CHEMISTRY
A EUROPEAN JOURNAL

Supporting Information

Evidences for the Key Role of Hydrogen Bonds in Nucleophilic Aromatic Substitution Reactions

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Supporting Information for the manuscript: Evidences for the Key-Role of Hydrogen Bonds in S_NAr

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1. Computational details

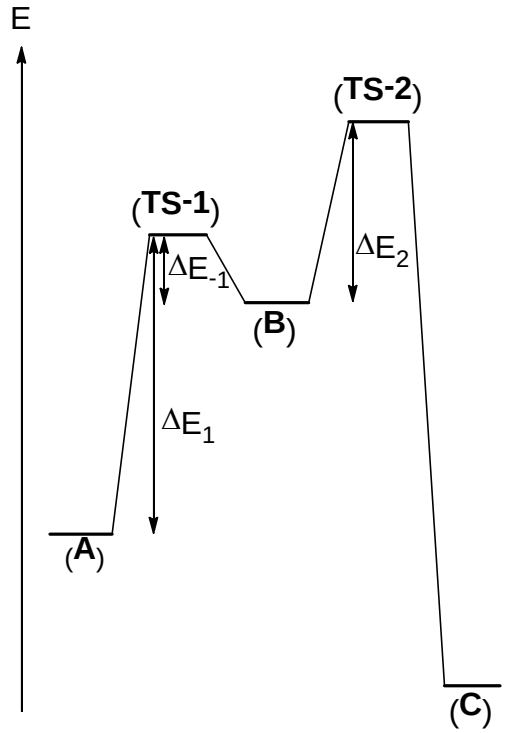
A comparison between the double-ζ 6-31+G(d,p) basis set and the larger aug-cc-pVTZ triple-ζ basis set was performed (see Table below). In the Table SI-1 are given the relative TS-2 energies for several phenols. No significant variations are observed.

TS-2 energy	(**1a**)	(**1b**)	(**1c**)	(**1d**)	(**2**)	(**3**)	(**4**)	(**5**)	(**6**)	(**8**)
6-31+G(d,p)	16.3	19.3	21.7	25.4	18.6	16.8	20.9	20.1	17.4	19.4
aug-cc-pVTZ	16.4	19.4	22.0	25.8	19.4	17.0	21.4	20.5	18.5	19.6

Table SI-1: Relative TS-2 energies of some structures with two basis set with the M06-2X functional in methanol.

2. Kinetic equations for A↔B→C

The energy profile of the Smiles rearrangement is schematised in the Figure below. The kinetic equations for such a system were solved. We assume that the rate constant for C→B is negligeable as the reaction is highly exothermic.



$$-\frac{d[A]}{dt} = k_1[A] - k_{-1}[B]$$

$$-\frac{d[B]}{dt} = (k_2 + k_{-1})[B] - k_1[A]$$

$$-\frac{d[C]}{dt} = -k_2[B]$$

Hence:

$$A(t) = -\frac{r_2+k_1}{r_1-r_2}e^{r_1 t} + \frac{r_1+k_1}{r_1-r_2}e^{r_2 t}$$

$$B(t) = \frac{r_1+k_1}{r_1-r_2} * \frac{r_2+k_1}{k_{-1}}(e^{r_2 t} - e^{r_1 t})$$

$$C(t) = 1 - A(t) - B(t)$$

With the following notations:

$$r_1 = -\frac{(k_1 + k_{-1} + k_2) + \sqrt{\Delta}}{2}$$

$$r_2 = -\frac{(k_1 + k_{-1} + k_2) - \sqrt{\Delta}}{2}$$

$$\Delta = (k_1 + k_{-1} + k_2)^2 - 4 * k_1 * k_2$$

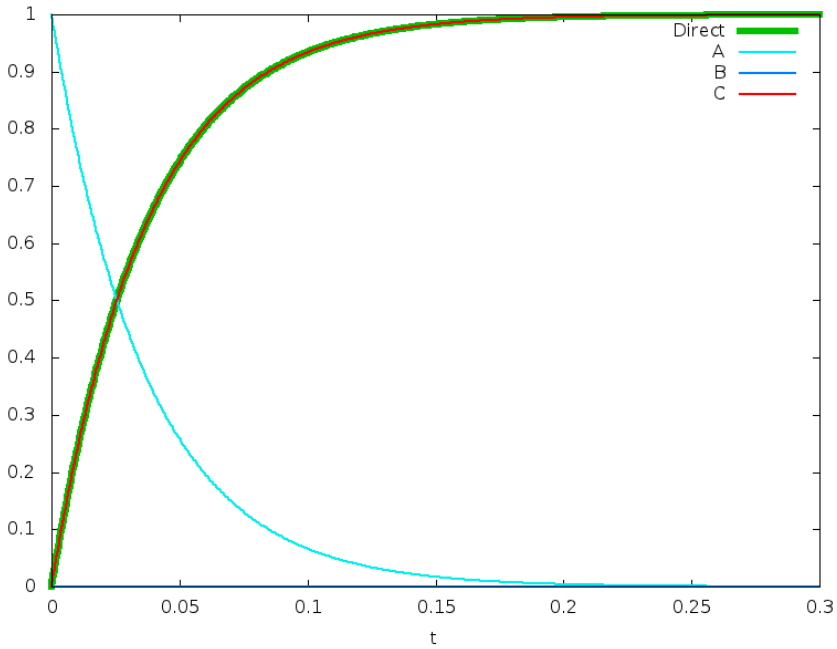
Rate constants were calculated with the Eyring formula:

$$k_i = \frac{k_B T}{h} * e^{-\frac{\Delta G_i^{\neq}}{RT}}$$

assuming the following approximation:

$$\Delta G_i^{\neq} = \Delta E_i$$

The time evolution of such a system is plot below, with the values of (**1a**) (E_1=11.5 kcal.mol^{-1}, E_{-1}=3.2 kcal.mol^{-1}, E_2=8.0 kcal.mol^{-1}). The plot for the kinetic of a single-step mechanism with only (**TS-2**) is also plotted. It appears clearly that the green and the red curves are superimposed.



3. Energy values for intermolecular processes

	TS-1	RI	TS-2	Prod
Ortho with HB	2.6	-4.0	4.2	-24.9
Ortho without HB	5.3	2.5	16.6	-23.2
Para	6.1	1.7	9.4	-25.9

Table SI-2: Relative energies with respect to reactants computed separately for the dimethylamine addition on 2,4-difluoronitrobenzene in methanol.

	TS	Prod
Ortho with HB	6.6	-29.1
Ortho without HB	10.2	-28.1
Para	11.2	-29.9

Table SI-2: Relative energies with respect to reactants computed separately for the dimethylamine addition on 2,4-dichloronitrobenzene in methanol.

	TS-1	RI	TS-2	Prod
Ortho	7.0	-0.1	7.9	-26.8
Para	10.1	5.2	12.5	-26.8

Table SI-2: Relative energies with respect to reactants computed separately for the methylamine addition on 2,4-difluoronitrobenzene in methanol.

	TS-1	Prod
Ortho	11.3	-30.2
Para	15.1	-27.1

Table SI-2: Relative energies with respect to reactants computed separately for the methylamine addition on 2,4-dichloronitrobenzene in methanol.

4. Cartesian coordinates of structures discussed in the text – Intermolecular processes

Cartesian coordinates and total energies of the at the M06-2X/6-31+G(d,p) level of theory in methanol.

Me2NH-2,4-DiFluoroNitroBenzene - Ortho with HB - TS1
Energy: -770.10214458 a.u.

C	-1.318805	-0.712202	-0.547966
C	-0.703040	-1.083239	-1.714057
C	0.678501	-0.989647	-1.949532
C	1.450822	-0.501980	-0.919954
C	0.868470	-0.095470	0.290375
C	-0.545753	-0.109552	0.481271
F	-1.465353	-1.616899	-2.686568
N	1.708867	0.462512	1.297945
O	2.924623	0.302567	1.216564
N	-1.117992	1.825164	0.558949
C	-0.412411	2.562734	-0.483694
F	-1.031638	-0.301081	1.738927
O	1.183428	1.109205	2.206310
C	-2.571318	1.907883	0.440796
H	2.526181	-0.414482	-1.022012
H	-0.807425	2.111489	1.485521
H	1.098878	-1.305004	-2.895382
H	-2.918909	2.944067	0.507725
H	-3.035952	1.318233	1.233190
H	-2.868570	1.504176	-0.531650
H	-2.379085	-0.875878	-0.397881
H	-0.763102	3.597605	-0.554261
H	0.658671	2.563599	-0.273024
H	-0.587902	2.060586	-1.441593

Me2NH-2,4-DiFluoroNitroBenzene - Ortho with HB - IR
Energy: -770.11278578 a.u.

