

Supplementary information (SI)

Self-catalytic mechanism of prebiotic reactions: From formamide to pterins and guanine

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Content

Figure S1

Reaction pathways from formamide to different precursors: formimidinic acid, water, hydrogen cyanide, ammonia, formic acid, carbonoxide, formyl cyanide, 2-iminoacetonitrile, 2-aminoacetonitrile, isocyanic acid, urea, cyanamide, guanidine, 2-aminomalnonitrile, glyoxylic acid, oxalic acid and glyoxal (above). Schematic potential energy profiles along the reaction pathways of the formation of the precursors from pure formamide. ΔH_0 is the zero-point energy corrected relative energy (in kcal mol⁻¹) calculated at SMD/SCS-MP2/cc-pVDZ level (below).

Figure S2

Detailed potential reaction pathways from 2,5,6-triaminopyrimidin-4(3*H*)-one to pterin, xanthopterin, isoxanthopterin and leucopterine. The plausible reaction routes are painted in black, whereas the implausible in red.

Figure S3

Schematic potential energy profiles along the reaction pathways of the formation of pterin, xanthopterin, isoxanthopterin and leucopterine from 2,5,6-triaminopyrimidin-4(3*H*)-one. ΔH_0 is the zero-point energy corrected relative energy (in kcal mol⁻¹) calculated at SMD/SCS-MP2/cc-pVDZ level.

Table S1

SMD/MP2/cc-pVDZ and SMD/SCS-MP2/cc-pVDZ calculated enthalpy at 0 K (H_0) and Gibbs free energy at 298.15K (G_T) for the reactants, products and transition states, and imaginary frequencies ($\nu^\#$) for the transition states of the reactions, shown on Figures 2-6, 8-11 in the main text. Solvent is formamide.

Table S2.

Cartesian coordinates (Å) of the geometries optimized at SMD/MP2/cc-pVDZ level of theory for the reactants, products and transition states, of the reactions, shown on Figures 2-6, 8-11 in the main text.

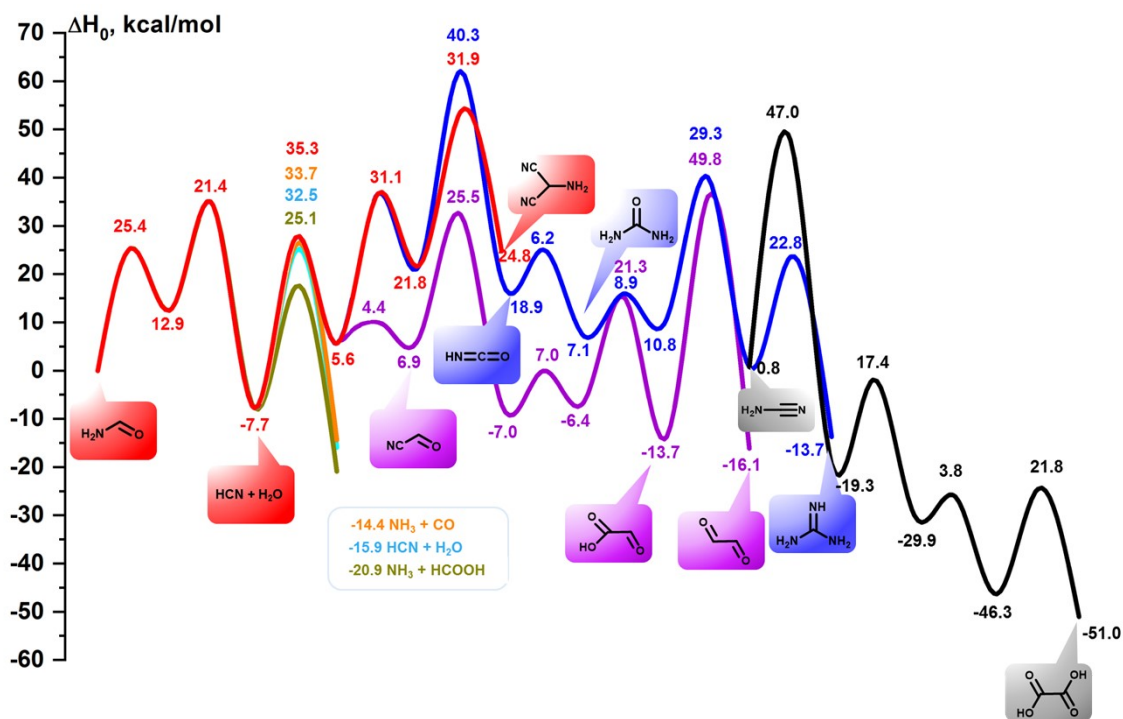
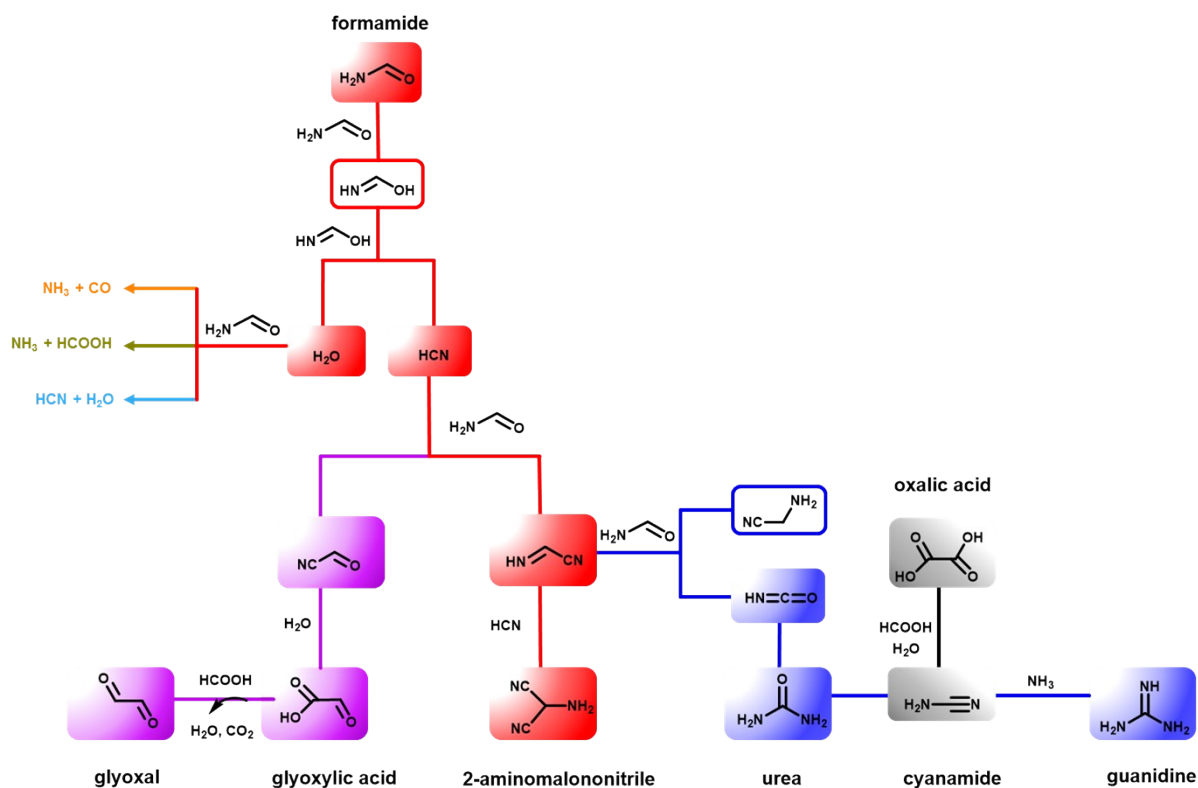


Figure S1

Reaction pathways from formamide to different precursors: formimidic acid, water, hydrogen cyanide, ammonia, formic acid, carbonoxide, formyl cyanide, 2-iminoacetoneitrile, 2-aminoacetoneitrile, isocyanic acid, urea, cyanamide, guanidine, 2-aminomalononitrile, glyoxylic acid, oxalic acid and glyoxal (above). Schematic potential energy profiles along the reaction pathways of the formation of the precursors from pure formamide. ΔH_0 is the zero-point energy corrected relative energy (in kcal mol⁻¹) calculated at SMD/SCS-MP2/cc-pVDZ level (below).

The formation of the precursors: water, hydrogen cyanide, formic acid, ammonia, formyl cyanide, urea and 2-aminomalonnitrile as a result of thermal decomposition of pure formamide was described in previous paper (Ref. 36 in the main text). Endothermic conversion of formamide to formimidic acid is followed by exothermic reaction of formation of hydrogen cyanide and water from formimidic acid. The obtained water reacts with formamide and the exothermic reactions of dehydration, hydrolysis and decarbonylation of formamide produce hydrogen cyanide, water, ammonia, formic acid, and carbon oxide. Interaction between hydrogen cyanide and formamide leads to the formation of unstable hemi-aminal, 2-hydroxylaminoacetonitrile. This hemi-aminal gives formyl cyanide by eliminating ammonia or 2-iminoacetonitrile by eliminating water. 2-Iminoacetonitrile reacts again with formamide producing 2-aminoacetonitrile and isocyanic acid which can interact with ammonia generating urea. 2-Iminoacetonitrile can also react with hydrogen cyanide forming 2-aminomalonnitrile (Fig. S1). Formation of cyanamide, guanidine, glyoxylic acid, glyoxal and oxalic acid is described in present paper.

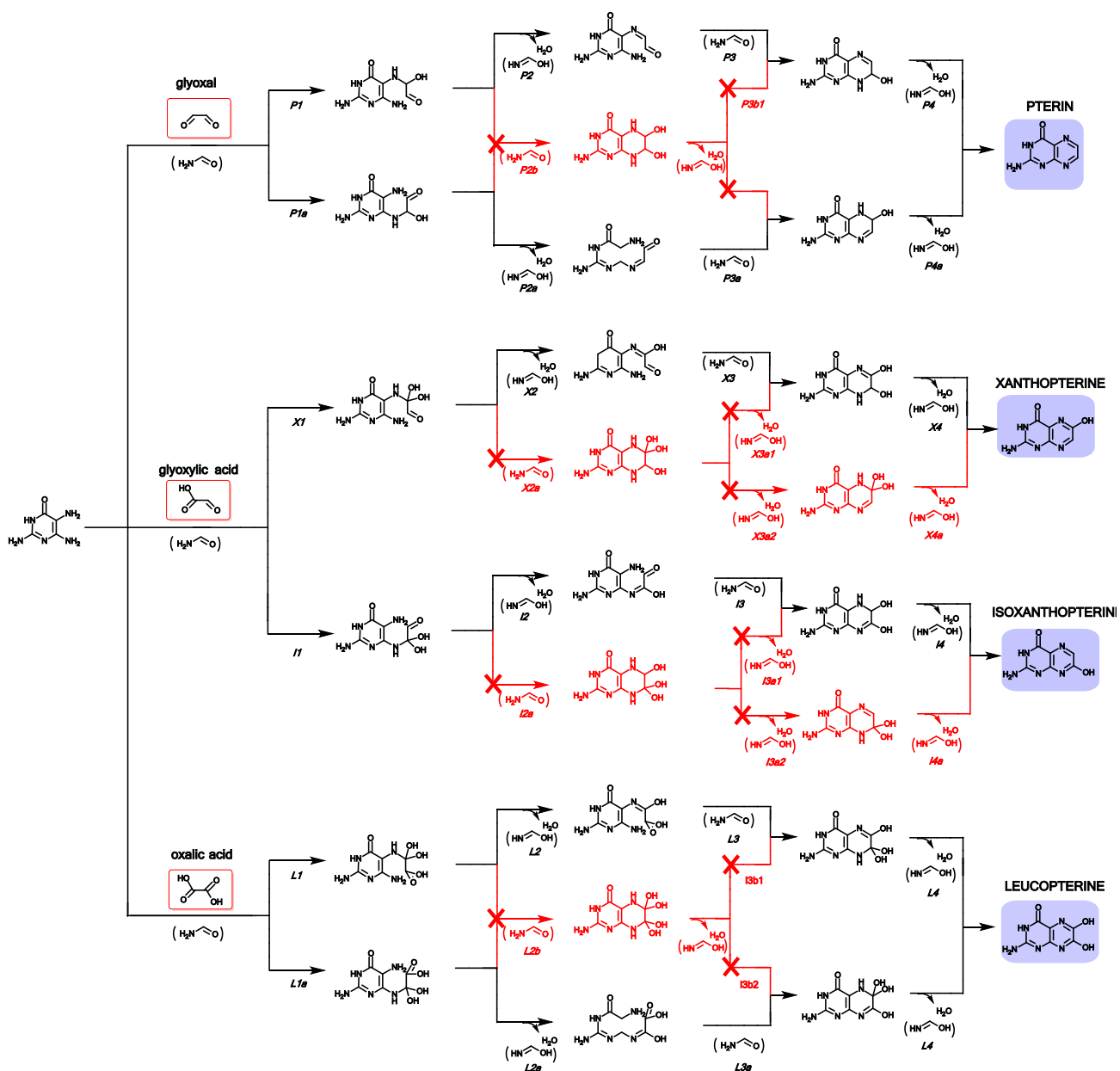


Figure S2

Detailed potential reaction pathways from 2,5,6-triaminopyrimidin-4(3*H*)-one to pterin, xanthopterin, isoxanthopterin and leucopterine. The plausible reaction routes are painted in black and the implausible in red.

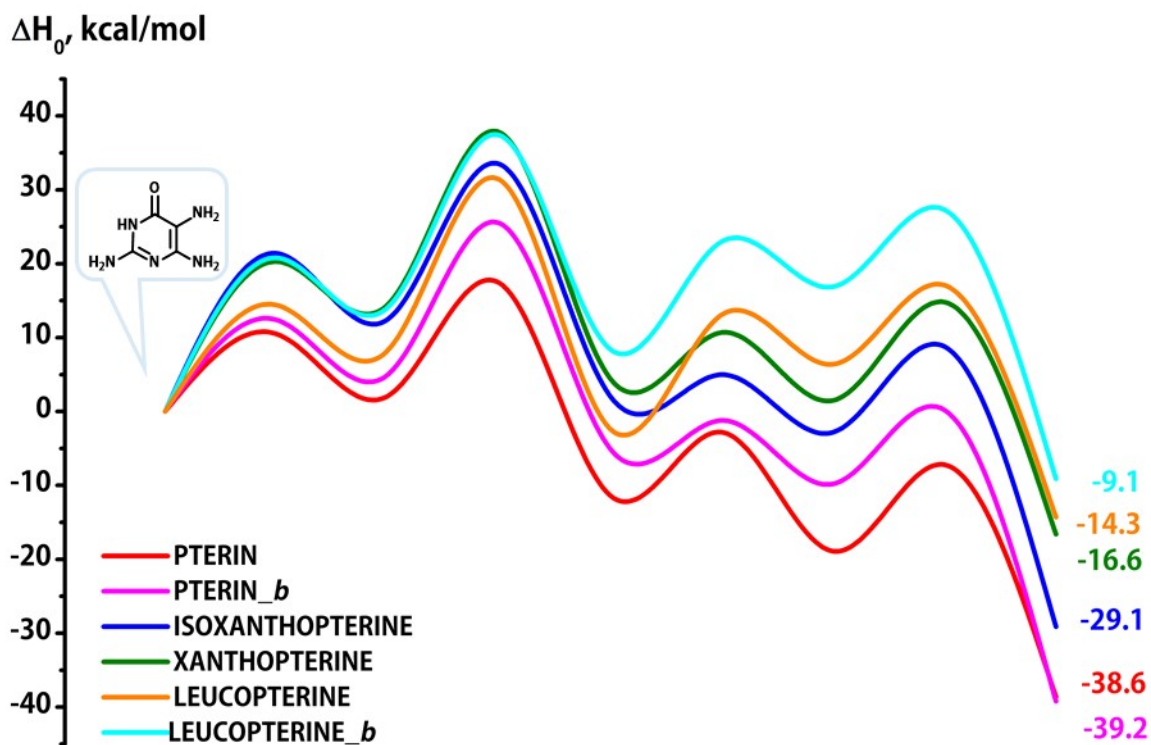


Figure S3

Schematic potential energy profiles along the reaction pathways of the formation of pterin, xanthopterin, isoxanthopterin and leucopterine from 2,5,6-triaminopyrimidin-4(3*H*)-one. ΔH_0 is the zero-point energy corrected relative energy (in kcal mol⁻¹) calculated at SMD/SCS-MP2/cc-pVDZ level.

Table S1.

SMD/MP2/cc-pVDZ and SMD/SCS-MP2/cc-pVDZ calculated enthalpy at 0 K (H_0) and Gibbs free energy at 298.15K (G_T) for the reactants, products and transition states, and imaginary frequencies (ν^\ddagger) for the transition states of the reactions, shown on Figures 2-6, 8-11 in the main text. Solvent is formamide.

Fig. 2a	H_0 [a.u.]	ΔH_0 (kcal/mol)	G_T [a.u.]	ΔG_T (kcal/mol)	ν , cm^{-1}
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-393.989599	0.00	-394.023486	0.00	
Product	-393.983944	3.55	-394.017305	3.88	
Transition state	-393.978432	7.01	-394.010322	8.26	1187.42i
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-393.956552	0.00	-393.990440	0.00	
Product	-393.950579	3.75	-393.983940	4.08	
Transition state	-393.942399	8.88	-393.974290	10.13	1187.42i

Fig. 2b	H_0 [a.u.]	ΔH_0 (kcal/mol)	G_T [a.u.]	ΔG_T (kcal/mol)	ν , cm^{-1}
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-393.956537	0.00	-393.990394	0.00	
Product	-393.971500	-9.39	-394.008003	-11.05	
Transition state	-393.913755	26.85	-393.946554	27.51	895.42i
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-393.923710	0.00	-393.957567	0.00	
Product	-393.939611	-9.98	-393.976113	-11.64	
Transition state	-393.877039	29.29	-393.909838	29.95	895.42i

Fig. 2c	H_0 [a.u.]	ΔH_0 (kcal/mol)	G_T [a.u.]	ΔG_T (kcal/mol)	ν , cm^{-1}
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-374.089367	0.00	-374.125874	0.00	
Product	-374.113371	-15.06	-374.147774	-13.74	
Transition state	-374.055695	21.13	-374.089197	23.02	330.05i
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-374.061101	0.00	-374.097608	0.00	
Product	-374.084275	-14.54	-374.118678	-13.22	
Transition state	-374.024806	22.78	-374.058307	24.66	330.05i

Fig. 3a	H_0 [a.u.]	ΔH_0 (kcal/mol)	G_T [a.u.]	ΔG_T (kcal/mol)	ν , cm^{-1}
<i>SMD/MP2/cc-pVDZ</i>					

Reactant	-451.765180	0.00	-451.803721	0.00	
Product	-451.789053	-14.98	-451.824124	-12.80	
Transition state	-451.729278	22.53	-451.764132	24.84	788.38 <i>i</i>
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-451.728681	0.00	-451.767221	0.00	
Product	-451.750877	-13.93	-451.785948	-11.75	
Transition state	-451.687990	25.53	-451.722844	27.85	788.38 <i>i</i>

Fig. 3 <i>b</i>	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-451.798965	0.00	-451.833420	0.00	
Product	-451.797804	0.73	-451.832262	0.73	
Transition state	-451.790450	5.34	-451.824252	5.75	1109.28 <i>i</i>
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-451.759889	0.00	-451.794344	0.00	
Product	-451.758949	0.59	-451.793407	0.59	
Transition state	-451.748765	6.98	-451.782567	7.39	1109.28 <i>i</i>

Fig. 3 <i>c</i>	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-528.011294	0.00	-528.050093	0.00	
Product	-528.022397	-6.97	-528.061932	-7.43	
Transition state	-527.981801	18.51	-528.017355	20.54	872.74 <i>i</i>
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-527.968327	0.00	-528.007126	0.00	
Product	-527.979956	-7.30	-528.019492	-7.76	
Transition state	-527.934299	21.35	-527.969853	23.39	872.74 <i>i</i>

Fig. 3 <i>d</i>	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-830.297440	0.00	-830.346864	0.00	
Product	-830.299945	-1.57	-830.352504	-3.54	
Transition state	-830.227111	44.13	-830.273289	46.17	509.69 <i>i</i>
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-830.224924	0.00	-830.274347	0.00	
Product	-830.228699	-2.37	-830.281257	-4.34	
Transition state	-830.145555	49.80	-830.191732	51.84	509.69 <i>i</i>

Fig. 4 <i>a</i>	H ₀ [a.u.]	ΔH ₀	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
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		(kcal/mol)			
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-506.971054	0.00	-507.010930	0.00	
Product	-507.005912	-21.87	-507.042760	-19.97	
Transition state	-506.900298	44.40	-506.936774	46.53	301.14 <i>i</i>
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-506.928549	0.00	-506.968426	0.00	
Product	-506.960582	-20.10	-506.997430	-18.20	
Transition state	-506.853600	47.03	-506.890076	49.16	301.14 <i>i</i>

Fig. 4b	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-583.215676	0.00	-583.254777	0.00	
Product	-583.233153	-10.97	-583.270626	-9.95	
Transition state	-583.191452	15.20	-583.227907	16.86	771.65 <i>i</i>
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-583.164344	0.00	-583.203445	0.00	
Product	-583.181182	-10.57	-583.218655	-9.54	
Transition state	-583.136070	17.74	-583.172525	19.40	771.65 <i>i</i>

Fig. 4c	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-583.226734	0.00	-583.264396	0.00	
Product	-583.250326	-14.80	-583.290787	-16.56	
Transition state	-583.223372	2.11	-583.259576	3.03	698.5 <i>i</i>
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-583.173602	0.00	-583.211264	0.00	
Product	-583.199743	-16.40	-583.240204	-18.16	
Transition state	-583.167520	3.82	-583.203723	4.73	698.5 <i>i</i>

Fig. 4d	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-603.095584	0.00	-603.135634	0.00	
Product	-603.101168	-3.50	-603.141920	-3.94	
Transition state	-603.064587	19.45	-603.100906	21.79	825.42 <i>i</i>
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-603.040620	0.00	-603.080671	0.00	
Product	-603.048145	-4.72	-603.088897	-5.16	
Transition state	-603.005908	21.78	-603.042227	24.12	825.42 <i>i</i>

Fig. 5a	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-525.094767	0.00	-525.134724	0.00	
Product	-525.117683	-14.38	-525.156013	-13.36	
Transition state	-525.058815	22.56	-525.096367	24.07	609.64i
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-525.049791	0.00	-525.089749	0.00	
Product	-525.071357	-13.53	-525.109688	-12.51	
Transition state	-525.009331	25.39	-525.046883	26.90	609.64i

Fig. 5b	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-525.120943	0.00	-525.159139	0.00	
Product	-525.119017	1.21	-525.156941	1.38	
Transition state	-525.112661	5.20	-525.150052	5.70	1022.49i
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-525.074301	0.00	-525.112497	0.00	
Product	-525.072380	1.21	-525.110304	1.38	
Transition state	-525.063259	6.93	-525.100650	7.43	1022.49i

Fig. 5c	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-729.852204	0.00	-729.897955	0.00	
Product	-729.864004	-7.40	-729.907471	-5.97	
Transition state	-729.804534	29.91	-729.847855	31.44	834.44i
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-729.787183	0.00	-729.832933	0.00	
Product	-729.796823	-6.05	-729.840290	-4.62	
Transition state	-729.733924	33.42	-729.777245	34.94	834.44i

Fig. 5d	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-729.843957	0.00	-729.886867	0.00	
Product	-729.855798	-7.43	-729.900109	-8.31	
Transition state	-729.814915	18.22	-729.856542	19.03	1066.15i
<i>SMD/SCS-MP2/cc-pVDZ</i>					

Reactant	-729.775359	0.00	-729.818270	0.00	
Product	-729.786486	-6.98	-729.830797	-7.86	
Transition state	-729.742101	20.87	-729.783728	21.68	1066.15i

Fig. 5e	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-729.832917	0.00	-729.876399	0.00	
Product	-729.815379	11.01	-729.857152	12.08	
Transition state	-729.781231	32.43	-729.821243	34.61	1096.62i
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-729.763933	0.00	-729.807414	0.00	
Product	-729.742657	13.35	-729.784430	14.42	
Transition state	-729.705664	36.56	-729.745676	38.74	1096.62i

Fig. 5f	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-673.511391	0.00	-673.551638	0.00	
Product	-673.535299	-15.00	-673.575348	-14.88	
Transition state	-673.512663	-0.80	-673.551451	0.12	1041.69i
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-673.441630	0.00	-673.481876	0.00	
Product	-673.465496	-14.98	-673.505545	-14.85	
Transition state	-673.440876	0.47	-673.479664	1.39	1041.69i

G1	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-842.919640	0.00	-842.966589	0.00	
Product	-842.918951	0.43	-842.963487	1.95	
Transition state	-842.892004	17.34	-842.936374	18.96	195.55i
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-842.834876	0.00	-842.881826	0.00	
Product	-842.833122	1.10	-842.877659	2.61	
Transition state	-842.804279	19.20	-842.848649	20.82	195.55i

