328797	0.6918444282
N	0.6536750299	-0.5339180186	0.9253895514
C	0.3173192133	-1.9127203258	1.3607452906
C	-0.9915873212	-2.3726692851	0.8218872546
H	1.0957999214	-2.6020596537	1.0284008758
H	0.2754774028	-1.9266388445	2.4528001912
O	-2.119913673	-1.7917354664	1.3402346331
C	-3.1900714753	-2.3774099223	0.7284669344
C	-2.7729343216	-3.3202805028	-0.1600574685
C	-1.3396970666	-3.3161430933	-0.1002136668
H	-0.655444678	-3.9299488214	-0.6689345926
H	-3.4029400253	-3.9408245279	-0.7817542695
H	-4.1626257723	-2.0188758283	1.0314703394
C	0.3284179544	-0.0701714743	-0.439474124
C	-0.3693383226	1.0269353622	-0.6184939401
C	1.0026127082	-0.9057556508	-1.4772979377
C	-0.7024473915	2.2930577675	-1.0068812213
O	0.6192098471	-0.577609354	-2.7252645475

O 1.8132337486 -1.7903328038 -1.2405547306  
C 1.2444094625 -1.3267833665 -3.7829205918  
O -1.9990794468 2.4697146271 -1.4466193326  
O 0.0946130197 3.2619195159 -0.8994049612  
C -2.3976984902 3.8317743492 -1.6256716856  
H -2.3355467675 4.3995282303 -0.6908830703  
H -1.7901006488 4.33763486 -2.3822893386  
H -3.4370826357 3.7941696905 -1.9592264235  
H 0.8205409468 -0.9365614655 -4.7085327513  
H 2.3280792215 -1.182820456 -3.775822164  
H 1.0226538754 -2.3930263076 -3.6877689713

#### TS2(1a\_t2)

C 0.5365006327 -0.6283455867 0.8246480122  
N 0.6287957107 -1.6507327073 1.7098930756  
C 1.9815388457 -2.2336676702 1.6430004881  
C 2.7939766747 -1.1121217113 0.9697499574  
N 1.7418485246 -0.2775785512 0.3491716611  
H -0.1631953828 -2.2736934672 1.8187039577  
H 1.9672360135 -3.1471669466 1.0396161264  
H 2.3515947531 -2.4719374779 2.6413414728  
H 3.4790557439 -1.487868896 0.2069622031  
H 3.353195122 -0.51469981 1.6913697896  
N -0.611216894 -0.0286100047 0.5061190073  
H -0.5946030903 0.6455066702 -0.2571407973  
C -1.9086061784 -0.3345133824 1.1274505645  
C -2.637606114 -1.4825410659 0.5124979309  
H -1.7520129181 -0.5081085534 2.1971159819  
H -2.5227887932 0.5614197461 1.0271311227  
O -2.1589668973 -2.7388300184 0.8006301173  
C -2.9527592794 -3.6366999147 0.140205419  
C -3.923831584 -2.9832527528 -0.5518303561  
C -3.718068047 -1.5828270291 -0.3115297736  
H -4.2982209255 -0.7576426187 -0.7005714853  
H -4.6940307864 -3.4381573537 -1.1587382957  
H -2.6984134118 -4.6779524825 0.2691552841  
C 1.9464060938 0.8362521057 -0.5724198596  
C 1.1698372776 0.985041343 -1.6223663338  
C 2.9905042014 1.7930852026 -0.0921662612  
C 0.2614818054 1.437717093 -2.5358949997  
O 3.3280060743 2.692693953 -1.0356648557  
O 3.4882435583 1.7833613224 1.0246374665  
C 4.2979032101 3.6770013081 -0.6340825706  
O 0.5792570421 1.1689488505 -3.8576340997  
O -0.8186608549 1.9997218778 -2.2246792404  
C -0.4615320923 1.4477293313 -4.7968665625  
H 4.4467353538 4.3143043712 -1.5061044678  
H 3.9272528174 4.2701948131 0.2060596202  
H 5.2406207742 3.2017283019 -0.3501832727  
H -0.0612929585 1.1678167878 -5.7740728461

H -1.3637316087 0.8609023249 -4.5919735892  
H -0.7313124126 2.508497598 -4.8045645913

#### 11a\_t1

C 1.4600831831 0.2739955056 1.9413281309  
N 1.9560086834 -0.2767413769 3.0795598672  
C 2.6862180811 0.7565235159 3.8395887151  
C 2.0999016702 2.0557267513 3.2587044794  
N 1.6154698935 1.6079183358 1.9461111268  
H 2.3330763719 -1.2161594468 3.0627306062  
H 3.7612437805 0.6784395992 3.6458929234  
H 2.5071071208 0.6524922911 4.9106882701  
H 2.8467066316 2.8448461654 3.157940063  
H 1.266005304 2.4287884433 3.8636725253  
H 0.9340917413 2.1194120675 1.3680824031  
N 0.8604932217 -0.4034367055 0.9569092613  
C 0.5480674769 -1.8456566288 1.1401928717  
C -0.8374182885 -2.1893299658 0.7151757038  
H 1.2517059551 -2.4504372234 0.5672114976  
H 0.6635044578 -2.0818149911 2.1999694504  
O -1.8661281664 -1.6770445096 1.4625690414  
C -3.0280055356 -2.1465014005 0.9215000208  
C -2.7657293058 -2.9500918151 -0.1450581657  
C -1.3378555496 -2.9765008871 -0.2808632885  
H -0.7569155639 -3.5079692449 -1.0215227262  
H -3.4938112632 -3.4588928956 -0.7611279588  
H -3.9388349527 -1.8219698233 1.4024686359  
C 0.4166897463 0.2767353796 -0.2684077765  
C -0.1483783973 1.4895909488 -0.2155568324  
C 0.8298935756 -0.4862831732 -1.4835040232  
C -0.4839520677 2.2932248676 -1.3611038545  
O 0.1523606649 -0.1054036139 -2.5838697525  
O 1.7002401739 -1.3456934472 -1.5092779008  
C 0.5615261105 -0.7270566382 -3.815011137  
O -1.8168271811 2.2143047532 -1.6714977845  
O 0.2641264494 3.0914261472 -1.9234417997  
C -2.2588001908 3.0980206198 -2.7092535185  
H -2.0784018228 4.1451843365 -2.4474603761  
H -1.7584422611 2.8824090918 -3.6584240324  
H -3.3315336937 2.9234719655 -2.812239271  
H -0.0730136976 -0.2926232433 -4.5877342662  
H 1.6125973281 -0.5155211478 -4.0282303999  
H 0.4135153163 -1.8092176071 -3.770971729

#### 11a\_t2

C -0.1014425753 -0.8098368241 1.2870585361  
N 0.171954135 -1.7027489362 2.2758444823  
C 1.6077400092 -2.0270283505 2.239649117  
C 2.2016449542 -0.8164745761 1.5014685569  
N 1.0283897368 -0.259528194 0.7881304013

H	-0.4877841154	-2.4594243106	2.4207490942
H	1.7729486278	-2.9602465491	1.6902249579
H	2.0121252376	-2.1309951766	3.2476875777
H	2.9842436379	-1.1008833228	0.7968680413
H	2.6037007649	-0.0724346195	2.1899470858
N	-1.3078062649	-0.4839563477	0.8526149034
H	-1.2349504183	0.1765205615	0.0124825637
C	-2.5695479416	-0.9692135235	1.4219793567
C	-2.9708265852	-2.3385174317	0.9800530007
H	-2.5120564185	-0.9301439934	2.5159209662
H	-3.3430281513	-0.2657403584	1.1089640921
O	-2.3095396544	-3.3913771175	1.5690774946
C	-2.8070905854	-4.5429229594	1.0210538528
C	-3.7697933265	-4.2478424029	0.1075916502
C	-3.8753391062	-2.8160353449	0.0797430722
H	-4.5387596168	-2.2190344422	-0.5304803712
H	-4.3389497318	-4.9585861982	-0.4750935632
H	-2.3804044857	-5.4642608121	1.3881693043
C	1.0571735795	0.74841209	-0.2470832434
C	-0.0547271613	1.0542820646	-0.9377489668
C	2.3597529689	1.4778120239	-0.3350401317
C	-0.1524681121	2.1197287065	-1.9057705615
O	2.5965900628	1.9326226296	-1.5802608715
O	3.1150342439	1.6922858601	0.6013610706
C	3.7472210877	2.7862371308	-1.7246575461
O	-0.1455952876	1.6461301394	-3.1908328202
O	-0.3698048754	3.3039535197	-1.6583043294
C	-0.3707986394	2.6283340663	-4.210223117
H	3.7757117021	3.0625095027	-2.7787021674
H	3.6473173582	3.6799137941	-1.1032253737
H	4.6611634793	2.2542365557	-1.4490835718
H	-0.345952271	2.0858226681	-5.1572209056
H	-1.3432339512	3.1149920775	-4.0882791534
H	0.4093106898	3.3957504011	-4.2051254841

### TS3(1a\_t1)

C	1.3909689297	0.2967786832	1.9362518792
N	1.8235219226	-0.2450805441	3.1193781513
C	2.3334042699	0.8621188432	3.9567363239
C	1.6715740217	2.0990293906	3.3096328679
N	1.3131229891	1.6149074086	1.9712786462
H	2.3845481506	-1.0877428085	3.0878937126
H	3.4258685427	0.9129082426	3.8942898108
H	2.0442353235	0.7245089079	5.0002041283
H	2.3474955288	2.9552884223	3.2561373522
H	0.768358376	2.4039039234	3.8509429424
H	0.708020638	1.9881577665	1.0440734166
N	1.0179806712	-0.4293293883	0.8530389454
C	0.8034216574	-1.8938007228	0.9916558351
C	-0.5977830924	-2.3126421115	0.6969824064

H 1.4754417372 -2.4259074045 0.3195522759  
H 1.0517502669 -2.1721042997 2.0157409197  
O -1.5794861746 -1.854862958 1.5374799988  
C -2.7589354238 -2.3932314071 1.1098686238  
C -2.5529854293 -3.1878130379 0.0245383916  
C -1.1451538781 -3.1331486777 -0.2464772353  
H -0.6078691669 -3.6359954273 -1.0381342292  
H -3.3058041654 -3.7404887054 -0.5198721456  
H -3.6370955061 -2.1158568983 1.6739387953  
C 0.5546262521 0.2496924734 -0.3448921076  
C 0.2213358317 1.5520198796 -0.3216324467  
C 0.7031436736 -0.5664911104 -1.5901781389  
C -0.0946694943 2.3500219918 -1.4922166249  
O -0.1998871514 -0.2222731069 -2.5255014256  
O 1.5680119255 -1.4087541801 -1.7759889102  
C -0.0305994972 -0.8384419404 -3.8165960288  
O -1.42964707 2.6100184001 -1.5812468069  
O 0.7220324672 2.8648655223 -2.2482544372  
C -1.8170014397 3.5006756308 -2.6387734079  
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H -2.8998924465 3.6065190653 -2.5555035769  
H -0.8291807905 -0.4353249724 -4.4391769881  
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H -0.1227909073 -1.9245930642 -3.7407020167

### TS3(1a\_t2)

C -0.1174906786 -0.7726897889 1.3814228674  
N 0.1716685957 -1.664120139 2.3726283445  
C 1.6129120237 -1.961440039 2.3383192116  
C 2.1898649189 -0.7287737042 1.6230639259  
N 1.01551784 -0.200341458 0.8945622647  
H -0.4708584698 -2.4371951368 2.5033224035  
H 1.8010748557 -2.8812268663 1.7732668373  
H 2.0151097448 -2.0750235439 3.3463366108  
H 2.994047958 -0.9880258313 0.9343479011  
H 2.5602851261 0.0177221981 2.3279134477  
N -1.3094374209 -0.4506695443 0.9249137813  
H -1.1652923439 0.2940493251 0.0565881509  
C -2.5634525109 -0.9934691347 1.4538863349  
C -2.9357099266 -2.3364409807 0.9146269595  
H -2.5175330643 -1.0284363984 2.5496976581  
H -3.3537139855 -0.2892901766 1.1846711612  
O -2.2119328103 -3.4092245676 1.379997332  
C -2.6973239083 -4.5284476421 0.7591775992  
C -3.712037127 -4.1942429947 -0.0816456429  
C -3.8658441575 -2.7698108182 0.0176696864  
H -4.5761867615 -2.1483972607 -0.5097849658  
H -4.2836530502 -4.8742329866 -0.6977443877  
H -2.2222754355 -5.4608144457 1.0252665615

C 1.0115628025 0.800017173 -0.1371980374  
C -0.1422686314 1.1276039478 -0.7501642407  
C 2.3269827352 1.4815795746 -0.3406453655  
C -0.2837724389 2.1145007803 -1.8008989772  
O 2.4659682955 1.9320283205 -1.6005037454  
O 3.1701105216 1.6583356684 0.5248102651  
C 3.6384903839 2.7297681223 -1.85482288  
O -0.3264224924 3.3920329817 -1.3122490704  
O -0.484513958 1.8689793502 -2.9851022197  
C -0.6141510473 4.4126875204 -2.2801364487  
H 3.5778627222 3.0097068994 -2.9064185806  
H 3.6429402806 3.6231163797 -1.2252695303  
H 4.5465002428 2.1508742662 -1.6694477601  
H -0.6408886883 5.3511833263 -1.7237043697  
H 0.1626240963 4.460013907 -3.0490215438  
H -1.5799522362 4.239921717 -2.764009539

## 12a\_t1

C 1.0069565394 0.1888632048 1.8353362512  
N 1.8055696703 -0.5215503062 2.7239442252  
C 2.7547359256 0.4659096878 3.2786861107  
C 2.0794435123 1.8104322387 2.892872754  
N 1.0582267804 1.4784062564 1.8841025389  
H 2.2194283018 -1.3784656322 2.372444639  
H 3.7402607298 0.3559276242 2.8112394002  
H 2.8689211782 0.3400331879 4.3585724815  
H 2.8003695519 2.5364779288 2.5013401009  
H 1.5960452696 2.2750436227 3.7627544197  
N 0.1454292935 -0.4838666035 0.9810597698  
C -0.0639946682 -1.9450405076 1.0976987705  
C 0.9079168669 -2.7569230284 0.3063891446  
H -1.0883673456 -2.1574920946 0.7960409384  
H 0.0201433549 -2.217823668 2.1505552958  
O 0.7846772686 -2.7168904753 -1.0575715965  
C 1.7555158759 -3.5257744088 -1.5754810975  
C 2.48795126 -4.0879715528 -0.5761633368  
C 1.9359090937 -3.5874821432 0.6506543743  
H 2.255068833 -3.8202779824 1.6575585067  
H 3.315699109 -4.7734684195 -0.692994707  
H 1.7892920669 -3.5948122924 -2.6526867102  
C -0.3851474181 0.2483308641 -0.0885854885  
C -1.677640553 0.270878698 -0.4880936077  
C 0.6438637616 0.9635999374 -0.9443577815  
C -2.8380648881 -0.2791792107 0.2325578295  
O 0.1417882383 2.0622054831 -1.5253346273  
O 1.7696645155 0.5467616346 -1.1249712926  
C 1.0275897583 2.7479959863 -2.4366610581  
O -3.967254744 -0.029508423 -0.4661220386  
O -2.8369679304 -0.8493759215 1.3130367685  
C -5.1938017818 -0.4727303723 0.1461180191



H -5.1775353387 -1.5541533474 0.3033419372  
H -5.3511116521 0.0302285409 1.1036562166  
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H 0.4610075127 3.6022379928 -2.8059709881  
H 1.9251806131 3.0844417252 -1.9128303172  
H 1.3099024809 2.092471926 -3.2638502338  
H -1.9085183624 0.8001982691 -1.4036114451

#### E-12a\_t1

C 1.012141576 0.4511045169 2.1184954934  
N 1.8740966592 -0.152153206 3.0371563293  
C 2.1966865142 0.8887461592 4.0325815413  
C 1.0947062036 1.9426359593 3.7556499453  
N 0.5164324657 1.5926476749 2.4464499976  
H 2.6722160864 -0.6411480199 2.6446659309  
H 3.2006191771 1.2912644292 3.8554723928  
H 2.1581673206 0.4886317508 5.0489568583  
H 1.4845335481 2.9655290283 3.7486545953  
H 0.3029952809 1.9022337574 4.5146045962  
N 0.7238785979 -0.249019308 0.9333275952  
C 0.8715305642 -1.7328809879 0.9622593395  
C -0.3713834085 -2.4777958108 0.6071655784  
H 1.674763804 -2.0500048468 0.2949627911  
H 1.1614539071 -1.98910712 1.980931568  
O -1.5101455264 -2.1728658704 1.3039500226  
C -2.4820421946 -3.0348438164 0.8817138096  
C -1.9857037543 -3.8880899381 -0.0548938449  
C -0.6095468471 -3.5244734874 -0.2354327367  
H 0.1087639957 -3.9787045649 -0.9035273509  
H -2.5293664716 -4.6734522507 -0.5611477988  
H -3.4549101079 -2.9070928975 1.3325994905  
C 0.3320018819 0.3907361024 -0.2397035684  
C -0.0595045636 1.6878290382 -0.3485394138  
C 0.453633715 -0.4541932337 -1.4996469203  
C -0.2435431199 2.3554194092 -1.6400165168  
O -0.7370828123 -0.6550765437 -2.0650156521  
O 1.5090174523 -0.8969441475 -1.9061771687  
C -0.7216378197 -1.3541611286 -3.3266612172  
O -0.8566313998 3.551430736 -1.4616624224  
O 0.1118144566 1.9575999631 -2.7415369097  
C -1.0589285056 4.3324661488 -2.6522273379  
H -0.1045171198 4.5652799556 -3.1322849929  
H -1.6978287533 3.8015978907 -3.3628935357  
H -1.5468795191 5.2502640933 -2.3230096235  
H -1.7661987021 -1.443273118 -3.6232259191  
H -0.1639757942 -0.7753690542 -4.0662929804  
H -0.2726506866 -2.3433375888 -3.2149188551  
H -0.1911470998 2.2813443262 0.5429378899

#### 12a\_t2

C	0.814686568	0.7614530555	0.5927385333
N	1.7086439656	1.7931250533	0.3887720687
C	0.9986203891	3.019045329	0.0041431992
C	-0.3083732536	2.47916191	-0.5913801495
N	-0.4173915718	1.1513046581	0.0427109029
H	1.5698027176	3.5985770585	-0.7246438392
H	0.8028418911	3.6504038962	0.8791889851
H	-0.239861685	2.3522607672	-1.6777722793
H	-1.1645073267	3.1051833978	-0.3478978957
N	0.9626945914	-0.3874576828	1.1468040883
C	2.2991801545	-0.7501086115	1.6301117325
C	2.6054163805	-0.2477605123	3.0077420187
H	3.1017357409	-0.3912517465	0.9701232104
H	2.3566617704	-1.8455023585	1.6316834151
O	1.8174304388	-0.7084347168	4.0308393465
C	2.2685240578	-0.1303698578	5.1842099884
C	3.3256287856	0.6849384209	4.9238232487
C	3.5448375445	0.6094968546	3.5061600132
H	4.3068132119	1.1189818701	2.9319931016
H	3.8815165838	1.2671821395	5.6457055138
H	1.738849234	-0.3984120486	6.0864144193
C	-1.4164881073	0.2328316463	-0.2207663072
C	-2.7525404767	0.4714419426	-0.2457592645
C	-0.959706707	-1.1317926475	-0.709674562
C	-3.4498691851	1.6811938056	0.2055097364
O	-0.1561501873	-1.2727437446	-1.6088589027
O	-1.6346829242	-2.1287374579	-0.1249260974
O	-4.7737481493	1.5727598261	-0.0569731484
O	-2.9675155669	2.6490958868	0.7770426203
C	-5.5917772429	2.6705286656	0.3874488771
H	-6.6084372457	2.4207056406	0.0835661952
H	-5.5390903205	2.7784638348	1.4740246675
H	-5.2759571793	3.6050409309	-0.0834127745
H	-3.394210922	-0.3324546033	-0.5851039906
C	-1.3356144809	-3.4547053214	-0.6139163325
H	-1.5709450246	-3.5342030629	-1.677809439
H	-0.2808287315	-3.6893474633	-0.4529505815
H	-1.9661357191	-4.1282666258	-0.0344055676
H	2.4521129815	1.8877308718	1.0695192493

#### **E-12a\_t2**

C	-0.4117845793	-0.7447301206	1.3444665296
N	0.1620426338	-1.6596976056	2.2118674537
C	1.6095821754	-1.7320258277	2.007425966
C	1.9161186527	-0.3413419895	1.4538460143
N	0.6380618185	0.0363731682	0.8087306163
H	-0.3297692281	-2.5393826416	2.3120909287
H	1.8731350315	-2.5145910519	1.285098109
H	2.1373893342	-1.9229634337	2.9440407538
H	2.7306753787	-0.3588707125	0.7290389345

H	2.1563966071	0.367082496	2.2523455471
N	-1.6501259531	-0.5562980853	1.0635770259
H	-1.5233851366	1.007170861	-0.4662011236
C	-2.6462737952	-1.3972391729	1.7423865518
C	-2.8933298395	-2.7159003092	1.0797796882
H	-2.3853643596	-1.5672567231	2.7983044676
H	-3.5950131098	-0.8529841731	1.7336066775
O	-1.946232833	-3.6959996482	1.2716140304
C	-2.3482023429	-4.7987902624	0.5669064154
C	-3.5257129237	-4.5465126023	-0.0638478337
C	-3.8786822199	-3.1941564601	0.2675335492
H	-4.7535169544	-2.6473234818	-0.0561493963
H	-4.0788179414	-5.2354643923	-0.6870696465
H	-1.6997783885	-5.6601728485	0.6247976717
C	0.5320754508	1.1217089832	-0.0387143488
C	-0.6072494119	1.54841824	-0.6481737903
C	1.8589735164	1.8410864938	-0.2282096872
C	-0.7414879633	2.6920034605	-1.5478197644
O	2.4583004199	1.4597352631	-1.3588601853
O	2.3233459773	2.6053938566	0.5905464112
C	3.7280339159	2.0931495798	-1.6422708752
O	0.3635123974	3.4729652725	-1.643242485
O	-1.7733359095	2.9436694334	-2.1559752882
C	0.2628159902	4.5992238955	-2.5323151886
H	4.0680548498	1.6546054881	-2.5795967592
H	3.5944927189	3.1714291197	-1.7521184899
H	4.4440484732	1.8889134036	-0.8433214373
H	1.2228716524	5.1117794284	-2.4689257677
H	0.0790683122	4.2699189572	-3.5583808047
H	-0.542117417	5.2688861417	-2.2190894697

#### TS4<sub>sc</sub>(1a\_t1)

C	1.4052179191	-0.1701762376	1.4064779512
N	2.1385876886	-0.8322449764	2.3069922595
C	3.3117992145	0.0049806146	2.6336589859
C	3.3531606391	0.957202725	1.4106783819
N	1.954704564	0.9411449261	0.9549018379
H	4.20855133	-0.6085560187	2.7313601741
H	3.1423646162	0.5504558492	3.5683681387
H	3.9992667908	0.5657067081	0.6162439655
H	3.6790671328	1.9631140901	1.6788166302
N	0.2351613155	-0.5295379556	0.8000873318
C	-0.4952035172	-1.7696840397	1.1509978559
C	-0.1837750253	-2.9159243562	0.2521841444
H	-1.5592252751	-1.5505287416	1.0838953561
H	-0.2562867631	-2.0061985668	2.1909598596
O	1.0422308889	-3.5166200442	0.3874873457
C	1.0982614416	-4.5252807298	-0.5309150273
C	-0.0601480146	-4.5849447723	-1.2429992006
C	-0.8945092427	-3.5348704828	-0.7343466767

H	-1.8923090192	-3.2707730808	-1.0548192964
H	-0.2939093344	-5.2862849499	-2.0317320613
H	2.0130955626	-5.0989966538	-0.5480738994
C	0.0123928775	0.3251912498	-0.2826488694
C	-1.0698015416	0.5342782223	-1.0629082581
C	1.3144214724	1.1702843745	-0.5809924238
C	-2.4262373905	-0.0093656117	-1.0108645372
O	1.1992217391	2.3448623673	-0.9775139349
O	2.187936673	0.2650305698	-1.3266971242
O	-3.1070935347	0.3600392545	-2.1230197461
O	-2.9534353249	-0.6707828087	-0.1221582301
C	-4.4798641418	-0.064086783	-2.1898574634
H	-4.5511945325	-1.1550390875	-2.1876845402
H	-5.0527048457	0.3352542572	-1.3488203353
H	-4.8644090539	0.3344506467	-3.1290124574
H	-0.902437594	1.2716133153	-1.8412446273
C	2.6547119624	0.7941777178	-2.5599192523
H	3.3487565386	0.0510606306	-2.9641861329
H	1.8430440145	0.9470108226	-3.2841543393
H	3.1804809754	1.7461798217	-2.4326146312
H	1.7819957947	-1.5523682657	2.9207598464

#### TS4<sub>sc</sub>(1a\_t2)

C	0.8725676343	1.2374215116	0.4994801252
N	1.8009972519	2.1645175265	0.7705741927
C	1.3019900815	3.5046543922	0.412994823
C	-0.2262771344	3.2939576604	0.3565540948
N	-0.3267040311	1.8369428756	0.13864852
H	1.7038667574	3.8156048905	-0.556800926
H	1.5853834478	4.2373330769	1.1698705076
H	-0.7079046375	3.8429006303	-0.4469380741
H	-0.7065290984	3.5544106562	1.3051872206
N	0.8222524315	-0.0530526567	0.5595729109
C	1.8161839902	-0.9701983687	1.091054025
C	2.9165737404	-1.2991877649	0.1383265082
H	2.2360358276	-0.5670610326	2.0215793913
H	1.2689501663	-1.8831072661	1.3450361702
O	3.8266090231	-0.2988597531	-0.1054918104
C	4.7402561192	-0.7906846615	-0.9972031077
C	4.4374535989	-2.0767364785	-1.3191266228
C	3.2498529035	-2.4068898866	-0.5819575075
H	2.7139466102	-3.345847063	-0.5867620363
H	4.9879521431	-2.7148625965	-1.9962748456
H	5.5275262863	-0.1126123886	-1.2908931077
C	-1.3612841084	0.9348958665	0.121139002
C	-2.6995840401	1.1132106809	0.0025055117
C	-0.7962534843	-0.5270667196	0.284818589
C	-3.4255577616	2.3405276609	-0.2991612709
O	-0.6615778554	-1.0638727412	-1.0477517138
O	-1.251303738	-1.2575845424	1.1879957075

O -4.7617775057 2.1457404519 -0.1386493635  
O -2.9685356587 3.411921579 -0.680628472  
C -5.5979292067 3.2711308405 -0.4524252248  
H -6.6213559232 2.9349074847 -0.2825751464  
H -5.3708156546 4.1209223099 0.1972268134  
H -5.471360424 3.5748813274 -1.4952168344  
H -3.3018969683 0.2205111054 0.1274868983  
H 2.787286015 1.9382947941 0.7739378121  
C -1.402121852 -2.2558146515 -1.2830195826  
H -2.4860277485 -2.0752305628 -1.3100499839  
H -1.0867534963 -2.6201493739 -2.2650274626  
H -1.1997197013 -3.0231828132 -0.5300727305

#### TS4<sub>6c</sub>(1a\_t1)

C 0.8874830869 0.2961590419 2.1322438096  
N 1.3663662653 -0.1480673424 3.335002299  
C 1.4010643256 1.0121109574 4.2493632732  
C 0.4252435525 1.9892106081 3.5641211646  
N 0.3944829813 1.5172993911 2.1722046556  
H 2.4138250908 1.4266688781 4.297128761  
H 1.0868759809 0.7253038546 5.254643832  
H 0.7602937894 3.0264216185 3.6233584044  
H -0.5856468609 1.9190602947 3.9813250026  
N 0.8656212502 -0.4568917458 1.001136512  
C 1.120884049 -1.9222044448 1.0578315448  
C -0.0500844348 -2.7359970072 0.6227694435  
H 1.9736565123 -2.1648600019 0.4260226511  
H 1.3730034865 -2.1700069853 2.0888011829  
O -1.1648022054 -2.706450895 1.4204343507  
C -2.0870868938 -3.5372554277 0.8532083563  
C -1.5868857725 -4.100264178 -0.2803282724  
C -0.2605333423 -3.5757121988 -0.4326422748  
H 0.4454421136 -3.7904783996 -1.2223070102  
H -2.0964448073 -4.7974165403 -0.9305943984  
H -3.0329302401 -3.6158502215 1.3685575688  
C 0.3116329457 0.1303465592 -0.1713258607  
C -0.4349331614 1.2490007419 -0.1345021003  
C 0.7642121001 -0.4452802308 -1.4717334164  
C -0.9011965387 1.9389915014 1.1325369294  
O -0.1012671728 -0.1844595783 -2.4647383984  
O 1.8125683146 -1.0483088392 -1.6308527173  
C 0.3126517894 -0.6007816192 -3.7829545806  
O -0.6556094856 3.3382088264 0.9325866276  
O -2.0052428829 1.5787439727 1.6149136951  
C -1.5318382437 4.2091794041 1.6373420738  
H -1.2975842889 4.2674959767 2.7092822255  
H -1.3928017705 5.2022868277 1.1997356034  
H -2.5772451007 3.9037009795 1.5310327704  
H -0.490504649 -0.2898930574 -4.4505266862  
H 1.2498314637 -0.1148002841 -4.0645380674

H	0.4374975772	-1.6854340814	-3.8197862043
H	-0.7865737614	1.6708533771	-1.0684919184
H	2.1698419374	-0.7658817325	3.3427491685

#### TS4<sub>6c</sub>(1a\_t2)

C	0.2368019703	-0.5665769531	1.1471069737
N	0.2084885607	-1.4469113083	2.1888637851
C	1.5748339741	-1.8994824234	2.4841365077
C	2.4247357534	-0.7585201332	1.9116864456
N	1.5275055931	-0.2020664811	0.8706320604
H	1.7876121004	-2.8483175414	1.9786187696
H	1.7242735774	-2.0256604806	3.5576750411
H	3.3577771247	-1.1037257951	1.4768425391
H	2.6387584903	0.0070555484	2.6657570028
N	-0.7906121157	-0.0643218639	0.5156213631
C	-2.1654339993	-0.3588431565	0.9252154731
C	-2.7228745506	-1.6359940478	0.391867272
H	-2.2369692104	-0.3473485466	2.0200029656
H	-2.7527144167	0.4815775953	0.5443476874
O	-2.2869734241	-2.7963648328	0.9902937978
C	-2.9132366018	-3.8402216117	0.3641470278
C	-3.7391554182	-3.3730140835	-0.6093959021
C	-3.6148430144	-1.9424071964	-0.5921051299
H	-4.1235138262	-1.2327091556	-1.2294738689
H	-4.3626511185	-3.9695128793	-1.2607570148
H	-2.6680909529	-4.8268018402	0.7277355857
C	1.7785214811	0.9278872981	0.0655534065
C	0.7936607306	1.5398478518	-0.6200366511
C	3.2033376657	1.3401504681	-0.0962114414
C	-0.6699203242	1.1632989805	-0.6604089492
O	3.3117552707	2.6019416439	-0.5438201045
O	4.1637610748	0.6212972691	0.1216270008
C	4.653252153	3.0523342997	-0.8276952994
O	-0.8474973383	0.343058156	-1.8536066356
O	-1.5123036775	2.0689590082	-0.4396966465
C	-1.7467909926	0.880757839	-2.8136738562
H	4.5450141718	4.075526313	-1.186233679
H	5.2642095861	3.0302404496	0.0776062978
H	5.1149061677	2.427434506	-1.5958859107
H	-1.923583637	0.0889398014	-3.5482179374
H	-2.6997413622	1.1830143467	-2.3700382209
H	-1.3251013656	1.7516241633	-3.3378029709
H	1.0500454062	2.3908413104	-1.2391255709
H	-0.5468405062	-2.1218475179	2.2220587869

#### 13a\_t1

C	1.4304025422	-0.2002710165	1.4805007565
N	2.1467790369	-0.8513704454	2.3956214832
C	3.3230138333	-0.019134995	2.7321420098
C	3.3879275439	0.9365656716	1.5123370692

N	1.9967220547	0.9118869802	1.037103099
H	4.2147265238	-0.6382872791	2.8373603935
H	3.1460955416	0.5242419846	3.6660691835
H	4.0492990722	0.5534078378	0.7282478833
H	3.6998075	1.9437582041	1.7913994918
N	0.2667759251	-0.5333722276	0.8564898305
C	-0.4748863316	-1.7788080808	1.1633017027
C	-0.1329483953	-2.9088731946	0.255177192
H	-1.5354671692	-1.5566335367	1.0642112642
H	-0.2671493101	-2.0312615914	2.2061775139
O	1.0848478512	-3.5167042921	0.4283259117
C	1.1755849877	-4.5071101273	-0.5069415178
C	0.0474384717	-4.5475502058	-1.267352594
C	-0.8040529415	-3.5046444427	-0.7724952465
H	-1.7864922175	-3.2295054846	-1.1288866663
H	-0.1558822585	-5.2321182901	-2.0789170085
H	2.088504497	-5.0840629854	-0.4974984088
C	0.0709876788	0.3659555818	-0.1993705741
C	-0.9848327659	0.6063363772	-1.0056492587
C	1.3940335388	1.2166877472	-0.4000420197
C	-2.3322598752	0.0392409121	-1.0426106757
O	1.2975056064	2.4098809839	-0.7655812518
O	2.2857020085	0.3238403631	-1.1963809234
O	-2.9781210111	0.4717534369	-2.1528279202
O	-2.8795637629	-0.6908565929	-0.2223559719
C	-4.3382223676	0.0282108283	-2.3018144325
H	-4.3865771218	-1.0614009879	-2.3767730042
H	-4.950494895	0.3580917204	-1.4584277237
H	-4.695477822	0.4833797336	-3.2258971143
H	-0.7972796947	1.3951407691	-1.7271361116
C	2.2501262306	0.5902448804	-2.5868677964
H	3.097576767	0.0626312614	-3.0371197815
H	1.3262925301	0.2221365248	-3.0606536003
H	2.3411307758	1.6624512384	-2.7916737744
H	1.7856914225	-1.5787662607	2.9990805916

