

Electronic Supplementary Information (ESI) for: Theoretical studies of the mechanism of 2-aminooxazole formation under prebiotically plausible conditions.

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Schematic Representation of the Selected Reaction Steps

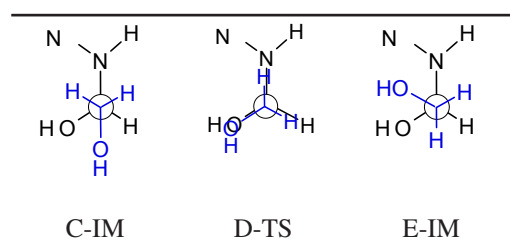


Fig. 1 Rotation of carbinolamine leading to an intermediate which can undergo the following step of the reaction – cyclization.

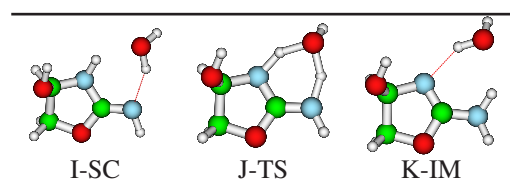


Fig. 2 The fourth step of the water-assisted reaction mechanism – proton transfer leading to the last intermediate K-IM.

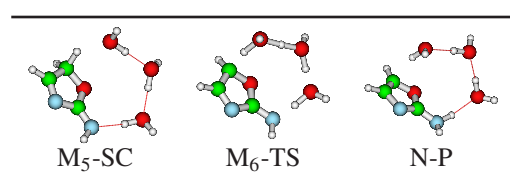


Fig. 3 The water-assisted tautomerism via three water molecules leading to the title compound.

Comparison of the Reaction Free Energy Profiles for Different Water-assisted Reaction Paths

Our preliminary calculations, performed at the M06-2X/6-31+G(d,p) level, indicated that the mechanism of water-assisted synthesis of 2-aminooxazole consists of five major steps. Since some of the intermediates can be formed as different stereoisomers there are also four distinct reaction paths possible. However, their energetics turned out to be quite similar and they all proceed towards only one possible final product which is 2-aminooxazole.

The greatest differences can be observed in the beginning of each path. The fourth and fifth steps of the reaction are identical for paths number 1 and 3. The same is true for paths number 2 and 4. The formation of 2-aminooxazole in the gas phase is exergonic. The total absolute Gibbs energy change for each of the investigated reaction paths is below 30 kcal/mol. The largest amount of energy is released in the first path ($\Delta G_1 = -28.4$ kcal/mol) and the smallest in the second ($\Delta G_2 = -24.2$ kcal/mol). The magnitudes of Gibbs free energy changes for paths number 3 and 4 are virtually identical and amount to -25.2 kcal/mol.

All the investigated reaction paths are qualitatively similar, and there are only small quantitative energetical differences observed. The most favorable in the gas phase are the paths 1 and 3 ($\Delta G_{1,3}^\ddagger = 46.7$ kcal/mol). However, the largest activation energies for the other two paths are only slightly higher ($\Delta G_{2,4}^\ddagger = 48.0$ kcal/mol). Thus in the case of the more elaborate calculations we focused on the first and most exergonic path.