G2	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-842.923004	0.00	-842.966639	0.00	
Product	-842.922535	0.29	-842.967437	-0.50	

Transition state	-842.893906	18.26	-842.936676	18.80	637.29i
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-842.836663	0.00	-842.880299	0.00	
Product	-842.834265	1.50	-842.879167	0.71	
Transition state	-842.804216	20.36	-842.846985	20.90	637.29i

<i>G3</i>	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-766.651600	0.00	-766.693475	0.00	
Product	-766.711711	-37.72	-766.756010	-39.24	
Transition state	-766.641556	6.30	-766.681354	7.61	1019.28i
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-766.567463	0.00	-766.609339	0.00	
Product	-766.628246	-38.14	-766.672545	-39.66	
Transition state	-766.554051	8.42	-766.593849	9.72	1019.28i

<i>P1</i>	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-900.729769	0.00	-900.776965	0.00	
Product	-900.728214	0.98	-900.772690	2.68	
Transition state	-900.717571	7.65	-900.761025	10.00	906.38i
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-900.638878	0.00	-900.686074	0.00	
Product	-900.635563	2.08	-900.680038	3.79	
Transition state	-900.622177	10.48	-900.665631	12.83	906.38i

<i>P2</i>	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-900.722452	0.00	-900.769137	0.00	
Product	-900.743956	-13.49	-900.791713	-14.17	
Transition state	-900.701791	12.97	-900.746583	14.15	845.16i
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-900.630051	0.00	-900.676737	0.00	
Product	-900.651619	-13.53	-900.699376	-14.21	
Transition state	-900.605611	15.34	-900.650402	16.53	845.16i

<i>P3</i>	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					

Reactant	-824.510534	0.00	-824.555430	0.00	
Product	-824.524613	-8.84	-824.565598	-6.38	
Transition state	-824.500452	6.33	-824.541047	9.03	926.92i
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-824.421899	0.00	-824.466795	0.00	
Product	-824.433831	-7.49	-824.474816	-5.03	
Transition state	-824.408254	8.56	-824.448850	11.26	926.92i

<i>P4</i>	H_0 [a.u.]	ΔH_0 (kcal/mol)	G_T [a.u.]	ΔG_T (kcal/mol)	ν , cm^{-1}
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-824.526828	0.00	-824.569245	0.00	
Product	-824.561204	-21.57	-824.606504	-23.38	
Transition state	-824.512843	8.78	-824.554442	9.29	798.60i
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-824.437293	0.00	-824.479711	0.00	
Product	-824.468740	-19.73	-824.514040	-21.54	
Transition state	-824.418645	11.70	-824.460244	12.22	798.60i
<i>Pl1a</i>	H_0 [a.u.]	ΔH_0 (kcal/mol)	G_T [a.u.]	ΔG_T (kcal/mol)	ν , cm^{-1}
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-900.728704	0.00	-900.775887	0.00	
Product	-900.723197	3.46	-900.768415	4.69	
Transition state	-900.714463	8.94	-900.758269	11.06	847.28i
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-900.638478	0.00	-900.685660	0.00	
Product	-900.630559	4.97	-900.675777	6.20	
Transition state	-900.618666	12.43	-900.662472	14.55	847.28i

<i>P2a</i>	H_0 [a.u.]	ΔH_0 (kcal/mol)	G_T [a.u.]	ΔG_T (kcal/mol)	ν , cm^{-1}
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-900.717495	0.00	-900.763509	0.00	
Product	-900.732887	-9.66	-900.780784	-10.84	
Transition state	-900.689472	17.58	-900.735343	17.67	758.46i
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-900.625359	0.00	-900.671373	0.00	
Product	-900.641407	-10.07	-900.689304	-11.25	
Transition state	-900.592707	20.49	-900.638577	20.58	758.46i

<i>P3a</i>	H_0 [a.u.]	ΔH_0	G_T [a.u.]	ΔG_T (kcal/mol)	ν , cm^{-1}
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		(kcal/mol)			
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-824.499785	0.00	-824.543683	0.00	
Product	-824.511112	-7.11	-824.553189	-5.96	
Transition state	-824.499534	0.16	-824.540012	2.30	894.97i
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-824.414065	0.00	-824.457964	0.00	
Product	-824.421482	-4.65	-824.463559	-3.51	
Transition state	-824.407882	3.88	-824.448360	6.03	894.97i

<i>P4a</i>	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-824.512867	0.00	-824.555212	0.00	
Product	-824.561785	-30.70	-824.606777	-32.36	
Transition state	-824.503186	6.07	-824.543902	7.10	399.71i
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-824.422368	0.00	-824.464713	0.00	
Product	-824.469170	-29.37	-824.514162	-31.03	
Transition state	-824.406472	9.98	-824.447187	11.00	399.71i

<i>X1</i>	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-975.816932	0.00	-975.867430	0.00	
Product	-975.797972	11.90	-975.842882	15.40	
Transition state	-975.791615	15.89	-975.835302	20.16	698.25i
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-975.717067	0.00	-975.767565	0.00	
Product	-975.693930	14.52	-975.738840	18.03	
Transition state	-975.684757	20.27	-975.728444	24.55	698.25i

<i>X2</i>	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-975.791788	0.00	-975.837043	0.00	
Product	-975.807931	-10.13	-975.855372	-11.50	
Transition state	-975.759054	20.54	-975.803690	20.93	574.27i
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-975.688794	0.00	-975.734049	0.00	
Product	-975.704920	-10.12	-975.752360	-11.49	
Transition state	-975.651720	23.26	-975.696357	23.65	574.27i

<i>X3</i>	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-899.570475	0.00	-899.616182	0.00	
Product	-899.578438	-5.00	-899.621276	-3.20	
Transition state	-899.566570	2.45	-899.608373	4.90	931.29 <i>i</i>
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-899.474047	0.00	-899.519754	0.00	
Product	-899.478731	-2.94	-899.521569	-1.14	
Transition state	-899.464004	6.30	-899.505807	8.75	931.29 <i>i</i>

<i>X4</i>	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-899.584459	0.00	-899.627919	0.00	
Product	-899.616358	-20.02	-899.662319	-21.59	
Transition state	-899.567679	10.53	-899.610269	11.08	796.93 <i>i</i>
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-899.485181	0.00	-899.528641	0.00	
Product	-899.513988	-18.08	-899.559949	-19.65	
Transition state	-899.464040	13.27	-899.506630	13.81	796.93 <i>i</i>

<i>I1</i>	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-975.805294	0.00	-975.855214	0.00	
Product	-975.789163	10.12	-975.835247	12.53	
Transition state	-975.777247	17.60	-975.822150	20.75	342.29 <i>i</i>
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-975.705691	0.00	-975.755611	0.00	
Product	-975.685705	12.54	-975.731789	14.95	
Transition state	-975.671616	21.38	-975.716519	24.53	342.29 <i>i</i>

<i>I2</i>	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-975.782120	0.00	-975.827697	0.00	
Product	-975.798223	-10.10	-975.847599	-12.49	
Transition state	-975.753086	18.22	-975.798885	18.08	490.26 <i>i</i>
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-975.679111	0.00	-975.724688	0.00	

Product	-975.695878	-10.52	-975.745253	-12.91	
Transition state	-975.645574	21.04	-975.691372	20.91	490.26i

<i>I3</i>	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-899.567067	0.00	-899.612765	0.00	
Product	-899.578155	-6.96	-899.621383	-5.41	
Transition state	-899.568404	-0.84	-899.610150	1.64	909.62i
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-899.470809	0.00	-899.516507	0.00	
Product	-899.478378	-4.75	-899.521606	-3.20	
Transition state	-899.466036	3.00	-899.507782	5.48	909.62i

<i>I4</i>	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-899.576505	0.00	-899.619838	0.00	
Product	-899.620466	-27.59	-899.667343	-29.81	
Transition state	-899.563515	8.15	-899.605454	9.03	433.30i
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-899.476416	0.00	-899.519748	0.00	
Product	-899.518332	-26.30	-899.565209	-28.53	
Transition state	-899.457873	11.64	-899.499813	12.51	433.30i

<i>L1</i>	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-1050.886489	0.00	-1050.936042	0.00	
Product	-1050.875956	6.61	-1050.921638	9.04	
Transition state	-1050.868940	11.01	-1050.914721	13.38	771.75i
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-1050.774435	0.00	-1050.823989	0.00	
Product	-1050.761218	8.29	-1050.806900	10.72	
Transition state	-1050.751473	14.41	-1050.797253	16.78	771.75i

<i>L2</i>	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	v, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-1050.866652	0.00	-1050.914384	0.00	
Product	-1050.884141	-10.97	-1050.932973	-11.67	
Transition state	-1050.835106	19.80	-1050.881601	20.57	792.40i

<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-1050.753780	0.00	-1050.801511	0.00	
Product	-1050.770813	-10.69	-1050.819645	-11.38	
Transition state	-1050.716973	23.10	-1050.763467	23.87	792.40i

<i>L3</i>	H_0 [a.u.]	ΔH_0 (kcal/mol)	G_T [a.u.]	ΔG_T (kcal/mol)	ν , cm^{-1}
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-974.648195	0.00	-974.694737	0.00	
Product	-974.636810	7.14	-974.681318	8.42	
Transition state	-974.628770	12.19	-974.672226	14.13	842.43i
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-974.541186	0.00	-974.587729	0.00	
Product	-974.527231	8.76	-974.571739	10.03	
Transition state	-974.516530	15.47	-974.559986	17.41	842.43i

<i>L4</i>	H_0 [a.u.]	ΔH_0 (kcal/mol)	G_T [a.u.]	ΔG_T (kcal/mol)	ν , cm^{-1}
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-974.638223	0.00	-974.682451	0.00	
Product	-974.673895	-22.38	-974.721569	-24.55	
Transition state	-974.625611	7.91	-974.669058	8.40	755.76i
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-974.529073	0.00	-974.573300	0.00	
Product	-974.562111	-20.73	-974.609786	-22.89	
Transition state	-974.511983	10.72	-974.555430	11.21	755.76i

<i>L1a</i>	H_0 [a.u.]	ΔH_0 (kcal/mol)	G_T [a.u.]	ΔG_T (kcal/mol)	ν , cm^{-1}
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-1050.888171	0.00	-1050.937166	0.00	
Product	-1050.868023	12.64	-1050.916338	13.07	
Transition state	-1050.860030	17.66	-1050.905993	19.56	597.46i
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-1050.776192	0.00	-1050.825187	0.00	
Product	-1050.753741	14.09	-1050.802056	14.52	
Transition state	-1050.743080	20.78	-1050.789043	22.68	597.46i

<i>L2a</i>	H_0 [a.u.]	ΔH_0 (kcal/mol)	G_T [a.u.]	ΔG_T (kcal/mol)	ν , cm^{-1}
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-1050.860710	0.00	-1050.908072	0.00	

Product	-1050.868774	-5.06	-1050.920374	-7.72	
Transition state	-1050.827965	20.55	-1050.874374	21.15	775.11 <i>i</i>
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-1050.747273	0.00	-1050.794635	0.00	
Product	-1050.756185	-5.59	-1050.807785	-8.25	
Transition state	-1050.710095	23.33	-1050.756504	23.93	775.11 <i>i</i>

<i>L3a</i>	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	ν, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-974.648076	0.00	-974.694683	0.00	
Product	-974.636629	7.18	-974.680135	9.13	
Transition state	-974.629203	11.84	-974.672392	13.99	760.74 <i>i</i>
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-974.540472	0.00	-974.587079	0.00	
Product	-974.527008	8.45	-974.570514	10.39	
Transition state	-974.517196	14.61	-974.560385	16.75	760.74 <i>i</i>

<i>L4a</i>	H ₀ [a.u.]	ΔH ₀ (kcal/mol)	G _T [a.u.]	ΔG _T (kcal/mol)	ν, cm ⁻¹
<i>SMD/MP2/cc-pVDZ</i>					
Reactant	-974.632183	0.00	-974.677086	0.00	
Product	-974.675794	-27.37	-974.723255	-28.97	
Transition state	-974.621117	6.94	-974.664795	7.71	406.53 <i>i</i>
<i>SMD/SCS-MP2/cc-pVDZ</i>					
Reactant	-974.522321	0.00	-974.567224	0.00	
Product	-974.563740	-25.99	-974.611202	-27.60	
Transition state	-974.505688	10.44	-974.549365	11.21	406.53 <i>i</i>

Table S2.

Cartesian coordinates (Å) of the geometries optimized at SMD/MP2/cc-pVDZ level of theory for the reactants, products and transition states, of the reactions, shown on Figures 2-6, 8-11 in the main text.

Reaction	Cartesian coordinates			
Fig. 2a				
Reactant	O	-0.998829687000	-0.216217377800	-0.253381965500
	C	-1.410561807800	-1.198859517700	0.405866984700
	N	-0.559906442800	-2.238994537100	0.708548365000
	N	-2.689775966700	-1.304695113600	0.842943438200
	H	0.421693442800	-1.972241070200	0.671902070000
	H	-0.788993870800	-2.793278125800	1.531574044500
	H	-3.038047839500	-2.214356320000	1.135895032100
	H	-3.360498925100	-0.655961258500	0.403027499200
	O	-2.382524631000	1.691199235200	-1.430306522700
	C	-3.704904529100	1.643970165700	-1.245426431700
	N	-4.291010867600	0.741225233800	-0.538934952000
	H	-5.301963953300	0.921772322500	-0.555305491100
	H	-4.216562642900	2.466579977500	-1.770021324500
	H	-1.949053292300	0.928453085900	-0.939203763300
Product	O	-0.846591774800	-0.278719588600	-0.342666561800
	C	-1.424087713900	-1.255801915200	0.375598448100
	N	-0.503590903000	-2.218779247600	0.737439608000
	N	-2.698580517600	-1.271963504300	0.610018482100
	H	0.458139306200	-1.885745799700	0.768904745800
	H	-0.749400782300	-2.763528737700	1.561936689200
	H	-2.945647105200	-2.104106911700	1.156327326700
	H	-3.895100269900	-0.037202091600	-0.041118080900
	O	-2.447811881500	1.584813694400	-1.358701288600
	C	-3.687025461700	1.633570180000	-1.200507003500
	N	-4.397222096000	0.750680460200	-0.499328325700
	H	-5.404170922400	0.853507668300	-0.407553915000
	H	-4.275709366100	2.452847826900	-1.661199603400
	H	-1.542818878800	0.363950716500	-0.664282442000
Transition state	O	-0.926551500300	-0.188323245400	-0.374875483300
	C	-1.478928646900	-1.153162535000	0.320268526700
	N	-0.604144502100	-2.120904900100	0.722178838600
	N	-2.769755503500	-1.203665818200	0.555706410800
	H	0.370680676000	-1.829822464600	0.743419384100
	H	-0.879804460400	-2.705559810600	1.508325576500
	H	-3.087781120900	-2.008845362300	1.095355622500
	H	-3.541491659800	-0.347880179100	0.113776035200
	O	-2.374494901300	1.541024070500	-1.367480825100
	C	-3.635271995200	1.533625422700	-1.149506343100

	N	-4.259885432000	0.633397949000	-0.424326745800
	H	-5.268669028300	0.787994649900	-0.367810300700
	H	-4.224003762800	2.351889608600	-1.614128398500
	H	-1.631148657400	0.520159787600	-0.762955413900
Fig. 2b				
Reactant	O	-1.773368085700	-0.198668354000	0.397720287600
	C	-1.734576009900	-1.530627950900	0.700415729900
	N	-0.508305984900	-2.067441103100	0.346671137000
	N	-2.686105175400	-2.250646428100	1.187299844200
	H	0.268518156600	-1.417730206600	0.466992503100
	H	-0.327904368800	-2.954771671800	0.812960328000
	H	-3.522655771200	-1.663213675100	1.285507621000
	O	-3.422257125000	0.379219063600	-1.899548267100
	C	-4.425963464100	0.660181274800	-1.052986345100
	N	-4.287959792700	0.627209391400	0.225383621700
	H	-5.166708111000	0.874371203800	0.692299275900
	H	-5.349661130200	0.914200556600	-1.592600295400
	H	-2.627312582000	0.161593650800	-1.365460484800
	H	-2.698436957700	0.140091146600	0.605253844100
Product	O	-0.728444442000	0.066257188000	-0.734543269200
	C	-2.054714982500	-2.359830926300	0.998569928600
	N	-0.727790722700	-2.291975334400	0.792756991100
	N	-3.235377984300	-2.439922094900	1.104546336600
	H	-0.524818045500	-1.442000142500	0.229968118700
	H	-0.193106059200	-2.320570136700	1.664200142100
	H	-4.448184777700	-1.010772776100	0.382440923300
	O	-3.352877326400	0.949607179600	-0.932704802800
	C	-4.552901960300	0.766692370500	-0.666898994000
	N	-5.051033976200	-0.269942204100	0.020196078700
	H	-6.057728196500	-0.345497221600	0.154747887400
	H	-5.325891897200	1.489433573800	-0.995631438800
	H	-1.682627315000	0.279294493100	-0.780017362300
	H	-0.349802427300	0.854331798700	-0.312382035400
Transition state	O	-1.423665502100	-0.077047287600	-0.089043733000
	C	-1.801831898900	-1.517494596200	0.662158865300
	N	-0.646464710100	-2.239818702900	0.380876231500
	N	-2.900502622500	-1.711841815900	1.170598697900
	H	0.198711570500	-1.671176793400	0.432961497700
	H	-0.572445186500	-3.056396606800	0.990435441200
	H	-3.889669272200	-0.771942029900	0.705174232300
	O	-3.285020124400	0.580375421600	-1.518935745000
	C	-4.433505056900	0.531117297700	-0.928926852300
	N	-4.670478550300	-0.086048106000	0.196102612900
	H	-5.633610292100	-0.034379011800	0.536244056600
	H	-5.251159039500	1.061068612700	-1.440322896000
	H	-2.448509638100	0.225967570500	-0.871781524600
	H	-1.515620806900	0.564526888800	0.640878816600

Fig. 2c				
Reactant	C	-2.049372567300	-2.111406247500	0.461488931500
	N	-0.796773154400	-2.219048623300	0.926622248500
	N	-3.124687042400	-1.962102080500	-0.023081256600
	H	-0.527843944900	-1.283841030200	1.354225056000
	H	-0.700256724800	-2.992040915300	1.591983533500
	O	-5.203609322200	-0.188380530900	0.658165064300
	C	-4.780285007900	1.010804806800	1.092233091000
	N	-3.541457434100	1.332413034300	1.206117663600
	H	-3.505556163500	2.299364049600	1.556183740600
	H	-5.635937419000	1.661766331700	1.330804922600
	H	-4.419386347800	-0.748808202300	0.435804419600
	N	-0.569576943800	0.388416765700	1.896123468900
	H	0.054816394300	1.066608779500	1.448233341800
	H	-0.476948879800	0.565187766000	2.901304549200
	H	-1.523487441600	0.693303384200	1.653901162600
Product	C	-1.605471956300	-1.377353453200	1.069841179100
	N	-0.354296618400	-1.788456998500	0.607985070800
	N	-2.685700667200	-1.904695638000	0.589580561800
	H	0.368738354900	-1.817644536900	1.325750183600
	H	-0.419878134000	-2.694545842900	0.144428220800
	O	-4.510014221500	0.266596769100	2.166201405000
	C	-4.553688848600	1.238948149700	1.395993541400
	N	-3.487224111500	1.826362116500	0.827554207700
	H	-3.604089290300	2.595557820700	0.174385131700
	H	-5.518925831700	1.713871817500	1.117624921400
	H	-3.481147962900	-1.403077668500	1.005798902200
	N	-1.555093270900	-0.281428879500	1.942359685500
	H	-0.740523810200	-0.250705370400	2.556418329900
	H	-2.425512408900	-0.189810242700	2.470914292500
	H	-2.556749852600	1.442398533100	0.999780084500
Transition state	C	-1.742660146200	-1.528352540400	1.020370561300
	N	-0.484372536600	-2.117788180100	0.856921533800
	N	-2.909495290600	-1.772376002800	0.769853059800
	H	0.138496525500	-1.953744401500	1.649827644600
	H	-0.589972841200	-3.124560171200	0.718657771000
	O	-5.047167404700	-0.320473854100	0.734493920200
	C	-4.879211152300	0.970939206200	0.975453715100
	N	-3.744608241800	1.521936616600	1.256674337000
	H	-3.896065121000	2.528040771800	1.400166548400
	H	-5.828694954200	1.530045878700	0.906647055000
	H	-4.138152861200	-0.840588856500	0.782165969500
	N	-1.280041677600	0.050235304100	1.666942579300
	H	-0.472894429000	0.475424385200	1.196380638900
	H	-1.079375362500	0.031570899900	2.674423611600
	H	-2.124751929400	0.651789308100	1.518202664400
Fig. 3a				

Reactant	O	-2.901813867000	-0.170717633000	1.217792177300
	C	-1.740478661900	-0.412614304000	1.488788327100
	C	-1.034302288200	-1.545809792800	0.830772042700
	N	-0.501271797800	-2.439581847700	0.267817469200
	H	-1.115468983400	0.146579067500	2.205981542700
	O	2.007632975300	-3.413973343300	-0.757453254200
	C	3.021216592300	-2.635430881000	-0.343727445600
	H	3.961943269100	-2.934356148200	-0.828982628400
	N	2.883962830300	-1.680295602200	0.503275832500
	H	3.801778921300	-1.240264602100	0.651068074000
	H	1.176225409600	-3.097881112100	-0.338864400000
	O	1.108886503000	-0.686967995600	2.541704677800
	H	1.646172698100	-1.022951690500	1.790458709600
	H	0.991339154300	-1.484135445000	3.079468935200
Product	O	-2.397346893100	0.067204022900	1.088634421600
	C	-1.394135848600	-0.255001391300	1.703352900000
	C	-0.500535183900	-1.394019627100	1.271876674200
	N	-0.801131240600	-2.083395841000	0.226962476400
	H	-1.066576836400	0.269527232000	2.628270995000
	O	2.137050029900	-3.211863581300	0.924183898800
	C	3.000483867400	-2.570633824700	0.289369770100
	H	3.656370805000	-3.079932684900	-0.441993425100
	N	3.232485288400	-1.260408752200	0.418890918900
	H	3.912755982600	-0.789393211100	-0.171366040700
	H	-0.086449249800	-2.815326233700	0.092696491200
	O	0.546976702500	-1.521139642000	2.115861220800
	H	2.680238941500	-0.691243672300	1.058842404400
	H	1.144726008900	-2.248540202400	1.759410777300
Transition state	O	-2.711232846600	-0.718618912800	1.586082593400
	C	-1.531724464100	-0.415669671400	1.636200324000
	C	-0.474754600700	-1.331305022900	1.078699689800
	N	-0.368823470500	-2.246624920400	0.298604711600
	H	-1.161485294100	0.528005306000	2.082067956700
	O	1.835061616000	-3.274272610100	-0.538551744200
	C	2.890564930700	-2.625938085000	-0.141621341600
	H	3.832115984500	-3.000388772300	-0.564914265200
	N	2.889852711900	-1.621399620000	0.683377065800
	H	3.816878109900	-1.232826589400	0.873834901600
	H	0.947685598500	-2.860753669400	-0.158604479800
	O	0.954197561300	-0.643634636300	1.948434287300
	H	1.962184192600	-1.169072507700	1.257307405400
	H	0.942416273600	-1.160434785400	2.776175435200
Fig. 3b				
	O	-2.645349633000	-0.542336523000	0.958948625000
	C	-1.571991351000	-0.418548867000	1.528492701000
	C	-0.432679753000	-1.379849256000	1.267123974000
	N	-0.532937343000	-2.357576580000	0.431681515000
	H	-1.369108516000	0.391225200000	2.261551742000