C	-0.585966	-1.183200	-1.782127
C	0.830894	-1.305315	-1.846251
C	1.535621	-0.721130	-0.835823
C	0.895544	-0.007232	0.206280
C	-0.577003	0.108365	0.306227
C	-1.276714	-0.528002	-0.824164
N	1.674967	0.561326	1.202292
O	1.124307	1.283314	2.071676
N	-1.050067	1.575922	0.509001
C	-2.528881	1.711042	0.638367
F	-1.052623	-0.442266	1.529254
F	-1.284750	-1.785509	-2.766988
O	2.899743	0.375223	1.227080
H	2.617283	-0.776839	-0.805119
H	-0.602654	1.827732	1.402196
C	-0.518078	2.477338	-0.547490
H	1.297326	-1.844129	-2.660046
H	-2.741290	2.710872	1.013994
H	-2.895402	0.961582	1.335984
H	-2.981087	1.585014	-0.344697
H	-2.359802	-0.533517	-0.834468
H	-0.898985	3.480897	-0.363647
H	0.569897	2.473235	-0.506300
H	-0.861702	2.110009	-1.515520

Me2NH-2,4-DiFluoroNitroBenzene - Ortho with HB - TS2
Energy: -770.09958367 a.u.

C	-1.194665	-0.394770	-1.013889
C	-0.552612	-1.329969	-1.791823
C	0.807193	-1.629405	-1.699544
C	1.533778	-0.924568	-0.763981
C	0.926552	0.044389	0.043610
C	-0.481726	0.261501	0.009071
F	-1.280714	-1.975012	-2.718583
N	1.752423	0.679679	1.032204
O	2.929719	0.360372	1.117434
N	-1.053863	1.551495	0.487223
C	-0.598784	2.694970	-0.362865
F	-1.008827	-0.497139	1.668036
O	1.252539	1.537955	1.766771
C	-2.543285	1.556621	0.621658
H	2.594246	-1.104062	-0.638804
H	-0.650275	1.657827	1.425430
H	1.256949	-2.372467	-2.345088
H	-2.805000	2.426503	1.222280
H	-2.837331	0.637162	1.119908
H	-2.991469	1.651103	-0.366392
H	-2.253116	-0.227325	-1.163034
H	-1.019445	3.608986	0.054281
H	0.488317	2.740429	-0.351767
H	-0.964680	2.532472	-1.376422

Me2NH-2,4-DiFluoroNitroBenzene - Ortho with HB - Product
Energy: -770.14606435 a.u.

C	-1.064345	-0.370659	-1.362518
C	-0.429169	-1.377188	-2.072684
C	0.838154	-1.844251	-1.763015
C	1.488428	-1.259938	-0.686362
C	0.876608	-0.229754	0.021971
C	-0.412250	0.237288	-0.289124
F	-1.082505	-1.924646	-3.109700
N	1.657386	0.338263	1.123472
O	2.331759	-0.429870	1.789631
N	-1.065042	1.252059	0.492485
C	-0.799256	2.613002	-0.032639
F	-0.572986	0.900752	2.945809
O	1.615727	1.543626	1.298616
C	-2.522674	1.045574	0.622577
H	2.477235	-1.589229	-0.389614
H	-0.687701	1.099793	1.978448
H	1.292229	-2.637045	-2.344705
H	-2.885837	1.734656	1.387589
H	-2.720342	0.021691	0.943485
H	-3.057501	1.254376	-0.310140
H	-2.064565	-0.075566	-1.655497
H	-1.176378	3.337880	0.691910
H	0.270831	2.756362	-0.161156
H	-1.314233	2.755530	-0.990471

Me2NH-2,4-DiFluoroNitroBenzene - Ortho without HB - TS1
Energy: -770.09790268 a.u.

C	-0.116388	0.728129	-0.675860
C	0.410669	-0.131071	0.344023
C	1.140404	-1.271289	-0.128213
C	1.127295	-1.578305	-1.457631
C	0.512289	-0.793802	-2.453667
C	-0.086220	0.369023	-2.035998
F	0.951435	0.449450	1.451495
F	1.778406	-2.687737	-1.856794
N	-0.774438	1.932347	-0.310528
O	-1.071023	2.744580	-1.187717
O	-1.043605	2.116218	0.878398
N	-1.058612	-0.929169	1.346547
C	-1.368277	-0.377363	2.675805
H	-0.682286	-1.870695	1.464346
H	-0.555290	1.040143	-2.745876
C	-2.230499	-1.007771	0.467751
H	0.539592	-1.099350	-3.491208

H	1.673935	-1.889133	0.585164
H	-2.124000	-0.994155	3.173891
H	-0.459774	-0.361076	3.276868
H	-1.738750	0.639262	2.553682
H	-3.014597	-1.622945	0.918179
H	-2.616016	0.001634	0.305846
H	-1.933134	-1.441058	-0.490117

Me2NH-2,4-DiFluoroNitroBenzene - Ortho without HB - IR
Energy: -770.10227792 a.u.

C	0.543929	-0.341648	0.106132
C	1.136949	-0.340832	-1.245190
C	0.732905	0.533011	-2.193658
C	-0.252815	1.539997	-2.013872
C	-0.793453	1.632882	-0.763747
C	-0.432297	0.751716	0.282765
F	1.316247	0.464314	-3.408627
N	-1.014392	0.938987	1.532841
O	-0.790394	0.100125	2.426680
N	-0.040468	-1.825842	0.333946
H	0.431228	-2.360069	-0.401923
O	-1.751429	1.915449	1.741035
C	0.279599	-2.526486	1.617077
F	1.565147	-0.320262	1.064648
H	-1.530519	2.392442	-0.531719
C	-1.495278	-1.889297	0.019726
H	-0.525605	2.196122	-2.829368
H	1.928886	-1.053454	-1.452511
H	-0.077334	-3.552266	1.519006
H	1.356271	-2.516815	1.763254
H	-0.222492	-2.012365	2.429727
H	-1.782142	-2.937972	-0.051153
H	-2.042077	-1.401775	0.825874
H	-1.675861	-1.385440	-0.929693

Me2NH-2,4-DiFluoroNitroBenzene - Ortho without HB - TS2
Energy: -770.07981465 a.u.

C	0.569916	-1.284834	-0.693375
C	0.933494	-1.292402	-2.061896
C	0.760935	-0.175799	-2.838471
C	0.141728	0.991066	-2.389974
C	-0.302030	0.983294	-1.085553
C	-0.116499	-0.129376	-0.251438
F	1.190378	-0.223320	-4.113528
N	-0.550221	0.089643	1.121651
O	0.178755	-0.258311	2.037344
N	0.278723	-2.671808	-0.187458
H	1.112531	-3.187339	-0.488180
O	-1.614437	0.671955	1.290423
C	0.194033	-2.917286	1.289052
F	2.270577	-1.454026	0.149127
H	-0.794188	1.853617	-0.667078
C	-0.933814	-3.236021	-0.865297
H	0.019982	1.846850	-3.041136
H	1.399430	-2.172517	-2.492592
H	0.217849	-3.998324	1.421807
H	1.044752	-2.436214	1.757120
H	-0.750488	-2.525527	1.661646
H	-1.060253	-4.263488	-0.527806
H	-1.793375	-2.630864	-0.577311
H	-0.794940	-3.202005	-1.943141

Me2NH-2,4-DiFluoroNitroBenzene - Ortho without HB - Product
Energy: -770.14337197 a.u.

C	-0.033440	-0.390133	-0.217945
C	0.629638	-0.320215	-1.444768
C	0.685266	0.882120	-2.130203
C	0.143496	2.061551	-1.640972
C	-0.512967	2.005886	-0.421184
C	-0.622443	0.792099	0.253432
F	1.323427	0.907464	-3.311047
N	-1.461556	0.811530	1.452345
O	-1.342409	1.752380	2.217827
N	0.014638	-1.651230	0.469289
H	1.267594	-2.365051	0.004509
O	-2.266302	-0.095181	1.594197
C	0.218700	-1.618100	1.931608
F	2.086506	-2.843530	-0.311349
H	-0.972187	2.890861	0.004204
C	-1.063902	-2.583913	0.072565
H	0.229242	2.983460	-2.203187
H	1.129908	-1.195448	-1.845697
H	0.689408	-2.561569	2.219562
H	0.899472	-0.802330	2.184114
H	-0.716615	-1.515259	2.486416
H	-0.826205	-3.566832	0.485350
H	-2.032495	-2.246919	0.452315
H	-1.093901	-2.654666	-1.016014

Me2NH-2,4-DiFluoroNitroBenzene - Para - TS1
Energy: -770.09668462 a.u.

C	-0.488442	0.983948	-0.182625
C	-0.340284	0.102641	0.910308
C	0.120343	-1.179024	0.753389
C	0.556304	-1.611513	-0.529340
C	0.271479	-0.785261	-1.661578
C	-0.198850	0.484579	-1.471488
F	-0.703305	0.468183	2.145155
F	0.483177	-2.959235	-0.745811
N	-0.952121	2.320193	-0.050376
O	-1.151219	2.784809	1.071349
O	-1.132814	2.980485	-1.076631
N	2.519527	-1.696230	-0.446319
C	2.944052	-2.569194	0.651771
H	0.475160	-1.170805	-2.654218
H	-0.374989	1.134996	-2.320081
H	2.786469	-2.104660	-1.342285
H	0.159127	-1.846941	1.605370
C	3.047292	-0.337835	-0.325517
H	2.536432	-3.568776	0.501072
H	2.562903	-2.156511	1.590133
H	4.035383	-2.622404	0.713566
H	4.139620	-0.339375	-0.267949
H	2.729206	0.254594	-1.184546
H	2.643332	0.105525	0.589903

Me2NH-2,4-DiFluoroNitroBenzene - Para - IR
Energy: -770.10357527 a.u.