### 13a\_t2

C	0.9503841481	0.6457617411	0.5505232512
N	1.8832248643	1.5761735842	0.769505064
C	1.3799830574	2.9028069487	0.3655118597
C	-0.149553506	2.6886597028	0.3224328802
N	-0.2481273186	1.2225624789	0.169751485
H	1.7792921218	3.1774401526	-0.615949582
H	1.6660067944	3.6617312329	1.0948344211
H	-0.6322233331	3.2007132962	-0.5045531251
H	-0.627718609	2.991460575	1.2590870606
N	0.8940144656	-0.6449791537	0.6783167366
C	1.8953922284	-1.5501032841	1.221486438
C	2.9989528106	-1.8847125895	0.275321148
H	2.3090811949	-1.1289376045	2.1460374605

H	1.3463157303	-2.4583681065	1.4857996996
O	3.9190591779	-0.8908483487	0.0407563178
C	4.8334892566	-1.3869452903	-0.8477476691
C	4.5214020838	-2.6690411667	-1.1766069855
C	3.32686268	-2.991962176	-0.4478989573
H	2.7823954141	-3.9258898988	-0.4600630014
H	5.0704808522	-3.3093398734	-1.8528301897
H	5.6284842867	-0.7146744257	-1.1338360362
C	-1.2706401189	0.3017663745	0.21259732
C	-2.6138038139	0.4540016447	0.1289333913
C	-0.6429691745	-1.1319021562	0.4024174493
C	-3.3629312466	1.6622659963	-0.1953701504
O	-0.4513100138	-1.6726338814	-0.947045226
O	-1.1131912104	-1.8933808088	1.2789257262
O	-4.6912702827	1.4611401749	0.0110601527
O	-2.9263854141	2.7231161359	-0.6264090677
C	-5.5475551486	2.5682546435	-0.3140175698
H	-6.5616133994	2.2305047466	-0.0974879317
H	-5.305882393	3.4424777416	0.296715566
H	-5.4588673919	2.8349977989	-1.3707420613
H	-3.1962051596	-0.4409200252	0.3150926964
H	2.8691905206	1.3497662661	0.794538168
C	-1.493525038	-2.5384025599	-1.3699627936
H	-2.4008984495	-1.9874472384	-1.6614095474
H	-1.1236081469	-3.0769142722	-2.2482907224
H	-1.7567955195	-3.2593393752	-0.5891496755

#### 14a\_t1

C	0.9423320182	0.2332475662	2.21397464
N	1.468592902	-0.2330782162	3.3803715594
C	1.4973838189	0.8847252004	4.3465901355
C	0.4746958898	1.8627708058	3.7423811308
N	0.4247353458	1.4493486025	2.3312340278
H	2.4996313716	1.3243093247	4.3834155717
H	1.2220938868	0.5408326228	5.3450060258
H	0.7791311353	2.9056870924	3.8316238035
H	-0.5241007287	1.7416827039	4.1739050636
N	0.897324703	-0.4648085129	1.0563651678
C	1.1736631362	-1.9284344118	1.0408952682
C	-0.0083615299	-2.741305977	0.6353649058
H	1.9939888774	-2.1290627039	0.3544073931
H	1.4841112034	-2.2143729035	2.0457783994
O	-1.0696293808	-2.7798154691	1.5028047919
C	-2.0109728149	-3.5985645144	0.9500399943
C	-1.5747046387	-4.0880562291	-0.242602824
C	-0.27111426	-3.5269281121	-0.449580196
H	0.3858832341	-3.6818413137	-1.2935252137
H	-2.11221478	-4.7600275978	-0.8968676855
H	-2.9194885056	-3.7265387638	1.5197643905
C	0.2858714531	0.1695131703	-0.0689688806



C -0.4495758872 1.2864647948 0.0780666168  
C 0.6669693486 -0.3478812528 -1.4113338036  
C -0.780776422 1.9063952633 1.42582233  
O -0.2344368236 -0.0124653999 -2.3499311878  
O 1.6908449145 -0.9674670086 -1.6511094938  
C 0.1084437443 -0.3707101067 -3.7046492294  
O -0.4443041941 3.3405870756 1.337814214  
O -1.9238431672 1.6094306022 1.8937538897  
C -1.5534528687 4.1496045698 0.9904505533  
H -2.4191590271 3.9491731066 1.63065211  
H -1.2407542662 5.1912426955 1.1179133713  
H -1.8643204253 4.0134133396 -0.0584959721  
H -0.7154632604 -0.0071261614 -4.3182264434  
H 1.0443949586 0.106238106 -4.0053320318  
H 0.2029480387 -1.4547639575 -3.8016902726  
H -0.8667663041 1.760946535 -0.8017792507  
H 2.273670304 -0.847619565 3.3487061309

#### 14a\_t2

C 0.1156040954 -0.4090983661 1.0278422923  
N 0.0650414549 -1.2728269992 2.0790157513  
C 1.4275264575 -1.7003016392 2.4269654708  
C 2.277775274 -0.5556993752 1.8625045213  
N 1.4054078525 -0.0348685555 0.7828041244  
H 1.6695846105 -2.6542873391 1.9450805544  
H 1.5415810169 -1.8056685414 3.5069244282  
H 3.2298822344 -0.8911281743 1.4628818455  
H 2.4525892326 0.2281223419 2.6079776811  
N -0.9087402359 0.0654036088 0.3592883972  
C -2.2878309058 -0.2692720908 0.7416406242  
C -2.7790950514 -1.5848328744 0.2399968767  
H -2.3883430566 -0.2268025106 1.8327717031  
H -2.8925237448 0.5393396178 0.3256403584  
O -2.3947975458 -2.6980718426 0.9543090966  
C -2.9446407683 -3.7896259802 0.3383835027  
C -3.672271342 -3.3988780896 -0.7416334323  
C -3.5635228167 -1.9687819427 -0.8061420579  
H -4.0110529356 -1.3098531049 -1.5367780227  
H -4.2224339129 -4.0455605956 -1.4108777386  
H -2.7295143191 -4.7466786461 0.7894099567  
C 1.6678003671 1.0712421589 -0.0538158865  
C 0.6729295372 1.6761769953 -0.7295398121  
C 3.0959723103 1.4411119217 -0.2582318644  
C -0.8000821271 1.3367545242 -0.665929285  
O 3.2235926454 2.6731719627 -0.7788813316  
O 4.0449665726 0.7162198238 -0.0100545045  
C 4.5702251734 3.0806395248 -1.0992953608  
O -1.1249672115 0.6195059233 -1.9124561421  
O -1.5757791387 2.275966284 -0.3292458177  
C -1.6920424358 1.4508607339 -2.9132610396

H	4.4779705776	4.0833228741	-1.5156626281
H	5.1891874819	3.0991216079	-0.1993175796
H	5.0132289626	2.4039278062	-1.8338708623
H	-2.0706284432	0.7886694501	-3.6986903924
H	-2.5157899871	2.055217088	-2.5201491086
H	-0.9517459879	2.1293369434	-3.3665529463
H	0.9191368451	2.50009937	-1.3874150811
H	-0.6882387357	-1.9500108933	2.1157537095

### 15a\_t1

C	1.6296645001	-0.6259157167	1.3098357307
N	2.3607694057	-1.4205270208	1.9957364746
C	3.5977091396	-0.6319861815	2.2463943792
C	3.5570934328	0.5725324606	1.2559934012
N	2.106925859	0.6376615123	1.0126561535
H	4.4847276705	-1.2536496419	2.0978483591
H	3.6059657257	-0.2827352671	3.2868086318
H	4.098673293	0.3584642839	0.328222103
H	3.9359352895	1.4988216602	1.692012963
N	0.3851381822	-0.8062732413	0.7183132558
C	-0.4811012254	-1.9286088407	1.1257273991
C	-1.4318149395	-1.5902780524	2.2264658622
H	-1.0506287063	-2.2502951568	0.257448405
H	0.1967301995	-2.7270278756	1.4377558392
O	-0.9096328626	-1.4498215721	3.4878282982
C	-1.9479872048	-1.1594870934	4.3244418307
C	-3.1185500601	-1.1173058876	3.6314838929
C	-2.7822851413	-1.3958059775	2.2650197486
H	-3.4492089124	-1.4456806314	1.4169580609
H	-4.0991318424	-0.9132731741	4.0385625892
H	-1.6924411693	-1.0167047746	5.3640612221
C	0.1019612597	0.274357856	-0.0954826589
C	-0.985206551	0.6449849781	-0.8186133097
C	1.3899137636	1.1484055743	-0.1309616062
C	-2.2238302917	-0.0699984484	-1.1186893696
O	1.040381574	2.4919914314	-0.0446043294
O	2.1929112463	0.8840705633	-1.2641861529
H	1.8598733461	3.0120242778	-0.1110723531
O	-3.1333797201	0.7941965257	-1.6326566426
O	-2.4623728829	-1.2671533333	-1.0006028365
C	-4.3851003036	0.2184868466	-2.0458556735
H	-4.2276196039	-0.555222417	-2.8017664551
H	-4.915983794	-0.2139844489	-1.1936683476
H	-4.9621054627	1.0427666933	-2.4658781331
H	-0.9191179792	1.6312208419	-1.2610671415
C	1.7212419584	1.3238553926	-2.5434617077
H	2.5597546171	1.1854860348	-3.2291651517
H	0.8728694639	0.723798386	-2.8888742344
H	1.4379527267	2.3804094343	-2.5295504965

### E-15a\_t1

C	1.7840984566	-0.6526709031	1.4886822652
N	2.4792422061	-1.5012848754	2.1477134498
C	3.7906849911	-0.8172917134	2.3161551047
C	3.7963105293	0.3634417309	1.2983545497
N	2.3470623939	0.5597766111	1.1404730165
H	4.6127971662	-1.5155070549	2.1382304509
H	3.8831810311	-0.4474236103	3.3454591551
H	4.2554913895	0.0704711402	0.3461866873
H	4.2904703405	1.2589188483	1.6794488062
N	0.5025425023	-0.7303719345	0.963246085
C	-0.4116809613	-1.8422949996	1.248185824
C	-1.5438445822	-1.4904436115	2.1556528817
H	-0.8194520778	-2.2146781642	0.3048722626
H	0.2068795452	-2.6306354104	1.6857512113
O	-1.2269384424	-1.1243649441	3.4370766521
C	-2.4026254689	-0.8852330306	4.0896411217
C	-3.4584189895	-1.0975531351	3.2580344603
C	-2.898710023	-1.489992876	1.9961881901
H	-3.4328126221	-1.7413873381	1.0903726638
H	-4.5047498952	-0.9869365611	3.506105453
H	-2.3161018217	-0.5765093212	5.1209499015
C	0.2817554959	0.3239826374	0.1069377802
C	-0.8728857781	0.5452090091	-0.574389141
C	1.6113100176	1.1384095649	0.0275542267
C	-1.1043770883	1.6627387113	-1.4738194746
O	1.466097251	2.4943592745	0.2218148469
O	2.1756849135	0.811092696	-1.231322668
H	0.8206953809	2.7811288643	-0.4729956248
O	-2.2649727232	1.5121532603	-2.1387884058
O	-0.3920617687	2.6598197106	-1.6456749218
C	-2.6298694282	2.5777633398	-3.0378657741
H	-2.7320428438	3.5219425459	-2.4973350679
H	-1.8835257617	2.6900833536	-3.82794083
H	-3.5881945744	2.2819274803	-3.4645978539
H	-1.6994749425	-0.1444226532	-0.4578003027
C	3.0995637975	1.7569249452	-1.7866995959
H	3.5586441248	1.2478195134	-2.6372861355
H	2.5892265636	2.6574064629	-2.142077161
H	3.8836516962	2.0471984367	-1.0805020893

### 15a\_t2

C	0.498140491	-1.6749327962	0.5108876721
N	0.5037083634	-2.9282378323	0.7680254137
C	1.2619488315	-3.5539755554	-0.3405416717
C	1.5489713645	-2.4450051805	-1.4030013723
N	1.1446139952	-1.2460984245	-0.6559602973
H	0.6852587519	-4.3758766902	-0.7759228854
H	2.1959858273	-3.9794089246	0.0452441143
H	0.9366402175	-2.5571617118	-2.3016574686

H	2.5964314909	-2.3909842688	-1.6941606029
N	-0.0609758407	-0.5962364939	1.1313758928
C	-0.5026773242	-0.6218773686	2.5279931907
C	-1.8034385065	0.0770512943	2.7473598604
H	-0.5863649799	-1.6775735678	2.80101046
H	0.2510521701	-0.163255019	3.1748946572
O	-2.9233250648	-0.4856295837	2.1949573234
C	-3.9835760731	0.3020258471	2.54164621
C	-3.5689402343	1.3496210315	3.3041658421
C	-2.1468196391	1.2042336364	3.4386277743
H	-1.4679885994	1.846964288	3.9821235371
H	-4.1916952037	2.1290313393	3.7202190681
H	-4.9476926517	-0.0138105074	2.1714808984
C	0.9909455085	0.0922199571	-0.8607593149
C	1.258959927	0.9359473015	-1.8928756608
C	0.3725333029	0.6274025364	0.4607421204
C	1.8974415887	0.7072908005	-3.1838299096
O	-0.6636564042	1.5028594456	0.1554980919
O	1.3227257734	1.2129304348	1.3255088048
H	-1.019005222	1.8446002499	0.9953394222
O	2.4903878917	-0.5046243415	-3.3137321005
O	1.9240910305	1.5469905466	-4.0746428341
C	3.1144805749	-0.7639476594	-4.5834138639
H	3.5237357302	-1.7719298168	-4.5101173349
H	2.3838871383	-0.7133045716	-5.3949661983
H	3.916241807	-0.0463765187	-4.7757820166
H	0.9220165885	1.9565757226	-1.764210731
C	1.8781766613	2.4813036549	0.9551410092
H	2.4367375408	2.8231773177	1.8288215244
H	2.5625191545	2.3872593284	0.1056729501
H	1.099186022	3.2113810999	0.7170764253

#### **E-15a\_t2**

C	0.3295406567	-1.6072453654	0.5056546516
N	0.3044514148	-2.8731981541	0.6979528108
C	1.0083912659	-3.4695047502	-0.464404512
C	1.358481563	-2.3096191634	-1.4593259913
N	0.9496479927	-1.1575243598	-0.6622039913
H	0.3710047813	-4.2188132878	-0.9437045874
H	1.9161553288	-3.9803999671	-0.1249386446
H	0.7829510708	-2.3578197134	-2.3891763655
H	2.422745043	-2.2569281599	-1.7024707298
N	-0.1468785153	-0.5282668005	1.1890342425
C	-0.5142797031	-0.6049019712	2.6026357204
C	-1.8867251198	-0.105760042	2.913053298
H	-0.4248464558	-1.6599325743	2.8811445364
H	0.205804988	-0.0450969545	3.2076067169
O	-2.9352635411	-0.7085254608	2.2723363932
C	-4.0815055865	-0.1353770035	2.7469170109
C	-3.7875909225	0.8089930908	3.6809078218

C	-2.3558343764	0.8286699203	3.789359694
H	-1.7546323601	1.453428226	4.4353158228
H	-4.4962788625	1.4197155982	4.2228049399
H	-5.0043770126	-0.5022764513	2.3226706845
C	0.9264740476	0.1841760972	-0.7901525438
C	1.3864979468	0.8982204977	-1.8586050638
C	0.3035904728	0.7166568408	0.5387908368
C	1.2677547119	2.3317525642	-1.9926577193
O	-0.7708305611	1.5539752132	0.3468262449
O	1.3576378581	1.3059087811	1.2774847778
H	-0.4219606088	2.2800147018	-0.2348547186
O	1.9521827164	2.7880430984	-3.0603446746
O	0.6165528016	3.1064021193	-1.2735815923
C	1.8613395259	4.2014885036	-3.3212385959
H	2.4530809316	4.3693993171	-4.221225475
H	0.8236417063	4.4993452101	-3.4909025969
H	2.2720402176	4.777252711	-2.4881662681
H	1.8585361846	0.3656735476	-2.6765347364
C	1.0685514405	2.4910817932	2.0334411618
H	1.9553000467	2.6586232706	2.649015276
H	0.9183879754	3.3567491265	1.3813962365
H	0.1968819367	2.3738139505	2.6828959292

#### 16a\_t1

C	0.8738242985	0.2076299076	2.2763306237
N	1.3614127605	-0.3188179121	3.3494773716
C	1.2766602423	0.7218983867	4.3882254587
C	0.3722475779	1.8374848357	3.8105850094
N	0.4039836877	1.5145179124	2.3718778575
H	2.2817789887	1.1097885164	4.6028403443
H	0.8807460385	0.3138021316	5.3235809549
H	0.7487311593	2.8441239032	3.9980430199
H	-0.6530784421	1.7652329288	4.1961781252
N	0.8426570288	-0.4178146675	1.0416818097
C	1.249933946	-1.8403328878	0.9655930348
C	0.1322294456	-2.7668120248	0.6249200209
H	2.036821793	-1.95177155	0.2210957211
H	1.6605354569	-2.0734718259	1.9487126315
O	-0.8614903485	-2.9257151773	1.5569869034
C	-1.7537028199	-3.8243505128	1.0471146329
C	-1.3525612294	-4.2470557332	-0.182502843
C	-0.1258909726	-3.5558778123	-0.45917847
H	0.4864007588	-3.6328564421	-1.3465270512
H	-1.8641566887	-4.9577893161	-0.816419071
H	-2.6050039295	-4.0515895387	1.6715766678
C	0.2594303153	0.2592330631	-0.033560866
C	-0.4083082818	1.4168377061	0.119472123
C	0.5392883023	-0.2521102468	-1.4176611494
C	-0.5946795336	2.0485801319	1.4705616844
O	-0.4699417196	0.0186247293	-2.2551230687

O 1.5737836903 -0.8008581556 -1.7500584782  
C -0.2463044958 -0.3265206452 -3.640755885  
O -0.3651757641 3.4446392924 1.4888567732  
O -1.9269790731 1.7686944568 1.8721356587  
C -1.2286047591 4.2477800807 0.6784978502  
H -2.2827060139 3.9971764829 0.8318099519  
H -1.0563818461 5.2805857217 0.9889090851  
H -0.9865923952 4.157027734 -0.3872197678  
H -1.1527579631 -0.0237675672 -4.1635695347  
H 0.6192118281 0.2109851355 -4.0346575048  
H -0.0891459512 -1.4024322762 -3.7433286487  
H -0.8218344624 1.9208753338 -0.7418413214  
H -2.1213116288 2.323523901 2.6472253464

### 16a\_t2

C 0.2590947781 -0.5599916299 1.4615403657  
N 0.2193481861 -1.2098840518 2.5769066791  
C 1.5996025428 -1.2498339635 3.0887115463  
C 2.4142535828 -0.2413611411 2.2435287887  
N 1.5090018206 -0.0603852868 1.0916204924  
H 2.0069185035 -2.2650317652 2.9873100979  
H 1.62453871 -0.995813232 4.1529503659  
H 3.381587865 -0.6223407496 1.923889945  
H 2.5608877749 0.7145882406 2.7607265302  
N -0.8038604117 -0.372641516 0.6043878077  
C -2.1110091902 -0.9195570552 1.0188678621  
C -2.6926596676 -1.9090913832 0.0624054462  
H -1.9523673774 -1.3821750553 1.9952944431  
H -2.8264936114 -0.1039533924 1.1503937061  
O -1.955341191 -3.0261711238 -0.2212508166  
C -2.7022326325 -3.8012967686 -1.0640217808  
C -3.8997885498 -3.2083403384 -1.3168240826  
C -3.8947537783 -1.9739456298 -0.5827695204  
H -4.6824637839 -1.2343802031 -0.5352935308  
H -4.6884909243 -3.5947545852 -1.9471588708  
H -2.2437732792 -4.7238061863 -1.3880184853  
C 1.6522164512 0.7763152976 -0.0008131639  
C 0.5814373748 1.1388915875 -0.7330129331  
C 3.0437139553 1.145052636 -0.4167788449  
C -0.8140499217 0.7398263383 -0.3487272482  
O 3.0510514658 2.2036233268 -1.2389185596  
O 4.0460005807 0.5516454275 -0.064072477  
C 4.3443397855 2.5888163249 -1.7543421596  
O -1.4642797897 0.3850700569 -1.5407344433  
O -1.5256678824 1.7865007671 0.3129378981  
H -2.3934596817 0.1833708659 -1.3380453848  
H 4.1559283553 3.4505586948 -2.3936176313  
H 5.0147460286 2.8609712868 -0.936105793  
H 4.7840378557 1.7737198304 -2.3337746386  
H 0.6968889784 1.7206835488 -1.6354596852

C	-1.7059183631	2.9966813968	-0.4284801266
H	-2.3811823946	3.6172524218	0.1647730145
H	-0.7595461097	3.5338387116	-0.5642964221
H	-2.1572850551	2.8089452972	-1.4080593904

#### 17a\_t1

C	1.7956272899	-0.809391473	1.1699670357
N	2.4288578082	-1.6136961215	1.9289061118
C	3.7672631539	-1.000808914	2.1275044014
C	3.8044281839	0.3485667821	1.3251331407
N	2.4574018772	0.342678178	0.7565213557
H	4.5394998686	-1.6926558543	1.7782424054
H	3.9334032713	-0.8309029226	3.1954622608
H	4.5571972392	0.3535715742	0.5337788659
H	3.9471420011	1.2219445016	1.9652889855
N	0.5231170907	-0.8054387511	0.630207461
C	-0.487511341	-1.7946812185	1.0568415413
C	-1.4298410709	-1.2815800128	2.0932095547
H	-1.0579567026	-2.0992711315	0.1824967422
H	0.0791302104	-2.6482644698	1.4363949788
O	-0.9268971944	-1.0683251663	3.3516320474
C	-1.9589059397	-0.626775564	4.1280448933
C	-3.1063953712	-0.5590421603	3.3994856096
C	-2.7612955083	-0.9829884353	2.0732200233
H	-3.4116600684	-1.0579522888	1.2140018952
H	-4.0772240001	-0.2461471856	3.7575220589
H	-1.7167395879	-0.4105915286	5.1580268313
C	0.3614650873	0.3522793829	-0.1266294552
C	-0.6461578458	0.847580662	-0.8842815009
C	1.66649237	1.131421614	-0.0092036599
C	-1.9143897166	0.2268101083	-1.2776738578
O	1.952552886	2.2157921584	-0.5090905064
O	-2.7425677244	1.1657570746	-1.7853096988
O	-2.2156758423	-0.959171054	-1.2278297456
C	-4.0082916673	0.6896791745	-2.2808414325
H	-3.8608577291	-0.0544341398	-3.0675220155
H	-4.6001185445	0.2504854329	-1.4737116015
H	-4.5139509487	1.5681176543	-2.681673483
H	-0.4740055093	1.8398991521	-1.2894879239
H	0.9644359713	3.4024828056	-1.5399514505
O	0.4137878789	3.9024288931	-2.1701655669
C	0.8971941264	3.5934007754	-3.4699633306
H	0.2631449069	4.1136513315	-4.1951339539
H	1.9332839176	3.9309474011	-3.6241151837
H	0.8532651739	2.5171967351	-3.6937778332

#### E-17a\_t1

C	1.7861939424	-0.7048588824	1.1237801919
N	2.304285428	-1.2351333954	2.1684585982
C	3.7704205521	-1.0219262626	2.0431197196

C	4.0283566857	-0.341491672	0.654387645
N	2.6514394938	-0.1308312496	0.2107612976
H	4.2888486773	-1.9813634025	2.1212409902
H	4.1154944997	-0.3879935977	2.8657820834
H	4.560741813	-0.992642637	-0.0439440628
H	4.5610063455	0.6078780468	0.7382752537
N	0.5048550439	-0.5722842819	0.6475058344
C	-0.6799070218	-1.08200722	1.3294132503
C	-1.5687146244	0.0075396365	1.8559670879
H	-1.2485270276	-1.7132753199	0.6377024245
H	-0.330043216	-1.7260496966	2.1441362243
O	-2.8890576588	-0.3304439659	1.9758396753
C	-3.5358901282	0.7501149896	2.5102872996
C	-2.6563719978	1.764319555	2.7253202902
C	-1.3715388439	1.2809640178	2.3019098575
H	-0.4335744655	1.8170780482	2.3263985476
H	-2.8861289821	2.7391210145	3.1325590434
H	-4.5979010901	0.6345086158	2.6669738331
C	0.5353133181	0.0567944802	-0.6060378327
C	-0.5674380935	0.2784860606	-1.3549387856
C	2.0099262717	0.317346152	-0.9164031648
C	-0.6488637074	0.9887091808	-2.6441515577
O	2.5275187866	0.7717350874	-1.9183489517
O	-1.7849590096	0.605500986	-3.2815255789
O	0.1131331112	1.8227406445	-3.094757425
C	-2.0392040998	1.2538322054	-4.540590499
H	-2.1348157773	2.3349220395	-4.4083218255
H	-1.2358034537	1.0485398525	-5.252849319
H	-2.978204674	0.8349092884	-4.9029738836
H	-1.5178596031	-0.0932209588	-0.9886488929
H	1.3676913547	-2.2349090351	3.4424696285
O	0.7565969762	-2.8121670559	3.9517468145
C	1.077837198	-4.1520217116	3.6139563406
H	0.3508293286	-4.8089656877	4.1033141688
H	1.0273597444	-4.3424053876	2.5311169541
H	2.0810109036	-4.4456474812	3.9609017252

#### 17a\_t2

C	0.6337205887	-1.0824383562	0.6384641725
N	0.6215243802	-2.2486106883	1.1491266072
C	1.1934971537	-3.1314158627	0.0994466962
C	1.6718464206	-2.2243953689	-1.0820862069
N	1.1395988207	-0.9233203027	-0.648398904
H	0.4255181309	-3.8402606992	-0.2274892496
H	2.0206822375	-3.7104754522	0.5192347293
H	1.2578849838	-2.5137515418	-2.0459669355
H	2.7601397968	-2.1786997312	-1.1613344284
N	0.2529698269	0.1608271007	1.1157947447
C	-0.3572895731	0.4178741789	2.4316903937
C	-1.8437482864	0.5299541568	2.3942108301



H -0.0376857723 -0.3961277125 3.0865128009  
H 0.0543733568 1.3550645925 2.8109999003  
O -2.5597097541 -0.6266405284 2.2237845617  
C -3.8808540608 -0.2831195997 2.2267289474  
C -4.02249315 1.0596123199 2.3993498457  
C -2.6943308224 1.5908642726 2.5076252624  
H -2.3967346807 2.6206756118 2.6495802491  
H -4.9541450321 1.6060394802 2.4454988504  
H -4.5806828286 -1.0960479282 2.1006807126  
C 1.1601604071 0.39255581 -1.0116956161  
C 1.5754304181 1.0769116132 -2.1069364925  
C 0.5488597647 1.1208846589 0.1690121853  
C 2.1379351106 0.4993536063 -3.3237268271  
O 0.3608777163 2.3262602527 0.2658124271  
O 2.5053433666 1.4798734227 -4.1828993068  
O 2.2667126318 -0.6899127206 -3.5814923342  
C 3.0596663328 1.0379474602 -5.4349986481  
H 3.2905449539 1.946728064 -5.991249555  
H 3.9696827436 0.4543394876 -5.2726902395  
H 2.3370554863 0.4315282279 -5.9874264657  
H 1.4601312613 2.1534199112 -2.0673500634  
H -0.0882989193 3.3710084656 1.771000608  
O -0.2491113896 3.7972945649 2.6317380405  
C 0.7010981436 4.8437431385 2.7830582159  
H 0.5522995048 5.2884755598 3.7718728655  
H 1.7378101855 4.4813900526 2.7253713737  
H 0.573786546 5.6369114829 2.0314342523

#### E-17a\_t2

C 0.484746677 -1.2809156102 0.5720035115  
N 0.2048855477 -2.5108999248 0.7615487895  
C 0.6322370992 -3.1949497024 -0.4887809665  
C 1.2370694761 -2.1125165998 -1.4506496379  
N 1.0605238078 -0.9163929931 -0.6306047839  
H -0.2310133671 -3.690895877 -0.9424606473  
H 1.3684894496 -3.96688948 -0.2462637308  
H 0.6884527681 -2.023471935 -2.3923758414  
H 2.2958039641 -2.2796527804 -1.668936047  
N 0.3544556699 -0.1371166505 1.3350819837  
C -0.2049298378 -0.0678884788 2.6935707743  
C -1.6320589155 0.3636644789 2.741493477  
H -0.0817271203 -1.0590703769 3.1358492216  
H 0.4027494684 0.6401915918 3.2594587012  
O -2.5830481116 -0.5852624643 2.465713977  
C -3.7986083363 0.0273608984 2.5630457978  
C -3.6448491538 1.3385092336 2.8954482826  
C -2.2320450219 1.559260749 3.0108963938  
H -1.7171625525 2.4818487563 3.248528695  
H -4.4363679664 2.0600396212 3.0426937781  
H -4.6591117817 -0.597478754 2.3747083929

C 1.3408233811 0.4199843292 -0.7032800371  
C 1.9293699495 1.0234704588 -1.7706402793  
C 0.8601532863 0.9571969765 0.6413189979  
C 2.2555824864 2.4382801047 -1.9555492019  
O 0.904226825 2.0940109475 1.0754276447  
O 2.8939810256 2.5834337696 -3.1516730683  
O 2.0248130142 3.3825577706 -1.2200778633  
C 3.278566324 3.9258968847 -3.4876013974  
H 3.7625346761 3.8592347451 -4.4625652109  
H 2.4044775381 4.5802090351 -3.5467084657  
H 3.9771807018 4.3290748023 -2.749198669  
H 2.1952072864 0.3792262739 -2.6023705804  
H 0.3772502382 3.3140351335 2.4369113131  
O 0.0413156288 4.0571672059 2.9665331998  
C -0.4162976075 5.034876924 2.0409285284  
H -0.7709138 5.8967053302 2.6150206507  
H 0.3832248302 5.3787142662 1.3686680508  
H -1.2502155473 4.6732533402 1.4212912669

#### 18a\_t1

C 0.473886546 0.4585830677 2.2532550421  
N 0.9418124866 0.0223463581 3.3649479199  
C 0.5787975707 1.0120546124 4.3986550786  
C -0.341968651 2.0625525328 3.7194991335  
N -0.2451809532 1.6559115761 2.3074425412  
H 1.4896927937 1.476084409 4.7942349342  
H 0.0751711505 0.517552466 5.234586132  
H -0.0116888242 3.0952416971 3.8426881025  
H -1.3839335866 1.989896834 4.0460346217  
N 0.6170236113 -0.1524534542 1.0140323851  
C 1.2856668315 -1.4823877526 0.9763202864  
C 0.3644503482 -2.6026525079 0.6361936941  
H 2.0946974517 -1.4489556634 0.2494112236  
H 1.7092892563 -1.6148821708 1.9721991315  
O -0.6081497523 -2.9159266772 1.5505652966  
C -1.3021394703 -3.9799967806 1.0517912214  
C -0.7930215787 -4.3576941763 -0.1523503176  
C 0.2907019257 -3.4584279933 -0.4252758115  
H 0.9337406097 -3.448214527 -1.2937640972  
H -1.1436739677 -5.1707559807 -0.7723885449  
H -2.1147135007 -4.3425838303 1.663782566  
C 0.0453515092 0.441964194 -0.0955038126  
C -0.6745832927 1.5920114819 -0.0206745012  
C 0.3493998235 -0.1356226868 -1.4555382293  
C -0.8637546353 2.2752589554 1.2497578634  
O -0.7204169771 -0.0830535365 -2.2493609099  
O 1.4477003308 -0.5340129924 -1.7912587537  
C -0.5131692727 -0.5057074986 -3.6195710499  
O -1.5162063667 3.3206473583 1.3861132965  
H -1.4780385034 -0.3780582501 -4.1078254992

H	0.2447647009	0.117733422	-4.0982155439
H	-0.2054551522	-1.5529246308	-3.6478146583
H	-1.0983362593	2.0395541064	-0.9080690881
H	-1.2233376429	4.6411835325	2.6372229956
O	-0.9163574947	5.3600534902	3.2233870378
C	-0.0500507257	6.175429654	2.4507965855
H	0.3475665429	6.9586378086	3.1049785704
H	0.8041924327	5.6180393087	2.0370852737
H	-0.5675963141	6.6689512442	1.6134138841