	O	2.686093430000	-2.688928366000	1.697106597000
	C	2.762092146000	-3.683859429000	0.944373185000
	H	3.681608374000	-4.301680691000	0.933865193000
	N	1.803140422000	-4.089768094000	0.112422915000
	H	1.935173363000	-4.928330928000	-0.442701886000
	H	-1.484933332000	-2.317343871000	0.037591887000
	O	0.647720995000	-1.085770350000	1.987022709000
	H	1.385476040000	-1.752793777000	1.804500344000
	H	0.907530781000	-3.576432480000	0.091332961000
	O	-2.653825437000	-0.560845908000	0.931950218000
	C	-1.586707751000	-0.424563476000	1.509411980000
	C	-0.409158094000	-1.367869615000	1.289085904000
	N	-0.625901763000	-2.341300741000	0.407582247000
	H	-1.386974642000	0.388743038000	2.240118600000
	O	2.839119561000	-2.693515287000	1.763763588000
	C	2.771127863000	-3.715417666000	0.905109860000
	H	3.707018130000	-4.295558928000	0.899665432000
	N	1.737686061000	-3.979751375000	0.184597883000
	H	1.934506125000	-4.813235017000	-0.381701378000
	H	-1.532660949000	-2.379182966000	-0.052524650000
	O	0.642445094000	-1.165433389000	1.933713181000
	H	1.980045302000	-2.183962638000	1.755125194000
	H	0.132132425000	-3.021302196000	0.207312129000
	O	-2.586139933500	-0.621491985200	0.924353756300
	C	-1.520037342800	-0.494539280700	1.508527418000
	C	-0.335055233100	-1.421737755900	1.273296303500
	N	-0.473105553300	-2.401152129600	0.408395585900
	H	-1.337049182300	0.308385682200	2.257241247300
	O	2.697685614900	-2.628922022600	1.751537266400
	C	2.621833257500	-3.629064305800	0.923005474300
	H	3.521587684500	-4.260595355600	0.894267764500
	N	1.592857187000	-3.903550636900	0.177422355200
	H	1.693668776500	-4.732302215800	-0.409378352700
	H	-1.410409314600	-2.403094012200	-0.006545358600
	O	0.714249232400	-1.152415354400	1.953793944200
	H	1.815624172000	-2.032590510700	1.781833782000
	H	0.572258279900	-3.234327909900	0.220341987900
Fig. 3c				
	O	-2.681139037400	-1.642425115400	1.023021963300
	C	-1.814280771300	-0.963537678900	1.550786223200
	C	-0.385353458300	-0.914930277300	1.014146250400
	N	-0.144360699300	-1.833568091600	0.026565019000
	H	-2.001781179600	-0.277830426400	2.401198575700
	O	0.646992800300	-4.598402527000	0.445263831000
	C	0.816351349700	-5.244535055300	1.609170056900
	H	1.161587538300	-6.274922187900	1.440180303400
	N	0.594909575600	-4.700895292600	2.750239218600
	H	0.793223197800	-5.380896868600	3.492865659000

	H	-0.972860101700	-2.176950525200	-0.458752484200
	O	0.435064110300	-0.120991688000	1.468033837000
	H	0.359159997400	-3.676774175100	0.634125152100
	H	0.677251117100	-1.670905166500	-0.555447903000
	O	-0.596318164200	-2.239136792700	3.501954946200
	H	0.169655740500	-1.660518335200	3.633092181300
	H	-0.177619187200	-3.087348822300	3.225405291200
Product	O	-2.056158316000	-2.481362034300	2.205054067900
	C	-1.621579111500	-1.397297838200	1.840215855900
	C	-0.238006991600	-0.884060355000	2.206554914800
	N	-0.388952723700	-1.850468908000	-0.275556178300
	H	-2.237198850600	-0.639143682200	1.316510290200
	O	0.994769499600	-4.508399318800	0.570016663500
	C	0.731271635900	-5.192953067700	1.567327141300
	H	1.249866314400	-6.158043273100	1.759058235600
	N	-0.185477154900	-4.895024256200	2.503920019500
	H	-0.299324291800	-5.499799696700	3.311767370400
	H	-1.044022445200	-2.075112773100	-1.031000255100
	O	0.085318765000	0.283577161400	2.076523155700
	H	0.082654326000	-2.735089233700	-0.044272685300
	H	0.327748931200	-1.259548407100	-0.708895622900
	O	0.531433545400	-1.854628403600	2.724178713000
	H	1.412138679600	-1.478860589600	2.931191624100
	H	-0.681705003900	-4.003346345000	2.478872025500
Transition state	O	-2.522784689400	-0.516007703800	0.940099865100
	C	-1.505664014900	-0.508313914200	1.618072195900
	C	-0.321241413200	-1.437340267500	1.393294145800
	N	-0.511417088300	-2.388265069900	0.295557823500
	H	-1.347865822800	0.217251194700	2.450938307800
	O	1.150849655500	-4.358754578600	0.402301926000
	C	1.202514294200	-4.929630695800	1.570063609000
	H	1.906149114100	-5.771988905100	1.638247584500
	N	0.495986622000	-4.568686626700	2.599109675100
	H	0.664332347800	-5.116967395900	3.445007665500
	H	-1.509642831200	-2.608429378900	0.205045402300
	O	0.825230260100	-1.053025906100	1.664437169400
	H	0.443110673400	-3.562730030200	0.389573321500
	H	-0.254172054400	-1.900268351600	-0.574049434800
	O	-1.009419269900	-2.581616844800	2.705346430300
	H	-0.677958525000	-2.141713856100	3.510487573100
	H	-0.249312595200	-3.619393408500	2.634556027000
Fig. 3d				
	H	0.343577811100	-0.780935077100	1.001506557000
	O	-0.685066896200	-1.697588517600	0.019345929200
	C	-1.910840851100	-1.384344914400	-0.402004417000
	O	-2.690842699400	-2.140433157000	-0.955039755300
	C	-2.278122351700	0.072404177600	-0.128435312200
	O	-1.501668978400	0.863335962300	0.382366154600

	O	1.094641437500	-0.271713043300	1.398377176800
	C	1.421434151100	0.655120736100	0.500956697300
	O	2.175179140500	1.579439809100	0.772932339500
	H	0.972901389500	0.513638053000	-0.500695453500
	H	1.832641684300	-2.554595547000	0.699117666600
	H	-3.307711705200	0.342922635900	-0.443076719800
	O	0.032827815700	-4.060614863400	-0.427856819400
	C	1.218382444100	-4.333410433800	-0.140425227400
	H	1.620887752800	-5.337201860600	-0.366319628700
	N	2.085718683200	-3.505222170800	0.445453569100
	H	3.046419320400	-3.790915429800	0.605110364200
	H	-0.453712689400	-2.695799284300	-0.189522170900
	O	2.067462656200	3.170250326600	-1.442740212400
	C	0.829505401800	3.722004393500	-1.452699834600
	H	0.640536067800	4.223397753700	-2.412599783400
	N	-0.075093972100	3.723421546700	-0.542799105000
	H	0.264008111700	3.217859340000	0.289294781300
	H	2.197655963700	2.685334290600	-0.590537918100
Product	H	-2.318328163300	-2.676674455900	1.364669981000
	O	-2.453075283000	-2.577953202300	0.410391586700
	C	-0.698848115300	-0.637434805000	-1.134823619300
	O	-1.520811631000	-0.724500357200	-2.031392963200
	C	-1.099381987200	-0.259307949700	0.284297162300
	O	-0.331322850500	-0.396294130300	1.230492745600
	O	2.642003316400	0.148337500300	0.222418262200
	C	2.229490418500	0.960433190000	0.966424878800
	O	1.823388206400	1.776805433600	1.708749412000
	H	0.387998334000	-0.829177729800	-1.282486318800
	H	1.021645724200	-1.933750351300	1.043595012000
	H	-2.121233248000	0.157572595300	0.390280195800
	O	-0.063150845000	-3.517445267300	-0.662671202000
	C	1.076302787000	-3.581597947800	-0.172923426000
	H	1.789558974600	-4.373885357700	-0.481284674200
	N	1.568626162100	-2.744393431000	0.752666183400
	H	2.535186465400	-2.823144695000	1.057234102400
	H	-1.637425572100	-2.970252810700	0.041364782400
	O	1.873893789600	3.203276362300	-1.175971499000
	C	0.886151688200	2.305586071600	-1.425100637500
	H	1.140605129800	1.705072117500	-2.308796068800
	N	-0.207498839900	2.098062339700	-0.788105132000
	H	-0.302076303800	2.734424509000	0.020558886300
	H	1.634163455900	3.775251131800	-0.420149048100
	H	-0.487354685000	-1.485254548000	1.254210190000
	O	-1.045699460000	-1.668448331000	0.446227101000
	C	-0.862260678000	-0.293511857000	-0.510697513000
	O	-0.748753349000	-0.510825758000	-1.690299832000
	C	-1.846059320000	0.668728725000	0.201107921000
	O	-1.635275390000	1.053145046000	1.333068980000
	O	0.916470833000	-0.791094400000	1.944919963000
	C	1.035751947000	0.215772931000	1.239149175000

	O	1.645484899000	1.271597680000	1.193763552000
	H	0.271069197000	0.076330885000	0.166947110000
	H	1.771262981000	-2.419056310000	1.012113038000
	H	-2.736797349000	0.938671494000	-0.403033419000
	O	0.182668906000	-3.453774856000	-0.769148651000
	C	1.370386667000	-3.751372901000	-0.502371533000
	H	1.870512857000	-4.548218939000	-1.081696747000
	N	2.119591471000	-3.190581856000	0.444704947000
	H	3.087682106000	-3.472559533000	0.569252660000
	H	-0.524204985000	-2.445477052000	-0.066538763000
	O	1.664430274000	1.765115497000	-1.568926108000
	C	0.446234844000	2.327949042000	-1.764851123000
	H	0.158941802000	2.268352646000	-2.823242641000
	N	-0.336742794000	2.877013428000	-0.908651628000
	H	0.096272231000	2.847101850000	0.028325540000
	H	1.851465203000	1.773868063000	-0.604331160000
Fig. 4a				
	N	-3.253165796100	-1.153123474600	1.424784691100
	C	-2.966013636100	-0.275131811300	2.167883620700
	H	-2.841847024000	-1.897142505700	-0.194943541500
	C	0.904773062700	-0.605750513700	2.001453166100
	O	1.235667749100	0.329633216300	1.310248359400
	N	-2.684054482600	0.660706289000	3.090726252800
	O	-2.653533259400	-2.183408644300	-1.122658733100
	C	-1.323936104300	-2.067127564900	-1.316991833500
	H	-1.062192821700	-2.297404942800	-2.362664864000
	N	-0.512750592100	-1.732710247900	-0.380772851900
	H	1.282343335300	-1.637564240500	1.884386212800
	O	0.034388822200	-0.438784012900	3.029184894200
	H	-0.069752051600	-1.273579150900	3.523764424100
	H	-3.209275925400	1.527400033200	2.973003163800
	H	-1.675945908000	0.812638374500	3.177285184900
	H	0.432615298000	-1.697692310600	-0.784652877000
	N	-2.796024201100	-0.656575435200	1.553131638600
	C	-1.998735218500	-0.143633442500	2.422060124400
	H	-2.273158907500	-1.284170019500	0.919576225700
	C	-0.510028587800	-0.444869256000	2.479286365900
	O	0.153735965200	-0.770918414100	1.512062489900
	N	-2.442761574700	0.641759205000	3.490591659100
	O	-2.052372006500	-2.567443008200	-0.737005868300
	C	-1.083388826500	-2.472311979800	-1.501140938100
	H	-1.027309323500	-3.058697308900	-2.443535121000
	N	-0.030572844700	-1.655218173400	-1.309990183700
	H	0.061013404800	-1.193879293600	-0.404236779900
	O	0.045169493300	-0.353420735300	3.702047424400
	H	-0.668469809100	-0.157629596700	4.343374774600
	H	-3.443074515100	0.841009014100	3.415828055600
	H	-1.929160488600	1.520387262200	3.590127040000
	H	0.795687736400	-1.747251857100	-1.892645047200
Product				

Transition state	N	-2.915080665100	-0.891628603100	1.115693337200
	C	-2.354843953900	-0.308151263400	2.002620081300
	H	-2.738504376400	-1.749307352500	-0.084628542900
	C	0.087108442800	-0.296245319700	2.131871091300
	O	1.088472590500	-0.068669868100	1.448196433500
	N	-2.386026113800	0.352228388000	3.196900409600
	O	-2.511762513500	-2.317533237600	-0.940714192200
	C	-1.249832364900	-2.264007518700	-1.182777646700
	H	-0.906223793400	-2.771669886200	-2.092099347100
	N	-0.366339132900	-1.655915088900	-0.436743168300
	H	-0.586205342100	-1.180763405100	0.456448639800
	O	0.379639003100	-0.321093917400	3.525306341100
	H	-0.455576985900	-0.571253834000	3.953825606100
	H	-3.317499303100	0.728755371300	3.388815668500
	H	-1.668110257200	1.074519505900	3.269949921800
	H	0.614284506000	-1.658110773600	-0.718274672100
Fig. 4b				
Reactant	N	-1.820362805800	1.455666739200	3.142931713800
	C	-1.909021217700	0.733737178200	2.075798684200
	H	-2.730968455600	1.866564700800	3.398396859300
	C	-0.623257435300	0.068760705500	1.611289227100
	O	0.302463067600	-0.182203056900	2.351600143700
	N	-2.980706958100	0.586445516600	1.213944627800
	O	-0.553060229600	-0.199005337000	0.286359878900
	H	-1.328068892900	0.182829211100	-0.169394077500
	H	-3.864057356800	0.977986873600	1.548922872500
	H	-3.116426671700	-0.383613565200	0.915511713900
	O	-2.142219625000	-1.970630817500	2.776514578300
	H	-1.709134960400	-1.599527783100	3.581102120400
	N	-0.966369296600	-1.106056612800	5.230701018600
	C	-0.176959448800	-0.195989229300	5.688019294900
	H	0.446640825800	-0.308503472600	6.589978321200
	O	-0.018649326200	1.010186495100	5.141956261200
	H	-0.623473549500	1.103003610800	4.344838997600
	H	-0.901302715600	-1.922483082400	5.852605254600
	H	-3.068194356800	-2.021720776100	3.056651605500
Product	N	-1.968951165400	1.319382965300	2.904255644500
	C	-2.053540108400	0.118871578500	2.121711168800
	H	-2.876001990600	1.501871875200	3.348899377200
	C	-0.621358973800	-0.163340268700	1.603684266700
	O	0.277791304900	-0.555723372700	2.324381534800
	N	-2.925646659300	0.341718529500	0.974370100600
	O	-0.467300608600	0.110866783200	0.306394782100
	H	-1.393542617500	0.369369292100	0.034431573600
	H	-3.561631709500	1.124397508200	1.135572184800
	H	-3.486203339500	-0.494940449500	0.795094498400
	O	-2.398095101500	-1.074842138200	2.835531759900
	H	-1.026905273300	-1.328240774300	4.341547484700

	N	-0.592823499400	-1.351444917000	5.266055845900
	C	-0.120226545600	-0.221961796800	5.815586956800
	H	0.364679315200	-0.381215200100	6.803145045100
	O	-0.198827202900	0.909735709600	5.314928076300
	H	-1.301002736600	1.162535038800	3.673640074400
	H	-0.473348773300	-2.241096871900	5.740074890300
	H	-3.244201108700	-0.914827369200	3.294021929100
Transition state	N	-1.873788437800	1.280917276800	3.125185450700
	C	-1.927755104100	0.406063138700	2.134198396300
	H	-2.763311125600	1.623172909700	3.496069905100
	C	-0.566363517400	-0.048794484900	1.609703244600
	O	0.371377071400	-0.300698634600	2.330835381100
	N	-2.947429725300	0.454262273300	1.208091937900
	O	-0.474608399500	-0.105935082600	0.267012061000
	H	-1.295693977900	0.251383533500	-0.126061194200
	H	-3.790847722500	0.942875861000	1.513789186900
	H	-3.194164076400	-0.451697890100	0.809627463400
	O	-2.152421544100	-1.439315593400	2.913500097500
	H	-1.579156085000	-1.326835967500	3.900308030600
	N	-0.920921106000	-1.220268455200	5.092174919200
	C	-0.219752923700	-0.209025204800	5.575157918400
	H	0.369117278300	-0.403343383900	6.502724194000
	O	-0.160476408900	0.968902199500	5.100008212700
	H	-1.090813089200	1.173222810500	3.853525704500
	H	-0.792547603100	-2.056533856600	5.668398680500
	H	-3.081233154300	-1.431034034600	3.206024865600
Fig. 4c				
Reactant	N	-2.206682082200	1.083435807500	3.241891253600
	C	-2.060374799600	-0.092421174700	2.391912123800
	H	-1.924177647200	1.912147991000	2.704738076000
	C	-0.620569776200	-0.080926160800	1.836202447200
	O	-0.040138155300	0.931037256300	1.488371387700
	N	-3.025194251300	-0.082154094400	1.300140222100
	O	-0.086601826300	-1.306706847500	1.673153221300
	H	-0.714556915000	-1.931925742800	2.097191369700
	H	-2.885882219700	-0.924098605000	0.730197660800
	H	-2.812709919500	0.710483926800	0.684851700400
	H	-3.207732806000	1.196996058800	3.442989035000
	O	-2.298323194200	-1.270998645100	3.107992412000
	H	-1.671126501000	-1.238361468800	3.903024487400
	N	-0.474551304800	-1.126667554500	5.060024761500
	C	-0.063020050200	-0.055933875400	5.650483928700
	H	0.696415830000	-0.041797111400	6.447740785400
	O	-0.513319180100	1.160846005300	5.363751431700
	H	-1.182593044300	1.094561330900	4.603281756900
	H	0.016715659700	-1.945049872200	5.438503022900
	N	-2.110829459400	1.057524140500	4.006064183800
	C	-1.654434120400	-1.131386798500	1.884363957000

	H	-2.272299676400	1.564671525400	3.131637657100
	C	-0.437237484000	-0.196616234600	1.856093239000
	O	-0.399664640000	0.861999682700	1.254640258800
	N	-2.665168579200	-0.718120638300	1.112458670600
	O	0.587263749700	-0.688233074900	2.554257461400
	H	0.240860477500	-1.525012047100	2.939964623400
	H	-3.529245823500	-1.253263175700	1.043946579400
	H	-2.560530652800	0.148026353900	0.595148375000
	H	-2.877295988400	1.352655597800	4.620385088200
	O	-1.596116928100	-2.162377420000	2.569711587600
	H	-1.330860785900	-0.640292704000	4.812050856800
	N	-0.604378043400	-1.076939285100	5.390845173700
	C	0.434699411000	-0.321354823800	5.800415092500
	H	1.224565179500	-0.906232211700	6.322120021600
	O	0.526394710700	0.903090105000	5.650655682300
	H	-1.272190154600	1.484079583100	4.417508776900
	H	-0.574739074300	-2.084211509800	5.508010677900
Transition state	N	-2.200615563300	1.057344157600	3.186780320100
	C	-2.065089841200	-0.113598645200	2.285663990100
	H	-2.046725912100	1.915842626100	2.642652538200
	C	-0.661772527200	0.005290453900	1.640069922700
	O	-0.201507708000	1.027376255200	1.154430507200
	N	-3.107976943700	-0.043397751000	1.259646573500
	O	-0.032365595000	-1.174528459200	1.633544441100
	H	-0.698833757800	-1.730634056900	2.135682818600
	H	-3.063297090400	-0.923714176000	0.734825862200
	H	-2.863436301600	0.687768010000	0.579986097900
	H	-3.178343587200	1.092182373400	3.504340721400
	O	-2.160104555000	-1.297930079600	2.963076510500
	H	-1.482125934800	-1.236774804000	4.089334175500
	N	-0.807483772600	-1.212195398300	5.061697795400
	C	-0.308377063300	-0.120313522200	5.567022661400
	H	0.359651718800	-0.167038169500	6.439181619600
	O	-0.541248380600	1.069851644700	5.110892498000
	H	-1.268823758600	1.048328787900	4.279487909700
	H	-0.526274148500	-2.079214715100	5.521401596000
Fig. 4d				
Reactant	C	-2.083324876100	-0.814898199800	1.683961382300
	C	-1.142677380800	0.357187010600	1.368556804900
	O	-1.164281761900	1.012403098000	0.346794977000
	N	-3.029402655100	-1.026872776700	0.764272992000
	O	-0.273505646200	0.566039227300	2.371918339400
	H	-0.436201165200	-0.172213847700	3.005934424900
	H	-3.707488066100	-1.772820732500	0.889716571100
	H	-3.839796427900	1.690348914100	1.368778557400
	O	-1.883613749200	-1.464628818800	2.721444148800
	N	-2.866864389000	3.719871362800	0.770096443300
	C	-3.551743208000	2.954678735000	-0.002540427200
	H	-3.761489897600	3.132737929100	-1.067880282600

	O	-4.113096868900	1.807391396600	0.424406837500
	H	-2.541518457600	4.534436106100	0.237194143300
	O	-3.094338142000	2.051601726300	2.931193152800
	H	-2.760785642000	2.837083352500	2.437750989000
	H	-2.324223359500	1.722419278000	3.417725844500
	H	-3.154135631100	-0.356988821000	0.009472072700
Product	C	-1.923568561900	0.772270582700	2.708903545600
	C	-0.957949590300	0.830539172200	1.527560822600
	O	-0.799805193000	1.799724043500	0.810235257500
	N	-3.253075501900	-0.161625378000	0.576759052700
	O	-0.232411711300	-0.288110068500	1.406574014500
	H	-0.552618024800	-0.910659782400	2.093983588000
	H	-4.082789841200	-0.544347412100	1.041652589100
	H	-3.605334637400	0.619478808000	0.008600713500
	O	-1.938068138600	-0.179838036100	3.471860438500
	N	-3.069501869000	3.782151678300	0.257496155000
	C	-4.067858903600	3.462800245300	-0.582250105700
	H	-4.673940523300	4.343742034100	-0.887988116200
	O	-4.328195382800	2.326097785400	-1.000142408900
	H	-2.926491367500	4.748730485300	0.534397021600
	O	-2.647377974700	1.886826854800	2.804848510200
	H	-2.422669604300	3.070035799000	0.598017893700
	H	-3.260649679800	1.809885908500	3.565050903900
	H	-2.981481974700	-0.883788504100	-0.098171839800
Transition state	C	-2.183854653400	-0.140712389000	2.022633568800
	C	-0.915408036400	0.441234917500	1.361130450000
	O	-0.874434531200	1.082638197900	0.327875884400
	N	-3.269430979600	-0.294097520600	1.056794888200
	O	0.170106507600	0.138823663700	2.090343767400
	H	-0.208462746300	-0.445971963000	2.796026720100
	H	-4.104905069500	-0.553209328600	1.596063283400
	H	-3.514756411900	0.941387364500	0.010635328600
	O	-1.984638229900	-0.956576765600	2.952181696600
	N	-3.157177195400	3.134042172300	0.981697027800
	C	-3.503022683700	2.864170299200	-0.236422549100
	H	-3.665320518700	3.656222686700	-0.981413260200
	O	-3.709213437100	1.656395563100	-0.705154200700
	H	-3.047560902200	4.135548568600	1.148122669400
	O	-2.819522594900	1.370605081600	2.705612518300
	H	-2.946256356400	2.219414890900	1.916595176700
	H	-2.181048189000	1.656946176800	3.385668210500
	H	-3.043892231000	-1.129181265000	0.498879896900
Fig. 5a				
	H	-1.622268223400	-0.217658945300	1.592652091100
	N	-2.260545996600	-0.564138405300	0.868906919700
	C	-1.563683433800	-0.525632099600	-0.410795019500
	C	-2.505629811600	-0.896110988100	-1.491705580000
	N	-3.257652968400	-1.169192891000	-2.362754115200

	H	-1.222994690800	0.505668562300	-0.619534312500
	H	-2.436152194700	-1.556906645100	1.064228426100
	N	0.593440711700	-2.101445715400	-0.498057837800
	C	-0.368934911800	-1.410783729700	-0.498160488800
	O	-2.647978311400	-3.317303403400	-4.236711566000
	C	-1.647404041800	-3.999778501700	-3.651866012100
	H	-1.063732770700	-4.558873023200	-4.398494812600
	N	-1.427985275000	-3.982580471000	-2.386502560100
	H	-0.607019153300	-4.566984177200	-2.183744067400
	H	-3.071887858500	-2.754174563600	-3.554878657900
	O	-2.683927557100	-3.364807478000	0.092451994100
	H	-2.276060030900	-3.568254978700	-0.780721008400
	H	-3.632412571800	-3.392573374100	-0.106919329600
Product	H	-1.753230492300	-0.215878826600	1.896150862600
	N	-2.305066163300	-0.625789428300	1.135114844000
	C	-1.471529270300	-0.689615345000	-0.066682711100
	C	-2.239745122500	-1.378144526900	-1.179966884500
	N	-2.424189857100	-0.790891017000	-2.306823555700
	H	-1.220574489100	0.328737257700	-0.398218456000
	H	-2.504681999900	-1.587223687800	1.431419111800
	N	0.787275031300	-2.070398884900	0.303389422300
	C	-0.201328263900	-1.441608105400	0.124419463400
	O	-3.219725313500	-3.900709077000	-2.955228642100
	C	-2.160188189700	-4.467250600600	-3.297137397400
	H	-2.090302590500	-4.989114210600	-4.270206126600
	N	-1.034985031800	-4.506524159800	-2.574590157400
	H	-0.212747626000	-4.998135771700	-2.916551300900
	H	-2.961522132400	-1.417812980700	-2.927013398800
	O	-2.632930610800	-2.609560622100	-0.781757507300
	H	-0.995841765000	-4.080576424800	-1.651438846400
	H	-3.014194851300	-3.096914004200	-1.578877247800
Transition state	H	-2.024106563400	-0.016974745600	1.686023187100
	N	-2.454850742300	-0.613427099800	0.971527865700
	C	-1.654103328000	-0.523129318000	-0.246731061400
	C	-2.274156501200	-1.345938373300	-1.343127682600
	N	-2.721922172200	-1.264808414400	-2.459209741500
	H	-1.632505617100	0.524356583500	-0.594677549700
	H	-2.367152714000	-1.577663746500	1.307936147900
	N	0.884232215200	-1.284846330100	0.093680673000
	C	-0.242663568600	-0.962449396800	-0.079064885600
	O	-2.758032866000	-3.228189161100	-4.110655019400
	C	-2.030978076800	-4.226340619500	-3.704585254300
	H	-1.829572904900	-4.978724260800	-4.478840615800
	N	-1.558102052200	-4.375398645700	-2.502666108600
	H	-1.006054690700	-5.218774817100	-2.351955140900
	H	-2.819532259500	-2.462953349700	-3.398102922800
	O	-2.173211021200	-2.978615724200	-0.487832539100
	H	-1.816307624000	-3.717102454700	-1.585520829800
	H	-3.127265875000	-3.176671021100	-0.429797128900