C	-0.895731	1.110038	-0.147085
C	-0.647089	0.243651	0.954121
C	-0.001793	-0.945006	0.835149
C	0.493829	-1.412519	-0.460860
C	0.167211	-0.535812	-1.597779
C	-0.482814	0.640949	-1.426014
F	-1.084506	0.567644	2.180522
F	0.055375	-2.736466	-0.724854
N	-1.521200	2.350354	-0.039404
O	-1.848282	2.790267	1.073783
O	-1.737287	3.004897	-1.075955
N	2.041945	-1.697192	-0.424175
C	2.435310	-2.648437	0.656688
H	0.458586	-0.874245	-2.587566
H	-0.706533	1.263859	-2.284060
H	2.248589	-2.143909	-1.324050
H	0.098191	-1.577889	1.708901
C	2.828539	-0.436683	-0.329987
H	1.787096	-3.520657	0.616809

H	2.341496	-2.136185	1.613532
H	3.472842	-2.936835	0.495000
H	3.886848	-0.693018	-0.313327
H	2.599883	0.192895	-1.187089
H	2.542743	0.065676	0.594973

Me2NH-2,4-DiFluoroNitroBenzene - Para - TS2
Energy: -770.09128256 a.u.

C	-1.119637	0.865796	1.090737
C	-0.249100	-0.199090	1.004552
C	0.166629	-0.650161	-0.262164
C	-0.141405	0.138062	-1.403806
C	-1.000296	1.199784	-1.291261
C	-1.525649	1.582853	-0.043878
N	1.436967	-1.438869	-0.342057
C	1.656027	-2.368820	0.809132
N	-2.418246	2.704471	0.015430
O	-2.632726	3.325155	-1.023025
F	-1.526425	1.210387	2.316601
O	-2.936943	3.001968	1.085599
F	-0.735216	-2.241126	-0.620854
H	0.248709	-0.144955	-2.375927
H	-1.283712	1.771895	-2.166006
H	1.303735	-2.031370	-1.167932
H	0.029497	-0.700705	1.921969
C	2.625876	-0.551772	-0.531702
H	0.734660	-2.920868	0.973664
H	1.941270	-1.782469	1.681914
H	2.470099	-3.039158	0.538419
H	3.510493	-1.183197	-0.601902
H	2.500055	0.030659	-1.441666
H	2.693952	0.108361	0.332971

Me2NH-2,4-DiFluoroNitroBenzene - Para - Product
Energy: -770.14758265 a.u.

C	-0.535610	0.618722	1.122321
C	0.400096	-0.403133	1.070516
C	0.951662	-0.779644	-0.155955
C	0.546778	-0.109541	-1.325922
C	-0.376757	0.913281	-1.260065
C	-0.932362	1.289159	-0.034319
N	1.879791	-1.850892	-0.263340
C	2.166721	-2.575328	0.982877
N	-1.912587	2.362815	-0.017339
O	-2.028662	3.035817	-1.031228
F	-1.007871	0.949693	2.324605
O	-2.573054	2.536767	0.993660
F	0.851111	-3.578621	-1.837165
H	0.934919	-0.408901	-2.292188
H	-0.698261	1.428758	-2.156736
H	1.223416	-2.912464	-1.216566
H	0.680433	-0.866142	2.007568
C	3.137545	-1.486997	-0.955016
H	1.237966	-2.943698	1.420846
H	2.695816	-1.943110	1.706663
H	2.796572	-3.430693	0.735824
H	3.714480	-2.399144	-1.112759
H	2.927705	-1.038780	-1.924375
H	3.720201	-0.786351	-0.346244

Me2NH-2,4-DiChloroNitroBenzene - Ortho with HB - TS
Energy: -1490.80695680 a.u.

C	0.054602	-1.210831	-2.017117
C	1.447172	-1.097382	-2.208814
C	2.183433	-0.597974	-1.161234
C	1.567343	-0.185509	0.031093
C	0.147769	-0.218738	0.206862
C	-0.581151	-0.842860	-0.858433
N	2.395312	0.399866	1.034672
O	1.862018	1.114001	1.886703
Cl	-0.507276	-0.629992	1.829719
Cl	-0.897958	-1.911776	-3.299374
O	3.608693	0.203336	1.001439
N	-0.461033	1.663972	0.247527
C	-1.910097	1.735781	0.061237
H	3.259743	-0.494774	-1.237349
H	-0.187083	1.983044	1.176519
C	0.276574	2.383712	-0.789051
H	1.909423	-1.404129	-3.137759
H	-2.256187	2.772496	0.108939
H	-2.411059	1.150753	0.834021
H	-2.155927	1.328686	-0.923494
H	-1.640578	-1.029284	-0.727946
H	-0.085720	3.411358	-0.887078
H	1.338863	2.400519	-0.542761
H	0.132114	1.859961	-1.740059

Me2NH-2,4-DiChloroNitroBenzene - Ortho with HB - Product
Energy: -1490.86378450 a.u.

C	-0.243726	-1.126722	-2.062631
C	0.991761	-1.654779	-1.706955
C	1.671520	-1.093066	-0.635181
C	1.121998	-0.017483	0.050608
C	-0.133068	0.500056	-0.293417
C	-0.816239	-0.068623	-1.359352
N	1.956428	0.573362	1.103371
O	1.907052	1.783348	1.247114
Cl	-0.373272	0.955319	3.349951
Cl	-1.111982	-1.801639	-3.401317
O	2.673562	-0.173357	1.738612
N	-0.761245	1.585628	0.464827
C	-2.239888	1.411664	0.638601
H	2.640768	-1.470841	-0.332047
H	-0.406064	1.521220	1.473067
C	-0.459471	2.939049	-0.108068
H	1.418785	-2.484019	-2.258146
H	-2.550907	2.128618	1.397170
H	-2.433230	0.398516	0.986739
H	-2.753376	1.617413	-0.299037
H	-1.796037	0.289799	-1.649762
H	-0.837155	3.682210	0.594260
H	0.615068	3.040995	-0.227870
H	-0.970252	3.026518	-1.067079

Me2NH-2,4-DiChloroNitroBenzene - Ortho without HB - TS
Energy: -1490.80129369 a.u.

C	0.005166	-1.144365	-1.994057
C	1.390421	-1.082758	-2.273204
C	2.206274	-0.652797	-1.258803
C	1.689766	-0.249497	-0.012842
C	0.278122	-0.210932	0.257540
C	-0.538361	-0.777197	-0.795540
N	2.618204	0.210192	0.959585
O	2.190560	0.851758	1.921304
Cl	-0.292783	-0.734869	1.881227
Cl	-1.054116	-1.770955	-3.230684
O	3.818710	-0.023846	0.804950
N	-0.325629	1.598093	0.308640
H	-1.281449	1.446215	-0.020112
H	3.280430	-0.603554	-1.393817
C	-0.388289	2.374777	1.563195
C	0.422339	2.303938	-0.742573
H	1.779843	-1.382963	-3.236747
H	-1.598669	-0.906038	-0.607856
H	-0.915442	3.315769	1.378267

H	-0.923707	1.803089	2.319133
H	0.625024	2.573420	1.905511
H	-0.024221	3.282785	-0.933328
H	1.453284	2.436697	-0.406831
H	0.407825	1.711025	-1.659376

Me2NH-2,4-DiChloroNitroBenzene - Ortho without HB - Product
Energy: -1490.86222847 a.u.

C	-0.406159	-1.370987	-1.677544
C	0.942946	-1.699935	-1.622865
C	1.784578	-0.923289	-0.839389
C	1.284179	0.170791	-0.142128
C	-0.078347	0.494157	-0.183808
C	-0.921227	-0.295874	-0.957743
N	2.277892	0.961362	0.589998
O	2.127406	2.172275	0.628026
Cl	-3.671063	1.151093	0.723390
Cl	-1.483324	-2.325955	-2.640540
O	3.212050	0.367073	1.091324
N	-0.740142	1.568045	0.562115
H	-1.789417	1.317641	0.562927
H	2.843057	-1.146394	-0.776058
C	-0.426263	1.655191	2.023814
C	-0.705414	2.902177	-0.122610
H	1.331883	-2.543075	-2.181356
H	-1.985655	-0.079385	-0.978508
H	-1.258731	2.187133	2.485356
H	-0.370988	0.643704	2.425283
H	0.500440	2.199328	2.184283
H	-1.398692	3.549811	0.414876
H	0.305756	3.298803	-0.096735
H	-1.047424	2.762280	-1.147705

Me2NH-2,4-DiChloroNitroBenzene - Para - TS
Energy: -1490.79967494 a.u.