#### 18a\_t2

C	0.017924878	-0.6750117522	1.4504349456
N	0.1860195191	-1.599490144	2.3228553698
C	1.6206099635	-1.6167684582	2.6554987981
C	2.3217139564	-0.5794560854	1.735984971
N	1.1610430515	0.0172171469	1.0351772385
H	2.0298263099	-2.6205683683	2.5034366547
H	1.7562893212	-1.3668678237	3.7138936423
H	2.9963379665	-1.038361485	1.0126214154
H	2.8678246877	0.1866885997	2.2871264516
N	-1.1991106326	-0.306379664	0.8944433234
C	-2.4240541436	-1.0247033119	1.3157634938
C	-2.8729225261	-2.0732442813	0.354215664
H	-2.2098561986	-1.4614184328	2.2913841893
H	-3.2127441433	-0.2799316989	1.4172214053
O	-2.2360205652	-3.2876422098	0.4005383219
C	-2.8122697799	-4.0816761885	-0.5476801689
C	-3.8024012667	-3.407447165	-1.1943379382
C	-3.8401925074	-2.0991584117	-0.6084521368
H	-4.4959696401	-1.2806332171	-0.868583252
H	-4.4285263566	-3.7904740558	-1.9880766213
H	-2.4144458577	-5.0821912631	-0.6320430531
C	1.096422545	1.0466504026	0.1428569409
C	-0.1028162407	1.4304999178	-0.3799149192
C	2.3833125152	1.7093186578	-0.2694108708
C	-1.3236579862	0.7473921534	-0.011677432
O	2.1541330448	2.8589139187	-0.907336183
O	3.4866207466	1.2459973958	-0.0569292755
C	3.3259301421	3.5560406159	-1.392013469
O	-2.4445338459	1.0510288977	-0.4502124054
H	2.946496772	4.4574832646	-1.8707020312
H	3.9845045963	3.8121652755	-0.5594846899
H	3.8637913128	2.9368242859	-2.1131567653
H	-0.1802062266	2.2411668518	-1.0892538525
H	-2.3979990954	2.4580286257	-1.6216374175
O	-2.2304781758	3.2701567119	-2.1415598839
C	-2.619501205	4.3640393363	-1.3262345074
H	-2.400226202	5.2873311406	-1.8729504596
H	-3.6964130469	4.3584673362	-1.0963167854
H	-2.071535686	4.4007674821	-0.3722617075

### S7.3. B3LYP Optimized geometries (from 1b tautomers)

#### **1b\_t1**

C	0.038522206	0.859363814	0.0191778037
N	-0.1386724416	1.9107697718	0.8936201726
N	1.1213767908	0.6082940438	-0.6539882001
C	-1.4542177983	2.3469764255	1.3750658068
H	0.5490914016	2.6468507902	0.8179925334
C	-2.3704914887	1.1421465004	1.5617497256
H	-1.3103802082	2.8790595665	2.3204990489
H	-1.9136640632	3.0529265981	0.6672531895
C	-2.3775764854	0.3134846439	0.2804960998
H	-2.0133443551	0.5261187135	2.3947950989
H	-3.3827156505	1.4821304591	1.7994103778
N	-1.0024183577	-0.0505866833	-0.0531023362
H	-2.9492225033	-0.6094633415	0.4153423083
H	-2.8605406357	0.884659202	-0.5285889198
H	-0.8790721664	-0.7109037038	-0.8099303852
C	2.2517821904	1.5117735893	-0.4685111069
H	2.034942639	2.543352884	-0.7942287037
H	2.5475145191	1.5880176645	0.593522317
C	3.4417300577	1.0636317442	-1.2543484503
C	4.1254806416	1.5983265006	-2.3073392657
C	5.1967104935	0.6903961837	-2.6113197433
C	5.0863081642	-0.3315608234	-1.7204115684
O	4.025351422	-0.1212155184	-0.8849323767
H	5.6491628775	-1.237910343	-1.5523983714
H	5.9432743455	0.7889181177	-3.3873362688
H	3.8921734051	2.5280012009	-2.8082107859

#### **1b\_t2**

C	-0.9048163869	0.0227717424	-0.4005870547
N	-1.5023260037	0.1502271863	0.7381154307
C	-1.0851754345	1.2571995962	1.6030021729
N	0.0107797254	0.9041724583	-0.9552622081
H	0.6315797388	0.5018735092	-1.6471579202
N	-1.1675146331	-1.073083983	-1.216715549
C	-2.302064283	-1.9434933355	-0.9086795801
C	-2.2781044927	-3.1836514959	-1.7355916535
H	-2.2476428703	-2.1908088787	0.1551582228
H	-3.2692272981	-1.4467993368	-1.0700224237
O	-1.2655211433	-4.0798341461	-1.5033289088
C	-1.4519259211	-5.1309177206	-2.3551248173
C	-2.5571477009	-4.9299135782	-3.1227465979
C	-3.093990828	-3.6606812906	-2.7201013496
H	-3.9728353356	-3.1660899245	-3.11041076
H	-2.9438999032	-5.5974337552	-3.8802104798
H	-0.7244187168	-5.926535545	-2.2912174624
H	-1.9597528689	1.5916878348	2.1755786829

H	-0.3633375288	0.8871970305	2.3485110089
C	-0.4731775554	2.4463073871	0.8533670609
C	0.5991318089	1.9413665292	-0.1085472724
H	-0.039490037	3.1661467918	1.5553623426
H	-1.2530857171	2.9665150698	0.2839160199
H	-1.0574026257	-0.8857236272	-2.207602095
H	0.9666601961	2.7469130462	-0.7522698914
H	1.4589078151	1.5544514354	0.459357082

# NCov(1b\_t1)

C	-1.1421325658	1.1953121045	1.661820871
N	-1.5710510027	2.5039329335	1.7170464463
N	0.0252180194	0.799841223	1.2435306124
C	-2.9756218493	2.8889157111	1.8914737057
H	-1.0131892795	3.1612977398	1.190833202
C	-3.6826615721	1.8931655942	2.8050938098
H	-3.0013733941	3.8970832448	2.3165659803
H	-3.4916024801	2.9284503424	0.9205879034
C	-3.4399071415	0.4787375749	2.2868183976
H	-3.2947025096	1.9811991112	3.8262820552
H	-4.7543670464	2.1114762597	2.8282718175
N	-2.0003294235	0.2481244863	2.1913067658
H	-3.8575508853	-0.2656613314	2.9712469115
H	-3.9428993985	0.3495305029	1.3148142782
H	-1.7069641795	-0.6970787629	1.9698174887
C	0.9600524338	1.8237411635	0.7898396932
H	0.5886280462	2.3837189973	-0.0850968466
H	1.1528392354	2.580094064	1.5719155283
C	2.2690592653	1.2273017453	0.3853177529
C	2.90693422	1.0905774084	-0.813267679
C	4.1517012024	0.424429766	-0.5473449028
C	4.1815720514	0.2065380786	0.7952364478
O	3.0456147812	0.6922499512	1.3802321102
H	4.9009221306	-0.2473032225	1.4608114047
H	4.9167297427	0.1490597818	-1.2602609396
H	2.5315599357	1.4204672909	-1.7723141228
C	-0.5984547125	-1.6271559177	-2.1909891988
C	-0.3065878201	-1.9490175777	-1.0606209736
C	-0.9279174761	-1.3157635194	-3.5695518447
C	0.0089395951	-2.2776586406	0.3174011118
O	-1.0970457395	-0.0014637931	-3.7376599141
O	-1.0274438552	-2.1637375201	-4.4342321875
C	-1.4259252072	0.4207546924	-5.0849421186
O	1.3234375263	-2.3421903039	0.5068196721
O	-0.8477456206	-2.4946541446	1.1566090103
C	1.7508311612	-2.5782611793	1.8710806839
H	-1.5292616067	1.5032550389	-5.0276250066
H	-0.6230872058	0.1482738132	-5.7732409928
H	-2.3633761721	-0.0374970475	-5.4069527517
H	2.8376512758	-2.6210897409	1.8261941548

H	1.4231711958	-1.7531777843	2.5051626594
H	1.3442143256	-3.5227641338	2.2382670043

#### NCov(1b\_t2)

C	0.0034886299	2.2549301685	0.6202572978
N	-0.0018345945	3.3511795176	1.4671705108
N	1.2598403844	1.8243001287	0.2135356874
C	-1.2690641426	4.0179991957	1.7750369447
H	0.7915056582	3.9730183179	1.3800876357
C	-2.3855440329	2.9789036268	1.804419187
H	-1.1693560274	4.5225670574	2.741831978
H	-1.4989220749	4.7886802109	1.024376956
C	-2.3532824862	2.1699474974	0.5036730184
H	-2.2384377124	2.3076414287	2.6594513375
H	-3.3526714427	3.475727975	1.9355080461
N	-1.0363245129	1.6117218497	0.1923802952
H	-3.067976623	1.3397266361	0.5610113898
H	-2.6994319145	2.8068875938	-0.3273549572
C	2.4744211237	1.937274285	1.0291096221
H	3.2685780105	2.447115993	0.4711755927
H	2.2518944089	2.5549384302	1.9043512637
C	3.0258429869	0.6212050044	1.4741420178
C	4.216264695	-0.0076377478	1.2506663743
C	4.1666924994	-1.2508686345	1.9678341573
C	2.9465512917	-1.2891396025	2.5704277911
O	2.2398493484	-0.1556393305	2.2859567698
H	2.4512651747	-2.0087053031	3.2055088158
H	4.9355626347	-2.0088725797	2.0250858058
H	5.0292787806	0.3691818763	0.6455158087
H	1.1993554868	0.9808144738	-0.3495302615
C	-1.9502684248	-1.567521675	-1.4956561711
C	-0.7515917205	-1.7342893717	-1.4602077904
C	-3.3871552741	-1.3674569031	-1.4409917294
C	0.6920001319	-1.8579537848	-1.4275966169
O	1.0681603315	-3.1344280849	-1.4684893674
O	1.4427492269	-0.8994401507	-1.3744986182
C	2.4984912079	-3.3763648926	-1.4245029256
O	-3.9162054349	-1.3423081229	-2.6654628214
O	-3.996703759	-1.2450204845	-0.3963886715
C	-5.3515829299	-1.1442875345	-2.7259946883
H	2.6048051567	-4.4586660519	-1.4779670294
H	2.9881813706	-2.8990722875	-2.2755378456
H	2.9142464382	-2.9936953738	-0.4901561927
H	-5.5969295621	-1.1581905295	-3.7867720095
H	-5.8666081446	-1.9520765838	-2.2021847662
H	-5.6186021635	-0.1827632376	-2.2825818412

#### TS1(1b\_t1)

C	-1.2895012539	0.8737918454	0.6255055582
N	-1.3565141538	2.223696989	0.8341022945

N	-0.3778000965	0.298102403	-0.1356659553
C	-2.4041251951	2.8915623985	1.610573718
H	-0.8522795853	2.8027959294	0.1790687441
C	-2.923330136	1.9571093982	2.6978714138
H	-1.9778767667	3.8008216875	2.0449970988
H	-3.2317803035	3.1946417322	0.9538691028
C	-3.3070083409	0.6213273817	2.0671518534
H	-2.1483619908	1.7983551394	3.4560873496
H	-3.7907741503	2.4085374355	3.1876682216
N	-2.1846312098	0.0974427794	1.2960635961
H	-3.558431082	-0.1167493629	2.8334751826
H	-4.1958940882	0.7507918064	1.4319059737
H	-2.0682150338	-0.908533606	1.2369141031
C	0.6261653031	1.1495848944	-0.7620073317
H	0.2041885608	1.7830209556	-1.5561091926
H	1.0762353912	1.8288068823	-0.0183435644
C	1.7213935845	0.3469589522	-1.38478785
C	2.1755135735	0.2214802485	-2.6661839739
C	3.2942223185	-0.6783372872	-2.6230418142
C	3.438564589	-1.0350844069	-1.3183158544
O	2.4925688497	-0.4184170517	-0.5489184618
H	4.1244715236	-1.6847141223	-0.794933247
H	3.9022522843	-1.0127466638	-3.4522409133
H	1.7619767859	0.7130020466	-3.5359133599
C	-1.0668096275	-1.4424487985	-1.3445989926
C	-1.1145437669	-2.5182334273	-0.7219019603
C	-1.3084568095	-0.7651730538	-2.6265729812
C	-1.0583184188	-3.1887447882	0.540470874
O	-1.2040962766	-1.6604451641	-3.6276134326
O	-1.5929486685	0.4038982433	-2.7910404049
C	-1.4900391154	-1.1489894069	-4.9480913466
O	-0.0985896305	-4.1274701568	0.5909672096
O	-1.8220090587	-2.9408337713	1.4724044335
C	0.0420355951	-4.8162607848	1.8524917605
H	-1.374670663	-2.0005949668	-5.6180520144
H	-2.5102303504	-0.761086867	-4.9981937888
H	-0.7845991767	-0.3582549523	-5.2141922236
H	0.8696925198	-5.5109514891	1.7114938998
H	0.2727523617	-4.1109567936	2.6544243386
H	-0.8725462919	-5.3618452273	2.0966699373

# TS1(1b\_t2)

C	-0.2761246797	1.1111999025	-0.0983792503
N	-0.3164608107	2.366800656	0.4435633766
N	0.9497473658	0.6517459258	-0.5009863816
C	-1.5864919466	2.9420384731	0.8989663609
H	0.5189938513	2.6980954525	0.9056808779
C	-2.5212981332	1.8277545018	1.3606505554
H	-1.3633619618	3.6461711571	1.7032583076
H	-2.0503746891	3.5081509899	0.0810821823

C	-2.6402544678	0.7903689379	0.240895721
H	-2.1155425553	1.3631221643	2.2669794038
H	-3.5089775956	2.2323338618	1.6033732238
N	-1.3427838585	0.3658828741	-0.2846619429
H	-3.1674376693	-0.0996381195	0.604892846
H	-3.251827098	1.1996525946	-0.574020219
C	2.1792698307	1.4420347293	-0.3943228627
H	1.9808562511	2.4525962814	-0.7618943934
H	2.5189830159	1.5302047445	0.6488301047
C	3.2815352349	0.8624665046	-1.2146232283
C	3.7660994295	1.1302695163	-2.4617234011
C	4.8414943093	0.2089590683	-2.6911841338
C	4.9320784125	-0.5528732428	-1.5666843947
O	3.9924193667	-0.168278414	-0.6552598598
H	5.578909482	-1.3637788946	-1.2663536584
H	5.4625884732	0.1300738057	-3.5725246981
H	3.4001607839	1.8935409135	-3.1345376894
H	1.0607290018	-0.3594921619	-0.5398431569
C	-1.2794752276	-1.1449046305	-1.760117026
C	-0.674056886	-2.2097120093	-1.5184170911
C	-2.0895644297	-0.4008185274	-2.7323686809
C	0.1900419847	-2.843157368	-0.5707021991
O	-0.3213203869	-3.9811780784	-0.0634266673
O	1.2997036093	-2.4061206687	-0.2662226146
C	0.4922793981	-4.6503799102	0.9218843356
O	-1.3254108383	0.0847603075	-3.7238778428
O	-3.2954889876	-0.2554261913	-2.6604109368
C	-2.0290656892	0.8168069988	-4.7530204994
H	-0.079516602	-5.5282802523	1.2226911475
H	1.4500430314	-4.9534425128	0.4918227011
H	0.6697864905	-4.0027132503	1.7840896899
H	-1.2626382115	1.1278319898	-5.4622149088
H	-2.7646780772	0.1762139296	-5.2448797276
H	-2.5299205209	1.6894709512	-4.3272773693

#### 10b\_t1

C	-1.4614505447	0.9000810117	0.3447911316
N	-1.3643984735	2.1886319131	0.7100428676
N	-0.6275727218	0.3722046055	-0.5874977299
C	-2.1037384179	2.8033807444	1.8231242881
H	-0.8945049246	2.8250356479	0.0818343111
C	-2.685780449	1.730794574	2.7362559109
H	-1.4158287303	3.4569065381	2.367180607
H	-2.904395139	3.4268691063	1.4090351836
C	-3.3525096645	0.6562347203	1.8806641311
H	-1.8949622995	1.2752495945	3.3418227002
H	-3.4106564927	2.188657616	3.4145960173
N	-2.3880664834	0.1175877781	0.9154428711
H	-3.7019625946	-0.1809661396	2.4871985043
H	-4.2182471278	1.0708907121	1.3500885832



H	-2.1923698473	-0.8926158387	0.9458599772
C	0.6316439591	1.0368083036	-0.9851279323
H	0.543480692	1.4021263341	-2.0115283048
H	0.8014227841	1.8978896692	-0.3353001161
C	1.8101861647	0.1271483184	-0.8929697687
C	2.6585193768	-0.3993211788	-1.8223138515
C	3.6335095618	-1.1659622639	-1.1002202692
C	3.3017702183	-1.0530424937	0.2148066418
O	2.1984544359	-0.2634115732	0.3624099237
H	3.7278391531	-1.4461203717	1.1258633976
H	4.4628745529	-1.7264761457	-1.508565784
H	2.5954603863	-0.2568590931	-2.8923164829
C	-1.0776224604	-0.7524184765	-1.4322115518
C	-1.0307278958	-2.0469811277	-1.1008367018
C	-1.6073898815	-0.2458935914	-2.7312989947
C	-0.6536307775	-2.5457229088	0.17582222
O	-1.9616918221	-1.2296561089	-3.5846686791
O	-1.7172735523	0.9391734317	-3.0201307155
C	-2.4872308597	-0.7902718829	-4.8486163078
O	0.5425909178	-3.1960740911	0.1895787017
O	-1.3882931714	-2.527541286	1.1849498346
C	0.9398662121	-3.7556157474	1.4497573747
H	-2.7145213397	-1.7008226717	-5.4041786254
H	-3.3962073587	-0.1981550431	-4.7115429251
H	-1.7506525133	-0.1929670534	-5.3928965033
H	1.9308279335	-4.180824055	1.2834079778
H	0.9914657738	-2.9890935355	2.228164678
H	0.2497324205	-4.5415769412	1.7705314096

#### 10b\_t2

C	0.1783441726	1.1538685648	-0.1774002736
N	-0.0061303519	2.3415528091	0.4239502315
N	1.3853079612	0.8491052023	-0.7033243182
C	-1.3117582838	2.7643292382	0.9401106777
H	0.8113018026	2.8379262411	0.7510458071
C	-2.0315249912	1.5443768332	1.5024899071
H	-1.1299615305	3.520567541	1.7049503886
H	-1.8966690369	3.2252429509	0.1357222962
C	-2.1232002839	0.4759074178	0.4192668445
H	-1.4813358341	1.1672593908	2.3712110672
H	-3.0406365603	1.8088972316	1.8303064894
N	-0.8381682315	0.279163125	-0.2874824341
H	-2.4058817582	-0.4895317012	0.8489903489
H	-2.8763307112	0.7517781254	-0.3253197337
C	2.4982662355	1.81036725	-0.7268768158
H	2.1144525881	2.78250823	-1.0458647457
H	2.9351096911	1.9325464569	0.2742634428
C	3.5589660593	1.3967262359	-1.6877669481
C	3.8844878685	1.7940583881	-2.9514791734
C	5.0184903514	1.0102419468	-3.3479842034

C 5.298457232 0.1921821137 -2.2968004276  
O 4.4220932627 0.414463981 -1.2744264135  
H 6.0493655543 -0.5635291372 -2.1203068948  
H 5.5516310769 1.0544402153 -4.2873700491  
H 3.376912534 2.5545784049 -3.5286198578  
H 1.6416860629 -0.1458906854 -0.6794605021  
C -0.8129488576 -0.8002030706 -1.2916095393  
C -0.1977695608 -1.978439024 -1.1409505637  
C -1.5662888761 -0.3999241191 -2.5146199001  
C 0.6533752618 -2.2964947161 -0.0451407353  
O 0.1217681821 -3.1819784155 0.8445266923  
O 1.8351078764 -1.9140457691 0.0518218603  
C 0.9999285216 -3.6190519853 1.8934135508  
O -1.6724027794 -1.3926536787 -3.4229719139  
O -2.0470352281 0.710270029 -2.7015944581  
C -2.3742307625 -1.0510776783 -4.630282359  
H 0.4066447841 -4.2950643396 2.5113936301  
H 1.8660951284 -4.1514327541 1.489724511  
H 1.350839208 -2.7772685361 2.4973388362  
H -2.3641571679 -1.9546368096 -5.2408956641  
H -3.40465566 -0.755929023 -4.4141742308  
H -1.8724499497 -0.2359864799 -5.1588864265

#### TS2(1b\_t1)

C -1.2382834117 1.0321196426 0.5462963088  
N -1.2744321696 2.3250972962 0.9226964224  
N -0.3855853153 0.6321771706 -0.4273786217  
C -2.1209481372 2.8525197741 2.0023078092  
H -0.8729151588 3.0106924876 0.3002632353  
C -2.4967686204 1.7390938518 2.9715257725  
H -1.5610748911 3.6445176031 2.5064327177  
H -3.0228327709 3.3000636059 1.5678706556  
C -3.0214539665 0.5453355281 2.1810620043  
H -1.6230056982 1.4371409656 3.5586753048  
H -3.262219876 2.1015170562 3.6624587645  
N -2.0381580907 0.1519508634 1.1671070408  
H -3.1820622792 -0.3211789875 2.8252039532  
H -3.9772605713 0.791642811 1.702068108  
H -1.8901228704 -0.838389887 0.9967602778  
C 0.6055503744 1.5768083996 -0.9981392853  
H 0.1592446453 2.1483356685 -1.8164284295  
H 0.9085694478 2.2721646212 -0.2097840914  
C 1.8237607084 0.8909539368 -1.5100837916  
C 2.3234597913 0.6881943797 -2.7635058767  
C 3.5713079485 -0.0004116562 -2.6005442359  
C 3.7379080889 -0.1661339801 -1.2599579518  
O 2.6868092112 0.3750794614 -0.5782881106  
H 4.5086440802 -0.6219789689 -0.6561931569  
H 4.2480934331 -0.3268442833 -3.3776948165  
H 1.8542317558 0.989491231 -3.6893942332

C	-0.5190683773	-0.7180037838	-1.0040808774
C	-0.3891820982	-1.7968871844	-0.267183668
C	-0.9251276146	-0.656907385	-2.4429667312
C	-0.6239291451	-2.9505014633	0.4229569376
O	-0.8910084723	-1.8639944219	-3.0395029464
O	-1.2593197437	0.3635080477	-3.0281178275
C	-1.2978391417	-1.8837860576	-4.4193226549
O	0.4482756514	-3.8243917049	0.4971783521
O	-1.7103341216	-3.1952509084	1.0074950905
C	0.2653273717	-4.9287835402	1.3857282783
H	-1.2050889168	-2.92247158	-4.73771463
H	-2.3331735773	-1.5491389716	-4.5261223901
H	-0.649850562	-1.2452277338	-5.0256617911
H	1.1878743544	-5.5110452505	1.3281447835
H	0.1079510426	-4.5993937135	2.4188466723
H	-0.5805043069	-5.5565559401	1.0884886287

#### TS2(1b\_t2)

C	-0.0581541444	1.4873370642	-0.1990768866
N	-0.1345368593	2.6912107539	0.3954171789
N	1.1425353533	1.0552557477	-0.632583044
C	-1.3755969263	3.2787723268	0.9057044781
H	0.724601447	3.1902433136	0.5723816235
C	-2.3178788643	2.1569003932	1.3177238225
H	-1.1117569103	3.9162247499	1.7519153104
H	-1.8365949355	3.9089156878	0.1354641363
C	-2.4772158598	1.1879133838	0.1537083914
H	-1.9162316099	1.6382530277	2.1948201415
H	-3.2964936018	2.5658905609	1.5829022241
N	-1.1658370813	0.7373410102	-0.3635886958
H	-3.0186537509	0.2917872777	0.4671314043
H	-3.0374804381	1.6539408906	-0.6617961002
C	2.382629942	1.8406465727	-0.5228680257
H	2.2731172914	2.7796918427	-1.0750642892
H	2.5874491014	2.0862318405	0.5278220331
C	3.5419933324	1.0930825427	-1.0803295149
C	4.1770620892	1.1085512736	-2.2877032743
C	5.2227988484	0.1305494143	-2.2107948365
C	5.1446165299	-0.4077021174	-0.9625037089
O	4.1312829084	0.1689602236	-0.2574209686
H	5.7118902997	-1.1653981574	-0.442579926
H	5.9347067717	-0.1319333158	-2.9807374099
H	3.9272835122	1.7399143642	-3.129173157
H	1.2227941318	0.0803139675	-0.9036428007
C	-1.1148696311	-0.5435387696	-1.0908949766
C	-0.3165159587	-1.5246068318	-0.742275159
C	-2.0042630547	-0.5187514878	-2.2967747919
C	0.6803485347	-2.44864765	-0.6186140497
O	0.3483768538	-3.5554395065	0.1516741699
O	1.8242458204	-2.3209188522	-1.1192910582

C	1.4247989216	-4.4619476203	0.3965330958
O	-2.1895069986	-1.7454171565	-2.8231903437
O	-2.5052793764	0.4887445143	-2.7744221865
C	-2.9962012548	-1.7916126254	-4.0134722224
H	1.006507417	-5.2577248634	1.0174281959
H	1.8160450685	-4.8928233274	-0.5308360909
H	2.2512145791	-3.9808552508	0.931193236
H	-3.0408034587	-2.8435366639	-4.29704468
H	-4.0026184137	-1.4120435017	-3.817436746
H	-2.5419186253	-1.2050670463	-4.8165254987

### 11b\_t1

C	-1.3577531111	1.1545754262	0.59341402
N	-1.4254541594	2.4871272146	0.7951194453
N	-0.6546754952	0.6576510877	-0.460699409
C	-2.1305667221	3.0970038405	1.9322770372
H	-1.260704606	3.0902817506	0.0014817288
C	-2.2457076681	2.1046641767	3.0846198895
H	-1.5728639455	3.9876059646	2.2342343163
H	-3.1276186515	3.4177377992	1.6072569889
C	-2.7820109785	0.7753234002	2.5582848569
H	-1.264784868	1.9462688102	3.5453492654
H	-2.9157589004	2.5119767525	3.8462683508
N	-1.9448657927	0.3205298886	1.4488397731
H	-2.7528267922	0.0007834126	3.3275917729
H	-3.8233094299	0.8828914823	2.2293208639
H	-1.6734894288	-0.6742365913	1.300575019
C	0.3585058893	1.5062357243	-1.1391515547
H	-0.0383309509	1.8962436441	-2.078377682
H	0.5846449364	2.3485868677	-0.4814613765
C	1.6228233604	0.7718038749	-1.4282968046
C	2.2531640266	0.4215665012	-2.5869343256
C	3.4741437934	-0.2301292789	-2.2085739023
C	3.4950692005	-0.2300203998	-0.8478833396
O	2.3786576518	0.380584862	-0.3536137936
H	4.1940480596	-0.6035263012	-0.1142112573
H	4.2287407551	-0.6436471594	-2.8629426601
H	1.8875211246	0.6040323445	-3.5877115861
C	-0.8178134342	-0.7229104658	-0.9127646326
C	-0.9305780686	-1.7392504013	-0.0442805327
C	-1.0011312159	-0.7877553069	-2.3957387473
C	-1.2566585089	-3.0974081798	-0.3969865293
O	-0.7636360621	-2.019193031	-2.889850091
O	-1.3521593364	0.1476631079	-3.1012799633
C	-1.0188018948	-2.187735903	-4.295147239
O	-0.1468313613	-3.901516284	-0.4257427563
O	-2.3907553912	-3.560658904	-0.5072373668
C	-0.4047124031	-5.2966194796	-0.6258409839
H	-0.7931619417	-3.232305515	-4.510952271
H	-2.0643004906	-1.9720705472	-4.5307460128

H -0.3740459032 -1.533514093 -4.8878653532  
H 0.5708708018 -5.7861346416 -0.6046105485  
H -1.0397108094 -5.7043856173 0.1667136991  
H -0.8870312776 -5.4800948333 -1.5909293082

### 11b\_t2

C 0.128858743 1.7278970857 -0.2444147215  
N -0.1129331184 2.9710983166 0.2175723051  
N 1.385505506 1.3488285236 -0.5085422448  
C -1.4421402751 3.4519986807 0.6003343662  
H 0.6819589967 3.5098488248 0.5301429522  
C -2.2615221489 2.2662656908 1.0879095008  
H -1.3067117636 4.2030765921 1.3806051851  
H -1.9298925597 3.9340765772 -0.2554847868  
C -2.2642279162 1.1932169221 0.0089863411  
H -1.8347897013 1.8797473476 2.0197957367  
H -3.2928829027 2.5703740326 1.2864761635  
N -0.8925671938 0.8608538831 -0.4552887854  
H -2.7060128651 0.2686056521 0.3894831824  
H -2.8564913582 1.5206558338 -0.8485174776  
C 2.5589717822 2.2064451377 -0.3299264269  
H 2.4202882196 3.1502045519 -0.8670938339  
H 2.7013246837 2.4470447049 0.7342874564  
C 3.7828737177 1.5500709832 -0.8676061268  
C 4.6131685043 1.8279699113 -1.9124181441  
C 5.6335497389 0.8184584128 -1.9034765709  
C 5.3455194313 -0.0014995343 -0.8568038598  
O 4.2227313819 0.4302353205 -0.2092573074  
H 5.8109075451 -0.888959537 -0.4545986434  
H 6.4650323924 0.7196746729 -2.5871709749  
H 4.5094670783 2.6515662225 -2.6051311924  
H 1.4688128331 0.3077117255 -0.5982349977  
C -0.6963589392 -0.4542659552 -1.0576110854  
C 0.4312167531 -1.1592814806 -0.8859667276  
C -1.795651914 -0.8004049839 -2.0136005472  
C 0.734612331 -2.3979318836 -1.5568168748  
O 0.5584686752 -3.4805219143 -0.734733776  
O 1.238179625 -2.512254163 -2.6728761035  
C 0.9687389532 -4.7401063456 -1.2809202032  
O -1.967339852 -2.13283989 -2.1305543719  
O -2.4476779182 0.0079806389 -2.6577150853  
C -2.8982764971 -2.556248501 -3.1427644512  
H 0.7750684819 -5.4800956628 -0.5019978409  
H 0.3960634052 -4.9925568953 -2.1786748659  
H 2.03369805 -4.7392959966 -1.5327350868  
H -2.9123530198 -3.6451235564 -3.0912456921  
H -3.8961316617 -2.1567009686 -2.9443847084  
H -2.5700632238 -2.2310739768 -4.1336036753

### TS3(1b\_t1)

C	-1.3255978396	1.4004308479	0.960321656
N	-1.624443195	2.7236400562	1.0239330166
N	-0.4474537413	0.9709320765	-0.014220383
C	-2.5696620024	3.2616123978	2.0113117402
H	-1.5100224903	3.2675497563	0.17977159
C	-2.6214324527	2.3571241294	3.2392023762
H	-2.2422161813	4.2701751653	2.2792602544
H	-3.5666542612	3.3419464595	1.5599489777
C	-2.8300764871	0.9089822945	2.7959068803
H	-1.6846672536	2.4354575902	3.8019597975
H	-3.4350554947	2.6810227945	3.8943483734
N	-1.8110006475	0.528122048	1.8196371054
H	-2.7491303563	0.2227076545	3.6436085609
H	-3.8334791791	0.7824380398	2.367280608
H	-1.3225310573	-0.5432247267	1.5987964923
C	0.5724871076	1.9213435364	-0.5356695686
H	0.3703076792	2.1698007097	-1.5784106152
H	0.4965801622	2.8371828901	0.0529051608
C	1.9665576922	1.4014051295	-0.4356779293
C	2.9245389196	1.1160155335	-1.3651419895
C	4.0921373301	0.7065148186	-0.638461514
C	3.7572850792	0.7697905245	0.6788979377
O	2.4684449666	1.1963107321	0.8235653028
H	4.2896636537	0.5547923294	1.5935585058
H	5.0466048388	0.4033333785	-1.0454959445
H	2.8113424185	1.1912675158	-2.4376991514
C	-0.2855122884	-0.4402713713	-0.2854460907
C	-0.5902247313	-1.3675483811	0.6405674963
C	0.081959557	-0.8170359118	-1.6872901454
C	-0.6249408156	-2.8003417368	0.3959998453
O	-0.2708020762	0.116226376	-2.6000244051
O	0.5820855302	-1.8840488504	-1.9962186396
C	0.0102167137	-0.2175087704	-3.9740059461
O	0.4811245366	-3.4242130734	0.8912755254
O	-1.5793769968	-3.4244124244	-0.0538278029
C	0.4769239798	-4.8563522344	0.7967745927
H	-0.3107416809	0.6459100552	-4.556841027
H	1.0779587679	-0.3977912587	-4.1197233141
H	-0.5503767146	-1.1058222395	-4.2754964244
H	1.4143448827	-5.1863792251	1.2475591025
H	-0.3690601975	-5.2878866611	1.3396103856
H	0.432717325	-5.1834659743	-0.2462613931

### TS3(1b\_t2)

C	-0.2994881478	1.8178358662	0.5909955296
N	-0.4635404388	3.1063085381	0.9728886355
N	0.9049578185	1.3101987106	0.3689066314
C	-1.737204071	3.6908962421	1.3943807523
H	0.3758411366	3.6227726074	1.1909406873
C	-2.6265443806	2.5796074513	1.9291967625