Fig. 5b				
Reactant	H N C C N H H N C O C H N H H O H H	-0.817586348700 -1.085066629600 -1.679938149700 -2.264980185100 -1.774447604500 -2.516915491500 -0.206823243400 0.057072450900 -0.736167340900 -4.507617496300 -4.173800488900 -4.734173480400 -3.166693432300 -2.923087293600 -0.917495008500 -3.373377257800 -3.724982563800 -2.577600944000	-0.636655254000 -1.227702414600 -0.373846722300 -1.252466632700 -1.429862586000 0.186186539900 -1.618625064700 1.370341872900 0.611088242900 -3.555357824300 -3.792195537300 -4.538294726300 -3.196984227400 -3.473588739500 -0.876054343700 -1.857386098900 -2.481121885300 -2.529501086800	2.320692212500 1.527604287800 0.497169699700 -0.608603631100 -1.786976463800 0.946781202900 1.168108787100 -0.532337946100 -0.087068971400 -1.837036121300 -3.017345635900 -3.615523058000 -3.657220468900 -4.602701481400 -1.901462871900 -0.179603025700 -0.888817145100 -3.133745141700
Product	H N C C N H H N C O C H N H H O H H	-0.733894806000 -1.028412468000 -1.682980727000 -2.332349824000 -1.664074661000 -2.511628490000 -0.160309350000 -0.028068585000 -0.784122017000 -4.700314653000 -4.209177448000 -4.809030748000 -3.164978664000 -2.990465845000 -0.761078792000 -3.429197614000 -4.155589884000 -2.090467170000	-0.654788650000 -1.235597986000 -0.371151752000 -1.258887003000 -1.440297713000 0.160876509000 -1.605068307000 1.431863887000 0.647095781000 -3.603704124000 -3.766427329000 -4.485137764000 -3.154335641000 -3.439772802000 -1.004596132000 -1.787271809000 -2.923795921000 -2.048602875000	2.257992249000 1.466754726000 0.480999967000 -0.593705413000 -1.735917635000 0.975126594000 1.062325536000 -0.584407581000 -0.118193060000 -1.822245101000 -3.054179780000 -3.634430114000 -3.491848496000 -4.462383734000 -1.886638660000 -0.325850911000 -1.331954713000 -2.464161450000
Transition state	H N C C N H H N C O C H	-0.668006460100 -1.043764549500 -1.718389994000 -2.372470526900 -1.771606046500 -2.533288519500 -0.220944931900 -0.066762025800 -0.822303624200 -4.613323560100 -4.096057654400 -4.629240092000	-0.718368375300 -1.296714674900 -0.420034135700 -1.293351237900 -1.503545213700 0.111478680400 -1.704953964000 1.384796094200 0.598942147700 -3.474448161800 -3.670110120900 -4.406392099400	2.165551265800 1.406318972000 0.442745234500 -0.643453992100 -1.794541314000 0.959780722200 0.948378084800 -0.623527854500 -0.157966487000 -1.767563365200 -2.944827925800 -3.563233759800

	N	-3.035761536800	-3.065889348200	-3.390962277500
	H	-2.736584552600	-3.335773397600	-4.328128908100
	H	-0.872860589700	-1.028565620500	-1.897245264900
	O	-3.492464052700	-1.808441851700	-0.309009037700
	H	-4.077977862700	-2.750995318900	-1.193846791800
	H	-2.393430637700	-2.310769244700	-2.695078190800
Fig. 5c				
Reactant	H	-0.015954804000	-1.075759262100	2.151765846400
	N	-0.266279525300	-1.241827972900	1.172704118300
	C	-1.500023294300	-0.526079212100	0.869765704700
	C	-2.225612980100	-1.041977744500	-0.391285976700
	N	-1.819853886800	-2.265150247500	-0.775391622200
	H	-2.222258673100	-0.676617320000	1.694426045100
	H	0.501214114700	-0.837587467300	0.614704300400
	N	-1.051444514100	2.091030467100	0.692036721100
	C	-1.310203538500	0.937820421900	0.736119148400
	H	-0.988626834500	-2.651759123700	-0.338096393100
	O	-3.145742961000	-0.391277622100	-0.892429747100
	H	-0.081217560900	3.583203651100	0.207463223800
	H	-2.205063553000	-2.682346611700	-1.619924914300
	C	0.932755113600	-0.517281549400	-1.860468853400
	N	-0.156332115900	0.327756358000	-2.036006208800
	H	0.078230253500	1.315462556600	-1.890099971700
	N	1.136145539600	-1.675997123700	-2.404082029700
	H	0.370374104200	-1.858772711500	-3.065981325600
	N	1.781207009600	-0.067362400300	-0.837811383200
	H	2.701716370300	-0.504188099500	-0.893850983800
	H	1.847231655100	0.954484703500	-0.813722680900
	O	0.389319124800	4.416072590800	-0.039836856400
	C	1.220062283000	4.150809967300	-1.057104282900
	H	1.736352018700	5.063676311700	-1.391545144000
	N	1.373784295500	2.975117022900	-1.557430524400
H	2.053461218400	3.037301055200	-2.327351232300	
H	-0.670182340700	0.178053006300	-2.903986460900	
Product	H	-2.161887970800	-2.281249519500	0.322015751400
	N	-1.227315545700	-1.873628351700	0.217194189100
	C	-1.309523155200	-0.434386375300	0.502313128300
	C	-2.131798348400	0.309184251100	-0.562596638900
	N	-2.367214180100	-0.385827757500	-1.697406100400
	H	-1.765390799600	-0.169252017200	1.472275404200
	H	-0.670757212900	-2.320483534700	0.955482652800
	N	0.406187075300	0.972680099400	1.479476952800
	C	0.088186901000	0.168690200600	0.525238650000
	H	-2.032667254400	-1.339242818500	-1.803303560800
	O	-2.516004953300	1.465979110600	-0.363341894300
	H	1.369166166700	1.304240624900	1.320714193600
	H	-2.940204900100	0.024203022000	-2.432253350200
	C	2.245712364500	-0.077709237100	-0.735142823300
	N	0.848384874700	-0.250532857700	-0.585056091800

	H	0.207064880800	1.194435201200	-2.462716341500
	N	3.056317744500	-0.976078988800	-1.189273635900
	H	2.550147813500	-1.863528085800	-1.301548552000
	N	2.682208248800	1.177144689500	-0.347933321100
	H	3.646580009600	1.352176025600	-0.631986922500
	H	2.038780334900	1.936081049500	-0.612125971900
	O	0.633135366400	3.185242924600	-0.906225798400
	C	-0.203962922700	3.084014059000	-1.811027842400
	H	-0.947543849100	3.885487494500	-2.004335275800
	N	-0.283143756600	2.058180738800	-2.683940530500
	H	-1.074410555900	2.006816800000	-3.318522049000
	H	0.491930892200	-1.128865351700	-0.967921861500
Transition state	H	-1.095500890300	-2.634792174300	0.760456993900
	N	-0.551363346000	-1.859250370100	0.364452639500
	C	-1.318507460500	-0.624814047000	0.565467143700
	C	-2.528693370200	-0.554562604000	-0.384776406700
	N	-2.470308693600	-1.398441134100	-1.442077051200
	H	-1.719885379000	-0.472097768600	1.583599765200
	H	0.290277751100	-1.822662425800	0.949986414400
	N	-0.317455528500	1.689861244900	0.823552893200
	C	-0.468538659700	0.600937334000	0.284133785400
	H	-1.778744400200	-2.142001067100	-1.458679674500
	O	-3.428860630200	0.266385522000	-0.194495963400
	H	0.390780274200	2.662238391700	0.206249685000
	H	-3.260405870100	-1.441585336300	-2.083137214000
	C	1.736390219400	-0.144427139600	-1.007200577400
	N	0.355240376200	0.247146038400	-1.197085443400
	H	0.257916855800	1.197292152900	-1.720361230300
	N	2.212857529900	-1.317329766400	-1.253972661900
	H	1.451130370100	-1.931045983800	-1.566664893700
	N	2.480192055500	0.853663627700	-0.442501765100
	H	3.486331801300	0.705767229300	-0.437401530200
	H	2.172389389500	1.819755420100	-0.521728367100
	O	0.970629028500	3.530925776400	-0.277293983700
	C	0.680553743800	3.667931406700	-1.555532316000
	H	0.938205681000	4.659690652900	-1.969829691200
	N	0.157763378200	2.725791786300	-2.278167024400
	H	0.024318475500	3.051572145300	-3.240795445000
	H	-0.156377276500	-0.482234710500	-1.703964629300
Fig. 5d				
	H	-0.199363556700	-0.427734888800	1.382316283500
	N	-0.692593803200	-1.109990405500	0.797131325200
	C	-1.475164763000	-0.366130615900	-0.183393907200
	C	-2.277002096500	-1.318841073500	-1.086059239500
	N	-3.545013671100	-0.942972061800	-1.287389543300
	H	-2.207474057900	0.240863886500	0.368420970100
	H	0.046123710200	-1.618478109400	0.302133723700
	N	-1.455499845300	1.777523272500	-1.231900099000
	C	-0.792587423300	0.665253325600	-1.090688441500

	O	-3.170103916300	2.989218743000	0.452531430500
	C	-4.319239901800	2.375366300700	0.736467441700
	H	-4.931375534800	2.967358286100	1.435292088600
	N	-4.664219731600	1.233164999800	0.249964474400
	H	-5.583863339600	0.979998352800	0.632884735700
	H	-3.942005083000	-0.113741656100	-0.812072493700
	O	-1.762675897900	-2.333310159000	-1.597116622600
	H	-4.125665800600	-1.514868623200	-1.897988413900
	H	-0.993092810300	2.431617642600	-1.880585896500
	H	-2.624220478500	2.441208631300	-0.202556203900
	N	0.413901719800	0.458676511100	-1.746979763500
	C	1.387252947500	-0.573651657500	-1.808999947700
	N	2.610442245500	-0.346044809900	-2.161851942400
	H	2.770481744900	0.664071563200	-2.262455463400
	N	0.976282395000	-1.839690931100	-1.467286280700
	H	1.677756511900	-2.545899103600	-1.683840119300
	H	0.713766273700	1.278576166300	-2.276164793000
	H	0.012181201000	-2.107012626200	-1.708633795300
	H	-1.863186255900	0.021214161200	1.296511625500
	N	-2.514879001700	-0.355382226600	0.597139792600
	C	-1.825728727900	-0.652669162500	-0.624112034500
	C	-2.102239734000	-2.021279198500	-1.138437370400
	N	-1.510079290200	-2.415824460500	-2.306033431600
	H	-3.881947215900	1.024705855400	0.810408137300
	H	-2.857773412200	-1.249902604700	0.964004324500
	N	-1.129873723500	1.664716238200	-0.818424234800
	C	-1.114945771500	0.345718800000	-1.242078472900
	O	-2.272155678800	2.794529922900	1.650282075100
	C	-3.514474001300	2.825995999900	1.692568815000
	H	-4.052888749000	3.672560612600	2.170564804700
	N	-4.318562799000	1.887554788900	1.173043913300
	H	-5.324506696900	1.950454870300	1.303781753700
	H	-1.165582562900	-1.669411227900	-2.908501327200
	O	-2.822336022900	-2.787180023600	-0.473509451400
	H	-1.915051348600	-3.238991751500	-2.750022594300
	H	-0.234279400900	2.143017119100	-0.921167734900
	H	-1.557672642500	1.868874915800	0.092116240600
	N	-0.375429067700	0.127419297100	-2.449347914400
	C	1.009503991000	-0.181158379400	-2.371043296500
	N	1.916638887700	0.243102521800	-3.187673323800
	H	1.505284340600	0.930421087500	-3.833239881800
	N	1.332864171300	-1.016539232300	-1.309898943100
	H	2.264523404400	-1.411339408500	-1.436972401200
	H	-0.548732542800	0.882480809300	-3.120254025300
	H	0.642859821300	-1.752181809100	-1.162720571200
	H	-2.007792899300	0.345610875900	1.739458527100
	N	-1.627837580700	-0.495892171300	1.292821269100
	C	-1.648527798700	-0.277639589000	-0.150882349700
	C	-1.876994990000	-1.540845750700	-0.939450596600
	N	-2.319469379800	-1.336104397300	-2.209097743500

	H	-2.741915718400	0.388821730700	-0.283203397900
	H	-0.663535587700	-0.562780871500	1.635336320000
	N	-0.682933788100	1.893701437900	-0.046707634000
	C	-0.722766598900	0.736027568000	-0.684490580900
	O	-2.769088987100	2.428062360300	1.517780516900
	C	-3.834243979100	2.090524203800	0.898460290000
	H	-4.786486604900	2.568064151500	1.225279497900
	N	-3.883309808100	1.224133452800	-0.096282437400
	H	-4.841268845400	1.066207669700	-0.423968164600
	H	-2.569006217100	-0.413194470100	-2.547919355600
	O	-1.727023088500	-2.674076504600	-0.463436163100
	H	-2.524126408300	-2.135304061900	-2.804868915100
	H	-0.059802856200	2.638076515600	-0.361768905600
	H	-1.460700729400	2.126326067100	0.642974979600
	N	-0.005134893300	0.608471354300	-1.840666590400
	C	0.575583780300	-0.576457014200	-2.383948796900
	N	0.828843760900	-0.726032103400	-3.637240040800
	H	0.449289369700	0.069245613100	-4.165503216900
	N	1.005108025300	-1.503491447700	-1.451123106800
	H	1.073416071700	-2.439587671700	-1.850975262600
	H	0.231004427000	1.466117958800	-2.345441630900
	H	0.489985010900	-1.529876010300	-0.576126839400
Fig. 5e				
	H	-3.116820479200	0.139556221000	0.089919677800
	N	-2.148626942800	0.225661800000	0.413634741600
	C	-1.335665388100	-0.353029376000	-0.610384653100
	C	-2.092460236300	-1.031639912300	-1.707391931400
	N	-1.454807965500	-1.985222315500	-2.435716951700
	H	-1.972627266500	1.234759038000	0.473887285300
	N	0.662579951300	0.168774648500	0.665707203900
	C	0.028318833600	-0.254779269800	-0.505691266000
	H	-1.809034220200	-2.137047405400	-3.392980655100
	O	-3.293016234300	-0.748339085900	-1.871168080000
	H	-0.445201360900	-2.023359873200	-2.317166051100
	H	1.326940338900	0.933280565100	0.530268719600
	N	0.933281018600	-0.662549454600	-1.529674486500
	H	1.795771446800	-1.034167339600	-1.125646870700
	H	-0.003502271700	0.412125874400	1.399951730300
	C	1.171837326500	0.108825120200	-2.687109350400
	N	0.042012715300	0.778323246700	-3.185375337900
	H	0.334743858400	1.590026490200	-3.736071733700
	N	2.276794866000	0.137505270000	-3.353171752900
	H	2.983051787100	-0.432981850700	-2.869584942000
	H	-0.590458180100	1.081705140200	-2.440399217300
	O	-1.154675911000	0.057531865100	-5.659391320800
	C	-1.870965338700	-1.003314008000	-6.059414987300
	H	-2.179559966300	-0.888861945000	-7.109964388100
	N	-2.148426558800	-2.007940223800	-5.308935324000
	H	-2.713704169900	-2.672762769000	-5.849269356800
	H	-0.884304611800	-0.030582276300	-4.712541985600
Reactant				

Product	H	-2.690703616900	-0.645491917600	0.615893013300
	N	-2.245503922600	0.200246677000	0.242299985000
	C	-1.210294607400	-0.194222418100	-0.675758914100
	C	-1.471569395100	-1.090814412200	-1.777454421000
	N	-0.357753461800	-1.446140446500	-2.526409356700
	H	-2.995909928700	0.657112303300	-0.286491479000
	N	0.444591110700	0.774651716600	0.799440718500
	C	0.106600151200	0.165851092900	-0.388022541600
	H	-2.761404950300	-1.752464430000	-3.851241989200
	O	-2.612003870900	-1.552965892800	-2.036993154700
	H	-0.546188676400	-1.957674679700	-3.389547860400
	H	1.182120825500	1.477031432400	0.732686872600
	N	1.100605174600	-0.159003703900	-1.262867636200
	H	2.058979208200	0.150263932800	-1.111704650900
	H	-0.390200745300	1.128994099700	1.270104848000
	C	0.797280117700	-0.537495893900	-2.660594334400
	N	0.214141370100	0.743649258000	-3.339383858200
	H	0.985888840300	1.368642193600	-3.603820618800
	N	1.830412300000	-0.910738126500	-3.454710260900
	H	2.183496052100	-1.781988837200	-3.035898967000
	H	-0.447715030800	1.244383785700	-2.731336431200
	O	-1.420495164100	-0.160058709300	-5.450194692300
	C	-2.157645918700	-1.117202555900	-5.742531582400
	H	-2.336336182500	-1.386697769700	-6.804729839000
	N	-2.802071206600	-1.907750385400	-4.871986303500
	H	-3.383252338200	-2.663092737300	-5.225042736700
	H	-0.306506021100	0.447880834200	-4.190892968900
Transition state	H	-2.477688230000	1.029662977700	0.470695426500
	N	-2.420090796700	0.016532242000	0.334319652100
	C	-1.422502857400	-0.321977705000	-0.643887119000
	C	-1.786644708500	-1.260531459600	-1.656099501500
	N	-0.756575245700	-1.523485759300	-2.679458596800
	H	-2.195802992000	-0.384522351000	1.250403156000
	N	0.377860388100	0.659971833300	0.636066468000
	C	-0.066122069700	0.041781521200	-0.498908264300
	H	-1.391236815600	-1.564834051700	-3.787398808600
	O	-2.860233308200	-1.863471577400	-1.776275347200
	H	-0.383040781200	-2.474741842400	-2.552895743300
	H	1.197007152500	1.258541497400	0.544333100600
	N	0.853792780300	-0.281827197800	-1.441504183800
	H	1.819276463300	0.029931680400	-1.335278634500
	H	-0.336384008400	1.042065356400	1.251013355900
	C	0.470507457000	-0.569283619100	-2.856213691400
	N	-0.163966789200	0.620648222000	-3.484258668700
	H	0.573067303400	1.329258685300	-3.572623549100
	N	1.474875209800	-1.014105307300	-3.647190480600
	H	1.958841752900	-1.734334193600	-3.090864691500
	H	-0.880962368300	1.023454595000	-2.865903117400
	O	-1.060403916000	0.245201945100	-5.857656882600
	C	-1.876485152300	-0.770734653600	-5.892840917400
	H	-2.418142111500	-0.892189426100	-6.843831079100

	N	-2.059411633600	-1.590528370200	-4.901884551300
	H	-2.749203099900	-2.323583255800	-5.089657894400
	H	-0.658908388300	0.361368140000	-4.859116877600
Fig. 5f				
Reactant	H	-1.360767022100	-1.038024003400	2.015680912400
	N	-1.546314414000	-0.232693274400	1.408546924800
	C	-0.841623645600	-0.427466917900	0.174589541000
	C	-0.794070708600	-1.703539761200	-0.485053628900
	N	-0.019425929700	-1.736053359600	-1.662048300100
	H	-2.556665021800	-0.279033892700	1.233949967800
	N	-0.241036031400	1.911461864600	0.145292845000
	C	-0.170688429400	0.647624075800	-0.383957203300
	O	-1.346379499600	-2.743494603600	-0.093559262400
	H	0.024470378600	-2.638666309400	-2.135419570900
	H	0.577146556900	2.501296032600	-0.002217802000
	N	0.540199304400	0.514997700700	-1.548545946900
	H	1.000534923000	1.350037981800	-1.998961160100
	H	-0.570627155000	1.902100495800	1.111142912600
	C	0.659173598000	-0.675824302300	-2.223952581100
	N	1.379780927200	-0.715939765700	-3.310687242000
	H	1.397152448100	-1.656251664800	-3.718746369200
	O	2.941494621200	1.185651135600	-4.310173765900
	C	2.720672023700	2.383535764200	-3.784000686700
	H	3.352297626200	3.160228692800	-4.244174452800
N	1.867354478900	2.614347235500	-2.841601936100	
H	1.879652968400	3.616685860700	-2.619909708300	
H	2.315600378600	0.489781025800	-3.889394527000	
Product	H	-1.676346450800	-1.241378167200	1.926064416900
	N	-1.575974233900	-0.323673603900	1.480843147600
	C	-0.889300466000	-0.521739419700	0.238198819400
	C	-0.892382720200	-1.793631158600	-0.415464619800
	N	-0.115026074200	-1.826849047700	-1.589806206300
	H	-2.542085728700	-0.030263514000	1.293448656400
	N	-0.174961998400	1.772053233800	0.270249938300
	C	-0.157929288000	0.522621746800	-0.317877674700
	O	-1.470928146200	-2.826928629900	-0.030578813800
	H	-0.090147280200	-2.723711747500	-2.076349008300
	H	0.674099177100	2.313867777100	0.109387499600
	N	0.554811574900	0.428170455600	-1.487106222200
	H	1.255942758100	1.988392904400	-2.440836106300
	H	-0.432977954800	1.729324675900	1.258176931100
	C	0.561047943700	-0.752907827900	-2.090836959000
	N	1.205841734200	-0.897537402100	-3.281126316700
	H	1.468803497200	-1.840500434600	-3.564952166000
	O	3.114050918100	1.203363321600	-4.015353787600
	C	2.756993190700	2.372088856000	-3.785881393400
	H	3.270427826400	3.231484718800	-4.266996139100
N	1.752786060300	2.720508973900	-2.969741073200	
H	1.523622082100	3.700869126600	-2.827070801200	

	H	1.909652162700	-0.175426420600	-3.488812835700
Transition state	H	-1.433312432200	-1.075766583500	2.028302753900
	N	-1.591263378000	-0.259068249900	1.428257603500
	C	-0.876079290800	-0.456441396400	0.201837791600
	C	-0.825928908100	-1.732371416400	-0.454410450300
	N	-0.033950976900	-1.763115159000	-1.625848746100
	H	-2.600552918000	-0.277221213600	1.241625079300
	N	-0.256647483400	1.876604634200	0.184913750400
	C	-0.191510920300	0.615779552600	-0.347375248300
	O	-1.380343059300	-2.773470183000	-0.074376844900
	H	0.016045322900	-2.664126876600	-2.102239263600
	H	0.559535767400	2.468114422000	0.034491478700
	N	0.531362694500	0.486824718000	-1.508148454600
	H	1.020092595500	1.351914978100	-1.968754541200
	H	-0.593680591800	1.872159600400	1.148040959100
	C	0.636692355100	-0.699570000000	-2.163297829900
	N	1.359087261000	-0.766675774500	-3.260172815100
	H	1.416997018700	-1.689736831200	-3.692284078300
	O	2.780180910500	1.031249114700	-4.219846692700
	C	2.609084467100	2.216567818800	-3.719610159900
	H	3.209508606000	3.011818301400	-4.204989661600
	N	1.806167414400	2.500344992000	-2.728933078800
	H	1.840266267000	3.504904722900	-2.529939556200
	H	2.056774352600	0.174837977000	-3.708344184200
<i>GI</i>				
Reactant	O	1.276834842600	-6.954706751200	-10.768584815700
	C	0.326843688500	-6.213445349500	-11.093971296400
	N	-0.050399489200	-5.966781894700	-12.351571963700
	H	0.432458462100	-6.412352152900	-13.128269750500
	H	-0.887061381400	-5.396302691500	-12.505024625300
	H	-0.277078131800	-5.693051543400	-10.328152763000
	H	1.481234284000	-7.035439145100	-9.136402326700
	O	1.700127639900	-7.084381297500	-8.155988975700
	C	0.676961028800	-6.559706927000	-7.464642582800
	H	0.894707431800	-6.542509053400	-6.383654621500
	N	-0.403778828900	-6.136802641400	-8.016300687700
	H	-1.027026845900	-5.749300913000	-7.296917621500
	N	-3.076989374500	-5.825004203700	-9.607457523600
	H	-3.749795473000	-5.942766147900	-8.841237605500
	H	-2.262255827900	-6.371090909700	-9.293763681800
	C	-2.670049630400	-4.450312221000	-9.611509521600
	C	-2.466281381200	-3.728968632100	-8.388668500700
	N	-2.074100145900	-2.392767896600	-8.581792736900
	N	-2.631381837700	-4.470789760200	-12.022654609700
	C	-2.487391575400	-3.785039741500	-10.818715861800
	O	-2.614047198900	-4.167575345100	-7.231874884000
	H	-1.910041745000	-1.851452321300	-7.730782012200
	H	-2.915250049500	-3.859397386800	-12.789832425500