C	-0.487512	0.969539	-0.147380
C	-0.351310	0.057374	0.926899
C	0.107467	-1.221031	0.706830
C	0.567331	-1.627822	-0.588147
C	0.264093	-0.756621	-1.688053
C	-0.211096	0.502449	-1.450842
Cl	-0.869150	0.400864	2.553688
Cl	0.344961	-3.377979	-0.941822
N	-0.917397	2.320496	-0.011934
O	-0.940787	2.846187	1.099355
O	-1.237204	2.936688	-1.033094
N	2.484379	-1.694010	-0.483400
C	2.923772	-2.411573	0.719647
H	0.450938	-1.097130	-2.700407
H	-0.390558	1.176107	-2.280342
H	2.772776	-2.201158	-1.321564
H	0.113618	-1.932671	1.523607
C	2.988578	-0.317441	-0.518135
H	2.522662	-3.424995	0.711872
H	2.553700	-1.873762	1.596050
H	4.015246	-2.449661	0.764004
H	4.075224	-0.303650	-0.399654
H	2.717853	0.149482	-1.464354
H	2.529190	0.234440	0.307935

Me2NH-2,4-DiChloroNitroBenzene - Para - Product
Energy: -1490.86521537 a.u.

C	-1.050669	1.384955	-0.150026
C	-0.188715	1.201051	0.934897
C	0.854011	0.288526	0.807668
C	1.000447	-0.419340	-0.379074
C	0.150112	-0.230226	-1.461560
C	-0.879889	0.693805	-1.342313
Cl	-0.303318	2.103356	2.403297
Cl	2.133766	-2.732276	-3.162372
N	-2.192244	2.307687	-0.086350
O	-2.834964	2.351363	0.945065
O	-2.440922	2.950357	-1.091412
N	2.088281	-1.390294	-0.507721
C	1.961544	-2.530256	0.449877
H	0.292680	-0.794183	-2.377899
H	-1.563681	0.876177	-2.163046
H	2.027514	-1.831754	-1.485817
H	1.535464	0.154727	1.640701
C	3.439507	-0.754907	-0.447887
H	0.969001	-2.964298	0.336581
H	2.110400	-2.171670	1.468433
H	2.725468	-3.263679	0.192374
H	4.174146	-1.519806	-0.699374
H	3.471515	0.052601	-1.178165
H	3.619638	-0.372364	0.556705

MeNH2-2,4-DiFluoroNitroBenzene - Ortho - TS1
Energy: -730.80888391 a.u.

O	3.563626	0.255655	1.022104
O	1.772255	0.965778	1.996513
N	2.340166	0.369456	1.078488
H	3.247015	-0.430194	-1.235996
C	1.546821	-0.190277	0.038209
C	2.172787	-0.554321	-1.164600
H	-0.090524	2.025993	1.068332
H	-0.014302	2.110236	-0.579502
N	-0.471470	1.646212	0.203243
C	0.124122	-0.234474	0.177202
F	-0.402258	-0.438870	1.415796
C	1.446352	-1.052354	-2.221440
H	1.902443	-1.338681	-3.159965
H	-2.242752	2.826444	0.139649
C	-1.928598	1.779851	0.130521
C	-0.595886	-0.878434	-0.870384
C	0.064152	-1.213891	-2.019905
H	-2.373411	1.263732	0.982827
H	-2.280973	1.315240	-0.793123
H	-1.653450	-1.078211	-0.747620
F	-0.646737	-1.775415	-3.016006

MeNH2-2,4-DiFluoroNitroBenzene - Ortho - IR
Energy: -730.82016560 a.u.

O	2.858739	0.491033	1.199388
O	1.039551	1.305779	2.045123
N	1.629184	0.633878	1.159587
H	2.649264	-0.681856	-0.825886
C	0.887706	0.064629	0.135224
C	1.568330	-0.642302	-0.887609
H	-0.561071	1.895328	1.252133
H	-0.759867	2.129914	-0.375823
N	-1.083262	1.573680	0.420426
C	-0.590369	0.131876	0.205998
F	-1.082762	-0.459947	1.402310
C	0.900991	-1.240673	-1.913938
H	1.397063	-1.775930	-2.712299
H	-2.730144	2.796666	0.852339
C	-2.550135	1.751985	0.605976
C	-1.248090	-0.490103	-0.958270
C	-0.519441	-1.132125	-1.896192
H	-2.873435	1.107984	1.420041
H	-3.063324	1.497437	-0.318763
H	-2.329859	-0.493289	-1.010877
F	-1.178044	-1.727036	-2.912388

MeNH2-2,4-DiFluoroNitroBenzene - Ortho - TS2

Energy: -730.80752030 a.u.

O	3.570509	0.715194	0.708013
O	1.816177	1.702917	1.465027
N	2.361561	0.901196	0.700004
H	3.278124	-0.828962	-0.992676
C	1.549933	0.172427	-0.231606
C	2.201270	-0.743405	-1.068422
H	-0.180411	1.578275	1.293396
H	-0.144066	2.311002	-0.179143
N	-0.514447	1.499999	0.327492
C	0.127925	0.265138	-0.197430
F	-0.332754	-0.541144	1.423663
C	1.496016	-1.505905	-1.972871
H	1.976659	-2.209755	-2.639647
H	-2.313412	2.406150	0.878032
C	-2.004522	1.532615	0.307160
C	-0.570474	-0.435568	-1.205242
C	0.112586	-1.314098	-2.010270
H	-2.358397	0.618470	0.777806
H	-2.351636	1.621085	-0.719683
H	-1.644115	-0.357160	-1.307716
F	-0.597148	-2.014991	-2.911540

MeNH2-2,4-DiFluoroNitroBenzene - Ortho - Product

Energy: -730.86761446 a.u.

O	2.942136	0.716980	0.879671
O	1.246904	1.902865	1.458391
N	1.754430	0.988415	0.813462
H	2.644115	-0.812316	-0.802139
C	0.909885	0.197310	-0.065798
C	1.566920	-0.734290	-0.874837
H	-1.279734	0.437052	2.187664
H	-0.651466	2.033066	0.997462
N	-1.204526	1.224064	0.733743
C	-0.497961	0.361435	-0.108234
F	-1.341495	-0.052826	3.018530
C	0.861546	-1.536748	-1.750523
H	1.349181	-2.263277	-2.388111
H	-2.917255	2.337105	1.089968
C	-2.596820	1.554420	0.403694
C	-1.200819	-0.459916	-1.001852
C	-0.517570	-1.370167	-1.784328
H	-3.237914	0.683958	0.554871
H	-2.698874	1.910367	-0.626131
H	-2.276602	-0.397772	-1.096589
F	-1.233401	-2.130138	-2.626789

MeNH2-2,4-DiFluoroNitroBenzene - Para - TS1

Energy: -730.80391607 a.u.

C	-0.342966	0.055142	0.910787
C	0.086282	-1.232935	0.729522
C	0.550334	-1.636870	-0.553893
C	0.294592	-0.781163	-1.673129
C	-0.143027	0.495778	-1.457785
C	-0.439740	0.970419	-0.160519
F	0.466634	-2.978531	-0.798591
N	2.483808	-1.726619	-0.446028
C	2.963203	-2.490117	0.712162
N	-0.866306	2.315261	-0.000362
O	-1.016772	3.005630	-1.011998
F	-0.726689	0.397850	2.145946
O	-1.063730	2.759128	1.130477
H	0.507271	-1.149306	-2.670272
H	-0.285731	1.172947	-2.291307
H	2.811418	-2.130660	-1.323108
H	0.097768	-1.924759	1.563048
H	2.802067	-0.759459	-0.411741
H	2.584650	-3.510428	0.640008
H	2.577723	-2.025268	1.621604
H	4.054202	-2.508960	0.760292

MeNH2-2,4-DiFluoroNitroBenzene - Para - IR

Energy: -730.81168900 a.u.

C	0.253213	-0.992792	0.820412
C	0.746211	-1.480048	-0.469785
C	0.481821	-0.584583	-1.608729
C	-0.144607	0.606714	-1.446249
C	-0.589530	1.075861	-0.178887
C	-0.375268	0.205530	0.926896
H	0.793619	-0.922859	-2.591885
F	0.262768	-2.789381	-0.731724
N	2.267673	-1.811304	-0.420877
C	2.704545	-2.714589	0.682028
F	-0.816485	0.542773	2.147920
H	-0.324424	1.241088	-2.306343
N	-1.197952	2.325871	-0.086236
H	2.518113	-2.226709	-1.324854
H	0.333386	-1.622702	1.698114
H	2.767251	-0.919486	-0.362203
H	2.113143	-3.626156	0.632350
H	2.553036	-2.203416	1.630125
H	3.760955	-2.935305	0.543983
O	-1.575776	2.757986	1.013783
O	-1.349909	2.996021	-1.124298

MeNH2-2,4-DiFluoroNitroBenzene - Para - TS2

Energy: -730.80016787 a.u.

C	-0.282040	-0.230842	1.010169
C	0.157140	-0.663972	-0.255910
C	-0.094821	0.156157	-1.387989
C	-0.943723	1.227375	-1.278604
C	-1.507361	1.585644	-0.041445
C	-1.142190	0.840811	1.091622
H	0.340098	-0.104205	-2.347206
F	-0.749000	-2.235042	-0.619596
N	1.409778	-1.469245	-0.332559
C	1.711822	-2.348097	0.835191
F	-1.582385	1.165577	2.311287
H	-1.185399	1.827834	-2.147108
N	-2.392777	2.712619	0.013782
H	1.293552	-2.063778	-1.158627
H	-0.036404	-0.759473	1.921835
H	2.198909	-0.837165	-0.500467
H	0.825125	-2.947509	1.026525
H	1.970110	-1.725322	1.688811
H	2.558026	-2.976440	0.564658
O	-2.933435	2.997952	1.076336
O	-2.579997	3.349882	-1.020076

MeNH2-2,4-DiFluoroNitroBenzene - Para - Product

Energy: -730.86275080 a.u.