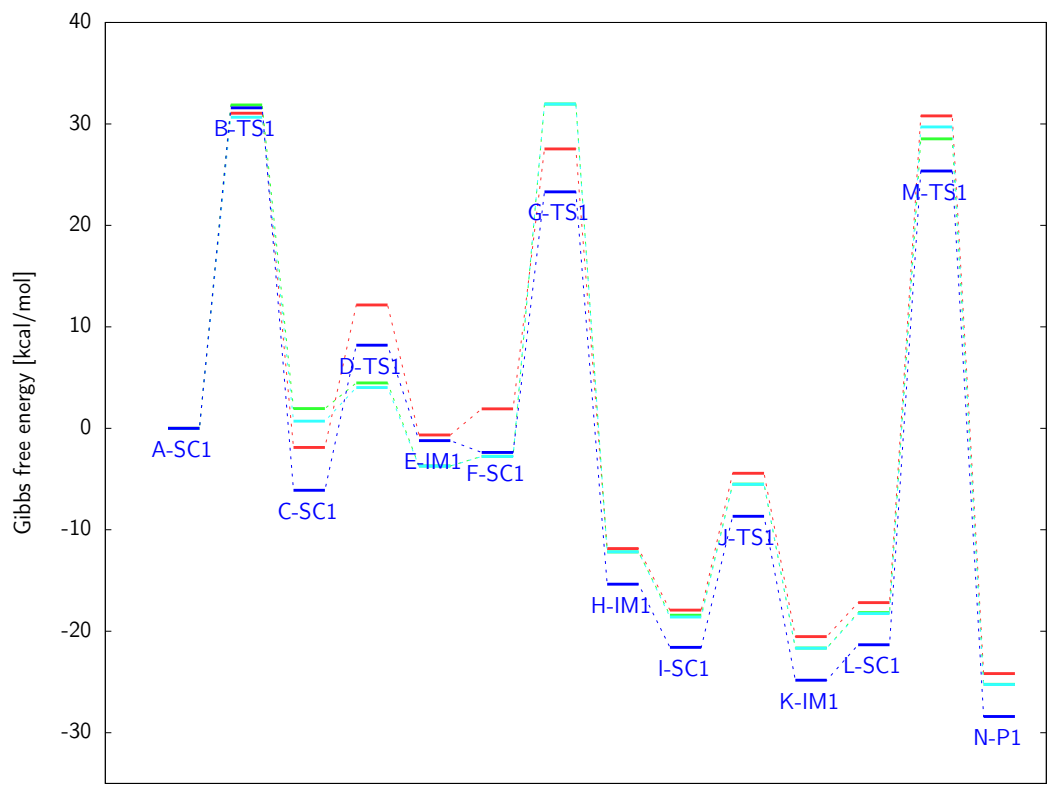


Fig. 4 A comparison of the energetics of the four considered reaction paths calculated using M06-2X/6-31+G(d,p) method. The consecutive reaction paths are plotted in blue, red, green and cyan, respectively, for the paths no 1-4.

Cartesian coordinates of the selected structures for the water-assisted reaction path optimized at the B3LYP/6-311++G(2d,2p) level

Carbinolamine formation

A-SC

C	0.583389	0.421929	0.130987
C	-0.125474	1.393215	-0.762853
C	-0.404395	-2.778118	-0.840689
O	0.315848	0.217870	1.292717
O	1.003878	-2.293314	2.286059
O	-1.113065	2.115388	-0.067418
N	-0.308269	-3.691678	0.126774
N	-0.428915	-1.991642	-1.689988
H	1.397697	-0.125710	-0.373495
H	0.961878	-2.365576	3.242303
H	0.819202	-1.357695	2.072836
H	-1.135839	-4.250431	0.269812
H	0.123946	-3.346260	0.989905
H	0.644862	2.047899	-1.197499
H	-0.530247	0.786952	-1.583158
H	-1.708777	2.518185	-0.703108

B-TS

C	1.209920	-0.334342	0.131583
C	1.465617	-0.136667	1.623011
C	0.554564	1.916067	-1.344847
O	2.259735	-1.242066	2.030226
O	-1.690392	-0.211447	-0.147580
O	0.431585	-1.258192	-0.263357
N	0.838420	2.349165	-2.379160
N	0.225972	1.343854	-0.172542
H	2.071231	-0.105827	-0.502482
H	-0.956812	0.689760	-0.141097
H	0.364332	1.996342	0.593488
H	-2.207585	-0.265696	0.662882
H	-0.792886	-0.925709	-0.118016
H	1.994494	0.807025	1.784131
H	0.511805	-0.116999	2.163676
H	2.677508	-1.039000	2.871209

C-IM

C	1.255066	0.427441	1.745329
C	1.767338	0.355442	0.312155
N	1.338543	1.539826	-0.450043
C	0.033648	1.767871	-0.660060
N	-1.087769	1.999342	-0.819463
O	1.706797	-0.681298	2.500523
O	1.309019	-0.862859	-0.223081
O	2.437871	-1.047223	-2.841028
H	2.858665	0.396912	0.310030
H	3.081891	-1.711615	-3.103800
H	1.922121	1.761069	-1.243211
H	1.715993	-1.117661	-3.473777
H	1.740186	-1.027918	-1.076670
H	1.642265	1.323040	2.225772
H	0.161673	0.484141	1.730584
H	1.441714	-1.476500	2.025707