H	-1.5217818846	4.4406693491	2.158653803
H	-2.2214339907	4.1974331878	0.5500304426
C	-2.7338249302	1.485480827	0.8768385256
H	-2.2079537404	2.1808936396	2.8597037572
H	-3.6281213752	2.9627278469	2.1429615729
N	-1.3996329599	1.0138946786	0.4264769556
H	-3.2660178756	0.6228385052	1.2843872281
H	-3.2982248061	1.8518953174	0.0152640678
C	2.1283742499	2.0971366844	0.496296636
H	2.1299323634	2.9416261951	-0.2048492684
H	2.2134065417	2.5182759161	1.5102527987
C	3.3329701095	1.2675867896	0.2060650025
C	4.2819460419	1.3066059603	-0.7721418409
C	5.2059763218	0.2445775192	-0.4898644616
C	4.748622534	-0.3640587756	0.6375322036
O	3.6094668966	0.2472508324	1.0794978982
H	5.0949261696	-1.2007411553	1.2260063853
H	6.0876464835	-0.026358701	-1.0537177475
H	4.3172448426	2.0065921906	-1.5954074081
H	0.8135142048	0.1467129954	0.2144927546
C	-1.2722070848	-0.3537473092	-0.0181269139
C	-0.0926784028	-0.9973904092	-0.0308791108
C	-2.5018870163	-0.9808336367	-0.608812617
C	0.1047641177	-2.3259704585	-0.5822010784
O	0.3048809969	-3.2546787929	0.3979447549
O	0.2240340119	-2.6036064887	-1.7710454786
C	0.6163831447	-4.5785995731	-0.06010484
O	-3.1782511785	-0.1350211964	-1.4166827563
O	-2.8151674405	-2.1480693109	-0.4605236424
C	-4.3414795966	-0.6856412868	-2.0681241081
H	0.7473969103	-5.1810537491	0.8403804406
H	-0.196352481	-4.9902613127	-0.6658077944
H	1.5372821484	-4.5879631261	-0.6504835277
H	-4.7590021963	0.1291368415	-2.659629197
H	-4.0603830288	-1.5186173883	-2.716960596
H	-5.0708350178	-1.0304620213	-1.3308738386

## 12b\_t1

C	-0.8735290925	1.1841783448	1.032493758
N	-1.7886006581	2.1829382048	0.8460702205
N	-0.2756170154	0.7476263721	-0.2044985266
C	-2.5168276482	2.751995238	1.9794870413
H	-2.1845550334	2.2874163899	-0.0786044796
C	-1.6613997941	2.605917529	3.2368698197
H	-2.7298981281	3.8039583568	1.7654365705
H	-3.4786002082	2.2380549673	2.1120019145
C	-1.1529673021	1.164771525	3.3562259957
H	-0.806337168	3.2895345392	3.1780913442
H	-2.2476196524	2.883775185	4.1180284482
N	-0.478384516	0.6806500625	2.1434944873

H	-0.4455766435	1.0812673648	4.1886244743
H	-1.9883788466	0.4901438792	3.5932101398
H	-1.1927817924	-1.4452811273	1.1378967053
C	0.5266522586	1.7665423694	-0.9343630416
H	0.6029085659	1.4694962701	-1.9797221809
H	-0.0332988799	2.7024843015	-0.9127166122
C	1.8900736073	2.0033773925	-0.3684762187
C	3.1017348897	1.3930735009	-0.5233592558
C	4.0268492261	2.0995525041	0.3131017935
C	3.3128089034	3.0891246946	0.9171159115
O	2.0103637328	3.0477649055	0.5146800627
H	3.567699917	3.8711937997	1.616865425
H	5.0811260291	1.8977347317	0.4420524849
H	3.2999364109	0.5368214077	-1.1514174046
C	-0.2723249918	-0.5779467709	-0.5701236258
C	-0.8037615181	-1.6102481543	0.1440866917
C	0.3659682	-0.8609104022	-1.9245982015
C	-0.8579537544	-2.9635194063	-0.3861350727
O	-0.5296774642	-0.7281215534	-2.906575967
O	1.5462102592	-1.0940736174	-2.0781092962
C	-0.0465252993	-1.008938569	-4.240887479
O	-1.4343502697	-3.8059569078	0.5104195346
O	-0.4537096515	-3.3483676338	-1.4789263607
C	-1.5419981034	-5.1776225358	0.0963364317
H	-0.8974824237	-0.8388072918	-4.899456562
H	0.7760337902	-0.3390872116	-4.5006335143
H	0.2850986997	-2.0472247709	-4.3064614962
H	-2.0234284153	-5.6988713142	0.9245227632
H	-2.151234992	-5.2673571325	-0.8072997254
H	-0.5549662279	-5.6080414367	-0.0936789972

#### E-12b\_t1

C	-1.2465179676	0.9773138589	0.4205094631
N	-1.065576942	2.2918961662	0.7852352617
N	-0.2215934505	0.4119929326	-0.3641363047
C	-2.1089941119	2.9265196778	1.6021367797
H	-0.6306555278	2.8873513638	0.0902229008
C	-3.4772337292	2.3360835025	1.2628785355
H	-2.0682695536	4.0018630167	1.4163621922
H	-1.88558859	2.7659273982	2.6644313506
C	-3.3989063975	0.8112963511	1.3896418855
H	-3.7472099895	2.616067054	0.2374427232
H	-4.245581474	2.7368760187	1.9319658917
N	-2.2303043602	0.2073955554	0.7454789817
H	-4.297486061	0.3485175806	0.962679806
H	-3.3929521481	0.5317539291	2.4536531883
H	-0.2226710153	-2.5425348409	-2.0377467978
C	1.1218579378	1.0257535625	-0.4543902217
H	1.8700990456	0.2361275807	-0.4551838092
H	1.2730412691	1.6070392844	0.4579876558



C	1.306216071	1.8852612972	-1.6598550073
C	2.0122536553	1.7437694416	-2.8175687623
C	1.776667139	2.9283376384	-3.5942516311
C	0.9421152769	3.708097972	-2.856469829
O	0.6466985797	3.0920418155	-1.6712446104
H	0.4909464657	4.676517351	-3.0125309243
H	2.1782485858	3.1641031654	-4.5699031552
H	2.6279841958	0.8962469294	-3.0849136881
C	-0.5628380401	-0.7063257446	-1.1232841593
C	0.1619830863	-1.8379915435	-1.3108734795
C	-1.8476828193	-0.6359716955	-1.9291325298
C	1.3456832282	-2.2856073285	-0.5698995631
O	-2.1012237382	0.6110785868	-2.3534731065
O	-2.50844049	-1.6078023986	-2.2388093902
C	-3.2926161655	0.7675109199	-3.1517100667
O	1.7626262747	-3.4800653357	-1.0502622008
O	1.8923735293	-1.7258924803	0.371165638
C	2.8881912324	-4.0694492623	-0.373379558
H	-3.3418407681	1.8277371359	-3.3982909184
H	-3.2254533256	0.1683613655	-4.0628471339
H	-4.1761501577	0.4684268757	-2.5826051239
H	3.0852477831	-5.0067568803	-0.8938447178
H	3.7613671396	-3.4144921173	-0.430843832
H	2.6510343274	-4.2637627001	0.6759322671

## 12b\_t2

C	-0.1368919183	1.8124300546	0.5445950496
N	-0.3761077546	2.9396250881	1.2875447046
N	1.0331062416	1.3598443854	0.24333247
C	-1.6566214882	3.5536388907	1.6494462071
H	0.4293967233	3.5317126146	1.4308903245
C	-2.8108367945	2.6132492162	1.3341016015
H	-1.6350425517	3.8159810999	2.7125460641
H	-1.7763976418	4.4855434593	1.0816209612
C	-2.5220170613	1.9461672973	-0.002636085
H	-2.9183892803	1.8409047382	2.1026953612
H	-3.7453750926	3.179352708	1.2872976652
N	-1.3002927252	1.1155973342	0.1143117406
H	-3.3551350378	1.3295300416	-0.3269079238
H	-2.3587026859	2.6982016676	-0.7833757711
C	2.196033436	2.0507260466	0.7904029003
H	2.2877940834	3.0793532968	0.4070051235
H	2.1282977273	2.138005921	1.8887604432
C	3.4637978679	1.3460479794	0.4339319163
C	4.558506118	1.702676358	-0.2977188516
C	5.4638609402	0.5879149736	-0.2580252135
C	4.8524026561	-0.3661971221	0.4941959371
O	3.6344073826	0.0782351811	0.9272023015
H	5.1288578269	-1.3637028447	0.8021407094
H	6.4343702041	0.511301408	-0.7284846957

H 4.7020788016 2.6461945943 -0.8061644001  
H 0.7195934344 -0.7303289341 -0.1980670981  
C -1.3406523129 -0.2424054651 -0.1531625043  
C -0.2894559313 -1.1023330616 -0.2629384794  
C -2.7541812384 -0.8080692556 -0.2389142776  
C -0.4854816946 -2.5363059854 -0.4469549114  
O 0.7122259447 -3.1616246746 -0.5837703404  
O -1.5480669541 -3.1476638967 -0.4792087788  
C 0.655097304 -4.585637595 -0.7676709211  
O -3.1456765367 -0.9546799359 -1.507990309  
O -3.4410929407 -1.0215222319 0.7377789483  
C -4.4488136272 -1.5500312425 -1.6963798497  
H 1.6918888189 -4.915058856 -0.8439017572  
H 0.1691518567 -5.0712689337 0.0830050132  
H 0.113338495 -4.840757259 -1.682664967  
H -4.5997739624 -1.5850035524 -2.7748060229  
H -4.4613690984 -2.5580694193 -1.2766379272  
H -5.2235925338 -0.941860089 -1.2239033575

#### **E-12b\_t2**

C 0.212151242 0.4067795676 0.6131563406  
N 0.3960848261 1.4925028836 1.4268876498  
N 1.1285366406 -0.1993247743 -0.0820603624  
C -0.6795245422 2.2469487124 2.0703430935  
H 1.2586804255 1.9975155193 1.2817863879  
C -1.8169970318 1.2998923992 2.4232711204  
H -0.2695069132 2.723349129 2.9656021833  
H -1.0472648675 3.0441689752 1.4083210114  
C -2.2339835048 0.5255081087 1.1813733257  
H -1.4965708477 0.6021484079 3.2041376891  
H -2.6714483203 1.8683359149 2.8015867221  
N -1.065306554 -0.1518942919 0.5848151067  
H -2.9729129805 -0.2341410508 1.4322036382  
H -2.6784604755 1.2052016083 0.4411181898  
C 2.5007217572 0.2658742205 -0.0047065104  
H 2.8085650737 0.5101602908 1.0276267821  
H 3.1561498046 -0.5609865977 -0.3114833503  
C 2.8077125979 1.4462016419 -0.8871103229  
C 2.0760189733 2.2178377291 -1.7419356981  
C 2.9837889632 3.1806330871 -2.3054773112  
C 4.1996688359 2.9236900672 -1.7555764802  
O 4.1122454936 1.868265312 -0.8873253729  
H 5.1780131467 3.3683477291 -1.8623375645  
H 2.7543531223 3.9558037486 -3.0236964064  
H 1.021413865 2.1124600985 -1.9466968508  
H -2.028021772 -3.0627179167 -0.8722284541  
C -1.2754789487 -1.2030357038 -0.3261764427  
C -1.833336637 -2.3980688441 -0.0386801408  
C -0.9731679877 -0.958577021 -1.7903196928  
C -2.1913652239 -3.0034184264 1.2596302296

O	-1.8870706324	-2.2622770412	2.3413790792
O	-2.6991027662	-4.1120612164	1.3313626594
C	-2.1869601251	-2.8704277573	3.6149805534
O	-1.1772749932	0.3257076499	-2.1281364015
O	-0.6899468056	-1.8332464786	-2.5852627303
C	-0.9854016212	0.6361425171	-3.5243246136
H	-1.8748817395	-2.1450766309	4.3657731658
H	-3.257213699	-3.0716329545	3.7035822519
H	-1.6310517403	-3.8032828716	3.7357218953
H	-1.2056756685	1.6988130586	-3.6216827186
H	0.0446996721	0.4315980981	-3.8246296135
H	-1.669070042	0.0500891026	-4.1432840372

#### TS4<sub>sc</sub>(1b\_t1)

C	-0.7848726758	1.2373986389	0.423895494
N	-0.3912331158	2.3689176981	1.0390995579
N	0.1458001859	0.290284674	-0.0171275185
C	-1.3791048009	3.4279839845	1.3052945173
H	0.5715932381	2.6642714769	0.9465600839
C	-2.7623045893	2.8143657699	1.5182014379
H	-1.0531280785	3.9749663598	2.1932969072
H	-1.3964572937	4.1300597804	0.4625343607
C	-3.1063254529	1.8433993215	0.3828775019
H	-2.7828089184	2.2778605223	2.473030477
H	-3.5067149759	3.6138984968	1.5692645905
N	-2.015819047	0.897017816	0.1897347087
H	-4.01223282	1.2803305942	0.6244965619
H	-3.2938418899	2.3842069578	-0.5537710759
H	-0.7049469727	-2.3871620253	-1.905491762
C	1.5930630946	0.4459014204	0.2448008286
H	2.0244036716	-0.5530692095	0.2672641324
H	1.7074099199	0.886121477	1.238810553
C	2.3168242693	1.2464998655	-0.7837760774
C	3.148195975	0.91274671	-1.8114997458
C	3.5319340514	2.1414317335	-2.4460904967
C	2.9059948392	3.1363303198	-1.7615125068
O	2.1615387763	2.61197083	-0.7415225839
H	2.8851213393	4.2114909112	-1.8587444301
H	4.1869280252	2.2635746484	-3.2973843984
H	3.4500829087	-0.0901841725	-2.0772115362
C	-0.445923043	-0.713300275	-0.7559597026
C	0.0401562475	-1.845530949	-1.3334290456
C	-1.950895114	-0.4021054363	-1.0369534854
C	1.3451347139	-2.4977775644	-1.3397252216
O	-2.2682008632	0.0498551852	-2.1535174943
O	-2.7075864641	-1.4329433877	-0.448363116
O	1.3304555872	-3.5155560769	-2.2397244064
O	2.3429004266	-2.2665597752	-0.6604308608
C	2.5378426089	-4.2894994168	-2.3318889595
H	2.3341586655	-5.0636489404	-3.0723921506

H	3.3760147256	-3.6687349929	-2.6600636433
H	2.7849612044	-4.7456576589	-1.3695602383
C	-4.0244049101	-1.5776800912	-0.9780424394
H	-4.4443320221	-2.4660628631	-0.4996275925
H	-4.6612894421	-0.715309702	-0.745378313
H	-4.0109749847	-1.7160726549	-2.0632939122

#### TS4<sub>sc</sub>(1b\_t2)

C	0.2375888805	0.6836892289	0.602319961
N	0.6402785687	1.6244387006	1.4767676606
N	0.8521370176	0.3024103329	-0.4741810795
C	-0.1221805755	2.0790114579	2.6456145691
H	1.391229827	2.2243693367	1.1575316045
C	-1.1182434295	1.007545836	3.068548603
H	0.5868323611	2.3014324854	3.4477626323
H	-0.64867162	3.0084846551	2.3945202156
C	-1.8913369937	0.4966904798	1.8572991118
H	-0.5984086588	0.1692886056	3.5452142306
H	-1.8158677353	1.429057487	3.7974093056
N	-0.9398438149	-0.0288764407	0.8593912184
H	-2.5621248084	-0.3092763578	2.1399424367
H	-2.4720311179	1.3048173834	1.3947360736
C	2.2497498373	0.5255055798	-0.7891318177
H	2.861167355	0.4566775249	0.1231511997
H	2.551390047	-0.2993425172	-1.4442983755
C	2.5462702862	1.8135174504	-1.4880461761
C	2.9977857259	2.1385257414	-2.7326720743
C	3.0962851619	3.5716230811	-2.7765723874
C	2.69745769	4.0192174363	-1.5568765684
O	2.3616734281	2.9616023927	-0.7540578124
H	2.5977803257	4.999351889	-1.1152006533
H	3.420454772	4.1815929645	-3.6082088534
H	3.2382198948	1.4403613784	-3.522308287
H	-1.9847861239	-2.7552630753	-0.8583111752
C	-1.1509965816	-1.0769866274	-0.0146063559
C	-2.018474881	-2.1229571135	0.0221203533
C	-0.2276303507	-1.0209923849	-1.2603513163
C	-2.9086785991	-2.6171280282	1.0680792956
O	-3.672634983	-3.6267866113	0.5754500995
O	-2.9843502653	-2.2686521382	2.2420951689
C	-4.5562376295	-4.2591135262	1.5162968132
O	-0.9313986285	-0.2640678679	-2.2076919697
O	0.4785953051	-1.9778496138	-1.6001128106
C	-0.3444108588	-0.2319914607	-3.507629532
H	-5.0789699913	-5.0333907396	0.9538399038
H	-3.9942498396	-4.7083836296	2.3396588356
H	-5.273555948	-3.5408179679	1.9221723264
H	-1.0879174571	0.2196609052	-4.1686665042
H	0.5633491138	0.3846454409	-3.5194717404
H	-0.0974397064	-1.2374846737	-3.8596831294

**TS4<sub>6c</sub>(1b\_t1)**

C	-1.3336596986	0.8039537652	0.4285765502
N	-0.8631186225	1.7834841357	1.2420840808
N	-0.4162632431	-0.1042726305	-0.0684887119
C	-1.793630094	2.743655358	1.8495761411
C	-3.1335948577	2.057761004	2.1109108668
H	-1.3319952896	3.1075869288	2.7691056024
H	-1.9292845384	3.6001663925	1.1785853469
C	-3.6416026337	1.4626696103	0.8024169077
H	-3.0011559136	1.274489439	2.8658020437
H	-3.8635253775	2.7760195818	2.495398359
N	-2.6015649236	0.7030616166	0.1033214672
H	-4.480218555	0.7776408081	0.9491251613
H	-3.995110495	2.2625602182	0.1408619722
C	0.984684196	0.3350056739	-0.31509294
H	1.3418870542	-0.1709842535	-1.2129085021
H	0.9456416895	1.4045338153	-0.5473485951
C	1.981876757	0.0951691958	0.7724612875
C	3.2163945614	-0.4792689175	0.7877672623
C	3.747419788	-0.2871819841	2.108009048
C	2.8011255101	0.3915000147	2.8080151705
O	1.7183841176	0.642263595	2.0047859305
H	2.7288408156	0.7500078652	3.8235897573
H	4.7049994519	-0.6197421765	2.4837863291
H	3.6881066349	-0.9895527018	-0.0399021818
C	-0.9067144803	-1.2732068633	-0.7076011785
C	-0.0335755551	-2.4827957994	-0.627165268
C	-3.1414688747	-0.2054217461	-1.2039806605
C	-2.1501353946	-1.3479424404	-1.2081917664
O	-4.3634931372	-0.4770857885	-1.0650772263
H	-2.5136588596	-2.2894172245	-1.602196451
O	-0.3390701003	-3.381871944	-1.5801106918
O	0.8369134757	-2.6526127329	0.2063160744
C	0.3812918194	-4.6298667651	-1.5151311663
H	0.0035770304	-5.2272830067	-2.344565285
H	1.4544100307	-4.4593322221	-1.6287978607
H	0.1912241987	-5.1367802637	-0.5658690286
O	-2.7379234379	0.6158684307	-2.3381545997
C	-3.7380412205	1.4995987332	-2.8213385926
H	-3.4695108838	1.7589892963	-3.8506835319
H	-4.7249272956	1.0260209314	-2.8067267265
H	-3.789148215	2.4293966724	-2.2344781965
H	-0.0217174345	1.5709673784	1.7655728022

**TS4<sub>6c</sub>(1b\_t2)**

C	-0.7801629908	0.9263013722	0.2111980959
N	-0.5258644377	1.9606411357	1.0467675229
N	0.2074765446	0.1934701273	-0.2977098809
C	-1.5696810737	2.7625666651	1.6890583435

C	-2.7825019579	1.8762047711	1.9258100676
H	-1.1560504162	3.1482937226	2.6223204878
H	-1.8343440428	3.6175363639	1.0549934821
C	-3.21905131	1.2813890954	0.5966624353
H	-2.5303177965	1.0885616719	2.6438538577
H	-3.6122669562	2.4585715504	2.3355905032
N	-2.0778766382	0.6633477788	-0.135543872
H	-3.9672826488	0.5013117302	0.75338576
H	-3.6615443724	2.0522444444	-0.0361880358
C	1.6020403931	0.5365347395	-0.0188871275
H	2.1822967459	-0.0217846095	-0.757087697
H	1.7769215873	1.6006959142	-0.2142596601
C	2.0742515276	0.2183728607	1.3741564614
C	1.9522396473	-0.8628995683	2.1965680236
C	2.6793653171	-0.5490796147	3.393532171
C	3.1918516029	0.6989675552	3.2153207321
O	2.830654445	1.187682405	1.9899399315
H	3.7976091182	1.3529202699	3.8249660826
H	2.8019785157	-1.171650921	4.2692388555
H	1.3959284858	-1.755254292	1.9466127527
C	-0.0729017109	-1.3515740064	-0.8509058179
O	0.0285421642	-2.2298845782	0.0525860377
C	-2.3480550148	-0.3147511201	-1.1252419135
C	-1.4266961759	-1.2159961388	-1.5022495424
C	-3.634350949	-0.1880086242	-1.8719761836
O	-4.0327058741	-1.3686747849	-2.3787243676
O	-4.2407384581	0.8555113279	-2.0436753096
C	-5.1972040533	-1.3220763588	-3.229296712
H	-5.3620624497	-2.3495941012	-3.5524455804
H	-6.0634156939	-0.9558867731	-2.6734038151
H	-5.0187375456	-0.6772453304	-4.0932650495
H	-1.6629117979	-1.9204148538	-2.2904092797
H	0.3910277322	1.9917835932	1.4668290874
O	0.9013273349	-1.3844393531	-1.939142335
C	1.6205553355	-2.6067662891	-2.0381723774
H	0.9710022121	-3.4516895879	-2.30740394
H	2.3540216097	-2.4630522182	-2.8374586606
H	2.1430050449	-2.862037971	-1.1110885336

### 13b\_t1

C	-0.8442405877	1.067272046	0.9018406646
N	-0.5490521434	2.1796778543	1.5829139965
N	0.1084319045	0.1146287825	0.5562786547
C	-1.6265211298	3.1220669938	1.9201594589
H	0.409207771	2.4989131924	1.6381912886
C	-2.9190507317	2.3435768181	2.1724017171
H	-1.3166111207	3.6708100564	2.8117052757
H	-1.7605335495	3.8421559572	1.1035226609
C	-3.2463437771	1.4408361854	0.9779269698
H	-2.8037796876	1.7355010115	3.0760126322

H	-3.7392789171	3.0458556862	2.3421549097
N	-2.0532662856	0.7243090621	0.5469150011
H	-3.9881933213	0.6812421119	1.2426531504
H	-3.6418536048	2.02906979	0.1419569122
H	-0.8129146071	-2.7914975966	-0.9164299149
C	1.5233897583	0.2546190965	0.9697487365
H	1.9616034131	-0.7385384026	0.9179834829
H	1.5405521585	0.5918099847	2.0106471853
C	2.3274993703	1.167038075	0.1072697905
C	3.1621275887	0.9635611256	-0.9509439684
C	3.6345079829	2.2560788295	-1.3572388345
C	3.054256192	3.1569804072	-0.5193237217
O	2.2549262561	2.5131082029	0.3844359528
H	3.1034700531	4.2316120082	-0.4266838006
H	4.3179199462	2.4807659922	-2.1641803923
H	3.4061140215	0.0026793896	-1.3802869531
C	-0.4956321907	-0.9775792562	-0.0390897363
C	-0.0254699987	-2.1512590848	-0.534235422
C	-2.0561046182	-0.7643793763	-0.064694072
C	1.3111411924	-2.7095060127	-0.6940862514
O	-2.3568210741	-0.5673725294	-1.4708541317
O	-2.7753622189	-1.564919786	0.593025096
C	-3.7221211194	-0.7600817615	-1.8127251442
O	1.2243215901	-3.9013669736	-1.3410251754
O	2.3984602089	-2.256134388	-0.343263688
C	2.4689668145	-4.5808595404	-1.5733124478
H	-3.7612416882	-0.880986769	-2.899832119
H	-4.1326344149	-1.6522165827	-1.3299012799
H	-4.3483956381	0.1026339789	-1.539572569
H	2.2063144909	-5.5083158203	-2.083331275
H	3.1307196782	-3.980827757	-2.2038034478
H	2.9760230334	-4.8016770009	-0.6301661912

### 13b\_t2

C	0.4920823315	0.7441398694	0.7633162401
N	0.8849801566	1.7118931578	1.5951419696
N	1.0875203182	0.3884718174	-0.3518609176
C	0.1841953594	2.0815587786	2.8326129614
H	1.6014524856	2.3410062394	1.2516869454
C	-0.6738749196	0.9165357813	3.3101582364
H	0.9379542752	2.3519339786	3.5762037485
H	-0.4371896301	2.96457041	2.6418518295
C	-1.5104388838	0.3609886221	2.1611171237
H	-0.0398069168	0.1219225371	3.7181467752
H	-1.3370210459	1.2604129934	4.1083189374
N	-0.6157957494	-0.0357205573	1.0562075954
H	-2.0726065786	-0.5199883312	2.4612152293
H	-2.2118190672	1.1170548764	1.7873089134
C	2.4909545715	0.6197782787	-0.6678777458
H	3.0917435614	0.5585911628	0.2499079821

H	2.779777124	-0.2206918201	-1.307110197
C	2.7751162528	1.9060358022	-1.3686129139
C	3.2512368156	2.2344705122	-2.6026436432
C	3.335807182	3.6683276111	-2.6458754657
C	2.9052031499	4.1133839231	-1.4361818824
O	2.563043173	3.0531385696	-0.6395392246
H	2.7844126163	5.0929030657	-0.9985515882
H	3.6718161862	4.2805571012	-3.4710528576
H	3.5164242634	1.5381803156	-3.3858356194
H	-1.4522145558	-2.7253230454	-0.821335766
C	-0.7635059645	-1.062088996	0.1434257316
C	-1.6010769558	-2.1265375383	0.0707237928
C	0.2817120611	-0.8942993822	-1.0101047109
C	-2.6221693619	-2.6505826885	0.9715642391
O	-3.2839588981	-3.6674692683	0.3582869847
O	-2.8913137742	-2.3171997751	2.1214175829
C	-4.2958918941	-4.3187414708	1.1433853964
O	-0.5093884758	-0.3047547096	-2.0688301896
O	1.0577305734	-1.841860163	-1.2962043727
C	0.130784573	-0.2776406943	-3.336527074
H	-4.7055070536	-5.1014689373	0.5040398867
H	-3.8667556255	-4.7594246738	2.0474027638
H	-5.0838349851	-3.615803933	1.4271069353
H	-0.6474098714	-0.0802049823	-4.0801032405
H	0.882964809	0.522258487	-3.4013826205
H	0.6151213681	-1.233640924	-3.5597067711

#### 14b\_t1

C	-1.2435133602	0.8550428915	0.516987055
N	-0.7341035826	1.8292671506	1.3047696922
N	-0.364642454	-0.0656409531	-0.0167605524
C	-1.5924513067	2.846848187	1.9227411596
C	-2.9576494023	2.2382896391	2.2239768469
H	-1.0871640429	3.1911164301	2.8268256523
H	-1.696304758	3.7035999205	1.2463387067
C	-3.516565544	1.6375945176	0.9426003741
H	-2.8539786826	1.4693625726	2.9976906316
H	-3.6436312486	3.0033119987	2.5985121569
N	-2.5378319812	0.7838768524	0.2580489679
H	-4.3914528903	1.0093210455	1.1203559198
H	-3.8187737575	2.4307242721	0.2485914778
C	1.0730338187	0.3090882483	-0.1839575147
H	1.4531031567	-0.2539156045	-1.033083584
H	1.1062006055	1.3680033995	-0.4572516573
C	1.9836690332	0.0757674555	0.9805803389
C	2.9214296527	-0.8643619333	1.2879810168
C	3.5291424643	-0.4632413044	2.5240231707
C	2.9223710929	0.6957681447	2.8923015045
O	1.9858384185	1.0486515424	1.9596258002
H	3.029083181	1.3654338018	3.7323537828



H	4.314131001	-0.9742481201	3.0637680542
H	3.1413555882	-1.7452461341	0.7051860526
C	-0.8974118506	-1.1534083128	-0.7645864464
C	-0.0310721833	-2.3578973746	-0.9211264225
C	-3.1785074371	-0.0693885798	-0.9355928388
C	-2.1711193429	-1.1655882859	-1.1904863502
O	-4.3611258857	-0.4443383699	-0.6830584832
H	-2.5491987814	-2.0421767684	-1.7011604159
O	-0.4647136921	-3.1604442438	-1.9089813374
O	0.9452809721	-2.6091519854	-0.2365808905
C	0.2588493941	-4.3976176065	-2.0724222018
H	-0.2247004311	-4.908213689	-2.9047844418
H	1.3076775927	-4.200505802	-2.3057726194
H	0.1942817114	-5.0050970478	-1.1664638775
O	-3.0123120665	0.9311412887	-2.0317259677
C	-3.959648096	0.7869260971	-3.0746036394
H	-3.8962230387	1.6878357143	-3.6948653881
H	-3.7531540663	-0.0837866302	-3.7187677553
H	-4.9782195643	0.6883248082	-2.6842693512
H	0.1626887638	1.6667217674	1.7453033739

#### 14b\_t2

C	-0.6788861167	0.9367305257	0.1698068309
N	-0.3939898309	1.9970884213	0.9584466751
N	0.2929168124	0.1438213546	-0.2822332612
C	-1.40063772	2.8792202839	1.5501499644
C	-2.6596386177	2.0674758677	1.8028017133
H	-0.9799358909	3.2788447053	2.4747849881
H	-1.611570502	3.7213882244	0.8794744655
C	-3.1001102885	1.4280622298	0.4962500173
H	-2.4626451041	1.3045944881	2.563529585
H	-3.4661681221	2.7106024083	2.164986009
N	-1.9831234392	0.7024365473	-0.1720273772
H	-3.8961446656	0.7041056107	0.6784596393
H	-3.4841579428	2.1861830769	-0.1886293953
C	1.6962111668	0.3856839638	0.0831576216
H	2.2660459899	-0.2815290804	-0.563288063
H	1.9821935866	1.4094572593	-0.1820080001
C	2.0466490863	0.1353897423	1.5199087728
C	2.1065597287	-0.9781861527	2.3031331183
C	2.5085346998	-0.5423838105	3.609890248
C	2.6606137708	0.8076435953	3.5349482409
O	2.3831623365	1.2430129955	2.2676739189
H	2.9511714801	1.5687782153	4.2436140396
H	2.6645643453	-1.1553730862	4.4869045891
H	1.8632994992	-1.9757113461	1.9685464059
C	0.0348606572	-1.3240502276	-0.887515199
O	0.3128768462	-2.2608642282	-0.0803317612
C	-2.288003135	-0.3582918519	-1.062537197
C	-1.3758683746	-1.2787753197	-1.4124175131

C	-3.6090490238	-0.3084996483	-1.7556756106
O	-4.0304554735	-1.5361958877	-2.1082486475
O	-4.2203974724	0.7131268384	-2.0175668341
C	-5.2300581203	-1.5787181123	-2.9089744349
H	-5.4087074587	-2.6350558431	-3.1082309413
H	-6.0719412656	-1.1487131958	-2.3614242349
H	-5.088170382	-1.0346406505	-3.8459591764
H	-1.6516108028	-2.0567596942	-2.1133285374
H	0.5466552247	2.0818288509	1.3130192077
O	0.9001236827	-1.2070691003	-2.090836479
C	1.3936874587	-2.4540014345	-2.5509443046
H	2.152416039	-2.2349476368	-3.3094953213
H	1.8453910254	-3.0371339076	-1.7421795643
H	0.6087073128	-3.0684249904	-3.0207821976

### 15b\_t1

C	-0.583517636	1.4158290082	0.0606155673
N	-0.1730851595	2.5843815011	0.3738494269
N	0.2779537939	0.3751584111	-0.3496501893
C	-1.2153855007	3.5602663851	0.7261441184
C	-2.5492641901	2.9430729623	1.1747344174
H	-0.8233437869	4.2054831336	1.5204717589
H	-1.3819585263	4.2125580066	-0.1430932663
C	-2.9893722371	1.8373522335	0.2109975371
H	-2.4394204588	2.5167959688	2.1784397219
H	-3.3217787496	3.7163456617	1.2260806183
N	-1.8647519899	0.9157693123	0.0690032915
H	-3.8461400292	1.2875153669	0.6116602133
H	-3.2761981189	2.253789196	-0.7624578011
H	-0.9099867061	-2.7425190837	-0.9717207528
C	1.7329353718	0.5340141885	-0.1938432054
H	2.2122967297	-0.1171105051	-0.9239160532
H	1.9591141364	1.5760681968	-0.4207626056
C	2.22202683	0.2332624093	1.1843923125
C	2.6738550629	1.0181084628	2.2054557615
C	3.0060844104	0.1359998679	3.2872845022
C	2.7260360228	-1.1214317285	2.8483235527
O	2.2502654241	-1.0839876882	1.5688542042
H	2.8062160105	-2.1017335243	3.2944783099
H	3.3987266887	0.4050332188	4.2580131043
H	2.7555788017	2.0959103013	2.1867583198
C	-0.4318434919	-0.7637489344	-0.63670417
C	-0.0837838035	-2.0434033718	-0.9378479567
C	-1.9245753788	-0.3664528638	-0.5808918668
C	1.2205253351	-2.6342921136	-1.2231502605
O	-2.4864677736	-0.1308416137	-1.8605177515
O	-2.6434431329	-1.3338938062	0.1198239464
C	-2.6920044793	-1.2530316523	-2.7270393219
O	1.1386027087	-3.9866773608	-1.1264099877
O	2.2576881948	-2.0745153408	-1.5595763355