C	0.557622	-0.660550	0.895098
C	1.179211	-0.950510	-0.321706
C	0.896795	-0.162023	-1.452510
C	0.012108	0.890709	-1.359385
C	-0.617998	1.186425	-0.145185
C	-0.332695	0.398030	0.972650
H	1.374170	-0.386099	-2.400478
F	0.536496	-3.969636	-1.373307
N	2.037318	-2.052338	-0.458609
C	2.656700	-2.619863	0.747721
F	-0.890461	0.630750	2.161299
H	-0.210357	1.504809	-2.223137
N	-1.542100	2.305127	-0.100443
H	1.109306	-3.251225	-1.060178
H	0.743394	-1.231164	1.796395
H	2.722045	-1.893051	-1.193449
H	1.901032	-3.130062	1.347833

H	3.145692	-1.849930	1.352760
H	3.394146	-3.356157	0.430987
O	-2.121634	2.549526	0.946130
O	-1.696776	2.953595	-1.126268

MeNH2-2,4-DiChloroNitroBenzene - Ortho - TS
Energy: -1451.51314990 a.u.

O	3.599130	0.241817	1.011031
O	1.841526	1.073704	1.949521
N	2.381076	0.406307	1.064284
H	3.244956	-0.377700	-1.245435
C	1.559457	-0.168401	0.050819
C	2.173325	-0.517395	-1.162654
H	-0.135475	2.007125	1.136401
H	0.061357	2.068147	-0.502966
N	-0.463131	1.624315	0.250239
C	0.138538	-0.228475	0.222336
Cl	-0.528931	-0.649520	1.833842
C	1.443493	-1.006211	-2.219973
H	1.907496	-1.268344	-3.161691
H	-2.195072	2.833885	0.042128
C	-1.906859	1.780488	0.060134
C	-0.577453	-0.869853	-0.844434
C	0.059183	-1.185747	-2.015969
H	-2.427389	1.277957	0.876895
H	-2.189278	1.319098	-0.888292
H	-1.629438	-1.089925	-0.707459
Cl	-0.877131	-1.897795	-3.304414

MeNH2-2,4-DiChloroNitroBenzene - Ortho - Product
Energy: -1451.57766220 a.u.

O	2.897028	0.511961	1.401459
O	1.588260	2.220529	1.270231
N	1.922023	1.084642	0.960845
H	2.798905	-0.768959	-0.649200
C	1.107535	0.382603	-0.033920
C	1.747812	-0.566425	-0.817111
H	-0.762412	1.190446	1.703617
H	-0.436906	2.500689	0.681747
N	-0.924155	1.599401	0.697008
C	-0.251865	0.677975	-0.208572
Cl	-0.438795	0.228515	3.244980
C	1.041343	-1.233194	-1.809948
H	1.530641	-1.969787	-2.435885
H	-2.703834	2.497364	1.288115
C	-2.387548	1.792188	0.521893
C	-0.961567	0.001357	-1.186967
C	-0.304731	-0.937234	-1.984199
H	-2.888724	0.837411	0.675152
H	-2.599506	2.195642	-0.466853
H	-2.017069	0.183063	-1.343270
Cl	-1.208500	-1.755870	-3.214672

MeNH2-2,4-DiChloroNitroBenzene - Para - TS
Energy: -1451.50706796 a.u.

C	-0.334165	0.015388	0.916556
C	0.048045	-1.286126	0.691639
C	0.534998	-1.689559	-0.594762
C	0.261507	-0.813380	-1.700587
C	-0.133518	0.471530	-1.457326
C	-0.382581	0.945598	-0.149403
Cl	0.352487	-3.437198	-0.937395
N	2.434056	-1.695692	-0.474281
C	2.971106	-2.346232	0.726790
N	-0.714003	2.323148	-0.001929
O	-1.002048	2.966078	-1.015582
Cl	-0.878418	0.375212	2.531488
O	-0.683228	2.841529	1.112563
H	0.438925	-1.162203	-2.711163
H	-0.267031	1.161629	-2.281741
H	2.794479	-2.118002	-1.330587
H	0.000897	-2.008854	1.496896
H	2.666752	-0.702665	-0.493796
H	2.717636	-3.406515	0.697206
H	2.514046	-1.885548	1.604624
H	4.055048	-2.231057	0.785902

MeNH2-2,4-DiChloroNitroBenzene - Para - Product
Energy: -1451.57250866 a.u.

C	-0.272754	0.764586	0.899853
C	0.666216	-0.262050	0.788359
C	1.158601	-0.600034	-0.462774
C	0.751845	0.066430	-1.616495
C	-0.164397	1.098460	-1.504933
C	-0.680826	1.429105	-0.255465
Cl	0.617697	-3.762317	-2.097115
N	2.099814	-1.701508	-0.633206
C	2.606397	-2.381798	0.587665
N	-1.677815	2.506737	-0.224589
O	-1.497178	3.446651	-0.979452
Cl	-0.810369	1.191512	2.484920
O	-2.629892	2.386622	0.522403
H	1.142721	-0.215951	-2.588401
H	-0.499542	1.646169	-2.377767
H	1.587669	-2.467459	-1.234333
H	0.992900	-0.763680	1.690540
H	2.891952	-1.377547	-1.195948
H	1.765402	-2.850434	1.097455
H	3.109038	-1.664410	1.234851
H	3.305779	-3.148862	0.260510

5. Cartesian coordinates of structures discussed in the text – Intramolecular processes

Cartesian coordinates and total energies of the at the M06-2X/6-31+G(d,p) level of theory in methanol.

(11) - Imidate
Energy: -613.27403189 a.u.

N	0.523304	-1.671614	-1.047463
C	-0.829901	0.405345	0.782303
O	-1.002063	0.750404	-0.549571
C	0.046748	0.651914	-1.436309
C	1.141136	-0.343155	-1.095409
C	-1.492978	-0.711440	1.278912
C	-1.375365	-1.021049	2.633182
C	-0.598193	-0.223577	3.474930
C	0.057271	0.895872	2.961484
C	-0.062471	1.220114	1.610289
N	0.020826	1.308383	-2.516381
C	-1.110668	2.199313	-2.743075
C	2.332401	-0.239879	-2.041795
H	-2.074773	-1.324991	0.600115
C	1.192112	-2.593370	-0.136190
H	-0.915561	2.803909	-3.629754
H	-2.030052	1.626328	-2.909885
H	-1.285837	2.861485	-1.887945
H	2.790488	0.751162	-1.996326
H	0.434036	2.091546	1.192582
H	2.016916	-0.420966	-3.072634
H	1.482297	-0.121635	-0.077046
H	0.658455	1.522996	3.612194
H	-1.888277	-1.891635	3.029829
H	-0.506343	-0.472496	4.527178
H	0.500341	-2.058500	-1.987839
H	1.053915	-2.235433	0.890210
H	3.083457	-0.984082	-1.762562
H	0.725492	-3.578020	-0.214052
H	2.271170	-2.707093	-0.321450

(11) - TS
Energy: -613.22818448 a.u.

N	1.879878	-4.384930	0.752568
C	0.894041	-3.614443	1.745479
O	0.379693	-2.621762	0.537094
C	1.308390	-2.439568	-0.390249
C	2.478191	-3.387121	-0.176545
C	-0.184209	-4.448304	2.188262
C	-0.606571	-4.434059	3.509200
C	0.022280	-3.650778	4.482110
C	1.114122	-2.874541	4.076288
C	1.568086	-2.862496	2.766725
N	1.281273	-1.610350	-1.354198
C	0.104149	-0.749702	-1.412904
C	3.035594	-3.998133	-1.447759
H	-0.698407	-5.060064	1.450826
C	2.850767	-5.230378	1.483250
H	0.199733	-0.067618	-2.259257
H	-0.814817	-1.335203	-1.539909
H	-0.010290	-0.157192	-0.496962
H	3.355304	-3.187758	-2.104407
H	2.413158	-2.236758	2.490962
H	2.267553	-4.575878	-1.970324
H	3.268782	-2.875380	0.383212
H	1.638382	-2.258491	4.803273
H	-1.450325	-5.063392	3.783274
H	-0.314390	-3.653363	5.512203
H	1.269876	-5.001244	0.203092
H	3.523985	-4.578395	2.039181
H	3.894605	-4.639183	-1.239473
H	2.293371	-5.863152	2.174102
H	3.404437	-5.840780	0.770603

(11) - Product
Energy: -613.27569755 a.u.