Rotation

C-SC

C	1.224707	0.223227	1.668819
C	1.775401	0.152550	0.257150
N	1.569153	1.446963	-0.412500
C	0.336038	1.893389	-0.627779
N	-0.735916	2.303516	-0.780248
O	1.568515	-0.983886	2.335978
O	1.143496	-0.913764	-0.411088
H	2.853394	0.011925	0.286321
H	2.240444	1.686084	-1.126623
H	1.653900	-1.145114	-1.192795
H	1.663958	1.087801	2.163283
H	0.140728	0.355466	1.625382
H	1.334440	-0.891824	3.262884

D-TS

C	1.470382	0.289818	1.720994
C	1.918827	0.236716	0.240812
N	1.408200	1.417096	-0.482929
C	0.097675	1.631540	-0.541977
N	-1.040542	1.843676	-0.546424
O	0.710032	-0.862187	2.059967
O	1.509458	-0.975521	-0.342089
H	2.998908	0.337540	0.182346
H	1.921342	1.677935	-1.312152
H	2.010545	-1.107427	-1.152400
H	2.362705	0.354043	2.342217
H	0.885074	1.195254	1.880819
H	0.515654	-0.812148	2.999599

E-IM

C	-1.535875	0.435410	0.404504
C	-0.653098	-0.793139	0.311212
N	0.696967	-0.550436	0.853088
C	1.612877	0.114799	0.157395
N	2.435379	0.697404	-0.412436
O	-0.958073	1.498033	-0.345531
O	-0.624946	-1.224487	-1.030093
H	-1.076327	-1.556123	0.962053
H	1.068092	-1.288334	1.431974
H	-0.234899	-2.103015	-1.067950
H	-2.520079	0.170167	0.015550
H	-1.630988	0.705116	1.455266
H	-1.411494	2.312622	-0.115126

Cyclization

F-SC

C	1.541133	0.236691	1.652832
C	0.017250	0.367202	1.761990
C	-0.594306	0.119427	-0.626282
O	2.106063	0.963697	0.595984
O	-0.304242	1.720510	1.889373
O	2.285647	-0.416089	-1.864195
N	-0.512786	0.417194	-1.742601
N	-0.745555	-0.244342	0.644790
H	-0.302444	-0.210459	2.637207
H	-1.025058	-1.203913	0.779627
H	-1.258286	1.812721	1.976988
H	1.951560	0.626246	2.587100
H	1.785763	-0.829492	1.599337
H	2.212775	0.410260	-0.197253
H	1.404908	-0.125896	-2.156489
H	2.915402	0.002959	-2.456828

G-TS

C	-0.728230	-1.211717	-0.588549
C	-1.675310	-0.034069	-0.337774
C	0.482925	1.032275	-0.056446
O	0.375151	-0.930604	0.221721
O	-2.339365	-0.120781	0.904318
O	2.739227	-0.695818	0.032778
N	1.578233	1.458268	0.105034
N	-0.804084	1.136657	-0.427918
H	-2.457570	0.056737	-1.087365
H	-1.218925	2.049630	-0.325681
H	-1.682622	-0.369958	1.566812
H	-1.223490	-2.140790	-0.295467
H	-0.472230	-1.266308	-1.653463
H	1.673277	-1.028270	0.040631
H	2.398771	0.456354	0.127805
H	3.155937	-0.981711	0.852257

H-IM

C	0.706027	-1.237019	0.557134
C	1.740240	-0.123046	0.382881
C	-0.415270	0.749363	0.228072
O	-3.385898	-1.090690	-0.502386
O	-0.554638	-0.624526	0.222424
O	2.318581	-0.258116	-0.913557
N	0.900441	1.028656	0.561097
N	-1.316156	1.595439	-0.001685
H	2.524632	-0.156546	1.139527
H	1.230516	1.959188	0.367795
H	3.045085	0.364460	-1.009074
H	0.889517	-2.059160	-0.127631
H	0.665552	-1.593899	1.585389
H	-2.446584	-1.186126	-0.299945
H	-2.217145	1.158622	-0.172434
H	-3.473539	-1.332263	-1.427814