C	2.3371326637	-4.7102864182	-1.4520768509
H	-3.288185476	-0.8750261792	-3.5603439578
H	-1.7448207613	-1.6441675676	-3.1126792593
H	-3.2416057307	-2.0581183068	-2.2296295975
H	2.0854171646	-5.764633398	-1.3330779809
H	2.6459336637	-4.5119846989	-2.4820853723
H	3.1522954825	-4.4406513702	-0.7753635334
H	-3.5889313786	-1.1270062664	0.019504392

#### **E-15b\_t1**

C	-0.8956222044	1.6364364144	0.2315103859
N	-0.6285635901	2.7897441417	0.7138861842
N	0.0917778353	0.7445106719	-0.2408491551
C	-1.7920476423	3.5834328009	1.1354778772
C	-3.0234890743	2.7430306177	1.5042301872
H	-1.4932109848	4.1971633981	1.9925413105
H	-2.049303128	4.2856467818	0.3291675839
C	-3.3403948467	1.7277977201	0.4017518486
H	-2.8335488637	2.2071072102	2.4413100721
H	-3.8897914509	3.3922834368	1.6633975741
N	-2.106833023	1.0126464584	0.0846179417
H	-4.0865004676	1.0022983434	0.7356549255
H	-3.7310091084	2.2364413031	-0.4891846746
C	1.5208661873	1.0564937303	-0.1747279122
H	1.9696980621	0.8784467986	-1.1560041439
H	1.5748880277	2.1266766224	0.0407185537
C	2.2822774536	0.2713885614	0.8433847336
C	3.3488949061	-0.574665963	0.7529250083
C	3.6707927982	-0.9725466786	2.0938032018
C	2.7741601917	-0.3421184632	2.8997001608
O	1.9227089446	0.424997725	2.1562935961
H	2.6098769879	-0.3317813271	3.9669246529
H	4.460189402	-1.6403208327	2.4092807029
H	3.8456409758	-0.8763404438	-0.15888895
C	-0.4653664856	-0.3989678569	-0.7333918327
C	0.2176809078	-1.4673256918	-1.2311576314
C	-2.0014068305	-0.2198947302	-0.6660719019
C	-0.4010174528	-2.6913187634	-1.701813673
O	-2.4159129621	-0.077902934	-2.0181270132
O	-2.6722963789	-1.2267727615	-0.001476657
C	-3.7899529834	-0.3503788686	-2.3144297239
O	0.4981854746	-3.4799905326	-2.3241370686
O	-1.5787251134	-3.0504110671	-1.5669267967
C	0.0133193094	-4.7505285249	-2.7981849086
H	-3.9134889621	-0.095582056	-3.3696838877
H	-4.0355858166	-1.407235067	-2.1733493279
H	-4.4809136504	0.2588617717	-1.7227132432
H	0.8763082937	-5.2413865919	-3.2482848953
H	-0.3740896034	-5.3513368249	-1.9716128822
H	-0.7726378601	-4.6117877034	-3.5446665452

H 1.29848022 -1.4335662666 -1.2796060235  
H -2.437631494 -2.0496955582 -0.5025056531

### 15b\_t2

C 0.4156191243 0.6411218109 0.8212510094  
N 0.8922562074 1.6171735584 1.4925749084  
N 1.028618435 0.0629125827 -0.267819319  
C 0.1190043956 2.0944574626 2.6434978784  
C -0.8811166045 1.0738688749 3.1935849094  
H 0.8250391258 2.3891184374 3.4284066816  
H -0.4105348448 3.0121805309 2.3487352188  
C -1.7111849404 0.4651633649 2.064330746  
H -0.345845229 0.2723116035 3.7164787298  
H -1.5513655576 1.549435974 3.9165130738  
N -0.7924970089 -0.0541258825 1.0402470032  
H -2.3376038789 -0.3539547097 2.4093048878  
H -2.3535978984 1.225637493 1.6012706154  
C 2.3029268767 0.5112213662 -0.7950659046  
H 3.0099731374 0.6074085125 0.0348412085  
H 2.6893930102 -0.2852696742 -1.4409690681  
C 2.2712815629 1.8229788828 -1.5306284063  
C 1.3878647267 2.4516620835 -2.3583811355  
C 2.008834876 3.6835754572 -2.7576198202  
C 3.2257240058 3.7117002762 -2.1506988734  
O 3.4019813235 2.5854071925 -1.3958594354  
H 4.0421186957 4.418441859 -2.1438922821  
H 1.5983428055 4.4431821007 -3.4086680419  
H 0.4152396283 2.0779354113 -2.6407030853  
H -1.6811745965 -2.7348914672 -0.8444008273  
C -0.9545502053 -1.0710188022 0.1392208879  
C -1.8405641135 -2.0969190983 0.0148607722  
C 0.1678283057 -0.8995466958 -0.910560347  
C -2.9295764874 -2.5328588538 0.8822023347  
O -3.6287945704 -3.5211368566 0.2636247886  
O -3.2182748534 -2.1536328574 2.0118369685  
C -4.7064406653 -4.0936379982 1.022790108  
O -0.2643557173 -0.2980959183 -2.1201302758  
O 0.7649379858 -2.1356650391 -1.1522326338  
C -1.1398844064 -1.0391869367 -2.9809883069  
H -5.1384332705 -4.8647365333 0.3841053593  
H -4.3377700985 -4.5386680716 1.9510173742  
H -5.4605146552 -3.3389960015 1.2620696667  
H -1.1580550307 -0.4891731921 -3.9240593718  
H -0.7708592708 -2.0526734773 -3.1653059697  
H -2.1555805073 -1.0882292728 -2.5754601326  
H 1.3334191826 -2.0420934961 -1.9360918939

### E-15b\_t2

C 0.4042799997 0.6701104158 0.7344845358  
N 0.8624043366 1.6230679668 1.4511528051

N	1.0406242001	0.0977739665	-0.3412168638
C	0.0215220055	2.0577619279	2.5726904903
C	-0.8608609382	0.9422842919	3.1412824478
H	0.6774366475	2.4473993678	3.3584457332
H	-0.6051448439	2.9009092386	2.2462953825
C	-1.6880972474	0.2783254057	2.0389919603
H	-0.2263472392	0.1875267305	3.6200083155
H	-1.5380539831	1.3376564699	3.9041946133
N	-0.8158019988	-0.0174054993	0.8985503695
H	-2.1261360227	-0.657814374	2.3939131699
H	-2.5028870638	0.9314457201	1.7051305526
C	2.3270447602	0.5352484636	-0.8503465295
H	3.0407131169	0.5757360336	-0.0211386267
H	2.6730751933	-0.2479823926	-1.5319396848
C	2.3310303285	1.8776471649	-1.5295742168
C	1.4790812538	2.550242404	-2.3559395564
C	2.1255420734	3.7887386277	-2.6883877367
C	3.3256276969	3.7766556392	-2.0481434779
O	3.4668735951	2.6193202762	-1.3340008284
H	4.1503425247	4.4714279723	-1.9913384761
H	1.7429477184	4.5785581355	-3.3202250248
H	0.5104729929	2.1992749162	-2.678476287
C	-0.9680483904	-1.0135115175	-0.0195468726
C	-1.9911654608	-1.9194253508	-0.0186284839
C	0.1901248842	-0.8371991506	-1.0359341574
C	-2.0604392083	-3.1114620338	-0.8368123691
O	-3.2295930168	-3.7553554645	-0.6664245318
O	-1.1862025505	-3.5652500188	-1.5919149705
C	-3.3899969309	-4.9939135026	-1.3856193568
O	-0.2839222167	-0.1375295574	-2.1901055884
O	0.8777305711	-1.9846994518	-1.3521779859
C	-1.0068770075	-0.8615976103	-3.1862160784
H	-4.3775687881	-5.3633118196	-1.1095959391
H	-3.3382063582	-4.8250063034	-2.4638848529
H	-2.6218926763	-5.7139288939	-1.0930354953
H	-1.113284038	-0.1755091415	-4.0296276194
H	-0.4651241553	-1.7518932182	-3.5174554883
H	-2.0066792226	-1.1477065302	-2.8394579616
H	-2.7929011988	-1.8016733522	0.7002852075
H	0.2011176577	-2.698089952	-1.5063795232

#### 16b\_t1

C	-1.2435395881	1.0101853507	0.5047423524
N	-0.6696315022	1.9795454766	1.1318394542
N	-0.4108799049	0.0281965196	-0.070163033
C	-1.5113593433	3.0184662637	1.7170274975
C	-2.8529471095	2.4661263022	2.1916686137
H	-0.9648098675	3.471305462	2.5522110927
H	-1.6799584392	3.8241529286	0.9856154513
C	-3.5333295643	1.7494866496	1.0337477053

H	-2.6888051348	1.7671275711	3.0202412635
H	-3.5091835339	3.2633646668	2.5552053647
N	-2.6122360375	0.7885819899	0.3944282846
H	-4.4023490615	1.1906666407	1.390330846
H	-3.8788574097	2.4790000691	0.2906016446
C	1.0256696106	0.3394499873	-0.1838345767
H	1.4220494535	-0.1728971377	-1.0611563677
H	1.0970625038	1.4146382455	-0.3663718627
C	1.8729429281	-0.0342142128	0.9977554149
C	1.7650948686	0.084911321	2.3532963929
C	2.9780991447	-0.4458833738	2.9091022019
C	3.7411748765	-0.8366957848	1.8529214862
O	3.0826930664	-0.5933113536	0.6811011586
H	4.7217579071	-1.279777318	1.7621257917
H	3.2418886254	-0.5202966302	3.9552346067
H	0.9273157177	0.5062433142	2.8876256577
C	-0.9673268138	-1.0789596048	-0.7071638544
C	-0.1065925622	-2.2923558109	-0.905137349
C	-3.1559517672	0.0413855945	-0.7360184277
C	-2.2749038321	-1.1353076884	-1.0138434041
O	-4.4370181893	-0.4531834147	-0.4473422973
H	-2.7157373571	-2.0243450674	-1.4402862567
O	-0.5251432045	-3.0244903322	-1.9488123445
O	0.8316065824	-2.5954894357	-0.1940088667
C	0.1717985629	-4.272825288	-2.155868967
H	-0.2964315485	-4.7244810952	-3.0297637434
H	1.2321656702	-4.0902408955	-2.3437801826
H	0.060487448	-4.9234444175	-1.2853143414
O	-3.2272049327	0.9710266524	-1.8176121975
C	-3.6447594155	0.4354034437	-3.0777771642
H	-3.7540809677	1.2897057876	-3.7493470273
H	-2.8970223624	-0.2502483634	-3.4935741737
H	-4.6059304456	-0.0848558393	-3.0017614259
H	-5.0618220712	0.285903827	-0.5360884176

#### 16b\_t2

C	-1.1971393144	0.9200951055	0.4952855566
N	-0.6383057615	1.89844668	1.1182753203
N	-0.3483683509	-0.0083016431	-0.1443302076
C	-1.4950455705	2.8704522557	1.7898151944
C	-2.7837817205	2.2369663473	2.3079385032
H	-0.9265549838	3.3151033894	2.6149631475
H	-1.7373454304	3.6958937615	1.102571571
C	-3.4888625366	1.5330080142	1.1571193111
H	-2.545395959	1.5157905226	3.0986144906
H	-3.4560973488	2.9876492467	2.7355978
N	-2.5599836572	0.6358892699	0.4405664502
H	-4.3160711471	0.9244417917	1.531808978
H	-3.8995931992	2.2731892001	0.4591419723
C	1.0768343333	0.345848585	-0.2387842115

H	1.5109870204	-0.2429850352	-1.0482683432
H	1.1520110328	1.3988810257	-0.5187960916
C	1.8539079716	0.1518996835	1.0300531954
C	1.8896939986	-0.8001437595	2.0062538766
C	2.9037087716	-0.3928951029	2.9377180166
C	3.4191670736	0.7699882486	2.4551111863
O	2.7887553687	1.1178528866	1.2931673473
H	4.1941273716	1.4419321125	2.792594984
H	3.2064822617	-0.9033202583	3.8417993268
H	1.2762742585	-1.687333081	2.0460182074
C	-0.8866018401	-1.0889162053	-0.8389322899
C	0.0029662467	-2.2572487809	-1.1521434425
C	-3.1208794604	-0.064686051	-0.7102147033
C	-2.2023227178	-1.1777942137	-1.1021739101
O	-4.3647622999	-0.635512449	-0.3982737977
H	-2.6225788601	-2.0529020537	-1.5753983492
O	-0.4202613906	-2.9169490997	-2.2394672866
O	0.9667217278	-2.5900308483	-0.4881446326
C	0.302703095	-4.126826493	-2.5592092201
H	-0.1744696033	-4.5202428614	-3.4559688346
H	1.3534664279	-3.9016690582	-2.7543190531
H	0.2269728831	-4.8461943967	-1.7405096375
O	-3.2843554332	0.9251706488	-1.7276062281
C	-3.7346755839	0.4477536213	-2.9996220081
H	-3.9180867862	1.3350747084	-3.6094249793
H	-2.9746880303	-0.1708110255	-3.4916011393
H	-4.6642913546	-0.1257324974	-2.9143830916
H	-5.0251295024	0.0772088084	-0.4192649781

#### 17b\_t1

C	-0.9021126239	1.5224096252	0.2436815279
N	-0.5829690675	2.6237958181	0.7911948885
N	-0.0016620582	0.5283096133	-0.1713734586
C	-1.689760824	3.5251349599	1.1445078482
C	-3.0265197464	2.8115504232	1.3897062673
H	-1.3944388371	4.0809726251	2.0398026831
H	-1.7972564556	4.2650431285	0.3391803144
C	-3.3707869001	1.8747201003	0.2309708092
H	-2.9649215596	2.2312933632	2.3171844636
H	-3.8271852201	3.5466456809	1.5099782812
N	-2.187411914	1.0595155369	-0.0549269364
H	-4.1933048836	1.1996457174	0.4753101223
H	-3.640110885	2.4374496321	-0.6695461703
H	-1.1461785388	-2.3702015751	-1.5546129322
C	1.4251824584	0.6164908802	0.1883578939
H	2.012311774	0.2715806012	-0.6596553692
H	1.6184674533	1.6763986352	0.3645953463
C	1.7934197074	-0.1926801691	1.3873324817
C	2.5444912724	-1.3202733229	1.5526782757
C	2.5586950442	-1.6018934268	2.959353175

C 1.8111985807 -0.6280233669 3.5465252511  
O 1.339213829 0.242160522 2.606761023  
H 1.5322680501 -0.4171533744 4.5682503304  
H 3.0571393921 -2.419728957 3.4608090779  
H 3.0260829035 -1.8780030682 0.7628277047  
C -0.6850168159 -0.5351568776 -0.7230929918  
C -0.3226873534 -1.7154386351 -1.2881330706  
C -2.149840894 -0.1760892575 -0.6254102193  
C 1.0060878407 -2.2193545985 -1.6386721946  
O -3.2394928328 -3.3489554771 -2.2714709262  
O -3.1236588142 -0.8275236605 -0.9926202193  
C -3.3612169028 -2.9963868932 -3.6424917575  
O 0.9319702812 -3.5406163941 -1.9187375416  
O 2.0512991573 -1.5869684833 -1.7340699602  
C 2.1550570368 -4.1627966852 -2.3537917644  
H -3.2866990332 -3.9157840735 -4.2321336786  
H -4.3296368103 -2.5261759684 -3.8710213973  
H -2.5647882762 -2.3152028914 -3.9770143359  
H 1.8957079769 -5.1999848898 -2.5667296108  
H 2.5386389722 -3.6766030286 -3.2544049479  
H 2.9141465705 -4.1191223842 -1.5685288222  
H -3.2709200538 -2.517082404 -1.7648154602

#### **E-17b\_t1**

C -0.9893296058 1.5113328647 0.2982494621  
N -0.7269325843 2.6000842177 0.9032401351  
N -0.058497692 0.5307041721 -0.0541280482  
C -1.8706031977 3.487914716 1.161131652  
C -3.2182905786 2.7589625836 1.2595287887  
H -1.6710729891 4.0288730185 2.0915046488  
H -1.9070916078 4.2430141488 0.3632775324  
C -3.4412863503 1.8481406856 0.0507695301  
H -3.2396625118 2.156397151 2.1746428573  
H -4.0340343829 3.4848073882 1.3208691589  
N -2.2274901459 1.053951206 -0.1449385274  
H -4.2752930791 1.1593932766 0.2008579609  
H -3.6367156246 2.4324129894 -0.8554807516  
C 1.372325203 0.6827197276 0.2222938333  
H 1.9363103002 0.5049749969 -0.6974688071  
H 1.5057513061 1.7296851837 0.5061724273  
C 1.8951174204 -0.2243571663 1.2881175652  
C 2.8763838872 -1.1722330197 1.3014036675  
C 2.9545365953 -1.6610323889 2.6485453208  
C 2.012811554 -0.9772711385 3.3532337284  
O 1.359905616 -0.0930184852 2.5421052728  
H 1.6924152021 -0.9975870188 4.3844019518  
H 3.6195195092 -2.4215020117 3.0333604151  
H 3.4723937216 -1.4826231409 0.4543113933  
C -0.6638180784 -0.5203124168 -0.7200868534  
C 0.0099173949 -1.5992998522 -1.1980632295



C -2.1373201064 -0.1595396758 -0.7832106262  
C -0.5160640781 -2.7638069559 -1.9131105265  
O -4.5392661553 -2.910363475 -2.6413217695  
O -3.0782358035 -0.7563393098 -1.2782225062  
C -4.4081398043 -2.6231231104 -4.019454958  
O 0.5266174415 -3.5612589996 -2.2658838169  
O -1.6711583167 -3.0543040154 -2.1818133339  
C 0.1807926915 -4.7645522424 -2.9725544277  
H -5.3132471327 -2.9767875054 -4.5262628956  
H -4.3114632055 -1.5446845727 -4.2247449914  
H -3.5455978419 -3.1288673384 -4.4805741676  
H 1.1256055021 -5.2731559444 -3.1658834689  
H -0.4709556827 -5.3988461514 -2.3658994329  
H -0.3210390108 -4.5320451595 -3.9156225756  
H -3.7275052355 -2.5864166691 -2.2156278624  
H 1.080471457 -1.6307775627 -1.0383637252

#### 17b\_t2

C -0.5867575517 1.67633881 0.4579142643  
N -0.21089744 2.724070143 1.0722079782  
N 0.267975712 0.6224629175 0.1018363858  
C -1.2608948494 3.7044251662 1.3745112696  
C -2.6346690771 3.0559545562 1.5649330127  
H -0.9657938304 4.2452810581 2.2789081815  
H -1.2968418079 4.4444501683 0.5625992816  
C -3.0110116587 2.1908984981 0.3614937686  
H -2.61827361 2.4385695412 2.4704107971  
H -3.4040741581 3.8215815385 1.7008151708  
N -1.8675402099 1.3281557822 0.0140877982  
H -3.8633489403 1.5519134576 0.5863793671  
H -3.2701409384 2.8054022119 -0.5043521261  
C 1.7104546193 0.5877187936 0.3752996033  
H 2.1999563442 0.1689038369 -0.5056692126  
H 2.0283310623 1.624888629 0.497377934  
C 2.0805650936 -0.228135181 1.5680104359  
C 2.6148575296 -1.4754395921 1.7102956285  
C 2.7439041182 -1.7070516936 3.1199203189  
C 2.2759799981 -0.5844472878 3.7310150366  
O 1.8695539203 0.3296044395 2.802448578  
H 2.1720003028 -0.2871163439 4.7639995335  
H 3.1330744311 -2.5897926066 3.6077387382  
H 2.8817879467 -2.1468319598 0.9061880022  
C -0.4205407691 -0.3677195879 -0.5376822975  
O 0.0631646337 -1.4137081187 -0.9618667099  
C -1.8477555108 0.1123566253 -0.6315268859  
O -1.1697788187 -3.500808888 -2.4210050718  
C -2.7774123774 -0.6362849922 -1.276907342  
C -0.8277842401 -3.1797776128 -3.7622837837  
H -1.3718432465 -3.8655818704 -4.4196673901  
H -1.1104744109 -2.152852713 -4.0374261544

H 0.2474962353 -3.3019784674 -3.9623002157  
H -0.7082253188 -2.8569121494 -1.8533670916  
C -4.1541460837 -0.2855759369 -1.6369375949  
H -2.4401136347 -1.6114008548 -1.6133192855  
O -4.8162279967 -1.3959666032 -2.0405526329  
O -4.666411627 0.8243585518 -1.639388272  
C -6.1710361308 -1.1915168334 -2.4808498119  
H -6.5393960403 -2.1777328142 -2.763789959  
H -6.7829380471 -0.7776988113 -1.6751650176  
H -6.2022606224 -0.5165658067 -3.3402422298

#### E-17b\_t2

C -0.8846711022 1.4990852511 0.3349967402  
N -0.6403559542 2.5826322419 0.9568515647  
N 0.0777528055 0.5728981176 -0.0744679577  
C -1.80298959 3.4282638425 1.2585635214  
C -3.1133433625 2.6448969164 1.3950859499  
H -1.5937122491 3.9716036249 2.185375076  
H -1.893998417 4.1851094703 0.4665870051  
C -3.3484255952 1.7366221147 0.1858409633  
H -3.0754763857 2.0314529231 2.3023500513  
H -3.9582967348 3.3320008411 1.4953840334  
N -2.1139905736 0.9970319697 -0.0890226089  
H -4.1462001127 1.0184421152 0.3908288896  
H -3.6279238495 2.3152231826 -0.7026785977  
C 1.5201433721 0.7100781735 0.152794142  
H 2.0279853091 0.4457770345 -0.7766545182  
H 1.7021535379 1.7651722102 0.3671886808  
C 2.0445573584 -0.1544893468 1.2501576431  
C 2.7387340106 -1.328903745 1.2569569228  
C 2.958893928 -1.6666886275 2.6335596043  
C 2.3792165103 -0.6744946181 3.3629577613  
O 1.818889752 0.25790882 2.5383536789  
H 2.284962178 -0.4869089457 4.4221794733  
H 3.478165929 -2.5311347688 3.0230748518  
H 3.0498167404 -1.8869944433 0.3850661001  
C -0.4860673126 -0.4681561355 -0.781495797  
O 0.140001102 -1.3849625056 -1.2846691166  
C -1.9740194473 -0.1766400933 -0.7976525323  
O 0.4833609638 -4.2323223037 -1.951034289  
C -3.0080091384 -0.8300419279 -1.3903749264  
C 1.0545398436 -4.0144826289 -3.2261221281  
H 1.7856848072 -4.8100383962 -3.4097039901  
H 0.3118051821 -4.0501539912 -4.0392147879  
H 1.5823532176 -3.0507644718 -3.2982059195  
H -0.1558386885 -3.5128794291 -1.8124440394  
C -2.9835816546 -2.0926384348 -2.1292931524  
H -3.9886981046 -0.3733051289 -1.3238478082  
O -4.2079597347 -2.298772305 -2.6811070938  
O -2.0709604423 -2.8933444683 -2.2654328836

C	-4.3583539071	-3.5175088539	-3.4292581258
H	-5.3896824796	-3.5192737615	-3.7828964545
H	-3.669828573	-3.5407772373	-4.2781542197
H	-4.1760211385	-4.3889992811	-2.7948417066

#### 18b\_t1

C	-0.9805291263	1.0993428396	0.3264164719
N	-0.4071339336	2.0401139189	0.9758359514
N	-0.1712614855	0.0612678326	-0.19171752
C	-1.2104657143	3.1144426665	1.549809238
C	-2.6437048792	2.6817276643	1.8469033097
H	-0.7127191187	3.4566098232	2.4638921448
H	-1.2121966484	3.9702098945	0.8593244346
C	-3.2486819377	2.0509074374	0.6023945806
H	-2.650403851	1.9582486021	2.6702916029
H	-3.2571765026	3.5355449016	2.149852672
N	-2.3582619424	0.9929809916	0.0719775674
H	-4.2112331279	1.5826515852	0.8063156335
H	-3.4013514539	2.8014868411	-0.1814972222
C	1.2894183063	0.2323025685	-0.0316811129
H	1.7763918198	-0.387097403	-0.7837797798
H	1.5251405345	1.2747765854	-0.2473584991
C	1.7902498052	-0.0900977606	1.3427338096
C	1.628745611	-1.1401654379	2.1993342927
C	2.4170327477	-0.8436751516	3.3609384642
C	3.0086028844	0.3584992108	3.1217933898
O	2.6352231292	0.8335961556	1.8975582367
H	3.6873006514	0.9821451892	3.6844366086
H	2.5284688057	-1.4491263991	4.2498889806
H	1.0300024058	-2.0197922851	2.0164798922
C	-0.720678283	-0.9524338766	-0.9369510162
C	0.1418742183	-2.1227078558	-1.3404489177
C	-2.9397923139	0.0121731165	-0.7204729227
C	-2.0472263483	-1.0028081557	-1.2236000872
O	-4.1602685254	0.0388319725	-0.9529137582
H	-2.4727368814	-1.807239784	-1.8062947361
O	-0.160123678	-2.5371953946	-2.5713338456
O	0.959587026	-2.647979266	-0.6105785025
C	0.5237810787	-3.7329892722	-3.0213992285
H	0.1580904606	-3.9091137561	-4.0318240811
H	1.6033800985	-3.5705178864	-3.0268615306
H	0.2781287101	-4.5759151424	-2.3721175787
H	-4.7096961773	-1.3358934174	-2.0200065573
O	-4.83560768	-2.0545879602	-2.6731932779
C	-4.8634563199	-1.4417185642	-3.9521794387
H	-4.962474586	-2.2322547188	-4.7037322035
H	-5.7156447192	-0.7549584707	-4.0741717312
H	-3.9437240594	-0.8797908389	-4.1761057337

#### 18b\_t2

C	-0.6204650259	1.0724900419	0.2266228497
N	-0.3294763278	2.0841060348	0.9537793918
N	0.4213817109	0.1825744844	-0.1205110043
C	-1.3837587443	3.0034456402	1.3656418726
C	-2.7401545924	2.3141753846	1.4542953939
H	-1.1013863813	3.430709179	2.3338958928
H	-1.4337207074	3.8428744911	0.6571081942
C	-3.0373090227	1.6170475768	0.1358905399
H	-2.7338934054	1.584077206	2.2716336991
H	-3.538861641	3.0342821143	1.6557694091
N	-1.8988023046	0.7429326777	-0.2623151357
H	-3.9251568069	0.9920675642	0.22404969
H	-3.2103768921	2.3471284667	-0.659065452
C	1.7744438153	0.5036705792	0.3534106398
H	2.4636245992	0.0175364881	-0.3397232487
H	1.9120658992	1.5830169001	0.2975521324
C	2.0254664906	0.0465448542	1.7591202926
C	1.6440317496	-1.0389760797	2.4917796644
C	2.2863684662	-0.9123515399	3.7703056337
C	3.0165723781	0.2337300078	3.7176865756
O	2.8671556267	0.8330654199	2.4970976636
H	3.6599072658	0.7438486364	4.4188921379
H	2.2101829057	-1.5877109728	4.611236729
H	0.9868404594	-1.8327843956	2.1658956638
C	0.255365853	-0.9726166152	-0.873722098
O	1.2189788765	-1.7235487281	-1.1019386804
C	-2.0864724865	-0.3593831532	-1.0599179965
C	-1.0797353266	-1.2172843828	-1.3628157582
C	-3.422554665	-0.5476761998	-1.7358110766
O	-3.7749247147	-1.8344139606	-1.7535262948
O	-4.0549735583	0.3561225039	-2.2442527683
C	-4.9903208539	-2.1456408189	-2.4781632558
H	-5.1163063209	-3.2226662565	-2.3784454892
H	-5.838176128	-1.6180402389	-2.0365174285
H	-4.8863934784	-1.8672915743	-3.5290294764
H	-1.2370685492	-2.083765933	-1.9891512158
H	0.7857252944	-3.1306045628	-2.1871909666
O	0.4335050859	-3.7562990694	-2.8527139702
C	0.8860191396	-3.301571277	-4.1181470095
H	0.4672741056	-3.9628724859	-4.8841661429
H	0.5580591999	-2.2755407387	-4.3448849547
H	1.9827680115	-3.3330572686	-4.211518643

#### S7.4. B3LYP Optimized geometries (from 1c tautomers)

##### **1c\_t1**

C	1.3094437249	0.2518891738	0.9728995236
N	2.5836556956	0.6275707707	0.5844909687

N	1.0798136485	-0.9840465936	1.3058930774
N	0.3618558878	1.2589974127	0.9778224592
C	0.6112821587	2.7072531712	0.8906344968
H	-0.4861618179	1.0292788301	1.4784364074
H	2.6434228565	1.4645877777	0.0193539722
C	3.6340839968	-0.3568872495	0.3005641838
C	-0.2536923306	-1.3178161041	1.7926913481
C	1.2764850024	3.274394612	2.1523160012
C	-0.7236152065	3.3966217365	0.5979960559
H	1.2685385667	2.8884410115	0.0318989428
H	3.5514611827	-1.1227028842	1.0765033816
C	3.4614525428	-1.0297551215	-1.068368491
C	4.99318228	0.3366990707	0.4213648483
H	-1.0362831674	-1.0645061792	1.0547928117
H	-0.5216399157	-0.7744025208	2.7146924898
C	-0.3681083785	-2.7738307372	2.1110724455
H	4.2516954958	-1.7697167943	-1.2383801298
H	2.497948913	-1.5432467844	-1.13008884
H	3.5127581755	-0.2886753864	-1.8752750468
H	5.8052941682	-0.377023174	0.2501907754
H	5.0917265295	1.1384857805	-0.3212836765
H	5.1235820453	0.7763686545	1.4154280238
H	-0.5793659555	4.4753091824	0.486675254
H	-1.1725658641	3.0098122447	-0.3221395511
H	-1.4315438484	3.2351066731	1.4202495338
H	1.4595141204	4.3487676007	2.0404904512
H	0.6302196497	3.1265132399	3.0252869306
H	2.2351999458	2.7849650592	2.3458326892
C	-0.5269326825	-3.4705638632	3.2736713173
C	-0.5752241241	-4.8624810765	2.9205658515
C	-0.442097554	-4.9112066536	1.567653521
O	-0.3165888221	-3.6495615075	1.0570561351
H	-0.4177896338	-5.7173633468	0.8493231229
H	-0.6926101387	-5.7068842883	3.5857434258
H	-0.5993731467	-3.0425667369	4.2641732896

# 1c\_t2

C	-0.8467828495	0.042184089	-0.4712704657
N	-1.4490860278	0.1820459512	0.6660835912
C	-1.0662536524	1.2517535864	1.5858097982
N	0.0823623398	0.9122601244	-1.0207394099
C	1.1244360211	0.5493765099	-1.9994735405
N	-1.1352085951	-1.0675914232	-1.2603861438
C	-2.2375025248	-1.9493798334	-0.8768139957
C	-2.2603531062	-3.1816345979	-1.7156311061
H	-2.1060525942	-2.2045606506	0.1784904978
H	-3.2176168028	-1.4599800186	-0.9631608909
O	-1.2209364084	-4.0655662177	-1.5700723192
C	-1.4574590662	-5.1113237144	-2.4159840521
C	-2.6204600992	-4.9190116295	-3.0953891967

C	-3.1422596584	-3.6613541823	-2.6400537996
H	-4.0548117254	-3.1757306544	-2.9574562495
H	-3.0545468743	-5.5848449146	-3.8282825818
H	-0.7161992496	-5.8967492329	-2.416140124
C	-1.328482809	0.7731238493	3.0190090131
H	0.0112610259	1.4880526629	1.5169637285
C	-1.8493115015	2.5424686025	1.2907008936
H	0.3833882358	1.6345398898	-0.378724054
C	1.737001054	1.8463874007	-2.5331979043
C	2.1930076706	-0.3836719172	-1.4146647261
H	0.6391199046	0.0409072923	-2.839336932
H	2.9423588864	-0.6336798516	-2.1739485185
H	2.706241596	0.0973529125	-0.5737960002
H	1.7472381022	-1.3174938289	-1.0598659209
H	-1.0468669289	1.5382416129	3.7511017194
H	-2.391272275	0.5408543883	3.1560234859
H	-0.7560531009	-0.1352891699	3.2356674206
H	-1.5983495817	3.3305731154	2.0099258646
H	-1.6313101552	2.920467261	0.2861970718
H	-2.9273589757	2.3529017762	1.3528702453
H	-1.080127825	-0.9060850076	-2.2589588209
H	2.4910022926	1.6275605333	-3.2951851006
H	0.9705800156	2.4888076059	-2.9780749447
H	2.2269722429	2.4054116808	-1.7264055323