N	0.619190	-1.085768	-0.271421
C	0.069618	-0.678325	1.030666
O	-1.072090	-0.315401	-1.958728
C	-0.204314	0.608465	-1.760553
C	1.091963	0.115082	-1.075842
C	-1.295317	-0.808591	1.254405
C	-1.813351	-0.432430	2.494383
C	-0.969498	0.064198	3.485571
C	0.398888	0.190070	3.241031
C	0.927178	-0.180014	2.007378
N	-0.231799	1.861850	-2.082047
C	-1.430901	2.262952	-2.804540
C	2.140623	-0.249356	-2.116847
H	-1.941676	-1.185123	0.467593
C	1.559498	-2.234689	-0.138100
H	-1.375247	3.328606	-3.041387
H	-1.551681	1.708712	-3.746468
H	-2.344169	2.089300	-2.217530
H	2.378986	0.664661	-2.664126
H	1.991021	-0.076136	1.815358
H	1.755604	-0.983047	-2.831449
H	1.480794	0.857648	-0.378508
H	1.058329	0.579025	4.009344
H	-2.877997	-0.527193	2.679480
H	-1.376141	0.356025	4.448148
H	-0.207919	-1.345413	-0.880650
H	2.469061	-1.910739	0.367223
H	3.061629	-0.627589	-1.667209
H	1.059150	-3.003027	0.449982
H	1.794610	-2.617491	-1.128843

(12) - Imidate
Energy: -1072.84174180 a.u.

O	0.962106	0.951486	0.406342
C	0.649847	0.437874	-0.829594
N	-1.254935	-0.778887	0.940391
C	-1.400321	0.667804	1.094767
C	-0.017799	1.250655	1.333511
C	1.097335	-0.838570	-1.176356
C	0.843654	-1.353524	-2.443255
C	0.145948	-0.586371	-3.375828
C	-0.282059	0.697022	-3.042314
C	-0.020917	1.211283	-1.773606
C	-2.182487	-1.372459	-0.014298
H	-0.053597	-0.992998	-4.361313
C	-2.394144	1.081632	2.175094
Cl	1.973532	-1.788922	-0.016347
N	0.284549	1.933692	2.351534
C	1.657149	2.411358	2.470844
H	-3.239390	-1.128961	0.175764
H	-1.923772	-1.025726	-1.022010
H	-2.070517	-2.459074	0.004842
H	-3.365782	0.628801	1.957567
H	-0.811830	1.303807	-3.768783
H	-1.757916	1.054632	0.133042
H	-0.332433	2.215326	-1.500758
H	-1.337583	-1.226538	1.848946
H	-2.513808	2.166521	2.214280
H	-2.053982	0.740749	3.156690
H	1.190394	-2.351176	-2.690705
H	1.962088	2.987179	1.589939
H	1.737395	3.045319	3.354556
H	2.356442	1.574018	2.575611

(12) - TS
Energy: -1072.79933667 a.u.

O	1.109242	3.391101	0.050249
C	0.252946	2.483656	-1.046734
N	-0.888378	2.196835	-0.002228
C	-1.113851	3.438644	0.793706
C	0.304996	3.970739	0.927915
C	1.003463	1.323226	-1.417824
C	1.435891	1.079520	-2.710056
C	1.089385	1.934944	-3.755570
C	0.281836	3.037025	-3.449506
C	-0.156160	3.292044	-2.162355
C	-2.096264	1.621891	-0.640177
H	1.421338	1.737614	-4.767401
C	-1.819948	3.186551	2.111818
Cl	1.464802	0.215086	-0.124162
N	0.611039	4.853524	1.790403
C	2.005006	5.286355	1.780822
H	-2.802336	1.332089	0.136900
H	-2.531306	2.372982	-1.298610
H	-1.791564	0.750603	-1.220426
H	-2.846504	2.847889	1.958852
H	-0.027336	3.717374	-4.238541
H	-1.703048	4.112846	0.162610
H	-0.777741	4.161163	-1.964820
H	-0.495770	1.488593	0.631852
H	-1.841845	4.125032	2.667480
H	-1.276593	2.449699	2.710549
H	2.043999	0.197971	-2.891509
H	2.286837	5.716218	0.811942
H	2.151622	6.042455	2.553545
H	2.686659	4.449692	1.976982

(12) - Product
Energy: -1072.83834730 a.u.

O	0.807935	0.227839	1.874255
C	-0.453295	-0.326744	-0.876454
N	-1.205756	-0.435869	0.383007
C	-1.336588	0.886967	1.120693
C	0.107475	1.235746	1.523338
C	0.484818	-1.311827	-1.190925
C	1.196504	-1.250850	-2.383650
C	0.956490	-0.206171	-3.272106
C	0.005152	0.765179	-2.971647
C	-0.702622	0.705541	-1.773769
C	-2.481548	-1.187677	0.172124
H	1.511866	-0.159459	-4.202576
C	-2.220297	0.726970	2.349855
Cl	0.757880	-2.648426	-0.107278
N	0.406850	2.498650	1.481351
C	1.754562	2.799213	1.942478
H	-2.894505	-1.469113	1.138092
H	-3.173662	-0.545653	-0.373144
H	-2.256918	-2.080816	-0.409886
H	-3.265952	0.543226	2.095058
H	-0.191424	1.574245	-3.665911
H	-1.758278	1.623779	0.439199
H	-1.444067	1.463952	-1.550637
H	-0.577910	-0.952300	1.031312
H	-2.169494	1.663268	2.909416
H	-1.854772	-0.076281	2.997443
H	1.926328	-2.020827	-2.607618
H	2.519590	2.258692	1.366879
H	1.944986	3.871100	1.841253
H	1.903891	2.525361	2.997219

(13) - Imidate
Energy: -727.75647240 a.u.

C	-0.038676	1.189995	-1.715357
C	0.607741	0.424009	-0.758995
C	1.040857	-0.880881	-1.051635
C	0.764551	-1.411679	-2.312754
C	0.086222	-0.644364	-3.265775
C	-0.312652	0.655047	-2.977892
N	-1.318587	-0.833170	1.006519
C	-1.436938	0.617670	1.163298
C	-0.049606	1.175663	1.430075
O	0.919550	0.955921	0.477881
C	-2.246326	-1.398677	0.034641
C	-2.446632	1.042363	2.224306
N	0.252822	1.793972	2.491175
C	1.626228	2.261756	2.635315
O	1.709191	-1.527573	-0.070448
H	-0.118830	-1.075503	-4.240445
H	-3.300693	-1.136373	0.215518
H	-1.968570	-1.045930	-0.965665
H	-2.156564	-2.487684	0.043346
H	-3.421937	0.610811	1.981112
H	-0.828064	1.254366	-3.720360
H	-1.766813	1.014120	0.195887
H	-0.332205	2.204213	-1.459196
H	-1.435585	-1.277797	1.913005
H	-2.545552	2.129212	2.270753
H	-2.137072	0.686480	3.210631
H	1.072816	-2.419903	-2.562162
H	1.913588	2.924923	1.811375
H	1.719651	2.806669	3.575495
H	2.332192	1.423395	2.643114
C	2.075552	-2.877797	-0.309418
H	2.565257	-3.220911	0.600568
H	1.190178	-3.492416	-0.505298
H	2.772226	-2.955406	-1.150921

(13) - TS
Energy: -727.70997392 a.u.

C	-0.138781	3.389844	-2.216375
C	0.317123	2.603613	-1.116661
C	1.095322	1.442230	-1.473462
C	1.464172	1.175737	-2.772758
C	1.057679	2.015066	-3.831525
C	0.253986	3.105913	-3.525160
N	-0.819323	2.186133	-0.044056
C	-1.078119	3.366779	0.815689
C	0.311737	3.972917	0.916421
O	1.111106	3.478632	-0.021782
C	-2.001450	1.597005	-0.702589
C	-1.711061	3.022480	2.150760
N	0.616190	4.833663	1.800205
C	1.984218	5.339555	1.748203
O	1.397237	0.663280	-0.371335
H	1.355469	1.795586	-4.849909
H	-2.687113	1.217079	0.054342
H	-2.480768	2.367177	-1.306786
H	-1.661371	0.784656	-1.346335
H	-2.713847	2.609919	2.021080
H	-0.090918	3.766861	-4.316536
H	-1.727146	4.038142	0.241414
H	-0.758389	4.258657	-2.008967
H	-0.356238	1.460839	0.518187
H	-1.783745	3.935125	2.744026
H	-1.091664	2.307035	2.699519
H	2.068516	0.299317	-2.983995
H	2.218104	5.775521	0.769456
H	2.112935	6.107056	2.512905
H	2.711844	4.539708	1.932668
C	2.045016	-0.571742	-0.611849
H	2.137462	-1.063377	0.355905
H	1.454580	-1.197530	-1.291455
H	3.042356	-0.414088	-1.037528

(13) - Product
Energy: -727.75969719 a.u.