Water-assisted proton transfer

I-SC

C	0.316778	0.870787	-0.004533
C	-1.186014	-0.839819	0.399120
C	-1.914546	0.502056	0.299826
O	2.974568	-0.910236	-0.029918
O	-0.911401	1.435353	-0.155555
O	-1.456617	-1.570965	-0.793912
N	1.427285	1.415796	-0.298996
N	0.168090	-0.382949	0.536192
H	-1.491544	-1.425330	1.267093
H	0.978098	-0.993113	0.520481
H	-0.959929	-2.394893	-0.784234
H	-2.714676	0.469091	-0.432830
H	-2.290048	0.834738	1.266460
H	1.305734	2.357487	-0.651067
H	2.709774	0.021574	-0.196188
H	3.743236	-0.869035	0.543557

J-TS

C	-0.320538	-0.550847	1.152111
C	1.740887	-0.066131	0.363095
C	0.773066	1.093868	0.089963
O	0.284799	-3.157464	2.010040
O	-0.443951	0.736442	0.807291
O	2.655832	0.359946	1.368012
N	-1.234183	-1.233917	1.784448
N	0.838287	-1.099715	0.796268
H	2.290671	-0.371833	-0.528125
H	0.883290	-2.171265	1.240517
H	3.130424	-0.408596	1.700847
H	1.139524	2.032601	0.491857
H	0.523552	1.191150	-0.964362
H	-2.097298	-0.784562	2.036668
H	-0.769396	-2.288133	2.022421
H	0.097395	-3.971644	1.537109

K-IM

C	-0.258964	-0.513752	1.072080
C	1.736029	0.012040	0.306362
C	0.780914	1.194351	0.084472
O	0.391724	-3.477891	2.154023
O	-0.436642	0.790278	0.761600
O	2.713783	0.403773	1.267470
N	-1.326952	-1.134789	1.609512
N	0.881792	-1.052382	0.800789
H	2.238231	-0.295495	-0.613045
H	0.823198	-2.793769	1.600698
H	3.078295	-0.398919	1.654523
H	1.146005	2.108574	0.542231
H	0.542729	1.355373	-0.965136
H	-2.073785	-0.563283	1.960479
H	-1.152240	-2.036897	2.034174
H	0.408241	-4.287321	1.637927

Elimination of water molecule and aromatization

L-SC

C	1.061110	-0.363337	0.838030
C	0.163498	1.559363	0.159364
C	-0.906024	0.554945	0.613738
O	-2.875283	2.593709	-1.452832
O	1.394576	0.792246	0.214345
O	-1.681890	0.158625	-0.532899
N	2.111431	-1.178860	1.113425
N	-0.166253	-0.568941	1.146651
H	-1.581201	0.970544	1.361973
H	-2.085544	-0.689372	-0.317711
H	0.009675	1.909223	-0.856351
H	0.260803	2.401758	0.840552
H	2.957559	-1.021121	0.594466
H	1.882087	-2.134047	1.324679
H	-3.175854	2.590502	-2.364373
H	-2.614329	1.679666	-1.258915

M-TS

C	0.951934	-0.172511	0.593901
C	-0.175226	1.714763	0.369289
C	-0.878590	0.707313	1.162532
O	1.079770	1.025359	0.066215
O	-2.590468	0.247406	-0.220172
O	-1.577992	1.675718	-1.890503
N	1.929345	-1.058353	0.413779
N	-0.157510	-0.409629	1.295074
H	-1.742239	0.893195	1.772966
H	-2.513735	-0.676241	-0.475622
H	-0.736909	1.906462	-0.661830
H	0.047469	2.650860	0.876157
H	2.706689	-0.838823	-0.182349
H	1.790833	-1.999314	0.734426
H	-2.099840	2.431546	-2.172025
H	-2.243600	0.868022	-1.068804