# NCov(1a\_t1)

C	-0.8965676164	2.4295161805	-0.3954149235
N	-1.8338104795	1.6033609524	0.1970250936
N	0.3238440802	2.0089014927	-0.5644911021
N	-1.3554659401	3.6768667839	-0.7753070835
C	-2.7607433857	4.1000727217	-0.8904076626
H	-0.7335471989	4.1788023238	-1.3945490909
H	-2.6344826185	2.0704450495	0.6027309478
C	-1.4664447031	0.3548813632	0.8740969946
C	1.2450560682	2.8879771247	-1.2776189359
C	-3.4870525592	3.4345701462	-2.0673641321
C	-2.7854743346	5.6263012671	-1.0006013529
H	-3.2736046566	3.8294390544	0.040182734
H	-0.7118839275	-0.1251713162	0.2466516259
C	-0.8664574242	0.5918438751	2.2670925915
C	-2.7023580959	-0.5458105376	0.9392147186
H	1.3600148379	3.8611989551	-0.7675833433
H	0.9058657534	3.1219788055	-2.3007677115
C	2.5992522692	2.2706750472	-1.4122609104
H	-0.5713450508	-0.3572916679	2.7272146122
H	0.0195840971	1.230054831	2.2080392769
H	-1.5971894223	1.0757745713	2.9266195184
H	-2.4510956369	-1.5061984122	1.4005920811
H	-3.4955799086	-0.0833674087	1.5399913239
H	-3.1019282039	-0.738316869	-0.0616890166

H	-3.8167049626	5.9881077796	-1.0503230831
H	-2.2960442788	6.0906862048	-0.1388568141
H	-2.2687436856	5.958110413	-1.9095590471
H	-4.5322814374	3.7602381647	-2.1079239146
H	-3.0075050491	3.7043316499	-3.0154393404
H	-3.4742784858	2.3451045609	-1.9719787427
C	3.3115698074	1.7911267621	-2.4727202316
C	4.5640217068	1.3174624654	-1.952622516
C	4.5234844352	1.5423793922	-0.6113726988
O	3.336226643	2.1252761546	-0.2637480637
H	5.2188403989	1.3654783182	0.1957842683
H	5.3801567278	0.8723165029	-2.504895695
H	2.9818916749	1.7755974172	-3.5025415632
C	0.5799850265	-4.0458816395	1.5922217549
C	-0.3212549111	-4.8426583331	1.7332135154
C	1.7112333994	-3.1427436977	1.4754010194
C	-1.3905317642	-5.8213322604	1.8122652068
O	1.3424107439	-1.9832344028	0.9274093426
O	2.8318178666	-3.4368151464	1.8417283668
C	2.3893495661	-0.9893098441	0.7718310218
H	1.8929582853	-0.1192283	0.3476214294
H	2.8271507894	-0.7512089652	1.7433785776
H	3.1623330945	-1.3640219307	0.0978653472
O	-2.0563406443	-5.71254515	2.9644455187
O	-1.6224768179	-6.6192970212	0.9258082504
C	-3.1517745316	-6.6445676996	3.1470662899
H	-3.5679613647	-6.4078304355	4.1250598818
H	-3.9021158015	-6.5034556463	2.3664352512
H	-2.7815713741	-7.671652647	3.1261834148

# NCov(1a\_t2)

C	-1.8882660798	0.604871229	-0.0864246531
N	-1.1938686497	1.5484846114	-0.6415719291
C	-1.3902003863	2.9402031722	-0.2332572537
N	-2.7404136884	0.747959059	0.9963993097
C	-3.8593053619	-0.149106776	1.3384361341
N	-1.8017584155	-0.6912652781	-0.582520188
C	-0.8044371003	-1.0079207109	-1.6041143053
C	-0.9764912407	-2.3993134079	-2.1109102208
H	-0.9215660934	-0.2882893102	-2.419443587
H	0.2242695797	-0.9039948876	-1.2345172498
O	-2.1084081288	-2.673283986	-2.8366066241
C	-2.0456513573	-3.9872356931	-3.2035295197
C	-0.9036610591	-4.5578405573	-2.7328618593
C	-0.208362217	-3.5236856483	-2.0200007201
H	0.7400698133	-3.6036853918	-1.5067466675
H	-0.5926420475	-5.5837857538	-2.8726833743
H	-2.8769119008	-4.3562670441	-3.7859967708
C	-1.0315965175	3.8506230749	-1.4138936394
H	-2.4474695684	3.1418966283	0.0184127623

C	-0.5377330038	3.2927700497	0.9987282335
H	-2.9145661352	1.7114294556	1.2514549082
C	-4.3501896322	0.2283608223	2.7378828841
C	-4.9957692478	-0.1066772752	0.3082563617
H	-3.4708324571	-1.1722239542	1.3888105529
H	-5.8011683939	-0.7913075038	0.5965706116
H	-5.4149350561	0.9038692285	0.2385957574
H	-4.6385350448	-0.4028040506	-0.6822205554
H	-1.2090724379	4.9038019675	-1.1683843843
H	0.0256858437	3.7352947936	-1.6788783885
H	-1.6318917332	3.5989328568	-2.2948670696
H	-0.6677796658	4.3446446187	1.2785619099
H	-0.8088762619	2.6786706723	1.8639229788
H	0.5232562312	3.1250146175	0.783167789
H	-1.9135409969	-1.4221520774	0.1096426349
H	-5.1562382532	-0.4408944271	3.0530529453
H	-3.5389702017	0.1628187479	3.4697530301
H	-4.7406734478	1.2534482369	2.7493214058
C	3.1915474714	0.7551580997	0.5036645353
C	3.5245668107	0.3167197046	1.5823563474
C	2.7909662666	1.367970774	-0.7493299414
C	4.013037368	-0.220989865	2.8393734469
O	2.5689984325	0.4458085674	-1.6882288502
O	2.6905473963	2.5712129794	-0.891881962
C	2.1342925921	0.9513004486	-2.9771035474
H	2.0307696654	0.0698772929	-3.6079151635
H	1.177121268	1.4644852446	-2.8704588898
H	2.8831188979	1.6316442894	-3.3873883419
O	3.0133200622	-0.4041817032	3.7047607188
O	5.1867764583	-0.4609005352	3.0421247469
C	3.3918526629	-0.9446000306	4.995891887
H	2.4620574303	-1.0186680511	5.5577026089
H	3.8462662459	-1.9301543758	4.8743782274
H	4.0906322855	-0.2717289487	5.4972399284

# TS1(1c\_t1)

C	-0.9423933577	1.0133482227	0.1039607118
N	-1.4171359916	0.8871559119	1.3723792418
N	0.2944230661	0.6315925074	-0.1819437011
N	-1.7938210734	1.5209909522	-0.8345413812
C	-3.0999746773	2.1637782888	-0.6271398422
H	-1.5536573116	1.3381359609	-1.7992916234
H	-2.4069526995	1.023798028	1.52073458
C	-0.6100892968	0.7238567424	2.5874561476
C	0.817540426	0.9614712953	-1.5085710933
C	-4.2500722126	1.1502464817	-0.7167812238
C	-3.2597014775	3.2923523971	-1.6491901575
H	-3.0859689983	2.6069424292	0.3738683779
H	0.4167317577	0.5732262849	2.2543036686
C	-0.6860297672	1.9917679262	3.4481494263



C	-1.0756979011	-0.5129321335	3.3630306731
H	0.4965560069	1.9711838501	-1.8058510146
H	0.4477753151	0.2729229629	-2.2838205104
C	2.3097046341	0.9128270708	-1.5553224129
H	-0.0799555284	1.8777385402	4.3534762335
H	-0.3177236477	2.8637959815	2.8981617073
H	-1.7187014236	2.1932181904	3.757792098
H	-0.4579640228	-0.660598867	4.2550880416
H	-2.1161632692	-0.3990720829	3.6914560277
H	-1.0102310048	-1.4122527856	2.7441573637
H	-4.2182138629	3.8004728636	-1.506677729
H	-2.4576889526	4.0299300091	-1.5485276229
H	-3.2378801249	2.8957117913	-2.6713085222
H	-5.2098798957	1.6422566597	-0.5270537216
H	-4.2868657592	0.7027602864	-1.7165351492
H	-4.129859829	0.3436488032	0.0138621056
C	3.1987298896	0.1292574997	-2.232576738
C	4.5110795767	0.6006996015	-1.8877267076
C	4.3225711884	1.637121014	-1.0258621884
O	2.9892424003	1.8458973909	-0.8169186109
H	4.9941438109	2.3023658261	-0.5034368205
H	5.4605575376	0.2177628771	-2.2354810907
H	2.9479913074	-0.6877786796	-2.894933783
C	0.6094318007	-1.4281441054	0.0810220842
C	-0.3005131773	-2.18741434	-0.3204712812
C	1.9676838961	-1.5399187077	0.6423901527
C	-1.5437362128	-2.5128007364	-0.9305397923
O	2.3497935854	-0.512588065	1.4100096998
O	2.6561443462	-2.5273332463	0.4479542559
C	3.663750636	-0.6304993265	1.9933446765
H	3.8217263864	0.2984369038	2.540516964
H	3.7063674552	-1.4835093426	2.6754289703
H	4.4211105069	-0.7470741504	1.215836537
O	-2.5118493429	-2.7587799448	-0.0094167309
O	-1.7229722926	-2.6089256082	-2.13999519
C	-3.7899417717	-3.1460857365	-0.5476565245
H	-4.4347092613	-3.3039491743	0.3173567464
H	-4.2030105535	-2.3596686687	-1.1845573777
H	-3.7060278321	-4.0701608497	-1.1259949503

# TS1(1c\_t2)

C	-0.5019641214	0.7295759258	-0.1495849302
N	-0.8137856799	0.152243205	0.9976846996
C	-1.9183853266	0.6986037352	1.809576201
N	-1.2824533624	1.6645995421	-0.7722377732
C	-0.8500828547	2.6740648325	-1.7574534807
N	0.6394460553	0.3861952783	-0.8069928077
C	1.7574785831	-0.366491553	-0.2507124215
C	3.0689170331	0.255698076	-0.599238231
H	1.6220403362	-0.409295396	0.8320377627

H 1.7561822698 -1.3952926188 -0.6262789975  
O 3.338367757 1.496676982 -0.0779013903  
C 4.5834989703 1.8556396252 -0.5116734221  
C 5.1150526956 0.8756175914 -1.2911763299  
C 4.1272960536 -0.1648270525 -1.3503539768  
H 4.1942866275 -1.1045469731 -1.8811011793  
H 6.0856995697 0.8887762051 -1.7671962885  
H 4.9386223976 2.8213817449 -0.1836174988  
C -1.5974818964 0.6040521741 3.30770645  
H -2.0084009069 1.7712900718 1.5878918113  
C -3.2701739854 0.0356015572 1.4975585542  
H -2.184636887 1.8370292782 -0.3535173674  
C -2.1078204068 3.3191986654 -2.3413271021  
C 0.0969495475 3.714062103 -1.1467769931  
H -0.3315828653 2.1629194472 -2.5770762663  
H 0.4055909315 4.4367811038 -1.9096922158  
H -0.4013524256 4.2590762381 -0.3373010248  
H 0.9980418956 3.2422617302 -0.7446925595  
H -2.336698416 1.1780971357 3.8768387768  
H -1.6375667174 -0.4263736818 3.6715807958  
H -0.6065261498 1.013439797 3.5239647546  
H -4.0693332032 0.514863377 2.0737274278  
H -3.52578295 0.1124377248 0.4355112811  
H -3.2527393809 -1.0264507265 1.7621942263  
H 0.7019488713 0.6149733024 -1.7884977899  
H -1.8343533041 4.0492544004 -3.1081449358  
H -2.760937811 2.5682187216 -2.7968935294  
H -2.6736040222 3.8430832301 -1.5615965117  
C -0.7050363391 -1.8785243466 0.9428388946  
C -0.8844170892 -2.4989741513 -0.131939429  
C -0.3807427799 -2.2364171447 2.3353702694  
C -1.0011994249 -2.6217599328 -1.5423989002  
O 0.7421831297 -1.6474053192 2.7756534403  
O -1.0306367339 -3.0297986235 2.9927915947  
C 1.1505497561 -1.9960980778 4.1151865203  
H 2.0724921483 -1.4423169654 4.2907949465  
H 0.388029817 -1.7007224502 4.8397403257  
H 1.3323845845 -3.0704368846 4.1944070585  
O -2.2999614214 -2.6646465583 -1.9456195604  
O -0.0552731592 -2.7339546299 -2.3180010969  
C -2.5002826155 -2.8439482462 -3.359097346  
H -3.5813453308 -2.8693574301 -3.5005446955  
H -2.0690958181 -2.0142166277 -3.9259131143  
H -2.0556786454 -3.7819574113 -3.7024516254

#### 10c\_t1

C 1.1357824444 -0.7699574542 0.2217579543  
N 1.4968028488 -0.8380484075 1.5132304214  
N -0.0465948505 -0.2279701074 -0.1703393839  
N 1.9833065116 -1.2547227997 -0.7081770816

C 3.1532931377 -2.1279983744 -0.492367256  
H 1.8952953889 -0.8836807361 -1.6459954854  
H 2.4825929382 -0.989360049 1.6853830374  
C 0.6595589685 -0.8509998344 2.727174727  
C -0.4897978127 -0.4282903764 -1.5802150473  
C 4.4481462842 -1.3082032366 -0.447350188  
C 3.1818682597 -3.187089449 -1.596816714  
H 3.003498091 -2.6291962816 0.4681942849  
H -0.3767799008 -0.7840673336 2.4013850255  
C 0.8581005707 -2.185468958 3.4548682864  
C 1.009494378 0.3440441691 3.6182568699  
H -0.1227647612 -1.3992760786 -1.9199933674  
H -0.0450753574 0.3520620394 -2.2084599921  
C -1.9661412677 -0.3935416408 -1.7680650196  
H 0.2425087728 -2.2140560854 4.3596656223  
H 0.5729258515 -3.0280960166 2.8173086006  
H 1.9046897805 -2.3162675963 3.7542570271  
H 0.3665097079 0.3551966475 4.5040575999  
H 2.0500796068 0.2802727833 3.9577983131  
H 0.8792014541 1.2862071047 3.0801691905  
H 4.0358864702 -3.8553941583 -1.4519646597  
H 2.26696447 -3.7870379043 -1.5902020698  
H 3.2830519303 -2.7185665199 -2.5826947959  
H 5.3021760934 -1.9621960881 -0.2451162234  
H 4.6192749402 -0.8086324317 -1.4075376382  
H 4.4092373687 -0.5413510161 0.3328034418  
C -2.8314931799 0.5749827593 -2.1883864524  
C -4.1382279839 -0.0158297274 -2.1912168306  
C -3.9695244607 -1.3025590827 -1.7776015322  
O -2.6540346576 -1.5531535784 -1.5235368604  
H -4.6465326432 -2.1315075243 -1.6331796028  
H -5.0718432715 0.4536916885 -2.4680322522  
H -2.5668509927 1.5877653095 -2.4587185248  
C -0.552162985 1.0138455429 0.4732431072  
C 0.0829967766 2.191274454 0.4106274361  
C -1.8809181218 0.8990282959 1.1399940058  
C 1.3580536367 2.4147879364 -0.1958545855  
O -2.3113592165 -0.3857496485 1.2519889625  
O -2.5388661065 1.8339967012 1.5643908968  
C -3.5993345 -0.5588396833 1.8658765678  
H -3.8029175588 -1.6293773223 1.8271757748  
H -3.584859782 -0.2169211935 2.9045564761  
H -4.3684041237 -0.0090033826 1.3186657276  
O 1.2474067881 2.7728493014 -1.5244014986  
O 2.4492937979 2.4292220663 0.3800822607  
C 2.4653888423 3.2002100091 -2.1489576194  
H 2.1985167162 3.459207847 -3.175357793  
H 2.8864486289 4.0758266981 -1.6452995696  
H 3.2157400794 2.4036937232 -2.1533045738

## 10c\_t2

C	0.0316275224	-0.8558980099	-0.0685966063
N	1.2804770928	-0.5220895864	-0.4677038478
C	1.9803907276	-1.2662114357	-1.5593334803
N	-0.4029636695	-2.1228082139	-0.210676633
C	-1.7758168238	-2.5921007046	-0.5000654968
N	-0.7542885446	0.0984786334	0.4697295499
C	-1.6655467519	-0.0659075109	1.6103361512
C	-2.9811542041	0.6071114634	1.405947915
H	-1.7934265534	-1.1307495811	1.8130813542
H	-1.2053830605	0.3787530129	2.4999719179
O	-3.8074259696	0.1124928378	0.4292595779
C	-4.9433137816	0.8726789766	0.4360230979
C	-4.8617195928	1.8347806893	1.3939971138
C	-3.5830039227	1.6636921789	2.0234462577
H	-3.1639393877	2.2498635765	2.8296039649
H	-5.6134146965	2.5767705266	1.6243190719
H	-5.6960121262	0.604127985	-0.2902759858
C	3.1157198657	-2.1561694528	-1.0419882736
H	1.2199225175	-1.9061504913	-2.0124621697
C	2.4701161335	-0.3021511644	-2.6438581612
H	0.317963963	-2.817838471	-0.3638575798
C	-1.8689341539	-3.0502479919	-1.9600603627
C	-2.1534100682	-3.7142403519	0.4697408724
H	-2.4436636971	-1.7422397505	-0.3567218521
H	-3.1729104451	-4.0569847945	0.2684189077
H	-1.4795361605	-4.5707601394	0.3513190292
H	-2.1011397435	-3.3810621844	1.5106159121
H	3.5339732221	-2.7246832974	-1.8789286954
H	3.9254902089	-1.5617053759	-0.6069692861
H	2.7636272135	-2.8633779287	-0.2865426596
H	2.8995690225	-0.883155557	-3.4665998491
H	1.6481882417	0.2994655969	-3.0407192881
H	3.2402876472	0.3756401131	-2.2666545343
H	-0.5015798304	1.0669632092	0.235798223
H	-2.8827087243	-3.4022013791	-2.1771214996
H	-1.6368460841	-2.2319828234	-2.6484142598
H	-1.1754949383	-3.8764279413	-2.1551621133
C	2.0211173482	0.5322285876	0.2582296555
C	2.0009556249	1.8390445685	-0.0281166488
C	2.7921357255	0.0406912674	1.4415612648
C	1.1177222966	2.4598717672	-0.9519018124
O	2.3806114615	-1.1850581854	1.8588198554
O	3.6676812194	0.658840942	2.0224393303
C	3.058466483	-1.7079761552	3.0137368571
H	2.6089814682	-2.6831028583	3.2043442308
H	4.1287866795	-1.8186934465	2.8204674407
H	2.9173027828	-1.0535959947	3.8780412635
O	1.7225125323	2.9867165679	-2.0554367664
O	-0.0954616218	2.6502072864	-0.7322622768

C	0.8673428896	3.7139290761	-2.9502119931
H	1.5043174086	4.0221620118	-3.7809457538
H	0.0514109461	3.0876223405	-3.3222316001
H	0.4426513075	4.5966915624	-2.4632803291

#### TS2(1c\_t1)

C	0.9788304484	-0.7834837963	0.3562806014
N	1.4116149582	-0.6701910588	1.6212647075
N	-0.197209762	-0.2372612902	-0.0536473577
N	1.7407744476	-1.4613493775	-0.5237733921
C	2.8768716597	-2.3563177596	-0.2285777847
H	1.604625892	-1.2539596935	-1.5048140489
H	2.382574207	-0.9116710915	1.7752639397
C	0.6528227994	-0.4034411166	2.8584464243
C	-0.7081547761	-0.6062780542	-1.4025598626
C	4.2120484433	-1.6113320771	-0.3464215895
C	2.8056384588	-3.5582519492	-1.1729773486
H	2.7448361603	-2.7115200046	0.7976982892
H	-0.3671576475	-0.1621747371	2.5670449483
C	0.6282181082	-1.6691636621	3.7228310818
C	1.2823290181	0.7830972	3.5936073935
H	-0.4299828066	-1.643919553	-1.6001892637
H	-0.2320626184	0.0302258728	-2.158910489
C	-2.1837900986	-0.485071374	-1.5595779238
H	0.0721334311	-1.4801085419	4.6468414236
H	0.1463920941	-2.4984428126	3.1955563087
H	1.6444438949	-1.9760036905	3.9963782577
H	0.6892868026	1.0322439323	4.4793907688
H	2.2953587556	0.5302865087	3.9300769092
H	1.3465638334	1.6648133395	2.9488572994
H	3.6291091945	-4.247083535	-0.9630055185
H	1.8619844891	-4.0985161286	-1.0522080493
H	2.891775058	-3.2376527101	-2.2177680202
H	5.0405511961	-2.283909308	-0.1029800992
H	4.357390978	-1.2442053986	-1.3684006433
H	4.2558404061	-0.7544733899	0.3333796375
C	-2.9869304247	0.4565291438	-2.1356772869
C	-4.3330287605	-0.0234527842	-2.0157146782
C	-4.2479510295	-1.2250615512	-1.3802071252
O	-2.9479095359	-1.5266124866	-1.1020710694
H	-4.9798710404	-1.959961567	-1.0791806208
H	-5.2366966811	0.4597090964	-2.3600929843
H	-2.6564531812	1.3814449409	-2.587650763
C	-0.5730733439	1.1367447744	0.4087524329
C	0.2259353716	2.1645281793	0.2675724797
C	-1.9342309117	1.24609454	1.0286651969
C	1.1302909073	3.1892098711	0.2506648654
O	-2.4299761466	0.050959696	1.4346393905
O	-2.5346376508	2.291774455	1.2032412271
C	-3.7257869416	0.0927937042	2.0589909296

H	-3.9830403209	-0.944660047	2.274175187
H	-3.6902439716	0.6710267387	2.9863406961
H	-4.4661432922	0.5340176749	1.3882698884
O	1.0884721809	3.927932148	-0.9343292057
O	1.9316572866	3.4902364918	1.163778528
C	1.9959331143	5.0278544897	-0.9853356281
H	1.8430759218	5.4932602544	-1.9622594157
H	1.7951345549	5.7635478863	-0.1986467703
H	3.0390768699	4.7051576084	-0.8969198734

# **TS2(1c\_t2)**

C	-0.1756082635	-1.1026548683	0.1198078412
N	1.0657848002	-0.7830344228	-0.2940175929
C	1.7929362574	-1.5979986296	-1.3154029117
N	-0.6207231425	-2.3730629518	0.0339251001
C	-1.9954897017	-2.8362948769	-0.2657527691
N	-0.9719397145	-0.1309799625	0.6223343927
C	-1.8766157412	-0.2641136086	1.7765482486
C	-3.1708730155	0.4465309712	1.5721447049
H	-2.0338779929	-1.3242250867	1.9805624365
H	-1.3949965272	0.1687749291	2.6599723715
O	-4.0149947652	-0.0348037098	0.6044055751
C	-5.1265148792	0.7603619857	0.6055121347
C	-5.0116203773	1.7317530343	1.5507762097
C	-3.7366439771	1.5291781206	2.178312949
H	-3.2965370113	2.1124215723	2.9752759219
H	-5.7389798347	2.4997496144	1.7739200451
H	-5.8898214224	0.5069753687	-0.1152382683
C	2.9371945495	-2.4114404267	-0.7024163542
H	1.0537833327	-2.2919287792	-1.7216271185
C	2.2761015767	-0.7267069103	-2.479505157
H	0.093316898	-3.0761212056	-0.1125590877
C	-2.0799822743	-3.3063540267	-1.7225040952
C	-2.3848359408	-3.9476705997	0.7111086946
H	-2.6609683524	-1.9824232199	-0.1355319191
H	-3.4034279782	-4.2896008948	0.5041252708
H	-1.7123052865	-4.8070134189	0.6063768974
H	-2.3404957816	-3.6045442586	1.7491434752
H	3.3808411473	-3.0473442828	-1.4755335648
H	3.7248683731	-1.7612819249	-0.3099414524
H	2.5839666737	-3.0526149846	0.1099381717
H	2.6705434265	-1.3810064958	-3.2637467085
H	1.4573951327	-0.1380093614	-2.9028551945
H	3.0729837971	-0.0425726455	-2.1767591741
H	-0.6218992849	0.8096532625	0.4713120182
H	-3.0943748089	-3.6537211226	-1.944167699
H	-1.8376231137	-2.4960036809	-2.4165598382
H	-1.390507127	-4.1387416088	-1.9045066242
C	1.6886186674	0.4788027839	0.1841724618
C	1.4292164206	1.6400175377	-0.36851297

C	2.584874765	0.3246907847	1.3789634794
C	1.0362016592	2.877598424	-0.7922706844
O	2.4071732373	-0.8557098922	2.0198996959
O	3.3662396675	1.1717542425	1.77447667
C	3.2166154198	-1.0551448729	3.1929997529
H	2.9478020106	-2.0409729595	3.5735212134
H	4.2797790369	-1.026070081	2.9406798586
H	3.005271392	-0.2906095572	3.9451563379
O	1.8273440304	3.3901878662	-1.8190050991
O	0.0605881844	3.5201790697	-0.3429116078
C	1.4032976284	4.6569029775	-2.3228334242
H	2.1076603895	4.9101573985	-3.1189406938
H	0.3890872865	4.6160350733	-2.735038344
H	1.4317855539	5.4349373109	-1.5524435763

### 11c\_t1

C	1.3463368044	-1.275982676	0.0436109793
N	1.7657832628	-1.149476014	1.3124052685
N	0.2487820302	-0.615313759	-0.4158503534
N	2.0270048617	-2.0913106778	-0.7822174402
C	3.0016312092	-3.1378838325	-0.4166916209
H	1.9345738314	-1.9192556117	-1.7754471679
H	2.7103195043	-1.4616574435	1.500172215
C	0.9986820483	-0.7698785866	2.5146488178
C	-0.3056488417	-1.0093607281	-1.7397170107
C	4.4398793263	-2.6231655847	-0.5445240926
C	2.7507144013	-4.3634007714	-1.2983942584
H	2.8006327556	-3.4075069174	0.624084929
H	-0.0164114874	-0.5490091206	2.1886171243
C	0.9559982659	-1.9648568835	3.4741697315
C	1.6204917031	0.4664500202	3.1702000095
H	-0.157293875	-2.0837455504	-1.8682650285
H	0.24412292	-0.484589184	-2.531136205
C	-1.7551018804	-0.7130165905	-1.9070115192
H	0.3829888659	-1.7054707916	4.3701716779
H	0.4837176766	-2.8325161833	3.0029504983
H	1.9663925756	-2.2497125575	3.7903819006
H	1.0481423561	0.7422846129	4.0619411788
H	2.6497562134	0.2568685957	3.4856263796
H	1.6336169453	1.3210486803	2.4882855731
H	3.4503006131	-5.1620967819	-1.0348472556
H	1.7312719411	-4.7391716603	-1.1697466939
H	2.9005534761	-4.1187555198	-2.3564272563
H	5.1464093836	-3.4066833402	-0.2530183219
H	4.6546855667	-2.3358166457	-1.579765006
H	4.6129678073	-1.7515872005	0.0947250344
C	-2.4371113576	0.2929248356	-2.5285665965
C	-3.8322966796	-0.0016748965	-2.3747647268
C	-3.8948226075	-1.1685804254	-1.6751464879
O	-2.6410146113	-1.6205693434	-1.3887403997

H -4.7116816426 -1.7865128051 -1.3323704545  
H -4.6706030724 0.574956226 -2.7400681005  
H -1.9955875102 1.1424612888 -3.0308187993  
C 0.0722097995 0.8094746951 -0.066437229  
C 1.0334410376 1.6820873275 -0.3965388642  
C -1.2086123468 1.1600465782 0.6091149084  
C 1.0087435671 3.0727982394 -0.0482918671  
O -1.9182451781 0.0789412483 1.0248970832  
O -1.5970684418 2.3003385799 0.8054999666  
C -3.1713502941 0.3658877254 1.670032978  
H -3.6159813415 -0.6040914346 1.8942179517  
H -3.0133714631 0.9294281073 2.5936321264  
H -3.8268201799 0.9370209644 1.0086327594  
O 0.5709040994 3.8668154413 -1.0800141986  
O 1.4865928388 3.5615854347 0.9795700813  
C 0.655364745 5.276826078 -0.8477658403  
H 0.2993080917 5.7523734031 -1.7640100161  
H 0.0245898171 5.5833404145 -0.007139531  
H 1.6842404697 5.590750021 -0.6457738302

#### 11c\_t2

C -0.6699145895 -0.9122634552 -0.0618201722  
N 0.624080166 -1.16187564 -0.3714721516  
C 0.9923927054 -2.3418534599 -1.2211063113  
N -1.5347320171 -1.9363302668 0.0788690035  
C -2.9763583247 -1.9640092712 -0.2547452801  
N -1.0642096116 0.3672280962 0.0840802458  
C -2.0027927942 0.890145854 1.0876507757  
C -2.9440483638 1.8998335651 0.5231318089  
H -2.5422807988 0.0560737262 1.5397301375  
H -1.4325476291 1.3779919452 1.8856320678  
O -3.8744639312 1.4641724196 -0.385525984  
C -4.6201374842 2.5489642506 -0.7531119563  
C -4.1903525993 3.6611985677 -0.098557152  
C -3.0971337377 3.238977813 0.7304106501  
H -2.5011721562 3.8505611324 1.393634748  
H -4.5952880615 4.6589725222 -0.193882576  
H -5.4003081017 2.3632677368 -1.4762513269  
C 1.7261617623 -3.4430276409 -0.4497474815  
H 0.0434585817 -2.7513203762 -1.573736647  
C 1.7810509333 -1.8956816298 -2.4566809407  
H -1.113381585 -2.8506735393 0.1919490002  
C -3.194214529 -2.7715461377 -1.5395341877  
C -3.7679395327 -2.544200077 0.9195379213  
H -3.2858783964 -0.9337459612 -0.4332707978  
H -4.8363279104 -2.5553662187 0.6832295506  
H -3.4561996291 -3.5750724795 1.1240139629  
H -3.6225176045 -1.9569323767 1.8312004413  
H 1.8576935338 -4.3083202626 -1.1080357062  
H 2.7178980825 -3.1186206443 -0.1224407389



H	1.1620306222	-3.7639837684	0.4301997035
H	1.8920908967	-2.7511160546	-3.1309002852
H	1.2591683967	-1.0987785468	-2.9942738887
H	2.780537474	-1.5368822813	-2.1964096933
H	-0.3493751721	1.0229807466	-0.2497591083
H	-4.2604892644	-2.8003171702	-1.786423258
H	-2.6600207278	-2.3256960218	-2.3839342108
H	-2.848337396	-3.8041664677	-1.4146014454
C	1.6622831868	-0.1709098599	-0.0662419757
C	1.6842893257	1.0153403176	-0.6925861792
C	2.5837701452	-0.5447394924	1.0500694246
C	2.6202616169	2.0632868837	-0.3674301619
O	2.04539365	-1.4557556592	1.8971252914
O	3.6829603258	-0.0498443667	1.2383542923
C	2.8697245974	-1.8308757485	3.0148879253
H	2.2889128707	-2.5620424264	3.578057593
H	3.8077456617	-2.2775379989	2.6747178409
H	3.0924382923	-0.9636231607	3.6419793099
O	3.6837254365	2.089189922	-1.2331558897
O	2.4428170743	2.9516480801	0.4650908835
C	4.592626649	3.1820115031	-1.0573873906
H	5.3481462811	3.0704671958	-1.837631535
H	4.0871662799	4.1462328961	-1.1681218951
H	5.0729994003	3.1478892864	-0.0744052505

### TS3(1c\_t1)

C	0.0019139417	-1.66046243	-0.2782634614
N	-1.0255299899	-2.5429227578	-0.1916520959
N	-0.3124162391	-0.3034362131	-0.3530671063
N	1.263319272	-2.0244892677	-0.3311522926
C	1.7805275989	-3.3512528431	0.0237628266
H	1.9323177382	-1.0263590812	-0.482567973
H	-0.7691915271	-3.5148896118	-0.3177834429
C	-2.3087585274	-2.3400048887	0.5154885245
C	-1.2487896776	0.0858111484	-1.4528121853
C	3.118909973	-3.1764398283	0.7490932919
C	1.9266216895	-4.2298282036	-1.2261172733
H	1.0746923788	-3.8336987475	0.7132490494
H	-2.4191471541	-1.2655422999	0.6663955979
C	-3.4628667463	-2.8527060063	-0.3489796126
C	-2.2737103789	-3.0357238186	1.8815159935
H	-1.7975394292	-0.8109587464	-1.7453620537
H	-0.6520442608	0.4029565628	-2.3162794222
C	-2.2041068948	1.1845536166	-1.1437102577
H	-4.4165049071	-2.7008233607	0.1662615484
H	-3.5062284933	-2.3317960961	-1.3101744703
H	-3.3538463775	-3.925777121	-0.5460567314
H	-3.2228477771	-2.8851597398	2.4065791448
H	-2.1198406187	-4.1149771662	1.7650671775
H	-1.4700647714	-2.6387472305	2.5093250151