	N	-2.087906348900	-2.479463343900	-10.939625480400
	H	-3.239391979300	-5.287607765100	-11.920429309900
	C	-1.894209186400	-1.825515251700	-9.809261675700
	N	-1.569319172900	-0.491067900500	-9.841837623400
	H	-1.015674597700	-0.142288829300	-9.058912764800
	H	-1.181372904800	-0.200011454100	-10.739206225900
Product	O	0.256975215700	-7.300324771800	-10.670462917100
	C	0.099183846000	-5.913540835000	-10.574897804800
	N	0.333338500100	-5.377017511400	-11.897697855700
	H	-0.416576024800	-5.714018870700	-12.510985083500
	H	0.194968271300	-4.362495484200	-11.854853658600
	H	0.826786883300	-5.443483531300	-9.885130718700
	H	0.275647813500	-7.665623787400	-9.751514816500
	O	0.493774965100	-8.373794833900	-8.193122660200
	C	0.130889530400	-7.739249294600	-7.182161120800
	H	0.414699891000	-8.088034098100	-6.167436359300
	N	-0.614265187700	-6.631918383100	-7.194262707000
	H	-0.777768731300	-6.120413717700	-6.332778044000
	N	-1.243635579900	-5.662178349300	-9.973270200500
	H	-1.902900327700	-6.282209062100	-10.455814878600
	H	-0.878727803100	-6.185762110600	-8.086781880800
	C	-1.652282402600	-4.290623890100	-10.028253166200
	C	-1.247385492600	-3.456473806500	-8.929068292700
	N	-1.663481615800	-2.117050717900	-9.051708951700
	N	-2.794906996400	-4.454155221200	-12.172227163600
	C	-2.401564238400	-3.726356547700	-11.062679042400
	O	-0.587879575000	-3.801920173100	-7.934943389700
	H	-1.440947433000	-1.513210630500	-8.258818066100
	H	-3.556440088500	-4.007942258800	-12.682723076800
	N	-2.763304309100	-2.403344090100	-11.117456198300
	H	-2.985442629300	-5.443590446300	-12.021540735200
	C	-2.375644774500	-1.641385885800	-10.112614681800
N	-2.751872407200	-0.323694141800	-10.079398674000	
H	-2.138177290100	0.312145481500	-9.575675682300	
H	-3.041518459400	0.039450035700	-10.986916290200	
Transition state	O	0.066428011200	-7.337005354100	-10.566537803600
	C	0.129845291300	-6.048366134200	-10.522485716400
	N	0.263476852700	-5.355990616000	-11.744204625300
	H	-0.402956121900	-5.703399715500	-12.438197822000
	H	0.127362516100	-4.348137853700	-11.632142027600
	H	0.743530461600	-5.560213258900	-9.734662407800
	H	0.517458241800	-7.832313323300	-9.294498476100
	O	0.950938494100	-8.188678679100	-8.399482292800
	C	0.353840031000	-7.665520848100	-7.337942829300
	H	0.809918894300	-8.012687358000	-6.394437845400
	N	-0.643738380600	-6.845548773100	-7.390690589200
	H	-0.901310914500	-6.571008015100	-6.435974980400
	N	-1.461111697000	-5.574368114500	-9.786832685600
	H	-2.099755685000	-6.246236762800	-10.228514652300
	H	-1.301601448700	-5.906639438000	-8.797928834400

	C	-1.862467283000	-4.209562041600	-9.878366141000
	C	-1.457513123200	-3.353710365200	-8.799245844400
	N	-1.803399150900	-2.006628932100	-8.998559702900
	N	-2.896688238000	-4.437416485600	-12.071497522600
	C	-2.528640324800	-3.673028315700	-10.977784156300
	O	-0.865117822600	-3.706393973200	-7.769005450700
	H	-1.584227047700	-1.383898721100	-8.221292297200
	H	-3.622347983800	-3.982265881600	-12.626115643100
	N	-2.816044238100	-2.338879480400	-11.103907847900
	H	-3.148175622700	-5.407127026000	-11.880781330500
	C	-2.444445291600	-1.549561218000	-10.112447472100
	N	-2.765698822100	-0.219096150100	-10.152255388800
	H	-2.153365454600	0.412321928100	-9.641739964100
	H	-2.984349524500	0.114492257000	-11.090012863400
G2				
	H	-1.986754467500	4.743192440600	-3.006900343100
	O	-2.795128521900	4.652743023000	-0.571011847300
	C	-1.789736762100	5.233706523700	-1.024827622200
	H	-1.107431278700	5.795306293600	-0.353426604900
	N	-1.423514195500	5.249204021300	-2.312152038700
	H	-0.575974879800	5.728580704700	-2.603035838800
	H	-3.304199246700	2.841949063500	-1.478293393900
	N	-3.676260949200	2.120828776600	-2.106469537900
	H	-4.061308390600	3.974543052000	-3.662571738900
	O	-3.198052660800	3.614665279000	-3.955919890900
	C	-3.082416820500	2.283406473900	-3.427827879800
	H	-1.998421733400	2.113800618400	-3.317590026100
	N	-3.610890934200	1.349411637500	-4.405045747700
	H	-4.582640940600	1.630863162200	-4.582759663800
Reactant	H	-3.706443323400	0.447934069600	-3.923055205000
	C	-5.109626924900	2.113829804100	-2.088455553800
	C	-5.770241638400	0.835510877900	-2.101529571600
	N	-7.175359302800	0.931461433300	-2.053275358200
	N	-5.293621850000	4.525069748900	-2.152677191700
	C	-5.890108527100	3.269688953300	-2.056360503300
	O	-5.242303091700	-0.285576772600	-2.181345311500
	H	-7.687049527500	0.048574035300	-2.114183793800
	H	-5.961802152800	5.270418176900	-1.955591950700
	N	-7.257503008300	3.287645170400	-1.995770476100
	H	-4.438051341600	4.629344789300	-1.591407950400
	C	-7.857002678900	2.109537009900	-1.995818102300
	N	-9.225703200300	2.053207459400	-2.003214576300
	H	-9.661985657200	1.255038968300	-1.547161432600
	H	-9.657607492000	2.940829889200	-1.751298973700
	H	-2.631516873500	5.163308724300	-3.377083593100
	O	-2.744134014700	4.057152654500	-0.546930258300
	C	-1.628732995400	4.661046848000	-0.944618613900
	H	-1.037755085200	5.036410202500	-0.092488553500
	N	-1.290070365800	4.792403499100	-2.184012878000

	H	-0.389524317800	5.284687429400	-2.228609513500
	H	-3.198944128600	3.620154396000	-1.358328155800
	N	-3.887260582400	2.688858191100	-2.497337564000
	H	-3.485945838600	4.765055061100	-4.578600434900
	O	-3.403030258800	5.465707949900	-3.914812289300
	C	-3.075967676600	2.047488814500	-3.294026467300
	H	-2.051094225300	2.441807684100	-3.337448105500
	N	-3.376052650400	1.023933487900	-4.143373086100
	H	-2.563440707300	0.536704743600	-4.518783514400
	H	-4.097189585700	0.388021204700	-3.775941397200
	C	-5.256287885500	2.356690545700	-2.356156151900
	C	-5.766907573600	1.030323899300	-2.227985450900
	N	-7.149533367500	0.973682547000	-1.969289512300
	N	-5.678115907700	4.719493953600	-2.199952475200
	C	-6.140172801800	3.441396296000	-2.164536839900
	O	-5.136329329100	-0.050947492600	-2.319003338400
	H	-7.541356586800	0.031965121900	-1.888330705500
	H	-6.401539728600	5.435272835900	-2.237528501500
	N	-7.474342578600	3.304094999400	-1.889635427300
	H	-4.826349992000	4.917725384900	-2.739110593600
	C	-7.934835889500	2.069981663000	-1.795035442300
	N	-9.276855175500	1.863828338100	-1.591707582400
	H	-9.535921553100	1.029283626600	-1.067082569500
	H	-9.748489039500	2.695472465700	-1.234568233600
Transition state	H	-2.405170396200	4.455866923400	-3.313653382500
	O	-2.891146684600	4.426924333400	-0.561197368400
	C	-1.907650518000	5.061377802800	-1.074778045900
	H	-1.249880115300	5.633557505500	-0.379543715900
	N	-1.614056793200	5.091316227200	-2.360201624800
	H	-0.786025117400	5.664350000600	-2.543714642700
	H	-3.276130315700	2.923906891500	-1.422065363900
	N	-3.679162534700	2.216000871500	-2.066735456900
	H	-3.959550958800	4.224819837200	-3.769740188000
	O	-3.073809642000	3.884776619400	-4.015683296000
	C	-3.027191945500	2.152593287100	-3.263986982500
	H	-1.936054095500	2.207686348200	-3.196084904900
	N	-3.513198687900	1.318590259200	-4.227609732600
	H	-3.042281488600	1.413513638400	-5.127386824800
	H	-4.529744957400	1.331510633100	-4.325357820500
	C	-5.106712027400	2.146412636200	-2.053878481300
	C	-5.736842062200	0.860079745000	-1.958497102900
	N	-7.145549411500	0.945274120200	-1.944741909300
	N	-5.293941542200	4.548728799200	-2.175114146900
	C	-5.890442693400	3.303585256500	-2.074405630200
	O	-5.190657362400	-0.250277470000	-1.912210475500
	H	-7.642860528800	0.052461180000	-1.915527181400
	H	-5.959772800800	5.301067114300	-1.999340599200
	N	-7.256721219700	3.303096308300	-2.044132848100
	H	-4.435798292300	4.640206537700	-1.605531034000
	C	-7.841494073300	2.116518372200	-1.980322622200
	N	-9.204562055000	2.041891295100	-2.005856907800
	H	-9.645664827800	1.246276326400	-1.551234111500

	H	-9.670638637300	2.929141361100	-1.819687441700
<i>G3</i>				
Reactant	C	-1.118391360500	-4.915254280700	-9.512906647400
	C	-1.746581635900	-4.705025734100	-8.215071706700
	N	-1.846775437300	-3.343838329000	-7.896004826500
	N	-0.269331902700	-4.183099302300	-11.500695227900
	C	-0.739089189500	-3.737833846600	-10.183842123400
	O	-2.189937822800	-5.570563977000	-7.442503210900
	H	-2.311304943000	-3.147580709400	-7.005296224700
	N	-0.866409771500	-2.432271045400	-9.839169631700
	H	0.599438738300	-3.681906971700	-11.849110813800
	C	-1.423411821300	-2.271114190200	-8.657413215600
	N	-1.702343125700	-1.002869959700	-8.127153885900
	H	-1.327770252500	-0.894328144700	-7.180282865800
	H	-1.269115518600	-0.289956691500	-8.717338630300
	C	-0.045063624800	-5.696873774400	-11.248753170200
	N	1.400770876900	-5.826294927800	-10.999251431300
	H	1.575364598600	-5.468021418000	-10.049977674100
	H	1.581498822200	-6.833990974200	-10.918197759900
	H	-0.264094531100	-6.227056545500	-12.188126176500
	N	-0.893361928200	-6.080924506000	-10.151059219600
	O	1.767990596500	-2.675332768100	-12.510382151700
	C	2.824922840400	-3.141262219500	-12.984555411000
	H	3.508628679300	-2.495333053000	-13.571904901800
	N	3.225930248500	-4.407817716600	-12.852914474600
	H	4.125069380800	-4.700931167600	-13.224389533800
H	-1.001389077100	-4.045200333000	-12.217065672200	
H	2.668925352100	-5.040782695900	-12.253410007700	
Product	C	-1.492146686100	-4.824848205400	-9.549279059600
	C	-2.579655138800	-4.736958651200	-8.608588780000
	N	-2.732810884500	-3.402282449000	-8.169869795400
	N	0.158798114100	-4.057630106400	-10.780901916100
	C	-0.785301121000	-3.657148244200	-9.874328123600
	O	-3.329820586500	-5.624299288300	-8.191945253000
	H	-3.539841164400	-3.239263353200	-7.563457144700
	N	-0.970041414300	-2.386001744900	-9.408030684300
	H	2.953713811300	-3.964920550100	-11.746634507300
	C	-1.976761076200	-2.316572374600	-8.558567857100
	N	-2.381755562300	-1.092433050900	-8.068814174400
	H	-2.696108932100	-1.080600055500	-7.098602670000
	H	-1.684590970000	-0.369028450500	-8.238869358100
	C	-0.009880276300	-5.408430483100	-10.964650624000
	N	3.695777193000	-5.084991225200	-10.925684067400
	H	4.662061816400	-4.865135631600	-10.662271940600
	H	3.246065778000	-5.410080568300	-10.064289822300
	H	0.616283251900	-5.964057414600	-11.663319623700
	N	-1.005835258400	-5.920532397500	-10.237775535200
	O	2.439919824600	-3.227711387700	-12.280795505200

	C	2.051276468600	-3.745265655200	-13.463654152200
	H	1.598690331400	-2.974519701700	-14.109703301800
	N	2.192993972300	-4.988571481600	-13.761343765100
	H	1.817424138100	-5.117712835700	-14.710573815800
	H	0.890111058400	-3.494551457200	-11.231316764500
	H	3.755885496600	-5.905779115300	-11.535618961700
Transition state	C	-1.040792779000	-4.922842772200	-9.571084101100
	C	-1.671854108400	-4.746081440700	-8.275833084600
	N	-1.788252261100	-3.390813789800	-7.933876659700
	N	-0.190032978800	-4.142167204000	-11.555862030400
	C	-0.692979551000	-3.737701687100	-10.252937411600
	O	-2.115952610100	-5.626351095900	-7.513533303500
	H	-2.256191671300	-3.215152111900	-7.040835891700
	N	-0.829732636700	-2.440996279600	-9.868986637900
	H	0.937252674000	-3.236923033800	-12.155511575600
	C	-1.381264730900	-2.305017058100	-8.680765564300
	N	-1.672339833500	-1.044117902300	-8.130764066800
	H	-1.293323159800	-0.946065153700	-7.184552232900
	H	-1.238987074000	-0.323941867700	-8.711963842700
	C	0.035353792900	-5.611836118900	-11.319716786400
	N	1.504033893400	-5.707921482200	-10.990403393900
	H	1.642688715300	-5.245335202300	-10.079858810900
	H	1.739600609600	-6.694754250800	-10.826638965700
	H	-0.097147399700	-6.168216609500	-12.260544471000
	N	-0.786716844300	-6.076408595500	-10.233048725100
	O	1.611665240200	-2.580493854700	-12.626089899600
	C	2.702863362300	-3.199911881400	-12.985331642500
	H	3.403656944100	-2.584725747600	-13.567110950100
	N	2.968982725200	-4.437980168100	-12.695274646400
	H	3.875852451500	-4.766580020000	-13.037511036900
	H	-0.953508657200	-4.042508971900	-12.246532260400
	H	2.285234913200	-5.099165109400	-11.909368320100
<i>PI</i>				
Reactant	H	-2.631647148500	0.940339178500	0.796056061800
	N	-2.226901067200	0.072769947300	1.165436906800
	C	-1.013038499100	-0.283702212400	0.530852493800
	C	0.079360015600	-0.725506221100	1.340116289500
	N	1.185324673300	-1.174137761100	0.605371320200
	N	-1.998241226300	-0.162068977200	-1.678813037700
	C	-0.921075606400	-0.419787752500	-0.854420185600
	O	0.129880719800	-0.729961216700	2.588936775000
	H	1.989855807900	-1.477270057600	1.156252601300
	H	-1.723588462000	0.013031067200	-2.644356525000
	N	0.199461622900	-0.862964231700	-1.508640544800
	H	-2.685943401400	0.511682871500	-1.350326282900
	C	1.217545995700	-1.227771354600	-0.757005860300
	N	2.402151875000	-1.605255745100	-1.348555440400
	H	2.974350011200	-2.267667739300	-0.830203095400
	H	2.276187018900	-1.890591474800	-2.318763483000

	O	-2.341301252100	-2.819460347700	0.256448359700
	C	-3.274483460700	-2.124333347400	0.643805677500
	C	-3.582107068300	-1.941021121600	2.118025379000
	H	-3.987210633200	-1.634013262400	-0.056938949000
	O	-2.976160267600	-2.551165389200	2.989672138800
	H	-4.420508400700	-1.247180937800	2.352022590900
	H	-0.840883696900	-0.852302562700	4.186395126600
	O	-2.914459333400	0.603786646100	3.957830668300
	C	-2.572456999200	-0.079871442500	4.934599429300
	H	-3.207352868800	-0.143860975900	5.845060186800
	N	-1.422294137800	-0.765516994600	5.026133166500
	H	-1.268456954700	-1.389902245900	5.810790379100
	H	-2.089235843900	0.233760865100	2.174135615200
	H	-2.896004502400	0.367753220700	0.979946445000
	N	-2.303160764300	-0.336303071900	1.432342163100
	C	-1.100811757700	-0.622622422300	0.701928291500
	C	0.087654396100	-0.822972683700	1.489078351100
	N	1.214245447100	-1.171799027300	0.715033557300
	N	-2.113231488100	-0.511129785900	-1.509664108500
	C	-1.017016181600	-0.701474460300	-0.688418906100
	O	0.201245614900	-0.718731712200	2.717413907800
	H	2.080574996700	-1.325982056300	1.236548696700
	H	-1.842127305300	-0.348759082800	-2.479081476100
	N	0.123885551500	-1.038610547600	-1.371212672400
	H	-2.810127971500	0.163116347100	-1.201245190700
	C	1.198243084300	-1.280545290200	-0.643246216500
	N	2.377084307700	-1.582467865400	-1.269620976500
	H	3.065630406000	-2.115171742900	-0.740744937800
	H	2.257431174800	-1.907735579200	-2.225698168000
	O	-3.212458173200	-3.380170401400	0.178941770600
	C	-3.569867310500	-2.258588731100	0.496651828500
	C	-3.101505374300	-1.557640452000	1.765533472200
	H	-4.268732345700	-1.669110773900	-0.141193364000
	O	-2.342259091200	-2.442508070700	2.516050139700
	H	-4.002855871600	-1.184410537900	2.298873596900
	H	-2.229586381500	-1.983679404300	3.397283672500
	O	-1.952983167300	1.011268444000	3.834060067900
	C	-2.102856028600	0.230819438900	4.903100655700
	H	-2.060981692700	0.809138502500	5.839707466900
	N	-2.289178273900	-1.042945696300	4.842189952300
	H	-2.384340847600	-1.410682989000	5.796488622600
	H	-1.961763028900	0.441249718300	3.004223723600
	H	-2.885707657200	0.399259515500	0.924595231500
	N	-2.256103218900	-0.233606004400	1.435274419200
	C	-1.028274973300	-0.498039698600	0.717988702100
	C	0.158221142700	-0.680971148100	1.506628467800
	N	1.270786302100	-1.054982242600	0.725043950700
	N	-2.096567594100	-0.475702156400	-1.467218239000
	C	-0.980494296300	-0.627579613700	-0.668737373400
	O	0.278890331200	-0.539031972500	2.727329154600

	H	2.144261734900	-1.198266269900	1.238635907900
	H	-1.860049948400	-0.404450764700	-2.458392894500
	N	0.146243980000	-0.993906090000	-1.350073138400
	H	-2.767464844200	0.244963921300	-1.208417876400
	C	1.233692041300	-1.211030009600	-0.628037401500
	N	2.397807700400	-1.533833069400	-1.260054039400
	H	3.102430140600	-2.042897400200	-0.730006912400
	H	2.273229963000	-1.866584322100	-2.212657091200
	O	-3.354127734100	-3.314760561500	0.251804194500
	C	-3.586529730100	-2.163019753100	0.573650642400
	C	-3.021715495200	-1.540296414000	1.849542279600
	H	-4.262361034100	-1.515287900300	-0.033517241400
	O	-2.209331398100	-2.350276799200	2.533363643100
	H	-3.883724250200	-1.115151905100	2.423186920400
	H	-2.166131687400	-1.832149935100	3.621812482200
	O	-2.206706046200	0.914563423200	3.730956648000
	C	-2.172670407100	0.141281296200	4.744476561500
	H	-2.120217764600	0.627348281300	5.742677785300
	N	-2.208836752400	-1.175227097500	4.711194847500
	H	-2.157705189200	-1.601798128700	5.637205180600
	H	-2.096057151200	0.269795780200	2.428720626800
<i>P2</i>				
	H	-2.820164986700	-1.106495288500	1.660073398000
	N	-2.094133557900	-0.379586178800	1.644238278900
	C	-0.992949428100	-0.610820634300	0.778008888500
	C	-0.255467623900	-1.809688856500	1.084234358500
	N	0.849984821000	-2.036108271800	0.248573620600
	N	-1.241683808900	1.312156883100	-0.701027420200
	C	-0.592190100300	0.158906596100	-0.319070995700
	O	-0.529027267400	-2.631619149200	1.976551033600
	H	1.406656344400	-2.867522260400	0.457980672200
	H	-1.032299272700	1.594916704600	-1.656567054700
	N	0.539548989400	-0.105766145100	-1.059989394500
	H	-2.230531019700	1.366230645600	-0.448225142600
	C	1.223236828300	-1.185549152800	-0.748870309800
	N	2.409993381800	-1.452839691700	-1.392261264800
	H	2.651362525700	-2.438004192800	-1.504262728800
	H	2.506076616800	-0.939267149300	-2.268744419300
	O	-1.744176145600	3.113234065400	1.942450463600
	C	-1.554902756000	1.937492062500	2.209060959000
	C	-2.627227472600	0.885504548000	1.954773025400
	H	-0.624728691800	1.578504795800	2.702560234400
	O	-3.550196445900	1.391960421700	0.940857001400
	H	-3.207479577700	0.792099633800	2.895675139400
	H	-3.659787578600	2.350232031900	1.116049453000
	O	-5.850835804100	-0.049513829200	0.668942006700
	C	-5.774771918700	-1.276518172300	1.205603823400
	H	-6.722406706500	-1.822740994100	1.077481423800
	N	-4.723965120800	-1.734239378600	1.788806225000
	H	-4.928896479900	-2.688372114400	2.113134682100
	H	-4.989635388400	0.423739167100	0.807198518000
Reactant				

Product	H	-3.666285778700	-1.639241437100	1.662330989200
	N	-2.095414899000	-0.526863937400	1.638804471400
	C	-0.909244391400	-0.675957441300	0.885217083200
	C	-0.238373591300	-1.937130346200	1.068862854400
	N	0.889000587600	-2.101002712900	0.244910006900
	N	-1.196702535800	1.296140825600	-0.526064014200
	C	-0.518365033400	0.161612633500	-0.179156073100
	O	-0.546797138700	-2.828147659800	1.872904631300
	H	1.438747233300	-2.945468914000	0.408675398300
	H	-0.943594839800	1.654120927200	-1.445519506300
	N	0.585486368100	-0.088525060700	-0.952444555600
	H	-2.192915828000	1.394253532200	-0.288695889000
	C	1.267078015500	-1.191670343200	-0.697180586300
	N	2.436671372000	-1.423568532600	-1.361620627600
	H	2.732080907200	-2.392162529600	-1.477383690100
	H	2.553475526100	-0.863814741800	-2.205841213200
	O	-1.952298630500	2.959346766800	2.332722028300
	C	-1.500323730400	1.826349486200	2.200731879900
	C	-2.395364624900	0.631842477700	2.145377113500
	H	-0.406083496000	1.624271760600	2.179563280400
	O	-3.971708003600	1.961346571000	0.098626213600
	H	-3.372568558900	0.735465428600	2.638856767100
	H	-3.871392594900	2.624609152100	0.799388664700
	O	-5.600789510600	0.060193725400	1.334546652600
	C	-5.672023100500	-1.169722498900	1.505760324800
	H	-6.659245040500	-1.678236753600	1.536211281900
	N	-4.633696511000	-1.998979461000	1.670411385800
	H	-4.802961887900	-2.991473441000	1.814238546200
	H	-4.516893372100	1.267569166900	0.526772907700
	Transition state	H	-2.939833970500	-1.172555434200
N		-2.140918871900	-0.436967557600	1.624690355600
C		-0.999154294400	-0.660542012900	0.811207860600
C		-0.323911424700	-1.899655682500	1.070582482600
N		0.790763198400	-2.113107448200	0.242935674100
N		-1.218155595300	1.318647133200	-0.586754420700
C		-0.583336929500	0.159805431100	-0.250423323300
O		-0.639008875500	-2.742877876900	1.924339066400
H		1.332580775600	-2.957929171300	0.431563295700
H		-0.934120113000	1.710038978300	-1.482883422900
N		0.537104086900	-0.114980924200	-0.992952084900
H		-2.208202919800	1.433341312100	-0.329371565800
C		1.192937615900	-1.226774477600	-0.712689422500
N		2.366807969800	-1.491152729000	-1.360080091900
H		2.640077171500	-2.467880063100	-1.462507243300
H		2.497490779500	-0.948591058500	-2.213260102800
O		-1.930251516400	3.021941869500	2.400154136800
C		-1.564143018300	1.872018892400	2.216000318900
C		-2.545433712100	0.736449118600	2.064220009500
H		-0.490246417700	1.582421672000	2.212311842300
O		-3.687405980600	1.512985510900	0.684619334900
H		-3.383041135700	0.715227124600	2.771087294300