C	-0.698666	0.723207	-1.670835
C	-0.447450	-0.322890	-0.799696
C	0.472998	-1.332486	-1.119955
C	1.170843	-1.261675	-2.324345
C	0.926911	-0.197505	-3.194412
C	-0.003275	0.787523	-2.879735
N	-1.151650	-0.478788	0.483241
C	-1.340420	0.823735	1.232633
C	0.086634	1.270669	1.598523
O	0.868194	0.318498	1.930254
C	-2.383372	-1.306964	0.305302
C	-2.175271	0.605150	2.487557
N	0.294530	2.553066	1.557168
C	1.629341	2.943082	1.987111
O	0.590180	-2.319896	-0.201739
H	1.473165	-0.148232	-4.130810
H	-2.760268	-1.607402	1.280450
H	-3.123407	-0.711493	-0.230343
H	-2.112338	-2.187885	-0.274963
H	-3.216248	0.363776	2.263059
H	-0.190656	1.608007	-3.562809
H	-1.829616	1.536567	0.570233
H	-1.422212	1.491293	-1.422972
H	-0.471805	-0.977139	1.090782
H	-2.161013	1.537331	3.056162
H	-1.744425	-0.182557	3.113507
H	1.892768	-2.024840	-2.588315
H	2.413349	2.492359	1.360963
H	1.730750	4.030113	1.928107
H	1.840548	2.635495	3.021759
C	1.568007	-3.331992	-0.426223
H	1.522545	-3.984732	0.442906
H	1.330971	-3.900182	-1.330252
H	2.565019	-2.890008	-0.508610

(1a) - Imidate
Energy: -817.70882443 a.u.

H	3.756068	2.445613	1.126238
H	1.977338	2.498203	1.259497
C	2.862914	1.859347	1.344607
H	2.924175	1.506352	2.380421
N	2.796373	0.733749	0.419923
C	1.743722	0.041473	0.405939
O	0.733895	0.321458	1.313323
H	3.416490	-2.108618	-0.252527
C	-0.537246	-0.165489	1.162843
C	1.507653	-1.110947	-0.549971
H	-0.231965	-1.568759	2.733717
C	-0.952706	-1.177282	2.023500
H	3.398396	-0.938049	-1.582170
O	-0.185459	2.167253	-0.395687
H	0.955773	-1.883938	0.001194
C	-1.456986	0.344449	0.235761
C	-2.253890	-1.670714	1.962335
C	-2.751964	-0.157433	0.157295
H	-2.558260	-2.457187	2.644749
N	-1.092525	1.411122	-0.697742
C	-3.156093	-1.162656	1.029207
C	2.812925	-1.705307	-1.069619
O	-1.741503	1.503610	-1.727061
H	-3.428600	0.253278	-0.582646
H	-4.169067	-1.544845	0.976672
N	0.609712	-0.619534	-1.598950
H	1.154508	-0.120726	-2.298799
H	-0.913270	-2.041786	-1.474410
H	2.592220	-2.514661	-1.770763
C	-0.206259	-1.656617	-2.219133
H	-0.784887	-1.214217	-3.033209
H	0.368701	-2.504273	-2.619993

(1a) - TS1
Energy: -817.69046567 a.u.

H	3.762317	2.234606	1.906593
H	2.022255	2.415424	1.575193
C	2.815397	1.700877	1.823632
H	2.575220	1.260746	2.797871
N	2.936083	0.670369	0.796965
C	1.896391	0.025001	0.503548
O	0.701428	0.220283	1.126107
H	3.802292	-0.807787	-1.342224
C	-0.473583	-0.324859	0.567789
C	1.841750	-1.097630	-0.511002
H	-0.396751	-1.979686	1.958886
C	-1.072727	-1.346887	1.392008
H	2.514021	0.048126	-2.208077
O	0.278775	1.661765	-1.112496
H	2.091642	-2.028340	0.013796
C	-1.414402	0.598311	-0.015039
C	-2.429203	-1.507859	1.466923
C	-2.809352	0.410090	0.076035
H	-2.824870	-2.304620	2.090506
N	-0.921157	1.672305	-0.784545
C	-3.327962	-0.641485	0.788146
C	2.772464	-0.882549	-1.694160
O	-1.681820	2.577834	-1.134567
H	-3.448833	1.120711	-0.435171
H	-4.398167	-0.792448	0.856623
N	0.428120	-1.173191	-0.879249
H	0.249763	-0.533743	-1.654882
H	0.006059	-3.138912	-0.294825
H	2.696940	-1.717108	-2.395161
C	-0.114461	-2.500666	-1.171681
H	-1.178388	-2.400073	-1.395553
H	0.398763	-2.949873	-2.025716

(1a) - Spiro
Energy: -817.69556749 a.u.

H	3.809511	1.964157	2.204399
H	2.265372	2.460561	1.475995
C	2.813004	1.623917	1.923589
H	2.275368	1.317754	2.827636
N	2.935691	0.513764	0.982053
C	1.865247	0.011400	0.552192
O	0.618142	0.438563	0.874680
H	3.815217	-1.161109	-1.032403
C	-0.431275	-0.361262	0.256291
C	1.781436	-1.157754	-0.406683
H	-0.120625	-2.048963	1.629486
C	-0.889837	-1.407713	1.207466
H	2.749261	-0.238150	-2.104815
O	-0.090982	1.537174	-1.644166
H	1.812127	-2.096499	0.157729
C	-1.543799	0.478221	-0.242263
C	-2.178013	-1.520649	1.600364
C	-2.883834	0.316583	0.213488
H	-2.432536	-2.285949	2.328230
N	-1.258260	1.467861	-1.154545
C	-3.216942	-0.656906	1.102106
C	2.830234	-1.146603	-1.501303
O	-2.130197	2.276262	-1.515333
H	-3.626111	0.997754	-0.186151
H	-4.238660	-0.783092	1.437930
N	0.391529	-0.994466	-0.920013
H	0.410510	-0.219157	-1.609333
H	-0.207712	-3.010486	-0.798954
H	2.736301	-2.023572	-2.144463
C	-0.233893	-2.194053	-1.519965
H	-1.266137	-1.948873	-1.773167

H	0.317540	-2.459752	-2.421071

(1a) - TS2
Energy: -817.68281124 a.u.

N	0.631575	0.832621	0.089265
C	-0.723507	0.260620	-0.207821
O	-0.130022	-1.417534	0.445674
C	1.155816	-1.477254	0.244970
C	1.717891	-0.147405	-0.259211
C	-1.830897	0.605735	0.621698
C	-3.154300	0.533262	0.142154
C	-3.406521	0.240805	-1.175504
C	-2.312451	0.025992	-2.043609
C	-1.017496	0.073991	-1.591575
N	1.945303	-2.473621	0.401166
C	1.297748	-3.703739	0.842027
C	3.047592	0.247088	0.353713
N	-1.650956	0.879273	2.010310
O	-2.630469	1.029452	2.727016
C	0.805469	2.185265	-0.514479
O	-0.497210	0.963532	2.470046
H	2.045743	-4.494538	0.926356
H	0.813766	-3.579428	1.819376
H	0.522364	-4.031561	0.137440
H	3.740813	-0.578345	0.188165
H	-0.197424	-0.084521	-2.283410
H	2.952230	0.397408	1.433481
H	1.791213	-0.164965	-1.351465
H	-2.490819	-0.163730	-3.097463
H	-3.959557	0.726901	0.840028
H	-4.423322	0.200197	-1.546057
H	0.625022	0.936769	1.120514
H	0.860266	2.084350	-1.598017
H	3.461053	1.146995	-0.105432
H	-0.050772	2.798567	-0.234935
H	1.722707	2.621115	-0.122339

(1b) - Imidate
Energy: -817.70711356 a.u.

C	1.705008	-1.326055	-0.284881
C	0.461535	-0.780344	-0.594017
C	-0.685134	-1.528553	-0.297972
C	-0.604255	-2.785253	0.299649
C	0.641169	-3.302939	0.624860
C	1.793777	-2.571973	0.326168
N	1.648841	1.431625	1.175444
C	0.238178	1.630553	0.832440
C	0.140954	1.605608	-0.677277
O	0.409920	0.393657	-1.297976
N	-2.018306	-1.018031	-0.609836
O	-2.192901	0.190933	-0.599690
N	-0.089197	2.621228	-1.385419
C	-0.118231	2.454644	-2.833672
C	-0.393879	2.883539	1.428241
C	1.853908	0.841868	2.493938
O	-2.894984	-1.832560	-0.849007
H	-0.871502	1.716263	-3.131272
H	-1.518841	-3.328987	0.505586
H	-0.358688	3.411771	-3.297463
H	0.850219	2.112140	-3.215178
H	-0.305302	0.754006	1.207640
H	1.464195	-0.182512	2.487677
H	0.713910	-4.272624	1.103879
H	-1.455115	2.945353	1.173440
H	2.925051	0.792158	2.701761
H	1.367775	1.391097	3.313851
H	-0.297725	2.858813	2.516941
H	2.134454	2.322830	1.106590
H	0.102934	3.778915	1.046337
H	2.770622	-2.976553	0.569739

H	2.586290	-0.743227	-0.524712

(1b) - TS1
Energy: -817.69037171 a.u.