N-P

C	-0.754136	-0.250989	0.319220
C	-0.817321	-0.625362	2.457076
C	0.458625	-0.498473	2.060349
O	-1.621230	-0.465936	1.334489
O	0.610854	0.935615	-2.887775
O	2.577521	0.252586	-1.107216
N	-1.268166	-0.106489	-0.919575
N	0.500166	-0.258169	0.687348
H	1.355316	-0.556866	2.650715
H	0.683500	1.858719	-3.141386
H	1.914849	0.030894	-0.406756
H	-1.317684	-0.807717	3.387264
H	-2.251478	0.091509	-0.977795
H	-0.669977	0.298161	-1.641118
H	3.071477	-0.553750	-1.274731
H	1.421289	0.733652	-2.370373

Cartesian coordinates of the structures in the phosphate-catalyzed reaction path optimized at the B3LYP/6-311++G(2d,2p) level

Carbinolamine formation

A-SC				C-IM			
C	-3.064043	-1.335561	-0.063260	C	-3.106067	-0.803878	0.256452
O	-3.643505	-0.658361	1.026945	O	-3.195698	-2.127288	0.757987
C	-1.565981	-1.526663	0.071312	C	-1.643382	-0.424137	0.035826
O	-0.960628	-2.404017	-0.505513	O	-1.094260	-1.342609	-0.824367
N	-0.620108	2.632763	-0.075676	N	-1.521738	0.944335	-0.603122
C	-1.871842	2.316572	0.192194	C	-2.120627	2.002999	-0.048815
N	-2.988994	2.038492	0.362383	N	-2.601908	2.923979	0.463780
O	1.854826	-1.561966	-0.689795	O	1.394745	-1.377921	-0.487253
P	1.905891	0.042656	-0.451169	P	2.266564	-0.278654	0.070737
O	0.699867	0.655195	-1.132447	O	1.770514	1.148984	-0.571164
O	1.545658	0.189750	1.165946	O	1.775812	-0.129699	1.643249
O	3.296771	0.509790	-0.671417	O	3.746228	-0.310897	0.006348
H	-1.043919	-0.807366	0.723697	H	-1.106236	-0.365277	0.986421
H	-0.124715	3.034552	0.708089	H	-1.625937	0.874715	-1.607879
H	-3.229452	-0.808235	-1.012056	H	-3.577491	-0.142972	0.982435
H	-3.527676	-2.319370	-0.153207	H	-3.635790	-0.709501	-0.700478
H	-0.044552	1.843435	-0.548559	H	0.806002	1.186728	-0.596030
H	-3.512095	0.301927	0.898764	H	-2.532458	-2.631186	0.267288
H	0.940858	-1.890981	-0.678596	H	-0.070356	-1.373757	-0.695455
H	2.371047	0.101674	1.651693	H	2.458167	0.353244	2.118715
B-TS							
C	-2.983742	-0.821889	-0.058378				
C	-1.462752	-0.788783	-0.104298				
O	-0.855238	-1.449075	-0.981090				
O	-3.437929	-1.999059	0.629930				
O	1.683193	-1.468154	-0.720553				
P	2.310157	-0.177942	-0.095260				
O	1.762612	-0.266203	1.443160				
O	3.774766	-0.071167	-0.182623				
O	1.580798	1.098473	-0.698705				
N	-1.178656	1.135861	-0.561128				
C	-1.784557	2.037637	0.193972				
N	-2.285876	2.773220	0.948087				
H	-0.997279	-0.646686	0.883023				
H	-1.471805	1.185844	-1.531412				
H	-3.382657	0.073217	0.420368				
H	-3.367397	-0.902562	-1.073518				
H	0.585134	1.115417	-0.604723				
H	-3.127395	-1.948353	1.538586				
H	0.662069	-1.476250	-0.822704				
H	2.162223	0.434039	1.968248				

Cyclization

F-SC

C	1.980875	-1.150779	0.797767
O	1.203524	-1.473261	-0.322051
C	3.168767	-0.283930	0.339687
N	2.877863	1.175038	0.431846
C	1.739360	1.680083	-0.062577
N	0.755269	2.159614	-0.433426
O	3.557252	-0.657439	-0.953707
O	-1.110821	-0.894467	0.493149
P	-2.392011	-0.283932	-0.022632
O	-3.475591	-1.073982	-0.664362
O	-2.008182	0.945518	-1.023176
O	-3.027945	0.491836	1.292519
H	4.026654	-0.420348	0.997050
H	3.681098	1.727456	0.162676
H	2.736083	-1.002471	-1.354999
H	2.398229	-2.058925	1.250464
H	1.392983	-0.631095	1.556515
H	0.230959	-1.249232	-0.110012
H	-1.173448	1.363948	-0.767196
H	-3.976570	0.540113	1.144585