	H	-4.005580549200	2.377718309500	1.006093826000
	O	-5.607978063300	0.046917514900	0.823763683800
	C	-5.523884654500	-1.164600048300	1.279904814300
	H	-6.493963918200	-1.703924189000	1.293119251200
	N	-4.440625748000	-1.766076086100	1.700001010200
	H	-4.682209917300	-2.715866465200	2.003791866700
	H	-4.590376018800	0.772231532800	0.757392742800
<i>P3</i>				
	H	-1.202663432900	0.567224430500	4.263045896900
	N	-0.479934722300	-0.070085808900	3.947569828100
	C	-2.050740523500	1.957328642000	2.323999860800
	O	-1.606477418400	0.959582728300	1.745747190900
	H	-3.084622534600	2.320960851700	2.118101114700
	H	-1.455413136800	-1.111268241400	1.796363281600
	O	-1.079313924500	-2.829175290700	3.724127441800
	C	-1.281115581000	-3.042160156700	2.518037709900
	H	-1.323365275100	-4.077550367700	2.119698769500
	N	-1.481061575100	-2.106266410100	1.576072058700
	H	-1.604547615100	-2.388427973100	0.609040403300
	H	-0.620570859700	-1.084893946900	4.047886500000
	N	0.028809071400	2.835439123400	3.425031407100
	C	0.866340923500	1.779553774700	3.139594186100
	C	2.228762105000	2.189821117000	2.835442764900
	N	3.100372006100	1.123722845400	2.556378744800
	C	0.631582824100	0.388207947000	3.359476021700
	O	2.651993518200	3.348165945400	2.751909336500
	H	4.019363331600	1.395806415200	2.202505492000
	N	1.552922583900	-0.586339140300	3.068522110200
	C	2.736133310100	-0.189117078200	2.640834301500
	N	3.643988374300	-1.116580301300	2.221255100000
	H	4.631114585400	-0.873027206600	2.269590218500
	H	3.432552584800	-2.071142479000	2.507079903700
	C	-1.272273044000	2.837990186500	3.210288648200
	H	-1.804203456400	3.742272599000	3.542503788600
	H	-0.846674015400	-0.276648321500	4.618337667800
	N	-0.627290385100	0.571307118300	4.092291883500
	C	-1.706006244700	1.223652581700	3.392635291600
	O	-2.085968855500	0.557317484600	2.176507576100
	H	-2.574168141800	1.280148908100	4.068038486700
	H	-2.243489195400	-0.397675644000	2.404577215700
	O	-0.047888296200	-0.868777494700	1.023159817900
	C	-0.431909301300	-2.004200052700	1.628370460500
	H	0.286811819700	-2.818791512000	1.451247813900
	N	-1.519254277500	-2.094941759600	2.312582217500
	H	-1.612264134400	-3.046687246200	2.685401137000
	H	-0.711440988100	-0.176242799800	1.275004733000
	N	0.004885134600	2.802139204300	2.574327621200
	C	0.888953969700	1.726780398800	2.695540021800

	C	2.171221047100	1.801300266700	2.044306658100
	N	2.992050409700	0.696389445000	2.345805575900
	C	0.611412709400	0.622300070500	3.510273869900
	O	2.583461423700	2.683170515500	1.281845156200
	H	3.872666005500	0.657286747300	1.828474016800
	N	1.492518891600	-0.369913221100	3.833767109200
	C	2.663439205600	-0.297887956500	3.224004280000
	N	3.593058126400	-1.288875138800	3.416115059100
	H	4.567943357800	-0.991375056100	3.401193659600
	H	3.383221775200	-1.875478428300	4.223345113200
	C	-1.215484436500	2.590488421100	2.983479426600
	H	-1.926758985100	3.426222066400	2.961956438100
Transition state	H	-0.486033554700	0.126207895600	4.625054063200
	N	-0.347445982700	0.069351254700	3.600895634800
	C	-1.455384973700	0.832385776000	2.853480596500
	O	-1.417897986700	0.514401504700	1.538211631200
	H	-2.379793776200	0.526595018100	3.388558694600
	H	-1.926789355800	-0.610029091700	1.481313026200
	O	-0.764498251300	-2.415745096700	3.078227151600
	C	-1.734635011100	-2.665957960700	2.291669147700
	H	-2.081206246400	-3.719121807000	2.234425672100
	N	-2.359214762300	-1.773413227800	1.548146221600
	H	-3.118138089100	-2.154683957200	0.983908411800
	H	-0.469200589700	-1.017103012300	3.327990294500
	N	0.007933436200	2.831650726300	3.030653796100
	C	1.074334136000	1.911732520200	2.953266625100
	C	2.390447910600	2.424369628500	2.619346798200
	N	3.376191445900	1.416268037100	2.625576460400
	C	0.968385578800	0.563103841800	3.238882113000
	O	2.691757214000	3.586947561200	2.347237220400
	H	4.324886176800	1.738105405000	2.411287556300
	N	1.949741137100	-0.361796345500	3.254295602400
	C	3.156919429300	0.104304037400	2.934517186600
	N	4.193749631400	-0.762511685300	2.856243837500
	H	5.153647300200	-0.426222326000	2.849549889000
	H	4.048154692400	-1.655980939000	3.319466356800
	C	-1.182960757700	2.311576484300	3.039437147100
	H	-2.043224043100	2.994037859400	3.087704886200
<i>P4</i>				
	H	-0.390822350200	-0.914305096300	2.609740214500
	N	-0.308734610900	0.119083046900	2.653507013200
	C	-1.449349621000	0.778381153800	3.211670792700
	O	-1.704718125900	0.392330632500	4.592502801900
	H	-2.361208566600	0.447367790800	2.693290778400
	H	-0.961874015900	0.711880049200	5.139812418700
	O	-2.305437613700	-2.241659416200	4.900828147200
	C	-1.825930294500	-3.052127613500	3.947746208500
	H	-2.124861855700	-4.094937570000	4.135142236200
	N	-1.118521469900	-2.647242895200	2.952414218800

	H	-0.873214445900	-3.462109215000	2.377205347800
	H	-2.015295773800	-1.307404646300	4.730315214300
	N	-0.097513444400	2.859654755100	3.158131940000
	C	1.025213823900	2.031093716200	3.115265603500
	C	2.329455220700	2.631906990700	3.237713402500
	N	3.371550493800	1.694033527900	3.081397271400
	C	0.930177858700	0.660442117500	2.829149117500
	O	2.602002329400	3.818228437000	3.453179009600
	H	4.319202588800	2.075973676800	3.114651146600
	N	1.991012946800	-0.183183611000	2.650081462200
	C	3.183624386400	0.374256415900	2.778374233100
	N	4.299619129100	-0.375583916700	2.541060289900
	H	5.164903547300	-0.112031221900	3.011344625600
	H	4.129116245300	-1.379846818200	2.531145686600
	C	-1.261715136700	2.269290462200	3.127093092300
	H	-2.161683476900	2.898201844600	3.128157475200
Product	H	-0.512489444200	-1.341932211900	3.864702267800
	N	-0.300576997500	0.610578774000	3.715146883400
	C	-1.212135645700	1.593156972900	3.714234138800
	O	-3.430749276800	-0.546038573200	4.694209640600
	H	-2.213197932400	1.319810312000	4.065533838600
	H	-2.917301130500	-0.621066854900	5.511426980200
	O	-2.574445142100	-2.864695119500	3.403509849900
	C	-1.372306369100	-3.180653646100	3.449936665400
	H	-1.050213791800	-4.222171113800	3.239418191900
	N	-0.364969837000	-2.354256664400	3.755975060200
	H	0.594222965100	-2.681597842500	3.696948110100
	H	-3.128412548900	-1.327456609100	4.184811506500
	N	0.300157387800	3.236545021300	2.796207011900
	C	1.210524674200	2.237679695800	2.792519496100
	C	2.549198121000	2.540405853200	2.246654940400
	N	3.406046327200	1.444366212900	2.309330812900
	C	0.942230037300	0.924112655500	3.255810942800
	O	2.909307152000	3.613114745300	1.772986948400
	H	4.325976376200	1.587616264100	1.885920289800
	N	1.868104669600	-0.094363507300	3.280104638900
	C	3.060565466500	0.201857992200	2.806285393600
	N	4.021764899800	-0.758729260200	2.720602619200
	H	4.995757521900	-0.464837212200	2.731800471200
	H	3.833814399000	-1.597712646600	3.265326298200
	C	-0.910308665400	2.896880021400	3.269869258500
	H	-1.675989033200	3.680566042800	3.291069289700
	H	-0.600898893900	-1.606333157400	2.777407753900
	N	-0.343015479400	0.059186458900	2.620059540200
	C	-1.432349054600	0.785982750000	3.093204252600
	O	-1.744439301200	0.347709390600	4.641033015800
	H	-2.393097600100	0.450885388600	2.672576068200
	H	-0.907859119800	0.492768381500	5.126440342200
	O	-2.320864223900	-1.992605329100	4.740725017600
	C	-1.779771819700	-2.852232618700	3.966487177100

	H	-2.074369880300	-3.901237610500	4.123363118800
	N	-0.917926881000	-2.598037392700	3.008701621000
	H	-0.575447192400	-3.388891824300	2.464988143600
	H	-1.990604349200	-0.863483179500	4.656463135600
	N	-0.097295875300	2.839293330700	3.225479160500
	C	0.997866090200	1.999059215600	3.161792760200
	C	2.309505969300	2.587978558000	3.313985940900
	N	3.343893553300	1.660714540800	3.107153123100
	C	0.866215741800	0.634413631500	2.803261486700
	O	2.586256939900	3.762158672700	3.593373503200
	H	4.294358793100	2.032553263600	3.159693072200
	N	1.956973637800	-0.189370297000	2.569697911300
	C	3.140525243200	0.355254583800	2.733785220500
	N	4.274030771700	-0.377474844800	2.463632321500
	H	5.106180758400	-0.153605345100	3.009325839700
	H	4.095689972900	-1.379840351000	2.424064536300
	C	-1.271940309800	2.254140423400	3.129188491400
	H	-2.167399297100	2.889467820300	3.119944605800
<i>XI</i>				
	H	-2.052493704300	0.862309234500	1.343793877800
	N	-2.112509321300	0.266290176900	0.505642007800
	C	-0.817684301700	-0.276874668300	0.235518001000
	C	-0.274587988600	-1.366562147700	0.950621466700
	N	0.981968989100	-1.796743870100	0.518170978800
	N	-0.503285975600	1.394732308700	-1.445235812600
	C	-0.041957197600	0.291269940900	-0.791288816700
	O	-0.797862327700	-1.977104567500	1.937769932600
	H	1.397384048700	-2.577121551600	1.033106660700
	H	-0.094771472100	1.579788882900	-2.358628055600
	N	1.193073029100	-0.160031849600	-1.164739844600
	H	-1.508803411300	1.541826228300	-1.358757973500
	C	1.664475275800	-1.198741603600	-0.498326210200
	N	2.924477047400	-1.667218795100	-0.770273458800
	H	3.080476560600	-2.665580019800	-0.644850912200
	H	3.286562210500	-1.333285727800	-1.663497848100
	O	-5.135163967400	-4.707381542400	3.189454635200
	C	-5.227857039900	-3.670346536600	2.556551893400
	C	-4.015843718400	-2.871877918000	2.085450115300
	H	-6.198398630900	-3.213571939200	2.265643538400
	O	-2.867309726300	-3.418666426500	2.444592877300
	O	-4.176216498300	-1.840355408400	1.442565758400
	H	-2.105843435600	-2.837392113100	2.122630933800
	O	-2.065812577200	1.678183291900	3.158332744400
	C	-2.291555740900	0.906710431700	4.102108014200
	H	-2.700323596700	1.279874097100	5.066114581500
	N	-2.093236960200	-0.423150520200	4.088539171100
	H	-2.242790102800	-0.962188537300	4.936961522500
	H	-2.738182954500	-0.498987499400	0.779757491500
	H	-1.645457321900	-0.877475841000	3.285460553800
Reactant				

Product	H	-2.865844699800	0.045121908900	0.814434115800
	N	-2.295342005700	-0.615307993600	1.352465144900
	C	-1.079110812800	-0.926528534900	0.653291977200
	C	0.019226777400	-1.384305413300	1.442741797300
	N	1.224299480900	-1.492519336800	0.746805554600
	N	-1.877536236400	-0.106620455600	-1.471650810600
	C	-0.861507397500	-0.616308879800	-0.694042522900
	O	-0.019135048800	-1.704173530200	2.655534145700
	H	2.008301704000	-1.877646898000	1.275446135900
	H	-1.649631762100	-0.105911733500	-2.466552375200
	N	0.358460325000	-0.714719202200	-1.305183934200
	H	-2.782868229000	-0.541889868700	-1.281751029100
	C	1.364031851600	-1.154077108100	-0.568081843300
	N	2.614649189100	-1.226859088000	-1.111089550900
	H	3.281663242300	-1.869836391700	-0.691680995700
	H	2.626181684600	-1.223506939300	-2.129267246900
	O	-3.970632020800	-1.948724565800	-0.536112662000
	C	-3.907313807300	-2.406584751300	0.594140813600
	C	-3.168180036200	-1.735273330000	1.756704239700
	H	-4.417287094400	-3.357594444800	0.868727407900
	O	-2.414577824200	-2.745371224800	2.356302280500
	O	-4.186192686700	-1.231688572000	2.561296676000
	H	-1.581105115200	-2.333707522200	2.706529200200
	O	-1.323206170600	0.929272034300	3.432523991000
	C	-1.851398937200	0.566959962400	4.600383367900
	H	-1.353775398000	1.057826118800	5.451053849800
	N	-2.837117351900	-0.257056203100	4.704318992200
	H	-3.071365602300	-0.391605591000	5.694438591600
	H	-1.742068392000	0.361549630400	2.716157203600
	H	-3.726284965900	-0.882772595200	3.387029756600
Transition state	H	-2.878486253100	0.031477363000	0.786867936500
	N	-2.284646631300	-0.583546236800	1.356847283300
	C	-1.056541832500	-0.885661434200	0.665175755400
	C	0.033921616200	-1.320583927400	1.477062930500
	N	1.240770346800	-1.455905460400	0.787517026500
	N	-1.850069959000	-0.150504223100	-1.494521630000
	C	-0.841243050400	-0.629308560500	-0.692660507900
	O	-0.011130793700	-1.596172022300	2.698533319600
	H	2.022253148500	-1.816520718700	1.334793914100
	H	-1.628586182600	-0.208228895700	-2.489150064300
	N	0.378141660800	-0.768779072800	-1.298645672500
	H	-2.771653971700	-0.537876458900	-1.276845629900
	C	1.380455671100	-1.183883989500	-0.542857497800
	N	2.630047767300	-1.299153106200	-1.081011553500
	H	3.271926014600	-1.958185503000	-0.647211709000
	H	2.642817868200	-1.311929020500	-2.099084100800
	O	-4.108938763600	-1.725410566700	-0.469131817700
	C	-3.970821805500	-2.292959181700	0.608199262700
	C	-3.182960007900	-1.745271111100	1.795159490800
	H	-4.519850440700	-3.235024272300	0.838674488700
O	-2.348426614600	-2.802740783800	2.227847790800	
O	-4.085774393400	-1.301083284500	2.667282914600	

	H	-1.574584562700	-2.398856655900	2.685290134500
	O	-1.565100595800	0.907878590900	3.249996652300
	C	-1.915572349500	0.524372258900	4.425326619200
	H	-1.425332336500	1.030553872700	5.271730882400
	N	-2.799149844600	-0.411245631300	4.662303571500
	H	-2.998732899200	-0.622109048900	5.640094821600
	H	-1.958268847200	0.201543455300	2.426603805100
	H	-3.392410505300	-0.860883996900	3.816955158100
X2				
	H	-3.200757793600	-0.251356960900	0.573052026900
	N	-2.396962007500	0.396033516600	0.608016440800
	C	-1.167298285000	-0.281528160900	0.349922221700
	C	-0.897362968400	-1.593393516100	0.829020811000
	N	0.343806082700	-2.105364424000	0.428477246700
	N	-0.469782686400	1.587315025800	-0.979960281900
	C	-0.226700320700	0.328908937300	-0.493486154400
	O	-1.630446709800	-2.341540314500	1.525837550100
	H	0.564102070300	-3.046412869300	0.765836251900
	H	0.089861176500	1.848830415800	-1.790339729900
	N	0.981169017300	-0.214762976000	-0.830366846000
	H	-1.460464095200	1.819055252200	-1.050453411600
	C	1.228579103700	-1.422373932700	-0.351817006400
	N	2.440325938400	-2.010237575100	-0.587242413300
	H	2.468855727900	-3.028368293400	-0.579297252200
	H	2.952933514400	-1.597079320200	-1.363543085000
	O	-1.963237879700	3.484752852300	1.860187856700
	C	-1.509347411400	2.352353960900	1.789750388900
	C	-2.444711243400	1.139415901700	1.860242393400
	H	-0.421279069900	2.149717689600	1.724669684900
	O	-3.767440473200	1.563163078100	2.017223758900
	O	-1.976327494500	0.450367376200	2.999866961900
	H	-3.710977191400	2.524308839200	2.190215161400
	O	-3.739797211500	-1.759987211400	2.893913956900
	C	-4.854248091000	-1.480339664900	2.187177354300
	H	-5.720074923500	-1.321197975100	2.848166233900
	N	-4.851395649500	-1.411856140600	0.904889994800
	H	-5.804478026400	-1.178013248500	0.595402262500
	H	-2.986116560200	-1.980886741500	2.254653742400
	H	-2.641523557000	-0.242240668600	3.188331575800
	H	-3.716823234000	-1.881751535100	0.972821745200
	N	-2.709269080600	0.294521354100	-0.283099386200
	C	-1.378935764200	-0.205709855600	-0.172288724900
	C	-1.225137459900	-1.613410079000	0.027045987900
	N	0.103564229600	-2.048478200800	0.003408323500
	N	-0.339363044700	1.943268867200	-0.592132553300
	C	-0.242273185300	0.572560706600	-0.392436624900
	O	-2.135474441300	-2.449442378200	0.216442670400
	H	0.235514419900	-3.053380097300	0.124900083600
	H	0.492266548000	2.326686135600	-1.044303894700

	N	1.034875114200	0.085777368700	-0.358985528200
	H	-1.187450346400	2.236582901000	-1.079885961900
	C	1.167268446300	-1.211491541000	-0.145058603900
	N	2.420914061000	-1.743635726300	-0.008670595400
	H	2.539867287400	-2.738459608200	-0.196335207700
	H	3.157308284500	-1.170539699600	-0.417634065500
	O	-2.569594281600	2.792060289700	2.260002357300
	C	-2.187758465200	1.776826180500	1.688604269600
	C	-3.029287761100	1.218003828600	0.561709718300
	H	-1.276787785900	1.220128276000	1.967642165400
	O	-4.261321301200	1.763680749400	0.495270129400
	O	-0.580304777400	-0.951510808300	2.898196456100
	H	-4.267073499000	2.488500790600	1.156898756200
	O	-3.317639870400	-0.290411806700	2.948198948600
	C	-4.406469035100	-0.721492306400	2.519067653900
	H	-5.364099225600	-0.402099892100	2.981003846500
	N	-4.546645816100	-1.579428354400	1.504949709600
	H	-5.475097830800	-1.850511523500	1.192611976900
	H	-1.550588709800	-0.888475265400	2.801460278300
	H	-0.447499064400	-0.515199975200	3.753780349900
	H	-3.664002154200	-0.629586189700	0.701821880100
	N	-2.466768074200	0.346033137300	0.573521611800
	C	-1.205351481900	-0.262191987800	0.327658707700
	C	-0.907443735500	-1.573154966300	0.836484519700
	N	0.339983303800	-2.068468491700	0.390012899800
	N	-0.529204912800	1.640581103600	-0.959605928400
	C	-0.281091662900	0.349143419700	-0.520536211000
	O	-1.606138861000	-2.280207133400	1.583296650300
	H	0.588970890800	-3.000365696200	0.731372374200
	H	-0.041596769200	1.874686204200	-1.824792956800
	N	0.916480970900	-0.194666101100	-0.918034779200
	H	-1.532120666700	1.833039058800	-1.005895584100
	C	1.181295785400	-1.396873236000	-0.445737561300
	N	2.388935390600	-1.995391578800	-0.735661953800
	H	2.386246823700	-3.015125596000	-0.748475205800
	H	2.825527799000	-1.609874201400	-1.572925204100
	O	-1.493739067600	3.233477459200	2.355838646300
	C	-1.307513066200	2.087553896900	1.960285699300
	C	-2.495772402700	1.203605154200	1.610698106900
	H	-0.298503188600	1.639814480700	1.883697350800
	O	-3.684164975500	1.895378905300	1.711702637700
	O	-2.391530996300	0.315615101900	3.086400431100
	H	-3.452190421600	2.741437676800	2.147695336400
	O	-4.071901722600	-1.455558634600	3.167688069700
	C	-4.702582922800	-1.807191617900	2.103699862300
	H	-5.492286870600	-2.559454377200	2.248998832800
	N	-4.492208011200	-1.336693128400	0.904685178100
	H	-5.062390802000	-1.719737040600	0.149638918300
	H	-3.284449501600	-0.684520327800	3.030904602100
	H	-2.750266498500	0.907671314400	3.777393978900
Transition state				

X3				
Reactant	H	-1.242771633400	0.752344764000	4.556170737700
	N	-0.766041954700	-0.006853396900	4.072543420700
	C	-1.919684154200	1.959739327500	1.768955916800
	O	-1.499527084400	0.869901728400	1.411238380600
	H	-2.825374277700	2.426651536100	1.322101333600
	H	-1.625712280800	-1.257210054000	2.502363988000
	O	-1.304378269200	-2.876841431000	4.471929875400
	C	-1.566423991200	-3.147518960900	3.291461833100
	H	-1.668263626600	-4.200054053900	2.948543239700
	N	-1.781225981400	-2.248051321000	2.313375236100
	H	-1.901525682400	-2.560436563900	1.357027704100
	H	-0.803238830500	-0.914521554700	4.546587977100
	N	-0.066803493000	2.729263900200	3.326219069400
	C	0.753509250100	1.598933013700	3.089027510800
	C	2.065971821600	1.879942826000	2.578655065000
	N	2.871668770100	0.734372144700	2.450805985900
	C	0.449442486200	0.303054753000	3.513160881700
	O	2.513459038200	2.985525288800	2.230827314600
	H	3.775241544900	0.890765408100	2.002275716800
	N	1.302162824800	-0.763528151500	3.371959941400
	C	2.476490116200	-0.514918969200	2.826721026000
	N	3.339664591400	-1.552415239900	2.560250216100
	H	4.331205336000	-1.322278208500	2.619696545200
	H	3.112724563000	-2.391963779500	3.091763656800
	C	-1.244000265800	2.823762697100	2.803706418700
	O	-2.027977156100	3.897192946100	3.074811685200
H	-1.534896711200	4.475050703100	3.691828650400	
Product	H	-0.798137708500	0.052927656700	4.699538735700
	N	-0.653104727500	0.216946795600	3.696939656100
	C	-1.664740604600	1.047702309900	3.034861497700
	O	-1.879730214700	0.610315261600	1.717782197700
	H	-2.578226576100	1.010607923600	3.652959271300
	H	-2.295257383000	-0.294442874500	1.802166581300
	O	-0.999271008800	-2.594969859800	3.210635677300
	C	-2.149399797600	-2.834456059700	2.569934264800
	H	-2.384418018800	-3.909177803500	2.547188430300
	N	-2.874016945400	-1.905604256700	2.054436640500
	H	-3.702975913400	-2.312801745500	1.608603654100
	H	-0.867850861900	-1.612326312400	3.264000857200
	N	0.068026947300	2.771644325700	2.653786047000
	C	0.970064067200	1.693368136200	2.711454919900
	C	2.313305726900	1.910122608500	2.222313528700
	N	3.169309088800	0.833941643200	2.511423892600
	C	0.680488236300	0.489757505300	3.342595349000
	O	2.738342223000	2.900159314200	1.616765281000
	H	4.130490630300	0.933931362900	2.170976953300
	N	1.584285662400	-0.484730898000	3.663663887400
	C	2.819170103600	-0.267470630500	3.245705062600
	N	3.790569973700	-1.205924335200	3.466745420600
	H	4.758367034800	-0.891901858900	3.488862353400