H	2.319552642	-5.2151795694	-0.9543429885
H	0.9646260299	-4.3745812369	-1.7290588503
H	2.6180378315	-3.7688672608	-1.9400500251
H	3.507103968	-4.1497965276	1.0645025919
H	3.8614691036	-2.7121873384	0.0904616119
H	3.0060308719	-2.5458028122	1.6364649131
C	-2.3129134459	2.464374445	-1.6057484268
C	-3.4805649213	3.0264708222	-0.9894381199
C	-3.99680698	2.0466496508	-0.1981198503
O	-3.2393280873	0.9142855132	-0.2879776687
H	-4.858460084	1.9904561504	0.4504058013
H	-3.8783634681	4.0232420449	-1.1197063863
H	-1.6400390336	2.9465813145	-2.3012924417
C	0.7159595296	0.6756248569	-0.0617350177
C	2.0088431366	0.4202933705	-0.3252349794
C	0.2740000555	1.8982487573	0.6811766864
C	3.1233669031	1.2591510751	0.0873064476
O	-0.8014022613	1.6764581737	1.4653194019
O	0.8669831281	2.9636832682	0.6540781709
C	-1.240734542	2.8001096758	2.2508451842
H	-2.1308619444	2.4590926388	2.7796382216
H	-0.4682147672	3.0959336495	2.965952267
H	-1.4841817683	3.6512337977	1.6111470119
O	3.5986633618	2.0154784399	-0.9402728558
O	3.6854266608	1.2046656737	1.1753773821
C	4.7743564698	2.7863953397	-0.6478490934
H	5.0214312204	3.3122874752	-1.5714256778
H	4.5837750078	3.5094345281	0.1505409409
H	5.6073445614	2.1421202151	-0.3520960421

### TS3(1c\_t2)

C	-0.3539258542	-1.0405115577	0.1978062057
N	0.9648660634	-0.8792444652	-0.1912200056
C	1.5563556916	-1.8804906615	-1.149908236
N	-0.7642777141	-2.3101932909	0.4553394975
C	-2.0870480785	-2.9108791707	0.1829689173
N	-1.1102327611	0.038750707	0.3022732132
C	-2.260989235	0.1953970512	1.192143793
C	-3.4788055278	0.7004969189	0.4885542416
H	-2.4755745623	-0.73391648	1.7279467518
H	-2.0031523296	0.944232972	1.9509374344
O	-4.0577860905	-0.113672846	-0.4514877065
C	-5.1482906978	0.5466341099	-0.946207758
C	-5.2787603553	1.7583694895	-0.3428281447
C	-4.1906731113	1.8595853868	0.5887431844
H	-3.9655702277	2.6869166971	1.2475371361
H	-6.048412661	2.4924395532	-0.5369334915
H	-5.7101063554	0.0270760538	-1.7080287364
C	2.6146823468	-2.802052644	-0.531964583
H	0.7148221042	-2.5084821733	-1.4469648045

C 2.0714987885 -1.1913667535 -2.4182981495  
H -0.0202377247 -2.9869171731 0.5735251344  
C -1.9940859705 -3.8569697061 -1.0205335246  
C -2.597275444 -3.6370219486 1.4306033669  
H -2.7672611666 -2.0972713237 -0.0699795468  
H -3.5816116666 -4.0753441725 1.2382691002  
H -1.9154375804 -4.4483568003 1.7113327845  
H -2.6837674769 -2.9561124743 2.2829014065  
H 2.8124377749 -3.6244587171 -1.227905456  
H 3.5583188044 -2.2849785208 -0.3471009201  
H 2.2732405966 -3.2333767136 0.4141357022  
H 2.3655660206 -1.958235688 -3.1421259816  
H 1.2958906254 -0.5699374554 -2.8757314445  
H 2.9469062471 -0.5645283077 -2.2241120893  
H -0.427221404 0.9995316349 -0.0106496224  
H -2.970051995 -4.312480747 -1.2182707596  
H -1.6786541244 -3.3221419002 -1.9216468531  
H -1.2781563427 -4.6646388672 -0.8277872516  
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C 0.8896159839 1.5499416275 -0.1599429005  
C 3.033793046 0.42929872 0.374448834  
C 1.4138053611 2.8732232867 0.1478344375  
O 3.2871469975 -0.4782933288 1.3404218451  
O 3.865157075 1.2268189512 -0.0231380844  
C 4.6317537245 -0.4807128934 1.8605961473  
H 4.6605989998 -1.2860703663 2.5946313979  
H 5.3566603153 -0.6678900267 1.0646263073  
H 4.8600384579 0.4747568265 2.3395122143  
O 1.6281600351 3.6056298389 -0.9798705432  
O 1.5326712497 3.3524811887 1.2698932581  
C 2.0459146508 4.9631237032 -0.766768227  
H 2.1607360772 5.3974273242 -1.7611129698  
H 1.2966909591 5.5233070934 -0.2000430399  
H 2.9992544442 5.0038179477 -0.2320123023

#### 12c\_t1

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N -1.5442746226 -0.6027126762 1.5257557622  
N 0.1572831491 0.2815209811 0.0373613512  
N -1.8237289715 1.4572259216 0.5059643474  
C -3.0907035863 1.7243987142 1.1982380696  
H -1.8167095737 1.7594444117 -0.4625397539  
C -0.7580059836 -1.72255194 2.0295514231  
C 0.7393098631 1.5697722032 -0.4405653477  
C -4.2744154987 0.9731123281 0.5734836548  
C -3.3281552048 3.236988913 1.2137319281  
H -2.9568267619 1.3692845376 2.2238977742  
H 0.2663834964 -1.7276494879 1.6388379513  
C -0.6646509683 -1.6065229397 3.5588182035  
C -1.4391334077 -3.0376367174 1.6256451722

H	0.3214511305	2.3523575634	0.1933045818
H	0.4170332107	1.7617393933	-1.4707769551
C	2.2259658422	1.6519535595	-0.4041673113
H	-0.1119549549	-2.4530036969	3.9822491718
H	-0.1502174186	-0.684354331	3.8500697106
H	-1.6657064329	-1.5909582886	4.0053220914
H	-0.8813397399	-3.9007387304	2.0059138619
H	-2.4560941219	-3.0807722248	2.0328041753
H	-1.5094380578	-3.1293295008	0.5368185226
H	-4.2521918402	3.4754086935	1.7504305695
H	-2.5002964352	3.7604122962	1.7027746169
H	-3.4240918737	3.6290728368	0.1936478144
H	-5.1957946494	1.1756384292	1.1310182408
H	-4.4307775359	1.2888810146	-0.4645561977
H	-4.0975050523	-0.1052461891	0.5853302946
C	3.184103455	1.594665032	-1.375849436
C	4.4451319192	1.7942144417	-0.7217420906
C	4.1597924418	1.9609204589	0.5994407102
O	2.8147698693	1.8858575382	0.8105296503
H	4.7671021696	2.1466404054	1.473065035
H	5.426194475	1.8143230046	-1.1754507472
H	3.0089886667	1.4325167451	-2.4305266434
C	0.5568693809	-0.8673679447	-0.6802203231
C	-0.2034381411	-1.5404239777	-1.5689618545
C	1.9373625387	-1.4479586719	-0.4405782921
C	-1.5231010114	-1.1115343358	-2.0813100581
O	2.4469317031	-1.1037235748	0.7481976452
O	2.4944357278	-2.1889795501	-1.2295043214
C	3.7440014138	-1.6572561899	1.0580686513
H	4.0184655069	-1.2316659028	2.0224424915
H	3.684216872	-2.7463804284	1.1260188692
H	4.4728441261	-1.3774894122	0.2954703452
O	-2.1956090124	-2.1691200174	-2.5717842859
O	-1.9472111572	0.0322614296	-2.1210466301
C	-3.4810239748	-1.8835248652	-3.1623797986
H	-3.8668171777	-2.844939854	-3.5001018475
H	-4.1540149603	-1.4433980979	-2.422955012
H	-3.3706471359	-1.2003954241	-4.0080272902
H	0.1825372	-2.4705952147	-1.9693375174

#### E-12c\_t1

C	0.2479265528	-1.657630835	-0.6646462071
N	0.1142239251	-2.1429554644	0.6108109568
N	-0.0096420399	-0.2463834861	-0.8083697372
N	0.5899416591	-2.3042027214	-1.719880139
C	0.7093367193	-3.7636046584	-1.698891078
H	2.1512708063	-0.5824719144	0.8082245303
H	0.3806683535	-3.1144486367	0.7144672817
C	-0.8116351594	-1.6698202382	1.6578607334
C	-0.7233224919	0.176507147	-2.0420802363

C	2.1567102783	-4.1771428612	-1.3882584609
C	0.2623406577	-4.3048203805	-3.0610972345
H	0.0535403599	-4.2067603226	-0.9306965808
H	-0.968368736	-0.6021869086	1.4956216123
C	-2.1648719042	-2.386877195	1.5671358277
C	-0.1547872889	-1.8718696692	3.0259390979
H	-0.7329938062	-0.7059445892	-2.6840813431
H	-0.1516666305	0.9481798118	-2.5593148431
C	-2.1080389118	0.6842523181	-1.8151079364
H	-2.8394694841	-2.029205062	2.3529266661
H	-2.6421243618	-2.203863174	0.6003533134
H	-2.0404269935	-3.4686771367	1.6948789778
H	-0.8177359839	-1.5185586547	3.8219521053
H	0.0489441021	-2.9343013247	3.2066737929
H	0.7896721087	-1.3241570957	3.0956499444
H	0.3275324247	-5.3979505525	-3.0871428088
H	-0.7735921602	-4.0196457048	-3.2731268159
H	0.8950289649	-3.9024700833	-3.8605588269
H	2.2623919382	-5.2670746173	-1.4174123635
H	2.8423646187	-3.7456993228	-2.1262874732
H	2.4677332354	-3.8334721952	-0.3958843633
C	-2.7383071165	1.8442643432	-2.1620111687
C	-4.1085183613	1.7056165439	-1.7569258581
C	-4.2119347135	0.4729739812	-1.1912138263
O	-3.0050440791	-0.1680410212	-1.2242553825
H	-5.0249699246	-0.073430903	-0.7367471263
H	-4.9030675774	2.430174327	-1.8685744783
H	-2.2801089281	2.6932163641	-2.6493155807
C	0.6877803909	0.6874516821	-0.0648827292
C	1.757070174	0.4211843039	0.7327959302
C	0.1768487275	2.1170761008	-0.183442112
C	2.4061694404	1.4461867081	1.5418953118
O	-0.7160084735	2.3738707407	0.7750515252
O	0.5071910473	2.882812384	-1.064302297
C	-1.2381034635	3.7210518485	0.8063356837
H	-1.9253675403	3.7463488799	1.6513465935
H	-0.4239887083	4.4334647619	0.9552164653
H	-1.7676210669	3.9491487057	-0.1207763503
O	3.4236001139	0.9078032393	2.2610650558
O	2.1204415763	2.6364866867	1.5960596123
C	4.1570281656	1.8270309947	3.0882577681
H	4.9264216435	1.2313611006	3.5803955632
H	4.6196799413	2.6121800024	2.4842101858
H	3.5041339801	2.2869387534	3.8349468227

## 12c\_t2

C	-0.0769897144	-0.7800839145	-0.6500513549
N	1.1960486156	-0.1802056975	-0.6824465356
C	2.204389509	-0.652161361	-1.6755935176
N	-0.2789362244	-1.879924007	-1.2851142293

C	-1.6271250286	-2.3763615702	-1.5568885512
N	-1.0231953851	-0.0109053376	0.037861034
C	-1.7872925326	-0.5320282774	1.1788819245
C	-3.1123362969	0.1387006628	1.3242238349
H	-1.9219293118	-1.6069974442	1.0438853706
H	-1.2439594464	-0.393440536	2.1231139953
O	-4.0488401613	-0.0845844459	0.3471239543
C	-5.1687454375	0.6185445229	0.6904130799
C	-4.9714974829	1.2814488851	1.8619025218
C	-3.6316191035	0.9701019121	2.2733953429
H	-3.1194795651	1.3186702888	3.1597460086
H	-5.685951396	1.9139629243	2.3702305147
H	-6.0025430828	0.5435720057	0.0081462925
C	3.1991139537	-1.6618645129	-1.0897858004
H	1.5982478494	-1.1736455334	-2.4179281931
C	2.9189469621	0.5138207308	-2.3630927119
C	-1.8006607034	-2.5015409906	-3.0782707559
C	-1.8210986948	-3.7419877306	-0.8818438632
H	-2.4009154603	-1.6887818299	-1.188710174
H	-2.8169151648	-4.1463131738	-1.0953874072
H	-1.0755161008	-4.4571571258	-1.2488258832
H	-1.7080165145	-3.6733926399	0.2054607541
H	3.8460154267	-2.043327658	-1.8872135702
H	3.8472138647	-1.2048632064	-0.3329403827
H	2.6785147687	-2.5087979835	-0.6364949588
H	3.5691083514	0.1227475963	-3.15295181
H	2.202117913	1.1994023304	-2.8239465999
H	3.5508047517	1.0797958271	-1.6704799659
H	-0.7427451689	0.956665706	0.1528037788
H	-2.7917279153	-2.8974019428	-3.3283431469
H	-1.6914187972	-1.5265551946	-3.5654525584
H	-1.0450803008	-3.1759813285	-3.4980461981
C	1.6658846202	0.5203907278	0.4646340291
C	1.8706850293	1.8487194868	0.5056817744
C	2.0266963105	-0.2395920259	1.7249749727
C	1.4235385379	2.8131076981	-0.5322489316
O	1.566924206	-1.4971911692	1.705212707
O	2.6370226852	0.2449213748	2.6604327422
C	1.8428524654	-2.288014406	2.8822043439
H	1.3935662996	-3.2615055139	2.6898741975
H	2.9206769832	-2.3874774396	3.0286526087
H	1.3938486743	-1.8278711943	3.7652259257
O	2.3134503705	3.8069040546	-0.6727567273
O	0.3644186626	2.7535468297	-1.131710235
C	1.9634490597	4.8427387212	-1.6180934446
H	2.7909206634	5.5509148125	-1.5931653917
H	1.8517832156	4.4240805899	-2.6208561806
H	1.0335968668	5.3323312021	-1.3195880042
H	2.3534383738	2.269341301	1.3821473752

# E-12c\_t2

C	-0.6020822314	-0.6739952843	-0.056456987
N	0.7952607986	-0.6917573935	-0.4822581715
C	1.0406753601	-1.5984613757	-1.6527582515
N	-0.8256141643	-1.7132183545	0.8009067946
C	-2.0761536264	-2.3167315404	1.2889928269
N	-1.3299449766	0.2516541	-0.5620720196
C	-2.7216496707	0.5073403747	-0.1902945123
C	-3.6845272813	0.1136575381	-1.2658928903
H	-3.0219763599	0.0579153625	0.7633716693
H	-2.8293558329	1.5913842673	-0.0680969735
O	-3.8190171304	-1.2258455756	-1.5343318005
C	-4.7439952785	-1.3511189046	-2.5341215794
C	-5.2013690384	-0.126304727	-2.9082065219
C	-4.5101036912	0.8264889871	-2.0852318907
H	-4.6136042053	1.9027260397	-2.0995962242
H	-5.9359076675	0.0776511514	-3.6750254776
H	-4.9567004407	-2.358958028	-2.8584163978
C	2.3040202729	-2.4595173705	-1.5383825776
H	0.1974959029	-2.2913787704	-1.5994004135
C	0.9478777551	-0.846643524	-2.986221408
H	0.0184702612	-2.1855336561	1.1005556216
C	-1.9386925632	-3.8411107339	1.2097596434
C	-2.3998315371	-1.8565233743	2.7155929778
H	-2.8765242909	-2.0152291274	0.6122156397
H	-3.3392122438	-2.3036689204	3.0577732688
H	-1.6053117379	-2.1619610909	3.4061195393
H	-2.4978982448	-0.7680702576	2.7735261585
H	2.2232294157	-3.275039499	-2.2641322965
H	3.2190706619	-1.9130593734	-1.7746664272
H	2.3981154188	-2.9005624201	-0.5422556909
H	0.9922595155	-1.5622402237	-3.8142244626
H	0.0028220576	-0.3011134534	-3.053654678
H	1.7708014989	-0.136456339	-3.0968742693
H	0.2609832046	1.2959528625	1.2652959146
H	-2.8536201489	-4.3230149941	1.567855405
H	-1.75700533	-4.1666700917	0.1808184162
H	-1.1075999368	-4.190024986	1.834616297
C	1.6349274782	0.2773943603	-0.0052457739
C	1.2802248422	1.2305377062	0.9116441395
C	3.0724248552	0.2668461539	-0.5073275955
C	2.2160296449	2.2098136678	1.4326446191
O	3.8619801494	-0.4016450664	0.3370013224
O	3.4302845055	0.7719447804	-1.5506491885
C	5.2697368909	-0.3974565048	0.0145753166
H	5.7514207732	-0.9708278867	0.8060383728
H	5.4468088631	-0.8676201463	-0.9555763067
H	5.6455580417	0.6276594415	0.0029125705
O	1.6079833519	3.0073712814	2.3539502344
O	3.3943520479	2.3584039963	1.1220336847

C	2.4332393171	4.0313593035	2.9300568166
H	1.7921596974	4.5684689312	3.6302116937
H	3.2850143844	3.5974278936	3.4613124304
H	2.803751662	4.7162207946	2.1621254127

**TS4<sub>sc</sub>(1c\_t1)**

C	-1.3018402781	0.6308783501	-0.2796831367
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N	-0.0015996548	0.1314085556	-0.4261322678
N	-2.1424780234	-0.281195645	0.1376380674
C	-3.5627696478	-0.041100521	0.4414093772
H	-2.6390537681	2.0160730524	-0.7270621171
C	-0.9743329201	3.1815435365	-0.2713458349
C	1.0913509118	0.890293354	-1.035855714
C	-3.982674513	-0.7098233023	1.7555324452
C	-4.4612137596	-0.4588126605	-0.7308403465
H	-3.6768958971	1.0397380182	0.586941191
H	0.0480279316	2.95954232	0.0307296239
C	-0.9647931078	4.0974173389	-1.4953235703
C	-1.6982958289	3.8226637011	0.9172157523
H	1.6574735208	0.2049718467	-1.6678200013
H	0.6627575545	1.6596181892	-1.6818878863
C	2.0174981616	1.4915178343	-0.0198130379
H	-0.4837205999	5.049066495	-1.2494145127
H	-0.4232842025	3.6419058741	-2.3299271616
H	-1.9877625252	4.310714269	-1.8267111374
H	-1.2163184265	4.770047714	1.1796392912
H	-2.7451110025	4.033216068	0.6690100409
H	-1.6740121561	3.1726995634	1.7970828092
H	-5.5007327785	-0.196342916	-0.5082948927
H	-4.1717184872	0.0535639092	-1.6538501022
H	-4.4069221098	-1.5360253863	-0.9056224124
H	-5.0188229782	-0.4301525405	1.9726228286
H	-3.9076203722	-1.7958204816	1.6965894067
H	-3.3535251567	-0.3741172732	2.5844698877
C	2.1180009798	1.4396944968	1.3394949588
C	3.2747693263	2.2191548261	1.6879514843
C	3.7876745903	2.684592998	0.5187110499
O	3.0297881242	2.2499740243	-0.5360261257
H	4.6344333194	3.305364962	0.2670301546
H	3.6643202242	2.4030013567	2.6795788551
H	1.4603212588	0.9084803719	2.0124057745
C	0.0601042217	-1.2065268998	-0.0823194434
C	1.0799220664	-2.0940943726	0.0158681992
C	-1.3672078366	-1.7473046578	0.2594696386
C	2.5087859494	-2.0316748197	-0.2877488953
O	-1.8082073898	-2.4040673696	-0.962121702
O	-1.5270336429	-2.3486121979	1.3480824024
C	-2.4469220251	-3.657671873	-0.7649595899
H	-2.5175770839	-4.1199316831	-1.7545014319



H	-1.8760399972	-4.3128502802	-0.0990528781
H	-3.461660665	-3.5603390155	-0.3553481385
O	3.1373003214	-3.0786812489	0.3113267782
O	3.1212908643	-1.2366212895	-0.9900472848
C	4.5474311674	-3.1882310604	0.0578466581
H	4.8742598778	-4.0799522676	0.5938288397
H	4.7454845233	-3.2996086857	-1.0117227462
H	5.0815967512	-2.3101664179	0.4308438067
H	0.7607662424	-3.0492172676	0.42058602

#### TS4<sub>sc</sub>(1c\_t2)

C	-0.5528061129	0.7604966712	0.1765829238
N	-0.8408097569	-0.3691016437	0.7862738013
N	-1.3733972738	1.7283196314	-0.242594234
N	0.8261803348	0.8821493008	-0.0539805734
C	1.5445082713	2.1805912458	-0.2636458555
C	0.501907908	-1.1616410139	1.1586078358
C	1.4692324864	-0.2936213268	0.3125822249
C	-2.8072896951	1.9423501168	0.0602921835
C	2.7101372689	-0.773416673	0.0598506587
C	-2.0943026351	-1.0762959675	1.0110075487
C	-2.6584481214	-1.7202256185	-0.2211636554
H	-1.8304700958	-1.8585683947	1.7289151692
H	-2.8464432759	-0.4384995134	1.4785852918
H	2.9028089879	-1.7376465864	0.518499577
C	3.7679243043	-0.2899040213	-0.8210499597
O	0.4358116121	-2.4055274076	0.958314037
O	4.8580420386	-1.0953577523	-0.7132135305
O	3.7421948559	0.6594072378	-1.5964532761
C	5.9638569453	-0.7663636168	-1.5698247491
H	6.7360606942	-1.5045431169	-1.3507111705
H	5.6751204422	-0.8275064183	-2.6226961783
H	6.3360918371	0.2398560097	-1.3588893592
O	-3.9520605706	-1.4065581455	-0.5526027387
C	-4.2617675564	-2.1128124945	-1.6821725274
C	-3.1960588145	-2.8630889575	-2.0747754544
C	-2.1531292554	-2.6103620267	-1.1225214841
H	-1.1533725908	-3.0185892981	-1.0902654716
H	-3.1570775887	-3.5192419464	-2.933406465
H	-5.2611116422	-1.9742654009	-2.0670536036
C	-3.3644165554	2.8872494981	-1.0047521725
H	-3.3219404535	0.9854720742	-0.0374453368
C	-3.0037955523	2.4905114363	1.4767184299
H	2.5894800817	1.8921351728	-0.2082142425
C	1.3441429694	2.7753690969	-1.6619203529
C	1.2744482	3.170585116	0.8753875225
H	-4.0728562913	2.6041853209	1.6837090752
H	-2.581749962	1.817199318	2.2288435203
H	-2.5266312722	3.4705432786	1.583361951
H	-4.4305682939	3.0530215664	-0.828379574

H	-2.8598395605	3.8598672027	-0.9677330626
H	-3.2419400855	2.4679328269	-2.0080208332
H	1.9534666825	4.0221980012	0.7666670692
H	0.2527541623	3.5592179255	0.8731172381
H	1.46698416	2.703980169	1.8461813038
H	2.094997311	3.5565670356	-1.8167157165
H	1.4874906228	2.0111530164	-2.4283284591
H	0.3674294384	3.2486915809	-1.811353571
O	0.7343937853	-0.6992978121	2.5435124411
C	0.8988854139	-1.7158656364	3.5186272738
H	1.8125275842	-1.5197980647	4.0952850146
H	0.0489413957	-1.7269491104	4.2169378283
H	0.9720505089	-2.69843383	3.0432661088
H	-0.9387012909	2.4794419441	-0.7602244208

### 13c\_t1

C	-0.8662092743	-1.4382509723	-0.2922970674
N	-0.320061543	-0.1604876602	-0.41572658
N	-2.1114654366	-1.7616756511	-0.6814974818
N	0.0083248182	-2.2970742179	0.1954181245
C	-0.2619387082	-3.6624702587	0.6858914888
C	0.9799233974	-0.15108058	0.0784268802
C	1.4149166616	-1.626234473	0.333590325
C	-3.3934578882	-1.0171544671	-0.5563816559
O	2.0955763308	-1.9085431953	1.3575457985
C	-0.9516990433	0.9358626685	-1.1533316366
C	-1.6446134402	1.9205778948	-0.2581841077
H	-0.1672480895	1.4528801222	-1.7077787263
H	-1.6458645412	0.5110822121	-1.8826298692
C	1.8708948985	0.832750309	0.341976108
O	-2.2620190607	2.9529637284	-0.9051254109
C	-2.808348621	3.762728642	0.0548099738
C	-2.5513015331	3.2625052242	1.2919549019
C	-1.7917143513	2.0584723867	1.0907895854
H	-1.402634463	1.3958377208	1.8504155823
H	-2.8605234713	3.6901404183	2.2355544002
H	-3.3383556943	4.6312765099	-0.3063308779
C	-4.2235144206	-1.6287666593	0.5766493585
H	-3.1586998059	0.0120941092	-0.2913880223
C	-4.1340272417	-1.0557469786	-1.8935380129
H	-1.2387240544	-3.9649393346	0.2970375756
C	-0.3376743849	-3.6755245264	2.2196108834
C	0.7771123704	-4.651559688	0.1491008386
H	-5.0827046986	-0.5165864919	-1.8112861188
H	-3.5431448475	-0.5954480619	-2.6910550697
H	-4.3553333227	-2.0893808243	-2.1836362011
H	-5.1747738728	-1.0952066197	0.6693450243
H	-4.4448026552	-2.6830000812	0.373491774
H	-3.6988579868	-1.5620063272	1.5344025103
H	0.5159590067	-5.6601012717	0.4854489518

H	0.8027109155	-4.6442066403	-0.9433984828
H	1.7720155064	-4.4002412598	0.5211248261
H	-0.5500641527	-4.6912700398	2.5696705817
H	0.6100767853	-3.3359493991	2.6404450879
H	-1.1366432719	-3.0192813859	2.579441946
C	1.8749987113	2.2714696789	0.0759003836
H	2.7466425011	0.4662222588	0.868751821
O	2.8054750087	2.8730267734	0.8626029662
O	1.213365956	2.9055052416	-0.7359760699
C	2.9597372671	4.2897089583	0.6746869186
H	3.7471114176	4.5942223632	1.3649679087
H	3.2525320043	4.5180280635	-0.3537060824
H	2.031517516	4.818207524	0.9082314619
O	1.9858214973	-2.0321236394	-0.9930583192
C	3.3865755923	-1.8563232535	-1.0859899149
H	3.729470936	-2.4411662188	-1.9465295938
H	3.6697175679	-0.8047588224	-1.2542422448
H	3.8957089698	-2.2125632623	-0.1834810452
H	-2.2621787613	-2.7635645461	-0.7310573954

### 13c\_t2

C	-0.2444553759	-1.0107898668	-0.2968741365
N	-0.8331792204	0.1357727852	-0.5771196539
N	-0.7894387634	-2.2208948628	-0.1542867258
N	1.1339581743	-0.8475203214	-0.1135396026
C	2.1521129732	-1.9342367948	-0.2861038552
C	0.2392827868	1.2825292089	-0.7280863929
C	1.4458677964	0.5090881531	-0.1396983399
C	-2.144912442	-2.6903256645	-0.5257180601
C	2.5426800285	1.2034699541	0.2468425466
C	-2.2290516777	0.5586148717	-0.5804852531
C	-2.8313755203	0.6822901682	0.7871541921
H	-2.1928980066	1.5500843817	-1.0406917428
H	-2.8481338559	-0.0810765485	-1.2115498609
H	2.4480001735	2.2742994054	0.1034233559
C	3.7548830599	0.7803183455	0.9423587004
O	-0.0930436052	2.4001779148	-0.2433700077
O	4.5902288709	1.8420539436	1.0919954851
O	4.0336232124	-0.3272722121	1.3872945132
C	5.8079467479	1.5818910288	1.8094455428
H	6.3457598283	2.5302975218	1.8305195054
H	5.5974922909	1.24776475	2.8290868996
H	6.4068537089	0.8219980604	1.3001953894
O	-3.9586209894	-0.0552046315	1.0471869023
C	-4.3358391346	0.2234749995	2.3317599567
C	-3.4741916118	1.1159878978	2.8921462906
C	-2.4968929907	1.4175424604	1.8862107643
H	-1.6475825356	2.0826844694	1.9467499111
H	-3.5294111209	1.5152957798	3.8955448555
H	-5.2224550323	-0.2822555502	2.6840671083

C	-2.3979463032	-3.9989641964	0.2229781474
H	-2.8682476339	-1.9549161671	-0.1707520689
C	-2.2817872289	-2.8558234889	-2.0419593677
H	3.0916045361	-1.3903604409	-0.2702775602
C	2.2086349549	-2.9135513078	0.8911023241
C	2.0317678314	-2.6188475019	-1.6526305922
H	-3.3026187692	-3.1654715648	-2.2881286909
H	-2.0752029387	-1.9184106453	-2.5671664137
H	-1.5910760394	-3.6201535551	-2.4135919216
H	-3.401240223	-4.3665932269	-0.0081074051
H	-1.6772724544	-4.7681593684	-0.0783476001
H	-2.3240881676	-3.8556300054	1.3053068862
H	2.9067178273	-3.2598613816	-1.7998892959
H	1.1421621422	-3.2479924314	-1.7406211163
H	2.0146674341	-1.8767609081	-2.4564811814
H	3.1316351374	-3.4967320375	0.813137818
H	2.227612909	-2.3741573307	1.8401999541
H	1.3851450179	-3.6361709181	0.9093835087
O	0.424538498	1.2232448576	-2.2041735181
C	1.0809844408	2.3601035912	-2.7374523688
H	0.9357066883	2.3357050823	-3.8226969634
H	0.6594269223	3.2890834804	-2.3382782112
H	2.1642478177	2.352822992	-2.5374045397
H	-0.163365168	-2.9480281751	0.162739889

#### 15c\_t1

C	-1.2759897955	0.700695065	-0.1468875232
N	0.0170172809	0.1447097166	-0.4156629393
N	-1.7282609268	1.888202442	-0.2003186492
N	-2.0780028816	-0.3651463839	0.246468569
C	-3.4599441711	-0.1695255048	0.7250273483
C	0.0481743547	-1.2010048708	-0.1377549358
C	-1.4131625516	-1.6253000197	0.0804345614
C	-1.0624550825	3.1548336606	-0.4833154819
O	-1.4973157463	-2.4881688292	1.1753732136
C	1.1461398655	0.9179548016	-0.9222663112
C	1.9369635997	1.586724855	0.1632438869
H	1.796019938	0.2298368701	-1.4643367726
H	0.7778723421	1.6546638024	-1.6380344928
C	1.0311347279	-2.1364012512	-0.0390087758
O	2.8303193836	2.529006751	-0.2672500752
C	3.4892359481	2.9974219743	0.8383923468
C	3.0313435338	2.3738705003	1.95574538
C	2.0187315404	1.4521213636	1.5178863295
H	1.4384160803	0.7789102573	2.1324480366
H	3.3652524396	2.544833565	2.9697762462
H	4.2329027171	3.7587948009	0.6567867659
C	-1.6017692571	4.1969080907	0.5064184349
H	0.0220907951	3.1108438677	-0.3408478788
C	-1.349503234	3.5809526347	-1.9304616567

H	-3.68346909	0.8593361539	0.4358019203
C	-3.5520661983	-0.2577759381	2.2563191024
C	-4.4810746518	-1.0819078504	0.0358931069
H	-0.9142651114	4.5649838567	-2.1360085041
H	-0.9327280185	2.8667695338	-2.6486214528
H	-2.4303375786	3.6395969817	-2.1025281758
H	-1.1396866072	5.1743210847	0.329406395
H	-2.6876663119	4.3025453932	0.4020457512
H	-1.3870058559	3.8992147817	1.5381203772
H	-5.4864858139	-0.7779974539	0.3457414257
H	-4.4148676863	-1.0047225753	-1.0517763717
H	-4.359641115	-2.1349153256	0.310012778
H	-4.559736803	0.0214529252	2.582773729
H	-3.3466144258	-1.2683356477	2.6206771949
H	-2.8416212197	0.426124025	2.7308080947
C	2.4743993593	-2.0907618867	-0.2717404522
H	0.6846163171	-3.0977174563	0.3187340472
O	3.0439970016	-3.1972720889	0.2743377673
O	3.1417597673	-1.2583662171	-0.8737549255
C	4.4645728282	-3.3226709321	0.0937766841
H	4.7396569051	-4.2624923518	0.5734303596
H	4.7222863556	-3.3532977643	-0.9682735431
H	4.9933584277	-2.4912276018	0.5673931208
O	-1.9621193271	-2.2269032423	-1.0891500207
C	-1.4867656211	-3.5190479196	-1.4814224697
H	-2.1655691596	-3.8542597427	-2.2688797108
H	-0.4690498063	-3.4742652058	-1.8837270219
H	-1.5168860556	-4.2380175754	-0.6563456247
H	-2.3793184052	-2.8965051194	1.1626697923

#### E-15c\_t1

C	-1.2447742231	-1.143954601	-0.1026871609
N	-0.5313270979	0.0462643294	-0.4570991525
N	-2.4874296361	-1.4179289063	-0.0751980999
N	-0.2788357953	-2.0562352979	0.2932632834
C	-0.6221986928	-3.378605979	0.8505680512
C	0.813201721	-0.0838892711	-0.2038899831
C	1.0537882312	-1.5883285244	0.0339002771
C	-3.6288415665	-0.5342801728	-0.2924996536
O	1.9115649337	-1.9073668636	1.0607521298
C	-1.0927182916	1.209052652	-1.1345389117
C	-1.4797056027	2.3217979918	-0.2038846709
H	-0.3462258121	1.5668702611	-1.8532920417
H	-1.9500939682	0.8884459256	-1.7287368211
C	1.7051977025	0.9462942365	-0.2497475293
O	-2.0324363785	3.4158549551	-0.8105031601
C	-2.3079579368	4.3269496119	0.1739465821
C	-1.9416657178	3.8334753235	1.3859965809
C	-1.4002090869	2.5242344528	1.142281186
H	-1.003023333	1.8347373196	1.8732220495