H-IM

C	1.665971	-2.086821	-0.492583
O	0.908220	-1.003202	0.054992
C	3.107134	-1.564878	-0.533458
N	3.063184	-0.651817	0.572638
C	1.766931	-0.117212	0.707362
N	1.455244	0.938757	1.289023
O	3.469879	-0.973011	-1.782632
O	-1.714317	0.076369	-1.018385
P	-2.409752	1.111979	0.061802
O	-3.184467	2.111542	-0.709755
O	-1.359140	1.449765	1.094461
O	-3.481245	0.115025	0.850097
H	3.843803	-2.352076	-0.388538
H	3.806994	0.020361	0.669551
H	2.840793	-0.269320	-1.981931
H	1.284852	-2.321609	-1.483377
H	1.579431	-2.960475	0.157199
H	-0.940123	-0.316247	-0.598466
H	0.438712	1.144768	1.258584
H	-3.077755	-0.077039	1.700869

G-TS

C	-0.812781	-1.008252	-0.583641
O	-1.421662	0.237142	-0.481015
C	0.599307	-0.777514	-0.037818
N	0.362322	0.052310	1.114709
C	-0.648440	1.004177	0.986233
N	-1.100749	1.985978	1.469968
O	1.456581	-0.164630	-1.011339
O	-3.960394	0.687187	-0.608071
P	-4.565428	1.687044	0.443807
O	-5.889880	2.228123	0.087543
O	-3.512031	2.812479	0.770671
O	-4.616443	0.741849	1.778813
H	1.113711	-1.691933	0.252375
H	1.186172	0.436324	1.550683
H	0.952640	0.571076	-1.382032
H	-0.752806	-1.357583	-1.621116
H	-1.317636	-1.781454	0.015726
H	-2.967541	0.496736	-0.532547
H	-2.575852	2.501389	1.049107
H	-5.022255	1.233821	2.498499

Elimination of water molecule and aromatization

L-SC

C	1.355218	0.421786	0.671553
C	0.197857	1.373705	0.323887
N	-0.977120	0.646668	0.601126
C	-0.648771	-0.647906	0.791967
O	0.751323	-0.856087	0.766911
O	0.269168	1.786419	-1.097972
N	-1.367153	-1.700389	0.994453
O	-1.726584	-4.625834	1.884641
P	-3.067850	-5.386134	1.347656
O	-4.232086	-4.433972	1.327896
O	-3.111287	-6.723821	2.011484
O	-2.689020	-5.669232	-0.264740
H	0.269922	2.323174	0.870930
H	-0.519004	1.361000	-1.457182
H	2.127911	0.409296	-0.099719
H	1.809990	0.689999	1.635243
H	-1.638770	-3.704970	1.566731
H	-2.345800	-1.432741	0.968328
H	-2.970789	-4.876600	-0.730454

M4-IM

C	-0.826043	0.745798	0.423676
N	0.225587	1.477679	0.301124
C	1.309868	0.603360	0.060211
O	0.910205	-0.693354	0.026244
C	-0.512309	-0.703660	0.264192
N	2.532158	0.913016	-0.112651
O	-3.659874	0.767626	0.657936
O	4.663797	-0.942647	-0.586278
O	-3.456009	-1.382153	-0.627740
H	-1.863096	1.091778	0.588076
H	-4.386847	1.309399	0.342780
H	-0.730096	-1.277489	1.166721
H	-1.060036	-1.159448	-0.561348
H	3.951139	-0.284857	-0.420843
H	2.626491	1.920848	-0.055400
H	-3.980136	-2.016273	-0.134237
H	-3.596697	-0.462767	-0.106903
H	4.189747	-1.771743	-0.682844