	H	3.566410424200	-1.870287542500	4.207029435700
	C	-1.161712283300	2.464998794900	2.905482874500
	O	-2.124718899000	3.405046107200	3.029444070600
	H	-1.704270628000	4.282614363800	2.926164726800
Transition state	H	-0.770324814000	0.429368944400	4.790843424600
	N	-0.633937657900	0.164482225300	3.798583634100
	C	-1.632414450100	0.894150363500	2.882357468400
	O	-1.557355310000	0.389308286200	1.629890378700
	H	-2.609474126300	0.773796390000	3.394430041400
	H	-2.133312780100	-0.677933751000	1.689261893200
	O	-1.301083045900	-2.299764560100	3.670877696500
	C	-2.187558735500	-2.611731860400	2.807046994300
	H	-2.589017340600	-3.645276810600	2.853502021300
	N	-2.659588292700	-1.807515057400	1.876634756600
	H	-3.367703874000	-2.239241588000	1.281632527200
	H	-0.880734538400	-0.947653022400	3.710292619600
	N	0.018720785700	2.756918386000	2.832054861700
	C	0.975624480900	1.725099607800	2.896537770500
	C	2.325532922200	2.024275325100	2.456276137600
	N	3.189295551700	0.923659206600	2.591136896100
	C	0.726947325200	0.451323137700	3.372186517800
	O	2.735083056400	3.090563239100	1.991286166600
	H	4.141861901900	1.072264452600	2.240778794000
	N	1.603775061800	-0.573253580000	3.500236491800
	C	2.834935563500	-0.302035994600	3.085420363700
	N	3.779022228400	-1.282592784400	3.073301703600
	H	4.759167720000	-1.012885478800	3.114355547900
	H	3.546358533300	-2.109717590000	3.618450304000
	C	-1.208899659000	2.350355787700	2.873336344900
	O	-2.245987714800	3.204936500000	2.837127691200
	H	-1.895747589800	4.117353665900	2.770988336800
<i>X4</i>				
Reactant	H	-0.095938397700	-0.648287347500	3.553138875300
	N	0.067322565200	0.376249923000	3.576120598000
	C	-1.077981704900	1.143975399300	3.225822985900
	O	-1.412586290300	0.877059941600	1.832513321000
	H	-1.929871073800	0.862222531100	3.864067606000
	H	-2.243345288700	1.346472624100	1.620763370600
	O	-1.888272847700	-1.739581063500	1.160007722400
	C	-1.529422811900	-2.631163696700	2.094244886600
	H	-1.821541462500	-3.652262911000	1.805204000100
	N	-0.921738862300	-2.310802110300	3.181594589800
	H	-0.757566406400	-3.164272627900	3.730577881400
	H	-1.642300040900	-0.828567811100	1.466798776500
	N	0.431956568400	3.118577289800	3.167336161700
	C	1.460020742400	2.193468759100	2.923979212900
	C	2.749736610700	2.683442745600	2.520178966600
	N	3.705327136900	1.652375859800	2.398362456200
	C	1.294509888300	0.825289649500	3.150075043700

	O	3.078108498500	3.853179928800	2.278036797900
	H	4.626762021900	1.948415871900	2.065572389200
	N	2.283846827100	-0.115495960700	3.063388203400
	C	3.464408972700	0.337598528700	2.683715328800
	N	4.493078557400	-0.551401631100	2.491203665600
	H	5.438362865500	-0.197264372400	2.634195782700
	H	4.338288937700	-1.435943966800	2.972456681600
	C	-0.736057092500	2.603450300500	3.374716069500
	O	-1.816237204800	3.368629417800	3.669719510100
	H	-1.523047930400	4.301624314600	3.704683482700
	H	-0.327771679900	-1.763587309300	2.986124767200
	N	0.422765331800	0.084356845200	3.134037669600
	C	-0.664841798000	0.848242432900	3.211944274300
	O	-2.569983768100	0.991870249200	0.841318182500
	H	-1.626913016500	0.344674406300	3.342198770500
	H	-2.818409191500	1.656362465500	1.499581627800
	O	-2.833557636900	-1.410253748200	2.398465636200
	C	-2.231498129800	-2.476522864100	2.611333225500
	H	-2.764675450200	-3.450233610500	2.567273344900
	N	-0.932057831500	-2.592271376900	2.919080831400
	H	-0.528911729500	-3.512612628600	3.068305860400
	H	-2.647130753300	0.157908372300	1.337879610400
	N	0.552847038700	2.921093581700	2.975555498500
	C	1.658817424900	2.135184553300	2.919838784000
	C	2.961634778700	2.810123475300	2.789770011000
	N	4.017658724500	1.905928525200	2.721337824900
	C	1.620899519700	0.722322604900	2.977138908000
	O	3.143020063800	4.024104359400	2.737919830500
	H	4.949845030800	2.312186567600	2.615376257300
	N	2.733804496600	-0.086296277600	2.912532644600
	C	3.885745347200	0.533028301400	2.794380008100
	N	5.046611458300	-0.186314875000	2.660093940500
	H	5.876926486600	0.201499378700	3.105058713700
	H	4.920438103000	-1.175048865300	2.877512025400
	C	-0.594219078300	2.260551685600	3.110299067600
	O	-1.766333001100	2.935338728300	3.147150934200
	H	-1.579301819900	3.886024044800	3.012469790100
	H	-0.229702559100	-1.354871388700	3.243850714900
	N	0.071736443000	0.289439464000	3.540827832200
	C	-1.018256953800	1.110240957500	3.313370643300
	O	-1.529778351400	0.820376816700	1.786418560900
	H	-1.907261564600	0.833454135600	3.901256042800
	H	-2.347504617100	1.337756996000	1.634101322200
	O	-2.239724911100	-1.472475953800	1.559968302900
	C	-1.592259581000	-2.431304503700	2.099472533900
	H	-1.918013382200	-3.449656679400	1.838859735900
	N	-0.579822550700	-2.312514189600	2.928029403400
	H	-0.152037801600	-3.169249915000	3.279763396500
	H	-1.850966971100	-0.369429893900	1.711675431900
	N	0.418796754700	3.088173294900	3.046665562000

	C	1.447120139400	2.165216994600	2.862645695200
	C	2.733803919700	2.666044242700	2.458465092300
	N	3.711921895000	1.658289167700	2.406454185100
	C	1.272515138200	0.797834722400	3.157048591100
	O	3.036270063800	3.832631715800	2.159315837300
	H	4.635336710800	1.950458143700	2.078177043500
	N	2.320861723100	-0.109641596900	3.147810848200
	C	3.488642883700	0.355043283900	2.768364732900
	N	4.563143533300	-0.503872275200	2.644815523300
	H	5.480403340800	-0.100334801200	2.839069712300
	H	4.417962064000	-1.369550973100	3.162200723000
	C	-0.738527101000	2.564108891900	3.317914227600
	O	-1.830397016100	3.339483153500	3.578666894300
	H	-1.544555788900	4.273456473500	3.536645753900
<i>II</i>				
	H	-2.623249828000	0.464083411200	0.471742878600
	N	-1.954214702900	-0.105358831100	0.993287589300
	C	-0.816255362600	-0.390297004900	0.266348998900
	N	0.277395814700	-0.777352840800	0.999706039100
	C	1.352686444800	-1.102426711600	0.307953841800
	N	-2.046954231800	0.087009399800	-1.795681275800
	C	-0.860468224700	-0.355126320800	-1.124261041200
	N	2.461207342000	-1.581991420600	0.964658719900
	H	-2.666427046200	-0.716886139200	-1.948377687300
	C	0.314640618100	-0.696160225600	-1.867222035100
	H	-1.764323463900	0.378911977400	-2.736795295100
	N	1.406291361500	-1.058749222900	-1.055446698500
	O	-3.909576466600	-2.213774170300	-0.412571629300
	C	-3.199083835000	-2.435076981800	0.553818036600
	C	-3.632974464700	-2.030648114700	1.958470428100
	H	-2.222967767100	-2.960848842100	0.489030817300
	O	-2.793055528000	-2.538801692400	2.871555962600
	O	-4.622811353800	-1.356865141500	2.190974903800
	H	-3.079426106600	-2.221792264200	3.758048289400
	O	-1.980507670800	0.651362293500	3.880100546900
	C	-2.442779452200	0.124124877200	4.892605640200
	H	-1.908650932900	0.156902962900	5.865461635300
	N	-3.607167532300	-0.580089656600	4.944403929000
	H	-3.995413373100	-0.819780149000	5.854668364000
	H	-1.805784250100	0.196715296000	1.959815600700
	H	-4.257941468500	-0.501051357500	4.161453584000
	O	0.438985886800	-0.675422600600	-3.105905915400
	H	2.469360848100	-1.344975712200	1.956562122500
	H	3.361173246100	-1.407652085700	0.521624877700
	H	2.261083420500	-1.326775531000	-1.548977929900
	H	-2.920381967500	0.276525992000	0.666491230100
	N	-2.321738167000	-0.335191522500	1.232732400900
	C	-1.175754923300	-0.687592942000	0.473041697600
	N	-0.265476151900	-1.468862849800	1.142262769300

	C	0.868831834000	-1.729499084000	0.514842148300
	N	-2.032622846800	0.539393995800	-1.456990148000
	C	-1.014129574200	-0.209960139800	-0.811452461500
	N	1.774202850600	-2.587089995700	1.074636504700
	H	-2.799825890600	-0.100589611500	-1.697336187700
	C	0.240675125300	-0.455375425300	-1.478853610300
	H	-1.653101589300	0.877836717300	-2.345974364900
	N	1.145649362000	-1.215001834500	-0.718869015300
	O	-3.564775130700	-2.067756793400	-0.557194823300
	C	-3.672772428700	-2.344112209500	0.626681452100
	C	-3.141939584900	-1.447942662600	1.758177324600
	H	-4.177576027500	-3.273135976300	0.978710562000
	O	-2.387291735500	-2.215906503500	2.658922142000
	O	-4.266793762300	-0.945540357000	2.377206072200
	H	-1.456930387700	-2.189080933600	2.330553732400
	O	-1.178747824500	0.842684269500	3.454795395800
	C	-2.067517842800	1.018408820200	4.434131765700
	H	-1.619924991900	1.532455977900	5.297925715300
	N	-3.293863594700	0.630746248800	4.361361527100
	H	-3.781412966200	0.884651211600	5.228183199900
	H	-1.643040240200	0.419421999400	2.674432016100
	H	-3.936323790200	-0.363096138200	3.133403798500
	O	0.546075992000	-0.055423488600	-2.611569181500
	H	1.661214612200	-2.707759913300	2.080654710200
	H	2.750147779200	-2.503693423900	0.791140158100
	H	2.042049307000	-1.396533408600	-1.174416418300
Transition state	H	-2.911367375600	-0.035465443300	0.795684718200
	N	-2.251483521100	-0.637239111400	1.307477806500
	C	-1.056973094700	-0.765098364000	0.526206063900
	N	0.029864899100	-1.254740703600	1.205162794900
	C	1.158092435600	-1.310667466800	0.532742447200
	N	-2.150128145800	0.288344049300	-1.409802114000
	C	-1.032375586600	-0.292571233500	-0.774577796400
	N	2.276018096800	-1.895130209400	1.094204323000
	H	-2.913135527000	-0.396490335100	-1.446567536200
	C	0.223693712300	-0.327471973500	-1.496196890500
	H	-1.878632731000	0.518157944100	-2.368775591400
	N	1.276045720200	-0.871770397000	-0.761071424400
	O	-3.712694230300	-2.085359862300	-0.672300445800
	C	-3.559331035300	-2.610072999100	0.422074223400
	C	-3.040105014500	-1.899760591200	1.674830222200
	H	-3.909078935700	-3.649643634200	0.621982737400
	O	-2.141465856400	-2.821729561600	2.267658220200
	O	-4.100278043400	-1.559722832200	2.396559708000
	H	-1.979669547100	-2.517538611800	3.177139226400
	O	-1.514838585100	0.636905965500	3.362585962500
	C	-2.298399152900	0.555736073100	4.381061697000
	H	-2.000372151200	1.131102895600	5.269692326500
	N	-3.392219840800	-0.158298973200	4.422296959600
	H	-3.934623511100	-0.143858620700	5.286657069700
	H	-1.879609085000	0.047144453000	2.480299087600
	H	-3.728986497300	-0.761438494000	3.555115116200

	O	0.385546878900	0.070415395700	-2.661065200000	
	H	2.181515849500	-1.994236352800	2.105502245600	
	H	3.167812035800	-1.464242556200	0.851780365400	
	H	2.162180159600	-0.976522530300	-1.263820104000	
<i>I2</i>					
Reactant	H	-3.131648071500	0.539683069600	-0.428385175000	
	N	-2.312262333100	1.065065460200	-0.106699475000	
	C	-1.183095922500	0.206841184400	-0.061551944600	
	N	-1.428221111900	-1.132266597800	0.1724444653000	
	C	-0.403633128200	-1.961108411400	0.171420515200	
	N	0.359807547600	2.075532149300	-0.490356231600	
	C	0.082591623400	0.715353287300	-0.279313677700	
	N	-0.593405763800	-3.318336178900	0.303347701300	
	H	1.243584424600	2.168176120300	-0.997538936900	
	C	1.216540818400	-0.189054596500	-0.272754939000	
	H	-0.385354783000	2.514629889100	-1.039373562900	
	N	0.874734813000	-1.522280261900	-0.036394859900	
	O	-3.007603986000	4.080101345800	1.238316299900	
	C	-2.209434125400	3.155568814100	1.179804237500	
	C	-2.696767871600	1.703681458300	1.175808132300	
	H	-1.112124544800	3.309696634400	1.137762151000	
	O	-4.096038087400	1.687190169600	1.208718547100	
	O	-2.108049406600	1.126175703600	2.293703969400	
	H	-4.359556035600	2.617690577000	1.358784660900	
	O	-3.531326167600	-2.521659995100	1.079821947300	
	C	-3.808397222600	-2.242155589100	2.359056327600	
	H	-4.454182406300	-3.009162139700	2.811943519400	
	N	-3.371083302300	-1.194049931800	2.962749625600	
	H	-3.708382454000	-1.197002526900	3.932921684900	
	H	-2.857098990500	-1.850247941600	0.738013722300	
	H	-2.561868799500	0.244961613000	2.460670070900	
	O	2.389932054300	0.144157723500	-0.491385912600	
	H	0.120621328900	-3.817369509600	0.834752747500	
	H	-1.530828860300	-3.548123326400	0.635287605900	
	H	1.632531638000	-2.203528708800	-0.119411069700	
		H	-3.381736794800	-1.577919409300	0.709992993900
	N	-2.566019611300	1.158958117300	-0.109372833000	
	C	-1.368624189000	0.400733232900	-0.105008582000	
	N	-1.505203675700	-0.865794045000	0.415458204400	
	C	-0.446560920600	-1.657901542500	0.361788887000	
	N	-0.067820902800	2.227962747800	-1.113892573200	
	C	-0.213814038700	0.890988202000	-0.682716716700	
	N	-0.528743426500	-2.942131320300	0.829002344000	
	H	0.782677495500	2.293623514100	-1.679150882600	
	C	0.932050286400	0.014644440300	-0.777565640400	
	H	-0.859181832800	2.516407387600	-1.696954332200	
	N	0.723739058500	-1.251643590400	-0.218695900200	
	O	-1.721834100400	3.619030839100	2.328946678400	
	C	-1.530502910900	2.604263193000	1.670476661100	

	C	-2.606061688000	2.162234726100	0.698586624100
	H	-0.606632495400	2.005880055500	1.733223260800
	O	-3.698560430200	2.943396748700	0.729055164900
	O	-2.398396743900	0.375705383000	2.975907950700
	H	-3.520343555900	3.623737207800	1.415145411800
	O	-2.822379665900	-3.168429551800	2.628536472000
	C	-3.945902045700	-2.811525796100	2.237015288600
	H	-4.867522500700	-3.148473346100	2.757874931900
	N	-4.178934614700	-2.030144375400	1.170582627900
	H	-5.126628473900	-1.728255689800	0.967355809000
	H	-2.201830205000	-0.284596912900	2.287680605300
	H	-1.728059804700	0.185688313900	3.650437253100
	O	2.018530102700	0.313242226600	-1.295577276000
	H	0.335248698600	-3.329419093800	1.208617428200
	H	-1.326768095800	-3.062486376100	1.471109875900
	H	1.493227062500	-1.913549935900	-0.336387275700
Transition state	H	-3.640690409000	-0.491017908400	0.650724205100
	N	-2.501457610900	0.557343956700	0.366402699200
	C	-1.256410095800	-0.040267290400	0.127840800100
	N	-1.124371821600	-1.366200283600	0.496608086700
	C	0.014255266500	-1.952049166200	0.197208269100
	N	-0.440179140800	2.019866908300	-0.903008131400
	C	-0.269675747000	0.658859197900	-0.557411653200
	N	0.189986962900	-3.300531057800	0.454871090800
	H	0.204613892100	2.261116889900	-1.660866795200
	C	0.978310374500	0.020101034400	-0.876022393900
	H	-1.401310824600	2.164540500600	-1.231574795300
	N	1.040332023700	-1.308500734300	-0.443729954100
	O	-1.543469757700	3.575396279600	1.987812357900
	C	-1.339945026100	2.407820234000	1.673042343800
	C	-2.526607630600	1.512318733700	1.315941938200
	H	-0.342274264700	1.936898028900	1.727895117400
	O	-3.702324637900	2.226901861900	1.337400921400
	O	-2.453384068100	0.746214089900	2.857814013900
	H	-3.461928265700	3.096166812900	1.722834104900
	O	-3.409320952200	-1.505319012300	3.035212871800
	C	-4.202116967600	-1.888818113100	2.095199238300
	H	-4.796800597900	-2.788625766300	2.309027505300
	N	-4.334188351300	-1.291277179700	0.943145647900
	H	-5.001124828700	-1.676073258300	0.274040332300
	H	-2.957828058900	-0.521198537400	2.864198162500
	H	-3.032943039700	1.276996779200	3.438318147600
	O	1.931872481600	0.541315360200	-1.486209911800
	H	1.145467227700	-3.587944950400	0.663256136800
	H	-0.454912992800	-3.634647859700	1.170819355900
	H	1.897819159800	-1.814606440100	-0.681665295900
I3				
	H	-0.410756509500	-0.122831582800	5.520313361700
	N	-0.609668846200	0.090502390900	4.534939929300

	C	-1.989789272200	1.012665854500	2.511545399900
	O	-1.473448431500	0.319998481700	1.643784454600
	H	-2.976809035200	0.781103388200	2.963283962800
	H	-2.372083542500	-1.389681391700	1.431998835700
	O	-2.173999728300	-2.411281885600	3.777733021300
	C	-2.799566182600	-2.852642857300	2.803195355900
	H	-3.372883187000	-3.802688750600	2.864911908000
	N	-2.867919046000	-2.268395970400	1.595428893700
	H	-3.402503242800	-2.692207045500	0.842982927400
	H	-1.028898908300	-0.780193794200	4.172449158600
	N	-0.073461552200	2.517397894100	3.070590171400
	C	0.829111800300	1.440835087400	3.064147211900
	N	1.969026633900	1.689686515400	2.343035020800
	C	2.937368204700	0.800975631200	2.451097101500
	C	0.630108522200	0.318503270400	3.861178516000
	N	4.056106327600	0.918762335300	1.662863049100
	C	1.725272037500	-0.609692142200	4.032625292400
	N	2.859431449400	-0.289239419800	3.271303923300
	C	-1.332787921400	2.292749029800	2.963262743700
	O	-2.257852174500	3.250759928000	3.176407517000
	H	-1.798407301700	4.072654358600	3.445893467100
	O	1.726935773700	-1.608213166600	4.768067243700
	H	4.941994046500	0.608253041500	2.060466438000
	H	4.129907940100	1.839657373500	1.232664331300
	H	3.650304797900	-0.934685144100	3.356178617000
Product	H	-1.017192497900	0.144735506800	4.802675042900
	N	-0.849942710900	0.028939294000	3.792538260500
	C	-1.782552896300	0.837321455700	2.993855834000
	O	-1.822867485400	0.378202713800	1.672667584500
	H	-2.765421849400	0.801893686000	3.496998655500
	H	-2.246167565100	-0.527883901500	1.735786771800
	O	-1.653538943700	-2.678038995000	3.855821831200
	C	-2.617141820000	-2.901512842700	2.962906569600
	H	-3.067873188900	-3.896910313900	3.097963457700
	N	-2.967601223700	-2.055580365800	2.056751282700
	H	-3.727058960400	-2.454975363300	1.493877314300
	H	-1.285803845000	-1.757818210600	3.727325359200
	N	-0.036983315800	2.592226900200	2.824287051100
	C	0.871342512200	1.519272788700	2.888516439200
	N	2.132834813800	1.812806303200	2.435996100700
	C	3.031710023500	0.859119396600	2.584030826900
	C	0.504545942300	0.302783037800	3.439318886800
	N	4.305796385000	1.033578621300	2.095931030600
	C	1.489151031800	-0.733269519800	3.629598027800
	N	2.753553873600	-0.355363682700	3.154566425000
	C	-1.281869369300	2.264643668100	2.940056503100
	O	-2.253651772600	3.189262424900	3.012039372100
	H	-1.838678730700	4.077012175200	2.996674267400
	O	1.301697370800	-1.844461646000	4.138950474400
	H	5.052616352400	0.573227693800	2.614875036400
	H	4.523807171500	2.013216484400	1.911149335800
	H	3.485956386100	-1.068715195900	3.226385620700

Transition state	H	-0.948054187200	0.239011317600	4.867816992800
	N	-0.801002566800	-0.032114192300	3.879209709500
	C	-1.780311291400	0.710120325200	2.959028792500
	O	-1.731952253100	0.195636553100	1.707864941200
	H	-2.759752015800	0.630837106800	3.473567224300
	H	-2.360830893700	-0.813837383400	1.781415778400
	O	-1.712945999800	-2.410520730100	3.868939706500
	C	-2.612943199300	-2.689426238300	3.007539974000
	H	-3.119549736600	-3.671141168500	3.118478956000
	N	-2.982540264900	-1.911751429200	2.011050274000
	H	-3.725599853200	-2.312278424300	1.437201664900
	H	-1.113854051500	-1.137101005200	3.816488960000
	N	-0.074582962700	2.529839491900	2.882485484100
	C	0.872190229600	1.489718098800	2.957460908900
	N	2.122808090200	1.840171800100	2.537470221200
	C	3.044002971500	0.891757340500	2.606646573700
	C	0.555570084900	0.239148683400	3.457017901500
	N	4.311148875000	1.136908188800	2.150750239100
	C	1.542161765500	-0.803051426900	3.543499782400
	N	2.791607361100	-0.370634710100	3.068276460900
	C	-1.310657241400	2.151371083200	2.929887524800
	O	-2.318790436200	3.028489443000	2.880490077100
	H	-1.948922993200	3.933345085700	2.803256581400
	O	1.376887705000	-1.955411137400	3.954446945100
	H	5.069808015400	0.671048731800	2.646734660800
	H	4.499728430300	2.127842388400	1.995130093200
	H	3.511770928600	-1.094311799700	2.998388875700
<i>I4</i>				
Reactant	H	-0.294076757500	-0.836137775800	3.620742050800
	N	-0.112958482200	0.182335849100	3.658017068300
	C	-1.221157366000	0.956557642100	3.232651632400
	O	-1.494710043400	0.705821749700	1.818568339700
	H	-2.113260731900	0.700045275700	3.824380527800
	H	-2.294405925600	1.209410026600	1.567503494900
	O	-2.079575042700	-1.890917212700	1.173611995800
	C	-1.856050229700	-2.758610256400	2.171328458900
	H	-2.174699224000	-3.775618212500	1.895591108400
	N	-1.334326300400	-2.417881860700	3.296194871400
	H	-1.261353950400	-3.253131487700	3.890916395300
	H	-1.806947876700	-0.983614941900	1.470804949700
	N	0.333836383900	2.902976788500	3.215434812500
	C	1.353113379000	1.967741991700	2.978347602600
	N	2.570389642800	2.490213709200	2.598124563300
	C	3.548249776500	1.627940274700	2.459587594200
	C	1.125750808200	0.619675913300	3.213208864100
	N	4.797248538400	2.033428783200	2.006225850400
	C	2.211262010000	-0.328708402700	3.089738953400
	N	3.398948741200	0.278358290300	2.681426894500
	C	-0.847172954700	2.408459826500	3.400202521100