H	-2.041138205	4.331986453	2.3401151349
H	-2.7549519181	5.2537807225	-0.153137791
C	-4.6481023428	-0.8046048999	0.8234766113
H	-3.3621056705	0.5269782864	-0.2302575595
C	-4.2485769602	-0.8096601081	-1.6698744941
H	-1.6663060144	-3.5192473923	0.5616470857
C	-0.5495796237	-3.3796596329	2.3845879558
C	0.2002982233	-4.5161335784	0.2369692483
H	-5.1450242998	-0.1982188767	-1.8196274654
H	-3.5450915725	-0.5877381427	-2.4794361159
H	-4.5337079705	-1.8646509013	-1.7533288937
H	-5.5334149342	-0.1709412564	0.7010629821
H	-4.9671646223	-1.8529755778	0.8081716459
H	-4.2121990539	-0.5967016209	1.8062653206
H	-0.1676351312	-5.4691737292	0.6316450512
H	0.1062628529	-4.5331237676	-0.8515356724
H	1.2604029923	-4.4302286212	0.4883465161
H	-0.9119496455	-4.3374082069	2.7745398639
H	0.475906001	-3.2290293048	2.7309884746
H	-1.1766507936	-2.5871510737	2.8055469819
C	3.1034776541	0.8859321924	0.132847311
H	1.3495350999	1.9350360491	-0.5133726762
O	3.7223758953	2.0542843047	-0.1110629822
O	3.710045863	-0.0630035391	0.6508849595
C	5.1084404211	2.139980153	0.2760674197
H	5.4212232175	3.1494392634	0.0096199084
H	5.2201124582	1.9807202024	1.3512353188
H	5.7071216235	1.4036024364	-0.2652531037
O	1.4405150192	-2.1738289675	-1.2213419599
C	2.7876278779	-2.0166148583	-1.6608665352
H	2.8908950781	-2.6615822345	-2.5370402365
H	3.0066983505	-0.9846905459	-1.9622042409
H	3.5081754843	-2.333592857	-0.9008663424
H	2.6864311966	-1.2871858132	1.0045493244

# 15c\_t2

C	-0.5409527215	0.8739615281	0.1957026329
N	-0.8340560801	-0.4443759047	0.5505701288
N	-1.2568848326	1.8896447939	-0.0787359678
N	0.8813859548	0.9621888196	0.1187308665
C	1.6109313662	2.2427314876	-0.0824622266
C	0.3777314188	-1.1727993624	0.8712230006
C	1.4665690639	-0.2608193747	0.2957931489
C	-2.7158424507	1.9314217541	-0.1702385209
C	2.7138874379	-0.7718581835	0.0845638554
C	-2.0999295486	-0.9303078305	1.0892391943
C	-2.9349127249	-1.6346106508	0.0594329648
H	-1.8643099774	-1.6133659755	1.9134579621
H	-2.6644648367	-0.113546551	1.5438905982
H	2.8236614733	-1.8105469876	0.367477334

C	3.8947276559	-0.2208544298	-0.5700319142
O	0.4540758845	-2.4324694671	0.2810283316
O	4.9142297574	-1.1193462186	-0.4802113238
O	4.0306583629	0.843761739	-1.1624718463
C	6.1385758369	-0.7399006338	-1.1283821134
H	6.8325403083	-1.5623577979	-0.9510903698
H	5.9874171944	-0.6027783447	-2.2026946862
H	6.5371582685	0.1850389966	-0.7028490788
O	-4.2175494306	-1.9245531364	0.4374222229
C	-4.8027540222	-2.5970842906	-0.6023243808
C	-3.9200886	-2.7378201687	-1.6263337901
C	-2.6996423159	-2.1114913323	-1.1964285873
H	-1.7716687127	-2.0325280293	-1.7433079178
H	-4.1077992126	-3.2230245881	-2.574146401
H	-5.8307131225	-2.8925099408	-0.4542921596
C	-3.0828583529	2.6877019074	-1.4547209737
H	-3.161467934	0.9330068254	-0.2483122158
C	-3.3007260921	2.6387138003	1.0602857608
H	2.6565786492	1.9605074575	0.0034334673
C	1.418032394	2.8160675659	-1.4890761178
C	1.3069413357	3.2514372433	1.0313282255
H	-4.3899660613	2.719055446	0.9759046916
H	-3.0690079672	2.0975780753	1.983669256
H	-2.8887113796	3.6503018995	1.1508101495
H	-4.1708092281	2.7470370207	-1.5693338959
H	-2.6821596467	3.7074936607	-1.430986757
H	-2.6743546845	2.1810636915	-2.3352765253
H	1.998484735	4.0955345936	0.9375039773
H	0.2861671111	3.6313955464	0.9739727703
H	1.4599423435	2.8007591615	2.0176404327
H	2.0782877883	3.6808033499	-1.6160668012
H	1.6899783827	2.0736258259	-2.2444810631
H	0.3888923997	3.1372740279	-1.6575355602
O	0.4187468415	-1.2561955348	2.2868531068
C	1.4857880127	-1.9989252438	2.8888615265
H	1.2274068523	-2.078396617	3.9468428943
H	1.5736006615	-3.003413066	2.4642067809
H	2.4440231558	-1.477526927	2.7929053452
H	-0.2100937114	-3.00423463	0.7040465692

#### E-15c\_t2

C	0.7322756369	1.052762455	-0.2196215598
N	0.5983493388	-0.3232860048	-0.3736484397
N	1.7299945623	1.8412484074	-0.157265599
N	-0.5900031351	1.5691435997	-0.063207234
C	-0.8900011476	2.9983829632	0.2123187722
C	-0.7984109066	-0.7221966586	-0.4536155813
C	-1.521249022	0.5749458047	-0.0368257008
C	3.1414459756	1.4577467811	-0.1590313002
C	-2.8497288225	0.713706135	0.2626727357

C	1.5945439427	-1.2113529875	-0.9590401778
C	2.3635355362	-1.9930286849	0.0660419912
H	1.0688534766	-1.8949506576	-1.633668599
H	2.2825690006	-0.6466942736	-1.5931330112
H	-3.2509237753	1.6959167449	0.4742980929
C	-3.814039824	-0.3573674587	0.3588843023
O	-1.0182206293	-1.8049262729	0.3644250146
O	-5.060977482	0.1271873184	0.5264479344
O	-3.6119706081	-1.5829882043	0.3293617785
C	-6.1107058012	-0.8459991851	0.6843538027
H	-7.0248550612	-0.267430014	0.8179662628
H	-6.1913783367	-1.4778283134	-0.2036090306
H	-5.9302134963	-1.4734819527	1.560664336
O	3.4510841	-2.6732888404	-0.4122810405
C	4.0049129545	-3.3450275394	0.6448652396
C	3.2948494145	-3.1024108675	1.7783613288
C	2.2226181746	-2.2218130744	1.4025573457
H	1.4438941916	-1.8229615445	2.0352927611
H	3.5028701525	-3.4971982944	2.7632736512
H	4.8835016013	-3.9322291681	0.4229208134
C	3.8331975014	2.203999247	0.9905042379
H	3.2872410726	0.3864017975	0.0192516676
C	3.7793891311	1.8250401181	-1.5059136855
H	-1.9782954649	3.0511411909	0.2077033989
C	-0.4133209301	3.4310973545	1.6027121054
C	-0.4101864521	3.9214352765	-0.91314369
H	4.8497566262	1.5920976346	-1.5007964671
H	3.3148382674	1.277202081	-2.3324460884
H	3.6622481555	2.8965663992	-1.7045374507
H	4.9002685534	1.9577595634	1.0220470465
H	3.7325851156	3.2879751524	0.8639939815
H	3.3921755541	1.9301756041	1.9546254248
H	-0.8220038825	4.921913784	-0.7445699207
H	0.6770990652	3.9889608761	-0.9452942158
H	-0.7708910024	3.5680744855	-1.8845789127
H	-0.7842345035	4.4398424645	1.8116500174
H	-0.8041019877	2.7604984835	2.3747097525
H	0.6762565733	3.4424297789	1.6655306728
O	-1.1337110353	-0.9621159637	-1.8225205138
C	-1.6370964943	-2.2500369891	-2.2005495213
H	-1.696103168	-2.2212430133	-3.2913152741
H	-0.9705074256	-3.0643684552	-1.9016997857
H	-2.6357947173	-2.4346738717	-1.7944148726
H	-2.0073285628	-1.9038012112	0.4238402034

#### 16c\_t1

C	-1.3107913802	0.468825768	0.1081258913
N	0.0611024817	0.7880197801	0.2943179345
N	-2.2352417928	1.3314964508	-0.1329181739
N	-1.6373936874	-0.8842202346	0.2545858987



C -3.0722774355 -1.2748963875 0.1906866167  
C 0.8699403918 -0.0839507531 1.0393654631  
C -0.5664638659 -1.8837464403 0.2417833483  
C -2.1058465573 2.7671666647 0.1045110687  
O -0.9720356575 -3.1054336767 0.793347646  
C 0.7372683206 1.7056418761 -0.6640473774  
H -0.0292213083 2.257430859 -1.1981646358  
H 1.3349430375 2.41771213 -0.0911992903  
C 1.5871725408 1.0189922483 -1.6818062015  
C 0.567667663 -1.3875688614 1.0985467823  
C -3.0917222695 3.160192279 1.2175561919  
H -1.1018990382 3.0505152361 0.4505850679  
C -2.425572736 3.5421288076 -1.1817856336  
H -3.5687237574 -0.3170262249 0.0429128793  
C -3.5986458659 -1.8562488677 1.5107075116  
C -3.4237136873 -2.1364796121 -1.0313021049  
H -2.3758696007 4.6226781318 -1.0087582813  
H -1.7303159376 3.296457751 -1.9917849799  
H -3.4362155455 3.2965826112 -1.5279374517  
H -3.046617842 4.2376761855 1.4137521748  
H -4.1184257399 2.9049576498 0.9310515646  
H -2.8594416468 2.6349295074 2.1499934226  
H -4.5139553688 -2.1866247624 -1.1258027463  
H -3.0216764668 -1.6989735688 -1.949029944  
H -3.0688263846 -3.1712412128 -0.9663036955  
H -4.6909382101 -1.9291664327 1.460925688  
H -3.1990889009 -2.8487772557 1.7263530378  
H -3.3443510749 -1.1972296609 2.3472994409  
H 1.0793301546 -2.0803610197 1.7524706763  
C 1.9767707007 0.5283750241 1.8404387527  
O 2.8386320823 -0.3980354311 2.2876875541  
O 2.0797605271 1.7196102267 2.0710847499  
C 3.9063981363 0.0904114792 3.1267808938  
H 4.4919433403 -0.7889967653 3.3932500234  
H 4.5241018977 0.8067566942 2.5802053786  
H 3.503732076 0.5648159534 4.0248867232  
O -0.2022390427 -2.056290194 -1.1243149437  
C 0.9282279246 -2.9017829645 -1.3659046716  
H 1.0185025366 -2.9836715718 -2.4507808888  
H 1.8516469604 -2.4707921981 -0.9634597035  
H 0.784988547 -3.9020603141 -0.941899635  
C 1.4193572445 0.7412641737 -3.0073968637  
C 2.6119577626 0.0737500821 -3.4440116659  
C 3.4209663513 -0.008031067 -2.352455968  
O 2.8168016215 0.5672674263 -1.2703599383  
H 4.4074264285 -0.4140439773 -2.1841785499  
H 2.8354265748 -0.2903666553 -4.4371904912  
H 0.5490252605 0.9848416423 -3.6009971615  
H -1.5177277625 -3.5608725284 0.132536616

**16c\_t2**

C	-0.0251115719	0.9723359626	0.1099441485
N	0.6936743776	-0.2538740929	0.1044819022
N	0.5026615191	2.1411497019	0.0850261643
N	-1.4330550019	0.8716202289	0.1332241208
C	-2.1977108485	2.0868111965	0.5578592145
C	0.0240980313	-1.3577725802	0.8144443513
C	-2.0366164461	-0.3832316499	-0.0270653098
C	1.9368376011	2.3548327501	0.2637153031
C	-3.3493803599	-0.4812929485	-0.7469955879
C	1.4402146783	-0.578993	-1.1319044782
C	2.9147999828	-0.7932953315	-0.9419254412
H	0.9901418621	-1.463831975	-1.5958284942
H	1.3131365175	0.2440205688	-1.8373969964
C	-1.3762545927	-1.5127653493	0.285288919
O	3.6966174315	-0.338943092	-1.9741526323
C	4.9947810421	-0.6402824981	-1.6682514835
C	5.0579635235	-1.2696232554	-0.4642665543
C	3.7052874572	-1.374798136	0.0066560241
H	3.3605627751	-1.8298617963	0.9225350256
H	5.953182961	-1.6194463727	0.0313057086
H	5.7340999339	-0.3413353115	-2.396230659
C	2.1361938049	3.2758672679	1.4767608274
H	2.4653444249	1.4125462242	0.4609750541
C	2.5284124826	2.9923948914	-1.0009888157
H	-1.4864272981	2.6222775798	1.1905490935
C	-3.41142252	1.7378063444	1.4240762755
C	-2.5503582097	3.0163985463	-0.608188781
H	3.5937103445	3.2076335259	-0.8623669442
H	2.4271975316	2.3332244123	-1.8683133991
H	2.0158571603	3.9341756046	-1.2292574921
H	3.2005307119	3.4815859032	1.6368909766
H	1.6197909601	4.2309014413	1.3258152931
H	1.7376296873	2.815489758	2.387268075
H	-2.9898989835	3.9403759167	-0.2153786257
H	-1.6493217848	3.2829520555	-1.166438339
H	-3.2638927826	2.5495668393	-1.2889823236
H	-3.7829444831	2.6586281265	1.8848072382
H	-4.2399758212	1.3108484254	0.8521882735
H	-3.1434730349	1.0454371323	2.2282079023
H	-1.7862523433	-2.4871607849	0.0598748654
O	-0.0672946871	-1.028339847	2.1779734134
O	-4.0545026769	-1.5468665863	-0.3330048092
O	-3.7173524146	0.271362936	-1.629268571
C	-5.2797054476	-1.8059173216	-1.0522297689
H	-5.7038919166	-2.6973247907	-0.5911151749
H	-5.9669417156	-0.9627270141	-0.9513694933
H	-5.0740772323	-1.9859999383	-2.1100399159
O	0.8309587646	-2.4853230405	0.5959300027
C	0.4376742169	-3.6742670659	1.2881930859

H	1.2265257025	-4.4041877524	1.0979558556
H	0.3545152221	-3.4987471853	2.3645951394
H	-0.511543413	-4.0730533761	0.9120238796
H	0.8324308778	-0.7849942473	2.4605109572

### 17c\_t1

C	-0.4776797355	-0.8282776364	0.5950110681
N	0.9208528486	-0.6399376003	0.4454805033
N	-1.2160889074	-1.8348231748	0.7977239322
N	-1.0542544083	0.46289647	0.4659019065
C	-2.5125821195	0.7103854994	0.5515941523
C	1.2133362465	0.6880021843	0.1992551523
C	-0.1120523703	1.404132805	0.2063853113
C	-0.8769066575	-3.254117479	0.8756172008
O	-0.3108200517	2.6047709675	0.018745873
C	1.9090559174	-1.693746691	0.6702958215
C	2.2224914131	-2.4706134453	-0.5735981098
H	2.8182376612	-1.2142455976	1.0342902553
H	1.5476582855	-2.3542393603	1.4604057489
C	2.3387232535	1.4130849964	-0.0316536113
O	2.9682567108	-3.5998454699	-0.3769943675
C	3.1973598302	-4.1524098887	-1.6090432732
C	2.6115157285	-3.3993582866	-2.5767989581
C	1.9751161625	-2.2999913167	-1.9037124884
H	1.4151090321	-1.493726619	-2.3553433306
H	2.6241480503	-3.5954433051	-3.6399367361
H	3.7778081982	-5.0627274427	-1.616958482
C	-1.9278695343	-4.0235966783	0.0653728098
H	0.1015206781	-3.4773697009	0.4395408699
C	-0.8808311868	-3.6970485256	2.3448792799
H	-2.9292589371	-0.2745913348	0.7669112532
C	-3.0629699039	1.2004447648	-0.7906933751
C	-2.834633151	1.6519966967	1.7151991298
H	-0.6967974995	-4.7741164263	2.414966503
H	-0.1074130367	-3.1793253666	2.9214659593
H	-1.8508187061	-3.4812834229	2.8062766141
H	-1.7207547317	-5.0984385254	0.0982607487
H	-2.9311630603	-3.8497497206	0.4696745165
H	-1.9209258565	-3.7058918042	-0.9822552041
H	-3.920711979	1.7429018068	1.8152736409
H	-2.4375121885	1.2591615671	2.6564337402
H	-2.419792439	2.6492815939	1.5489287566
H	-4.1515649976	1.2912787875	-0.7229807727
H	-2.6521994011	2.1773163202	-1.0579764818
H	-2.8297678323	0.4906922187	-1.5905761081
C	3.7546738209	1.0400629935	-0.1145880199
H	2.15022941	2.4648347575	-0.2202849835
O	4.4572516241	2.0890084185	-0.6033187125
O	4.2953053256	-0.0118796579	0.1997626295
C	5.8769727657	1.8890495388	-0.7291602137

H	6.2716670044	2.8295106397	-1.1139005007
H	6.3239612363	1.6606791526	0.2417693459
H	6.0936653306	1.0758458968	-1.4266960979
H	0.7469525035	4.067223851	-0.3893890174
O	1.3776323127	4.8053212447	-0.4741997097
C	1.4890475983	5.3954653689	0.8128690331
H	2.2333495701	6.1961085789	0.7511936296
H	0.5425907085	5.8410873865	1.1553229012
H	1.8249074642	4.6813959715	1.5794552673

#### **E-17c\_t1**

C	-0.6369392915	-0.5960663838	0.3770257556
N	0.7410374534	-0.3670794237	0.1562753677
N	-1.3086132475	-1.5983052824	0.7643444887
N	-1.2777085722	0.6188308867	0.0390875878
C	-2.7428639394	0.8139043389	0.1169060505
C	0.9644608498	0.9220853819	-0.3082820058
C	-0.3964448754	1.5521076776	-0.4376447427
C	-0.8378798392	-2.9599095288	1.0156739444
O	-0.6854423861	2.6450692383	-0.906125531
C	1.8263110114	-1.1988380201	0.6654458668
C	2.444397867	-2.0668783336	-0.3906727502
H	2.5843856143	-0.5316719197	1.0925543565
H	1.4536721023	-1.8016750405	1.4950029238
C	2.1831366381	1.4315096079	-0.6133413873
O	3.5222206189	-2.8011064997	0.0192103916
C	3.9532904301	-3.5220891775	-1.0624642155
C	3.1733401316	-3.2582439592	-2.1435544756
C	2.1866435085	-2.3077901454	-1.7077230874
H	1.3983005131	-1.8651532881	-2.2993744062
H	3.2799472559	-3.6823325451	-3.1322083576
H	4.8081075115	-4.1597705741	-0.8936085827
C	-1.8232049123	-3.9205060228	0.3367813447
H	0.1514816316	-3.1471298234	0.5828336834
C	-0.7812426619	-3.2129920229	2.5284494461
H	-3.1113468059	-0.1301023276	0.5216773759
C	-3.3531762666	1.0243046287	-1.272103223
C	-3.0720473259	1.9414508583	1.1014133424
H	-0.4899795283	-4.2491328221	2.7297037898
H	-0.0595356188	-2.5527420656	3.0207170493
H	-1.7635249983	-3.0362067918	2.9803825554
H	-1.5173021998	-4.9591552349	0.501221986
H	-2.8326867565	-3.7869928751	0.7410889718
H	-1.8610012969	-3.7418197676	-0.742649572
H	-4.1579727444	2.0616822074	1.1687440134
H	-2.6944774336	1.7025850028	2.1009583844
H	-2.6350922283	2.8924299295	0.7850405386
H	-4.4437900035	1.0589524695	-1.1850940585
H	-3.0120005652	1.9598618465	-1.7209494642
H	-3.0922413036	0.1981771779	-1.9412849387

C	2.5032986221	2.8241679284	-0.9580179643
H	3.0386881284	0.7660126062	-0.6053914009
O	3.6973882882	2.8578694011	-1.5981118678
O	1.8750181779	3.8376598493	-0.6960197228
C	4.1824274023	4.1664106676	-1.9507842369
H	5.1435392207	4.0013913391	-2.4381204161
H	3.4926922997	4.6639708044	-2.6373709515
H	4.312394599	4.7851233566	-1.0590493928
H	-0.0672296708	4.3548321871	0.1842494921
O	-0.4513343168	4.9431894436	0.8567077163
C	0.3625794704	4.8416016281	2.0106675578
H	-0.0729715198	5.4835727492	2.7843366733
H	0.4077126591	3.8173594371	2.4137580203
H	1.3952803034	5.1775792258	1.834583077

### 17c\_t2

C	-0.012660545	-0.4996300236	0.4519429254
N	1.3619307906	-0.1780426252	0.2916875567
N	-0.6369031749	-1.5882826961	0.618043724
N	-0.7051093781	0.7391331932	0.3940346286
C	-2.1898110839	0.8328635628	0.3175996129
C	1.5306155445	1.1725250875	0.1505156163
C	0.1655797308	1.7895308549	0.2436572968
C	-0.1017656012	-2.9491384492	0.6508966358
C	0.0720507901	3.1484179353	0.1838141576
C	2.5478293302	-1.0522912466	0.3606519056
C	3.0743646897	-1.4630542011	-0.9735412682
H	3.3259693458	-0.4730764501	0.8610940166
H	2.3152299162	-1.9072736435	0.9928878573
H	1.0120538891	3.6475752444	-0.025815125
C	-1.0440181073	4.0615342052	0.4277319433
O	2.6145124169	1.7334039743	0.0170256466
O	-0.6714683629	5.3219056879	0.0944855339
O	-2.1488154559	3.8147957115	0.8963126979
C	-1.6534404162	6.3472205708	0.3259726803
H	-1.1846613704	7.278812655	0.0084176049
H	-2.5563035407	6.1606783638	-0.2615545219
H	-1.9182322255	6.4007506292	1.3852336939
O	2.3442562358	-2.369757988	-1.6983523339
C	3.0224030787	-2.5953407064	-2.8628860144
C	4.1655856862	-1.8584425195	-2.8944683018
C	4.1978446255	-1.1184915636	-1.6658385687
H	4.9553175634	-0.4202244063	-1.3385450807
H	4.8950490147	-1.8389656514	-3.6920123931
H	2.5652729067	-3.2936482899	-3.5480529213
C	-1.0969886304	-3.8614516643	-0.07683539
H	0.8561571932	-3.0335939698	0.1298016958
C	0.0828899417	-3.3908649138	2.1098023561
H	-2.3730714073	1.8962367001	0.1934131062
C	-2.7522743672	0.1123117813	-0.9124382835

C	-2.8603946517	0.415467053	1.629502641
H	0.4167944576	-4.4329807673	2.1493301227
H	0.8263145148	-2.7739624693	2.6251320918
H	-0.8630875962	-3.3110457309	2.6566019469
H	-0.7406888483	-4.8970140534	-0.067026724
H	-2.0792305319	-3.8280624021	0.4074325809
H	-1.2176983311	-3.5533387658	-1.1204194053
H	-3.9315845595	0.6343141783	1.5665463541
H	-2.7355295824	-0.6499577299	1.8300436939
H	-2.4499716286	0.9843176223	2.4697032428
H	-3.8115883492	0.3709612809	-1.0137306406
H	-2.2396639503	0.4377284074	-1.823671981
H	-2.6691249569	-0.9725126943	-0.8308557844
H	3.1484560924	3.5075737203	-0.208385865
O	3.3505024321	4.4602422828	-0.2064100245
C	3.6954534267	4.8016912231	1.12872352
H	3.8892339615	5.8787999114	1.1589243465
H	2.8883175565	4.5840896874	1.8438662748
H	4.6042845217	4.2857050971	1.4739429195

#### E-17c\_t2

C	0.856592133	-1.1624657596	0.3016186279
N	0.5317985256	0.2091056559	0.4250874776
N	1.9374126069	-1.8189662503	0.3815468688
N	-0.3733621518	-1.8166180969	0.0439322066
C	-0.4197394081	-3.2884901003	-0.1257246962
C	-0.8170323599	0.4224144466	0.2442782346
C	-1.4287882974	-0.9301817457	0.0163601188
C	3.2976475226	-1.3399885664	0.6178358097
C	-2.7309900842	-1.2257741652	-0.2420942839
C	1.4266958533	1.3460290764	0.703827303
C	1.9102333167	2.0566977143	-0.5170513273
H	0.8531600674	2.0634091279	1.293593081
H	2.2462918554	0.9927053997	1.3279203102
H	-2.9796732156	-2.2363427776	-0.5341397503
C	-3.8962914483	-0.3336583406	-0.1546160108
O	-1.3634943373	1.5167056523	0.2438462514
O	-4.8954947966	-0.8478894547	-0.9247631382
O	-4.0415394399	0.672176913	0.5161473877
C	-6.1379478583	-0.1263595316	-0.8896138036
H	-6.818302432	-0.6781042691	-1.5391345627
H	-6.538133972	-0.0870261466	0.1272735369
H	-6.0081636936	0.8933574327	-1.2623610418
O	2.7584762284	1.3839097806	-1.3592587766
C	3.0733961125	2.2374010328	-2.379273181
C	2.4513567616	3.4343776288	-2.2031331147
C	1.6910035061	3.3167026709	-0.9918247496
H	1.0598301661	4.0615728889	-0.5272979273
H	2.5198406228	4.2945722807	-2.8543569432
H	3.7371738936	1.8450812859	-3.1352695654

C	4.2455116221	-2.204193766	-0.2226193044
H	3.4348028949	-0.3025305916	0.2990493661
C	3.6302998982	-1.4501289792	2.1127427435
H	0.6171305954	-3.5826193535	0.0386250516
C	-0.7923386889	-3.6943136036	-1.5568755165
C	-1.2703764725	-3.9708408946	0.9517831178
H	4.6727447506	-1.1659417743	2.2909483369
H	2.9904809891	-0.7965968389	2.7147584007
H	3.488803382	-2.4793121089	2.4607659352
H	5.2831546071	-1.8847389839	-0.0790752999
H	4.1636462077	-3.2587833962	0.0634194749
H	4.0061029395	-2.1197990111	-1.287679076
H	-1.131406791	-5.0538585374	0.8750831219
H	-0.9522068978	-3.6587032476	1.951342924
H	-2.3389695515	-3.7664798768	0.850292767
H	-0.6585278704	-4.7754879894	-1.6642335822
H	-1.8294092024	-3.4626782248	-1.8132678809
H	-0.1392429715	-3.1986122246	-2.2816351311
H	-0.9403219744	3.2314530188	0.83684576
O	-0.629379861	4.053297987	1.2571076961
C	-1.5127873125	4.3501128274	2.3301518226
H	-1.1302446196	5.2389634507	2.8417019676
H	-2.5334038404	4.5710216259	1.9838054099
H	-1.5711555096	3.53413371	3.0650955534

# 18c\_t1

C	-0.2805396825	-0.8482218178	0.4628062791
N	1.0882546033	-0.581453823	0.1514944127
N	-0.8181464932	-1.9295343683	0.8469576902
N	-1.1548928708	0.2856376172	0.3204039468
C	-2.6300222258	0.0420454023	0.4495143525
C	1.5210753999	0.7046477502	-0.1216176423
C	-0.7193926779	1.5871679483	0.1586001534
C	-0.4216539843	-3.3197089381	1.011408129
O	-1.5090934977	2.5488849746	0.1972520118
C	2.0960847162	-1.6187038025	0.4324516691
C	2.2961623758	-2.5846190972	-0.6964147258
H	3.0383932988	-1.1235117324	0.6748031357
H	1.8064074842	-2.146286568	1.3424830387
C	0.6907349045	1.7686355869	-0.0961809342
O	3.0428959519	-3.6867647703	-0.377873284
C	3.1380277184	-4.4504820352	-1.510732979
C	2.4655129753	-3.8581294214	-2.5326571529
C	1.9169336168	-2.6398206538	-2.0040131454
H	1.3326326303	-1.9016036401	-2.5333764944
H	2.3686214581	-4.2342439961	-3.5416114034
H	3.7062571839	-5.3638024007	-1.4175466252
C	-1.4602799402	-4.1932897043	0.2927266046
H	0.5502834569	-3.5595806365	0.5740012519
C	-0.3728265545	-3.649665457	2.5100950472

H	-2.7043182756	-1.0416683662	0.4645366686
C	-3.4043300095	0.5470290491	-0.7725156351
C	-3.1764388916	0.5624327048	1.7823333578
H	-0.1438363699	-4.7102014317	2.6587140605
H	0.3936185568	-3.0589017499	3.022918233
H	-1.3384521504	-3.4340432073	2.9808352638
H	-1.2038789761	-5.2530488344	0.3989394354
H	-2.4600736342	-4.0347600893	0.7118372726
H	-1.4938848982	-3.956058942	-0.7756305108
H	-4.2261653616	0.2652939204	1.880600343
H	-2.6258224121	0.1280904458	2.6230443409
H	-3.1178999433	1.6505614617	1.8470113251
H	-4.4282902952	0.1621502008	-0.715773561
H	-3.4454477754	1.6354876835	-0.822166903
H	-2.9577121856	0.1691173931	-1.6983743665
H	1.0392285957	2.7697669963	-0.3071277224
C	2.9411812829	0.9270289569	-0.5816033748
O	3.4542947496	2.0278069123	-0.0249792282
O	3.5123623564	0.2285634244	-1.3940245397
C	4.7721052165	2.4114759108	-0.4877656346
H	5.0222515442	3.3114711215	0.0720665888
H	5.4923183969	1.6178517698	-0.278711851
H	4.7513958306	2.6205470352	-1.5594986967
H	-0.7351075865	4.1588199402	-0.1127002513
O	-0.1793178256	4.9620793933	-0.1931844116
C	-0.0056882642	5.4693121562	1.1197942695
H	0.6456973811	6.3478605225	1.0600103249
H	-0.9544703493	5.786961506	1.5799742845
H	0.4707294461	4.7445666994	1.7978455822

# 18c\_t2

C	-0.0574174078	-1.0076193018	0.5413978383
N	1.342277713	-1.07902995	0.3011153057
N	-0.8786290988	-1.9446914121	0.7916538911
N	-0.6021702498	0.3224675801	0.5084474655
C	-2.1032353241	0.4227491949	0.5927710746
C	2.1421344045	0.0056509987	-0.0835875969
C	0.1958533343	1.4013399238	0.2477082779
C	-0.79007339	-3.3980208663	0.7232502096
C	-0.2943457848	2.8079607044	0.5044026862
C	2.0968828221	-2.3052301938	0.5966059585
C	2.3756875447	-3.1414170166	-0.6167195329
H	3.0483907014	-1.9944867491	1.0352432141
H	1.5642737045	-2.8727626769	1.3582972522
C	1.5038972483	1.2883580452	-0.1040730386
O	3.1779538495	-4.2262584124	-0.3927393306
C	3.3425127632	-4.8630523487	-1.5941770514
C	2.664193133	-4.2043282688	-2.5701675548
C	2.0326532252	-3.0798460713	-1.9348388235
H	1.4147954524	-2.3274017092	-2.4034272003



H	2.6146730259	-4.4769188006	-3.6152079096
H	3.9570360612	-5.7506800886	-1.5774136183
C	-1.9840618414	-3.8980988638	-0.1039034804
H	0.11402951	-3.7543432904	0.220224619
C	-0.8354820082	-3.9817990575	2.142473898
H	-2.4217154719	-0.5623087707	0.2589260216
C	-2.7081843644	1.4430920494	-0.3768892028
C	-2.5797695898	0.5940609316	2.0369836383
H	-0.8294984636	-5.0762112133	2.1052786621
H	0.0207125463	-3.6560890226	2.7425724599
H	-1.7476230657	-3.6586310702	2.6566413088
H	-1.9639920196	-4.9908754416	-0.1790281634
H	-2.930663739	-3.5999822127	0.3603730569
H	-1.954822153	-3.4861133799	-1.1179582514
H	-3.67442975	0.5629488561	2.0607071519
H	-2.2065512953	-0.2207937977	2.6634448717
H	-2.2489582823	1.5457036986	2.4575013856
H	-3.7692932483	1.199062924	-0.4883246068
H	-2.6606203689	2.474927323	-0.022898406
H	-2.2492268992	1.3805959288	-1.3683101641
H	2.117168409	2.1540161966	-0.3115357086
O	3.3481040431	-0.171844425	-0.3211278706
O	-0.072651054	3.5937584543	-0.5506987738
O	-0.7399865186	3.1803662776	1.5708218421
C	-0.3713493875	4.9998342509	-0.3671126843
H	-0.1268523741	5.471392525	-1.3177660606
H	-1.4294776989	5.1356086615	-0.1340984171
H	0.2415687667	5.4153827982	0.4354476288
H	4.2499273382	1.3849295162	-0.6497345999
O	4.6172051736	2.2913620801	-0.6933807027
C	5.2236032969	2.5456901298	0.5635905851
H	5.6075353416	3.5713667195	0.5520708528
H	4.5165540844	2.4618188147	1.4031459882
H	6.0711373557	1.873151829	0.768639605

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