M2-TS

C	1.057979	0.267902	0.661747
N	0.042341	1.229457	0.477547
C	-1.088839	0.584113	0.170928
O	-0.967662	-0.813353	0.245702
C	0.333682	-1.081495	0.755706
N	-2.262139	1.021844	-0.169308
O	1.993042	0.258404	-0.496415
O	-4.419521	-0.660672	-0.648126
O	4.729487	-0.277993	-0.525395
H	1.699364	0.463995	1.525110
H	1.665267	0.992427	-1.030467
H	0.808802	-1.857058	0.155235
H	0.257112	-1.417684	1.795346
H	-3.676589	-0.013818	-0.482068
H	-2.227362	2.033076	-0.218778
H	4.713083	-1.098386	-1.022978
H	3.783947	-0.023988	-0.462349
H	-3.980365	-1.509310	-0.554892

M5-TS

C	-2.604977	0.407350	-0.099425
O	-2.141620	-0.080946	1.080081
C	-1.782938	-1.458811	0.872839
C	-2.303148	-1.693528	-0.504825
N	-2.776815	-0.635300	-1.057584
N	-2.799149	1.656734	-0.264643
O	0.144011	2.546478	0.285797
H	-2.252319	-2.645634	-1.026134
H	-2.252466	-2.080066	1.644260
H	-0.678135	-1.550935	0.871300
H	-3.144203	1.808025	-1.211355
H	0.561509	2.050617	-0.445274
H	-0.812928	2.386563	0.212921
O	2.139473	0.561279	1.291537
H	1.354214	1.140708	1.299244
O	0.948307	-1.313141	-0.048540
P	2.151397	-0.393409	-0.056616
O	1.788716	0.772665	-1.241929
O	3.558353	-0.865399	-0.281959
H	2.633594	1.144259	-1.531554

M3-TS

C	-0.968885	0.654019	-0.447013
N	0.052573	1.423990	-0.280831
C	1.168112	0.583508	-0.130919
O	0.833438	-0.729130	-0.244087
C	-0.592338	-0.789840	-0.455560
N	2.380568	0.924194	0.067356
O	-2.559027	-0.077615	1.393574
O	4.602136	-0.857288	0.234688
O	-4.158138	-0.402059	-0.540519
H	-1.963985	1.009747	-0.645455
H	-2.916437	0.498844	2.073890
H	-1.082546	-1.311651	0.364009
H	-0.794837	-1.278647	-1.410563
H	3.852594	-0.220237	0.172682
H	2.430046	1.934865	0.127248
H	-4.559871	-1.263030	-0.408223
H	-3.553239	-0.261390	0.306702
H	4.167685	-1.703170	0.365736

M6-TS

C	0.989200	-0.018175	-1.207303
O	-0.018652	-0.757280	-0.672844
C	0.522096	-1.419759	0.473843
C	1.911406	-1.170031	0.350027
N	2.207115	-0.314131	-0.602395
N	0.711887	0.859659	-2.109445
O	-1.607674	2.017640	-0.927059
H	2.674979	-1.563060	1.009148
H	0.125230	-2.421412	0.601827
H	0.027720	-0.672843	1.586235
H	1.566369	1.335960	-2.374458
H	-1.199199	2.498733	-0.197403
H	-0.853723	1.656910	-1.452366
O	-2.505297	0.343974	1.114430
H	-2.181655	0.778957	0.292065
O	-0.385205	-0.025867	2.494813
P	-1.702271	0.773862	2.428803
O	-1.210593	2.312314	2.073460
O	-2.570211	0.786519	3.625967
H	-1.813124	2.910530	2.526152

N-P

C	1.698923	-0.650988	-1.974187
O	1.229567	-1.084208	-0.773314
C	2.179357	-1.995860	-0.336096
C	3.137087	-2.056210	-1.278704
N	2.833321	-1.193138	-2.327905
N	0.930732	0.223668	-2.657872
O	-0.866709	2.001253	-1.399007
H	4.031349	-2.655000	-1.281928
H	2.001148	-2.451773	0.618042
H	-0.391008	-0.744249	0.750998
H	1.396362	0.650406	-3.439398
H	-0.471270	2.495665	-0.672929
H	0.270653	0.828481	-2.143309
O	-2.457872	0.600335	0.174498
H	-1.553882	1.462529	-0.907850
O	-0.783354	-0.644490	1.626203
P	-1.898048	0.561301	1.570652
O	-0.931834	1.917707	1.671244
O	-2.712691	0.483250	2.809351
H	-0.865318	2.145763	2.602723