	O	-1.905514188100	3.192994225900	3.695540579300
	H	-1.591642443700	4.118907627200	3.754349877100
	O	2.135246918500	-1.547057278400	3.302836423100
	H	4.875616352900	3.050144762600	2.059578383200
	H	5.579257741500	1.603476402000	2.503640697900
	H	4.188007686100	-0.352021496300	2.522671095800
Product	H	-0.339219036200	-1.833297476100	3.268262717500
	N	0.018752749000	0.061010845000	3.632515512400
	C	-1.008761610000	0.905168308900	3.638646340700
	O	-2.323560579100	0.923563454100	0.917148182900
	H	-1.994029073500	0.520112637300	3.917207466200
	H	-2.838062462000	1.520321536100	1.478364667500
	O	-2.668411030000	-1.594122561800	2.198120211000
	C	-2.004476499700	-2.631390242800	2.365429185000
	H	-2.395875206700	-3.621196899000	2.044310645000
	N	-0.793533218100	-2.692864774600	2.934756002800
	H	-0.309350491200	-3.579686193900	3.022019208100
	H	-2.402915440700	0.068062373600	1.378637215800
	N	0.343072467100	2.794678013800	2.955834703800
	C	1.405683780700	1.938995088000	2.952470881700
	N	2.625962169100	2.486557521200	2.632465768800
	C	3.640013135800	1.649039179000	2.596231312000
	C	1.220749678300	0.576016882700	3.272472052200
	N	4.884296536900	2.095280666400	2.231122904300
	C	2.353885905800	-0.352487102600	3.192081995000
	N	3.538696711700	0.295908758900	2.844005850700
	C	-0.829014108100	2.267967939100	3.277753743800
	O	-1.939535973400	3.038429282900	3.251588315400
	H	-1.679032661300	3.943730167300	2.987423023300
	O	2.308606764000	-1.566368557500	3.382402049900
H	4.943639853000	3.113093089000	2.249542618000	
H	5.675413843000	1.659272531200	2.704042273000	
H	4.352383216500	-0.305524153300	2.700485445300	
Transition state	H	-0.496285282900	-1.405632778500	3.360023510700
	N	-0.180027026000	0.156203539500	3.632106715700
	C	-1.233510268300	0.998444147000	3.335400178300
	O	-1.702830525400	0.691307878100	1.792337937200
	H	-2.153356586200	0.770106193700	3.896187684400
	H	-2.543539892300	1.171190150700	1.647611632000
	O	-2.273154060100	-1.672068885400	1.419939045700
	C	-1.685008541500	-2.594036226700	2.101511680200
	H	-1.963840507200	-3.622951203500	1.836502794400
	N	-0.812824321600	-2.396325030800	3.052780473500
	H	-0.407016760000	-3.216029847600	3.505361485800
	H	-1.976917751200	-0.642981352400	1.640195805600
	N	0.309113969500	2.906580281900	3.085564222900
	C	1.306826645800	1.960668165400	2.913431678500
	N	2.546220363200	2.446241737600	2.534203017300
	C	3.514670542100	1.569663209300	2.479299976900
	C	1.044119948000	0.617360152700	3.241062306100

	N	4.784168711500	1.923165253600	2.018850116200
	C	2.151630327700	-0.330787809100	3.230348319300
	N	3.349789897700	0.239039873300	2.801920312500
	C	-0.876306936800	2.431085934100	3.347863788800
	O	-1.913978567400	3.267560986000	3.633207923000
	H	-1.561648026600	4.179592930600	3.642562541600
	O	2.085385719400	-1.531511407300	3.535827710100
	H	4.865767579200	2.940973511700	2.000725161200
	H	5.542186552000	1.540946268900	2.587111259000
	H	4.131725388400	-0.408115311700	2.688877499900
<i>L1</i>				
	H	-2.715216340600	0.472321229700	0.310624012100
	N	-2.352670891500	-0.330618095000	0.837082921900
	C	-0.998490514900	-0.544612223000	0.470275009900
	C	-0.062361170400	-1.042720453400	1.417169659300
	N	1.241595681400	-1.160274362500	0.932831622300
	N	-1.515527910200	-0.078791200500	-1.824142512700
	C	-0.581032351500	-0.425273152600	-0.856946505700
	O	-0.311672029000	-1.407910344500	2.604010181100
	H	1.925106694200	-1.517417836600	1.604720261800
	H	-1.184124303100	-0.282913039500	-2.766494456400
	N	0.709484577700	-0.571334958500	-1.279042146600
	H	-2.424735773700	-0.514307762100	-1.655730380000
	C	1.596254079400	-0.907537597200	-0.359508305900
	N	2.932051066400	-0.942748724900	-0.676647167600
	H	3.529187079900	-1.545016136800	-0.112709848700
	H	3.106187068400	-1.045218229800	-1.675595514400
	O	-5.428867478100	-2.887643472100	1.013782079600
	C	-4.126877468900	-3.022753533200	0.707530056500
	C	-3.259597538800	-2.717543330100	1.930442004000
	O	-3.682399364200	-3.320886912100	-0.383139221200
	O	-2.016089507600	-3.124445888100	1.742324545700
	O	-3.713909649600	-2.170256977300	2.925497620500
	H	-1.409588088600	-2.571250351900	2.331770332700
	O	-2.069858365900	1.071235859400	3.483812768500
	C	-1.764179724600	0.550987172900	4.564023946300
	H	-1.089619340900	1.064968801300	5.283808495700
	N	-2.226557802500	-0.629147887500	5.016221392800
	H	-1.815334362400	-1.039612456700	5.850122173700
	H	-2.377366843600	-0.036701451400	1.824662138500
	H	-2.732381907600	-1.236906169900	4.368895118100
	H	-5.950965041400	-3.069966774000	0.205008899900
	H	-2.808646034300	-0.047666277200	0.859142847300
	N	-2.207896943500	-0.691234907700	1.383731430200
	C	-0.980707579500	-0.934304075400	0.675032281500
	C	0.139839646700	-1.354818549700	1.453923051100
	N	1.347003839900	-1.401457245600	0.753745844700
	N	-1.812799116600	-0.103053146000	-1.435196452900
	C	-0.780120376100	-0.584262403900	-0.666257907500

	O	0.120170660600	-1.693801103400	2.661942892600
	H	2.142717810600	-1.777605186800	1.270203819400
	H	-1.587871137100	-0.064849180200	-2.429581910700
	N	0.443948441200	-0.611103084100	-1.277381290200
	H	-2.711941152600	-0.551392450600	-1.248591253700
	C	1.468789262700	-1.021907269400	-0.551119851200
	N	2.722108485900	-1.013813712900	-1.094498659800
	H	3.417703723200	-1.644005009000	-0.699387700800
	H	2.728589265200	-0.997477815300	-2.113147723800
	O	-4.143835273000	-3.742108797100	0.813600983900
	C	-3.717445025100	-2.502556207600	0.541753725800
	C	-3.026251266200	-1.861213024700	1.760324355700
	O	-3.901154055100	-1.931768701900	-0.521984010100
	O	-2.226423890400	-2.825845114600	2.364619481000
	O	-4.081793106200	-1.415495550600	2.550814106400
	H	-1.420216108200	-2.366354548700	2.718103919400
	O	-1.315899274300	0.870279580200	3.485304663000
	C	-1.866741455800	0.495615444800	4.639033747400
	H	-1.407770411500	1.005706343000	5.499742647200
	N	-2.827653298300	-0.359562332900	4.716856342600
	H	-3.088003659200	-0.499730984600	5.699524458200
	H	-1.700913296100	0.290911032800	2.759628701700
	H	-3.650754127800	-1.035991937800	3.378289802700
	H	-4.620798765000	-4.082882884100	0.027384508900
Transition state	H	-2.783181889700	-0.037161521700	0.867899207800
	N	-2.169734815100	-0.655098375200	1.413010060000
	C	-0.948136747400	-0.909701034700	0.688200092200
	C	0.174571727600	-1.331928312200	1.461748603100
	N	1.369498164300	-1.412087995900	0.741455999800
	N	-1.803359153700	-0.102777618900	-1.423209008000
	C	-0.767465620700	-0.585344247000	-0.661938193400
	O	0.168922352800	-1.638054762700	2.676687137500
	H	2.167843121700	-1.788760768100	1.253365218600
	H	-1.588831148800	-0.077477953600	-2.420441691200
	N	0.444439166800	-0.651567699200	-1.292656187600
	H	-2.707171652300	-0.537478464400	-1.222875024600
	C	1.474394807200	-1.066237108100	-0.574335083000
	N	2.715080141200	-1.099186629400	-1.140476004800
	H	3.409328744400	-1.729409495400	-0.744071363000
	H	2.709489536400	-1.090831571700	-2.159046817200
	O	-4.087759395700	-3.715705536400	0.773952156000
	C	-3.685419954100	-2.451699315000	0.566306276200
	C	-3.043813072500	-1.847775832100	1.827768437900
	O	-3.912676948300	-1.835877532800	-0.467561417900
	O	-2.183892815000	-2.829897800200	2.370873689700
	O	-4.021810187100	-1.409384497800	2.609955027800
	H	-1.397621672700	-2.369655747800	2.748005332900
	O	-1.483591727500	0.770676544900	3.369020717900
	C	-1.958401989900	0.431113469200	4.513285468800
	H	-1.520824954900	0.931503186200	5.391044832500
	N	-2.906659744700	-0.454138239100	4.681986320400
	H	-3.215370734300	-0.649886754500	5.630120933400

	H	-1.856454860500	0.086042002400	2.504223667800
	H	-3.421688049700	-0.917626421200	3.798715240100
	H	-4.574087094800	-4.013313551500	-0.023164825500
<i>L2</i>				
Reactant	H	-3.342051824000	-0.155816681600	0.695484707100
	N	-2.526680171400	0.486638707300	0.697745761400
	C	-1.319147865400	-0.215680400400	0.394880159700
	C	-1.071209048800	-1.537414307900	0.866787933400
	N	0.146931783100	-2.079311917300	0.419852097400
	N	-0.602175924900	1.641964623600	-0.944801143700
	C	-0.390796700300	0.373433472200	-0.473664745900
	O	-1.795545167800	-2.260806341300	1.589660349500
	H	0.358176660200	-3.023805527300	0.751639771200
	H	-0.093082162600	1.879705003600	-1.794110991900
	N	0.786347355500	-0.207017889200	-0.863483446500
	H	-1.576998590300	1.939358220800	-0.926144917000
	C	1.015938776800	-1.421614221100	-0.397710857200
	N	2.202660419100	-2.042606957100	-0.683444140200
	H	2.205778480400	-3.061337076800	-0.684082322200
	H	2.690391224300	-1.641320875200	-1.482886638400
	O	-1.854304075300	3.447419470000	1.414970699100
	C	-1.530168094400	2.362424967900	1.868038572300
	C	-2.531696494800	1.189060661400	1.962702954500
	O	-0.310933139200	2.052590338400	2.329014020800
	O	-3.810488017000	1.727823903800	2.189145461500
	O	-2.233721351200	0.314093245000	3.012853135200
	H	-3.864521777100	2.532492773800	1.641737838100
	O	-4.142242204600	-2.100650455900	2.783621410000
	C	-5.123641671000	-1.780250369100	1.936180125600
	H	-6.115524795700	-1.989830139800	2.369408753200
	N	-4.912827773800	-1.289189940100	0.764721519200
	H	-5.819942497300	-1.121954790300	0.311197223200
	H	-3.264706585400	-1.966291454000	2.321101443800
	H	-2.267193642900	0.821828874700	3.844152548300
	H	0.273840689700	2.830063503900	2.201573359400
	H	-4.075990383600	-0.488107549800	0.504971963000
	N	-2.335665973500	0.515107838600	0.620048995200
	C	-1.073567601400	-0.061433183200	0.321125050600
	C	-0.463132103600	-1.024203555500	1.182354940200
	N	0.691660377400	-1.603894338400	0.634522297100
	N	-1.094713053700	1.085420902200	-1.791296472300
	C	-0.533174245200	0.155285948300	-0.949543034300
	O	-0.836559577000	-1.398241825300	2.313849525600
	H	1.176652463300	-2.265591622000	1.243064634200
	H	-0.881532559600	0.942029134600	-2.777773462800
	N	0.598005061200	-0.457096230800	-1.420391728200
	H	-2.078141649300	1.289601070200	-1.610049948700
	C	1.174962938600	-1.321842569000	-0.608366052000
	N	2.348506298800	-1.930977966800	-0.980200558000

	H	2.511943978200	-2.874142739200	-0.625894087400
	H	2.527484836000	-1.859563946200	-1.981625784600
	O	-1.870984948800	2.948380543200	3.222547714900
	C	-1.508505999400	2.015515965600	2.521525088100
	C	-2.507118972000	1.347303156800	1.589966951000
	O	-0.268033589700	1.543103248400	2.436809924500
	O	-3.751936170400	1.812285161900	1.792080319300
	O	-2.611404436900	-0.055453393500	3.941126600100
	H	-3.686700635100	2.446782480500	2.536179034700
	O	-5.011785504700	-1.044161258000	2.869383289600
	C	-5.480274101900	-1.339350022600	1.760159917900
	H	-6.427732854200	-1.914688380400	1.677508154600
	N	-4.944093728300	-1.033031567000	0.568746718500
	H	-5.413521479800	-1.324190906700	-0.284098743100
	H	-1.971497240900	-0.560255956300	3.398166066000
	H	-3.460793086900	-0.323096169300	3.537522677800
	H	0.302556688700	2.067320376700	3.039964107600
	H	-3.795132835400	-0.565464573900	0.646509168200
	N	-2.563354854700	0.434359999300	0.625236228200
	C	-1.333425451800	-0.211034392700	0.343453644100
	C	-1.017905121100	-1.495535648800	0.902478151000
	N	0.202924228300	-2.022637145900	0.420515767600
	N	-0.709175469800	1.618776918600	-1.073297419800
	C	-0.453520633300	0.348290716200	-0.582610156500
	O	-1.681366237000	-2.158757561700	1.720209560000
	H	0.494352510100	-2.909507051900	0.836361755100
	H	-0.306825320200	1.784530751100	-1.995794224200
	N	0.711935244800	-0.232641885600	-1.023176906600
	H	-1.706082392700	1.839174760500	-1.027030118600
	C	1.001043245100	-1.403518587200	-0.493392733100
	N	2.196648117400	-2.022302278400	-0.803241515100
	H	2.178561519600	-3.042610102500	-0.802773640900
	H	2.601786813200	-1.662445628900	-1.667311946200
	O	-1.676217533100	3.375221107800	2.244250043400
	C	-1.471498586600	2.179465642200	2.072887487200
	C	-2.623532235900	1.230173504200	1.712827638600
	O	-0.277488122300	1.594947999100	2.186323331500
	O	-3.828606560700	1.917361736700	1.776974461000
	O	-2.620084202700	0.310604639900	3.117187775300
	H	-3.616782397700	2.794956535500	2.150495817800
	O	-4.312335722800	-1.415448943100	3.067599755800
	C	-4.890390275700	-1.751038439800	1.976742589200
	H	-5.700517271900	-2.492349507400	2.064407447200
	N	-4.610183470600	-1.283668939100	0.786207367600
	H	-5.166054770300	-1.630298809100	0.004826527500
	H	-3.474221978000	-0.621175730600	2.990752554500
	H	-3.003761685700	0.880934529300	3.813486929100
	H	0.378386293800	2.295419838400	2.390127098800
L3				

Reactant	H	-1.110223815300	0.692276119100	4.618722428300
	N	-0.679940630100	-0.059491470100	4.080980113900
	C	-1.872073519100	1.633131693200	2.060072176800
	O	-1.325896725900	0.980589275800	1.192466361500
	O	-3.164650569800	1.537569480100	2.416610903300
	H	-1.478003107700	-1.363349082300	2.495687357400
	O	-1.176824781500	-2.952708186400	4.484858118800
	C	-1.427763926000	-3.240911749900	3.307080444000
	H	-1.528245505000	-4.297499861700	2.977274635200
	N	-1.630282614100	-2.354521605200	2.313225173900
	H	-1.740707701700	-2.674689617300	1.358849989100
	H	-0.706365228100	-0.970773403000	4.551415986800
	N	0.050065101800	2.670962974000	3.309253580100
	C	0.865326046500	1.530062176500	3.094588114300
	C	2.168253195000	1.790992161100	2.549123191200
	N	2.960502105500	0.636270872200	2.424380134300
	C	0.550491206400	0.240702507300	3.521898726400
	O	2.618013164600	2.887386613900	2.179055993600
	H	3.860781787400	0.780988753800	1.965901061100
	N	1.385878098200	-0.837279694800	3.374718114500
	C	2.557824406700	-0.605925522000	2.815195104900
	N	3.407330167300	-1.653848813800	2.550201277400
	H	4.401867843500	-1.435237596700	2.601311979000
	H	3.173248184900	-2.489377500600	3.084920247600
	C	-1.165656279800	2.690238272300	2.887173298100
	O	-1.965938450500	3.754916202900	3.115641725600
H	-1.437319961500	4.408280335100	3.618899966300	
H	-3.604028078900	0.878692055400	1.837276022400	
Product	H	-0.772420972500	0.168070598200	4.767157976200
	N	-0.644627796700	0.125972867000	3.746482396100
	C	-1.623968619500	0.955874403400	3.038572809300
	O	-1.771532651000	0.525529680900	1.730007198600
	O	-2.784934575000	0.847800567500	3.818523094000
	H	-1.984561631800	-0.459212300000	1.755889379800
	O	-1.005287881100	-2.673681293400	3.571500534400
	C	-1.803539691200	-3.004156639800	2.553448051000
	H	-1.991319462700	-4.087852439500	2.520694244400
	N	-2.283509772400	-2.144519913000	1.725036465500
	H	-2.864969078700	-2.619993174000	1.024184199600
	H	-0.877471798200	-1.685938334700	3.563975489000
	N	0.131988753400	2.674897217900	2.694222040900
	C	1.012767387800	1.578566326300	2.748208301100
	C	2.362201541500	1.775034739400	2.261440606100
	N	3.192142129000	0.672848032600	2.525432589500
	C	0.698807169400	0.371822898000	3.358383102000
	O	2.806786612900	2.768391096900	1.677638301100
	H	4.155997811100	0.759661311200	2.187387904500
	N	1.574862890400	-0.634237865800	3.645876442300
	C	2.813405330400	-0.441089034200	3.224715095500
	N	3.756173159500	-1.416973454200	3.403730906600
	H	4.730990255500	-1.124912130100	3.437349241100
	H	3.519284001400	-2.091976416200	4.130774028500

	C	-1.105377328700	2.383048851500	2.919099078400
	O	-2.067486971700	3.320548732100	3.025928036200
	H	-1.652467310300	4.203258636100	2.943040637200
	H	-3.449960222600	1.439993848900	3.424907788100
Transition state	H	-0.723476038700	0.342943904800	4.787824918800
	N	-0.619397769900	0.081512542700	3.791785104800
	C	-1.618001543300	0.875312249100	2.952867320900
	O	-1.685306714100	0.437828362300	1.715368903700
	O	-2.798122428700	0.726259197700	3.744080232400
	H	-2.052230972100	-0.998581396500	1.715185149900
	O	-1.189349763500	-2.361741444000	3.765792829100
	C	-1.857495392800	-2.803200915400	2.765554591400
	H	-2.096110737700	-3.878340983100	2.766457478900
	N	-2.271721782500	-2.070665870300	1.762501923200
	H	-2.779511149800	-2.527864975900	1.006092293900
	H	-0.928422528200	-1.209119833900	3.727683317800
	N	0.120376152200	2.673454598800	2.833693393600
	C	1.029788146700	1.599944872200	2.872141097700
	C	2.381974081000	1.848647955500	2.409874943000
	N	3.214953345800	0.727450327100	2.556503261100
	C	0.732059284300	0.336883742600	3.356637279500
	O	2.820754998900	2.895076870100	1.922239560200
	H	4.170293494600	0.842580008600	2.201929191300
	N	1.590712693600	-0.709584039700	3.491956499600
	C	2.826906864200	-0.476874900900	3.077911291700
	N	3.750491245300	-1.481889984600	3.087023767600
	H	4.733975722600	-1.230832239600	3.156497254800
	H	3.489793352900	-2.292031868800	3.645007058600
	C	-1.122355503000	2.323761447100	2.944963280900
	O	-2.110147585400	3.239878948100	2.935393781300
	H	-1.701058249800	4.120232215800	2.809126920300
	H	-3.526758610800	0.990873484200	3.156647284800
<i>L4</i>				
Reactant	H	-0.035765528900	-0.574203351400	3.502437726900
	N	0.136458585700	0.453616537500	3.563274997700
	C	-0.999306453400	1.229164480000	3.208790926300
	O	-1.324623818400	0.922622141300	1.831139596700
	O	-2.052433251200	0.859609995600	4.048597668500
	H	-2.111855947500	1.438997962000	1.564769518000
	O	-1.828737611800	-1.717475275900	1.182801413000
	C	-1.303475768900	-2.609514449400	2.034966713600
	H	-1.522291718400	-3.641065574300	1.719118711700
	N	-0.634293552000	-2.279113857500	3.081739729500
	H	-0.334485499500	-3.134622050100	3.565657997400
	H	-1.610594035600	-0.804674679000	1.497617159100
	N	0.531838795600	3.194077350200	3.089490008700
	C	1.551842688100	2.250665478500	2.878606444100
	C	2.846025932500	2.715391535100	2.461277096100
	N	3.785201322600	1.668717376900	2.343073646800

	C	1.367512009600	0.888661196200	3.128997697900
	O	3.190626284900	3.877096381700	2.204294302200
	H	4.706535925000	1.950259665000	1.998636819200
	N	2.339618848500	-0.066458438200	3.046000128000
	C	3.523848818900	0.360671288000	2.640187456000
	N	4.518813272500	-0.552950549400	2.436617509900
	H	5.484880997300	-0.234777010200	2.448480443500
	H	4.370478465600	-1.434743193700	2.922337344700
	C	-0.640533508300	2.698293011100	3.295670223900
	O	-1.735515971700	3.460258174300	3.538412059800
	H	-1.474329233600	4.403294978500	3.556029072700
	H	-2.684987090300	1.599747019200	4.082962162800
	H	-0.221003353000	-1.525853878100	3.204293836400
	N	0.277848215100	0.346167305400	3.643289261400
	C	-0.734534017800	1.186596773200	3.691745235400
	O	-1.716225768200	1.153946805700	1.019490751000
	O	-1.920154605300	0.698546128400	4.108459279300
	H	-2.543183913400	1.556376942000	1.319903073600
	O	-2.220878744900	-1.551463893700	1.540525934000
	C	-1.613120138600	-2.512090336500	2.038658217800
	H	-1.910418097300	-3.555693244800	1.801008262200
	N	-0.571628310000	-2.434653076700	2.879526747200
	H	-0.152628414400	-3.290167983100	3.233441319000
	H	-1.840127380600	0.213938392000	1.262567746800
	N	0.544802698600	3.084508418700	2.918155877300
	C	1.591598496800	2.207546387000	2.859035496300
	C	2.882504946700	2.719137816000	2.394806762900
	N	3.862977291400	1.725326984000	2.358040777400
	C	1.474964686700	0.847276712100	3.204834695400
	O	3.129998934900	3.875611487900	2.054705601900
	H	4.781182129900	2.019089669700	2.011134052100
	N	2.512016551900	-0.056465793000	3.157004164200
	C	3.664911961800	0.416031636800	2.739133360000
	N	4.738975335700	-0.427173191900	2.597849698800
	H	5.664750473600	-0.026380222600	2.752832087800
	H	4.607820643400	-1.302525033600	3.101955232000
	C	-0.596513096600	2.562309521800	3.317822944900
	O	-1.732028080100	3.290969603800	3.394118118900
	H	-1.547460690600	4.212289480100	3.122255831400
	H	-2.561407017800	1.432881856400	4.165344807600
	H	-0.163518147600	-1.333632499300	3.178504498900
	N	0.192751570400	0.319825143400	3.475577867200
	C	-0.893255799700	1.131273709100	3.273838459600
	O	-1.363457635500	0.848918069800	1.703183018700
	O	-1.974750356700	0.716064954600	4.031781592500
	H	-2.152046774200	1.397442348300	1.511633118100
	O	-2.187816581000	-1.416926233000	1.513980511200
	C	-1.561713392600	-2.385500272400	2.063008454700
	H	-1.917860002600	-3.396635431400	1.817959986000
	N	-0.537208037800	-2.280606941100	2.876625252300

	H	-0.122815713500	-3.140324559300	3.236505479200
	H	-1.759174297500	-0.353220985100	1.652681619500
	N	0.522207334700	3.121119208000	2.981674153300
	C	1.557653725900	2.204029852300	2.801717504500
	C	2.840197193100	2.710426662900	2.394041689200
	N	3.822881494900	1.706436440000	2.340356501800
	C	1.389275744700	0.834818442200	3.096901012700
	O	3.136682634000	3.877775426900	2.093007690400
	H	4.744125745800	2.002166190400	2.008605635300
	N	2.440061962100	-0.067468758600	3.083904135900
	C	3.605512327500	0.402515418500	2.701621005300
	N	4.680582466200	-0.453389247800	2.575912120600
	H	5.598991994400	-0.049692499000	2.763509971700
	H	4.537900046100	-1.320805567700	3.090879525000
	C	-0.627837985600	2.593049334800	3.259022999800
	O	-1.742262883900	3.339120693800	3.504336739700
	H	-1.501131375500	4.285836959700	3.461757468600
	H	-2.632785012100	1.435090196100	4.043728160200