C	2.023655	-0.822473	-0.290304
C	0.675162	-0.311932	-0.151705
C	-0.309022	-1.325342	0.130898
C	0.050112	-2.658572	0.436983
C	1.359362	-3.057867	0.414628
C	2.346691	-2.112215	0.019112
N	0.770986	0.923852	1.284104
C	0.088045	2.127633	0.803090
C	-0.030657	1.916357	-0.694893
O	0.369243	0.678760	-1.103484
N	-1.676005	-0.978772	0.167589
O	-1.982287	0.223216	0.145860
N	-0.429978	2.800416	-1.496910
C	-0.524394	2.433907	-2.906468
C	0.807149	3.421391	1.161989
C	0.290062	0.342224	2.541237
O	-2.532383	-1.865102	0.239218
H	-1.187323	1.572566	-3.047264
H	-0.748903	-3.345707	0.690355
H	-0.919751	3.279423	-3.469754
H	0.457633	2.168574	-3.313907
H	-0.923990	2.120418	1.216637
H	-0.773293	0.119598	2.441487
H	1.635513	-4.076330	0.658377
H	0.253953	4.268419	0.753281
H	0.841676	-0.581447	2.729028
H	0.442201	1.035353	3.372474
H	0.867340	3.530104	2.247809
H	1.777270	1.089671	1.349572
H	1.817370	3.434622	0.742528
H	3.381970	-2.427332	-0.073647
H	2.774267	-0.119702	-0.639772

(1b) - Spiro
Energy: -817.69257952 a.u.

O	-2.535710	-1.998029	0.298420
H	-1.243895	1.298464	-3.211249
N	-1.675537	-1.103800	0.215331
O	-2.006869	0.104469	0.198249
H	-0.727080	-3.487979	0.539921
C	-0.611176	2.186092	-3.097508
H	-1.029974	2.996683	-3.693965
H	0.382828	1.939970	-3.487595
N	-0.540315	2.607969	-1.701398
C	0.062067	-2.772595	0.339513
C	-0.329132	-1.418597	0.160191
H	-0.995778	2.021623	1.056649
O	0.318480	0.519205	-1.194558
C	-0.119739	1.762255	-0.869986
H	-0.807095	0.082744	2.378001
H	1.660780	-4.186563	0.420617
C	0.001528	2.020180	0.614957
C	1.367552	-3.155447	0.268458
C	0.641940	-0.335234	-0.081985
H	0.207863	4.141052	0.557057
N	0.697293	0.789603	1.094144
C	0.260451	0.291064	2.421508
C	0.762709	3.290353	0.956051
C	2.347451	-2.158347	-0.053440
H	0.822198	-0.614763	2.651681
C	2.019934	-0.857360	-0.241468
H	0.468025	1.062081	3.164008
H	0.850676	3.409022	2.038764
H	1.698763	1.000343	1.166407
H	1.759477	3.289718	0.506227
H	3.385929	-2.452799	-0.176927

H	2.766820	-0.122886	-0.533399

(1b) - TS2
Energy: -817.67425173 a.u.

O	-2.928975	-2.233593	0.294990
H	-1.736704	1.139371	-3.382263
N	-2.091366	-1.339877	0.325850
O	-2.394717	-0.151785	0.425005
H	-1.208732	-3.724915	-0.075436
C	-1.144737	2.049294	-3.214713
H	-1.605999	2.865975	-3.774648
H	-0.146664	1.863857	-3.634232
N	-1.086546	2.404371	-1.802158
C	-0.387684	-3.020785	-0.019518
C	-0.698918	-1.675388	0.237147
H	-1.452340	1.878833	0.878130
O	-0.037351	0.370377	-1.377333
C	-0.545196	1.514952	-1.048708
H	-1.279845	0.090150	2.460854
H	1.150818	-4.466475	-0.385903
C	-0.455725	1.814522	0.444884
C	0.916227	-3.426186	-0.196912
C	0.300801	-0.665311	0.241296
H	-0.163116	3.916341	0.316160
N	0.221856	0.607349	1.066751
C	-0.223023	0.345644	2.474046
C	0.357109	3.062760	0.751864
C	1.932176	-2.458646	-0.112121
H	0.374990	-0.469610	2.877875
C	1.636986	-1.136153	0.132735
H	-0.060836	1.255506	3.050557
H	0.457055	3.231901	1.827602
H	1.208102	0.878563	1.140296
H	1.352057	3.004588	0.298826
H	2.971894	-2.750151	-0.221718
H	2.443722	-0.411674	0.201192

(1c) - Imidate
Energy: -817.70825536 a.u.

C	0.804452	-1.066914	1.073178
C	-0.407209	-1.299626	0.406815
C	-1.373198	-2.078744	1.036622
C	-1.140758	-2.611552	2.301796
C	0.064180	-2.365082	2.958343
C	1.036096	-1.583887	2.343441
N	-0.028126	1.759788	0.647776
C	-1.276839	1.389418	-0.030390
C	-0.928192	0.456191	-1.175312
O	-0.670686	-0.869573	-0.865694
N	-0.895126	0.817572	-2.382662
C	-0.500705	-0.170481	-3.379996
C	0.802885	2.728073	-0.063259
C	-2.138757	2.559487	-0.499836
N	1.872333	-0.268728	0.467089
O	2.701539	0.225674	1.213419
O	1.903704	-0.160971	-0.747228
H	-1.906141	-3.218153	2.774219
H	-0.431058	0.315526	-4.353585
H	-2.307676	-2.250992	0.513132
H	-1.237896	-0.978883	-3.444243
H	0.249997	-2.778010	3.943261
H	-0.249058	2.105267	1.577312
H	-1.852049	0.801565	0.695654
H	0.466327	-0.620230	-3.129937
H	-3.091606	2.198517	-0.895427
H	1.765713	2.804652	0.449138
H	1.980931	-1.373049	2.829666
H	0.362007	3.732008	-0.131298
H	-2.338270	3.221565	0.348073
H	0.987336	2.364277	-1.078033

H	-1.639984	3.127823	-1.286918

(1c) - TS1
Energy: -817.68727872 a.u.

C	0.927484	-0.546770	0.723142
C	-0.490941	-0.538756	0.454970
C	-1.261590	-1.378404	1.353889
C	-0.711800	-1.951510	2.463051
C	0.676387	-1.831868	2.760590
C	1.474105	-1.160149	1.874925
N	-1.185165	1.192022	0.695672
C	-1.608469	1.645317	-0.646264
C	-1.284732	0.475405	-1.560811
O	-0.916566	-0.646553	-0.881891
N	-1.419493	0.506635	-2.811093
C	-1.082108	-0.704775	-3.551342
C	-0.276143	2.029880	1.491523
C	-1.002608	2.953403	-1.134471
N	1.800355	0.124014	-0.153044
O	3.022350	-0.008968	-0.027104
O	1.312174	0.856190	-1.029855
H	-1.349517	-2.539611	3.116801
H	-1.099937	-0.487188	-4.619694
H	-2.310761	-1.513569	1.107581
H	-1.805008	-1.502994	-3.347557
H	1.092749	-2.291572	3.648319
H	-2.007938	0.991626	1.262600
H	-2.698610	1.743153	-0.633095
H	-0.087977	-1.076515	-3.277995
H	-1.402341	3.152442	-2.130069
H	-0.032597	1.480363	2.402917
H	2.543782	-1.073961	2.027261
H	-0.753428	2.975612	1.755450
H	-1.282134	3.778847	-0.476540
H	0.635813	2.221785	0.928237
H	0.083796	2.886061	-1.206874

(1c) - Spiro
Energy: -817.68883828 a.u.

H	-1.325958	-2.649246	3.075747
H	-0.921089	-0.770523	-4.633967
H	-2.284663	-1.468563	1.169999
C	-0.676799	-2.044094	2.448977
H	-1.601661	-1.752217	-3.322020
C	-1.225430	-1.383226	1.401206
C	-0.897346	-0.946553	-3.558253
H	1.136714	-2.529910	3.582900
O	-0.791856	-0.788834	-0.868405
H	-1.929719	0.827214	1.175243
H	-2.593718	1.545502	-0.704920
N	-1.258414	0.286164	-2.864508
C	0.728725	-1.996576	2.733485
H	0.105708	-1.283969	-3.273416
C	-1.151276	0.288095	-1.611532
C	-0.443223	-0.509885	0.495580
N	-1.079180	0.998732	0.634109
C	-1.503255	1.468598	-0.731858
C	1.532468	-1.295740	1.885516
C	1.001122	-0.578075	0.780621
H	-1.286152	2.949209	-2.219341
H	-0.038979	1.407915	2.402198
H	2.606695	-1.255495	2.025247
C	-0.250597	1.914552	1.460288
C	-0.921411	2.789317	-1.202759
H	-0.818989	2.824546	1.648014
H	-1.268746	3.615648	-0.579897
N	1.871449	0.088801	-0.062071
H	0.672604	2.141455	0.932705
H	0.167642	2.762808	-1.225957
O	1.388912	0.832022	-0.948837

O	3.102608	-0.029624	0.068483

(1c) - TS2
Energy: -817.66831208 a.u.

H	-0.798836	-2.910671	3.133796
H	-0.385352	-0.917940	-4.746010
H	-1.788816	-1.130709	1.795826
C	-0.152732	-2.303683	2.507514
H	-1.099096	-1.902203	-3.451523
C	-0.715392	-1.294174	1.755558
C	-0.362729	-1.116953	-3.672022
H	1.674516	-3.322020	3.089048
O	-0.419037	-1.073124	-0.958447
H	-1.486483	0.751747	1.106109
H	-2.088478	1.238753	-0.774715
N	-0.641863	0.115001	-2.945540
C	1.232595	-2.534289	2.491336
H	0.624782	-1.526344	-3.418368
C	-0.630749	-0.013589	-1.665029
C	0.055154	-0.489767	0.879715
N	-0.590905	0.862747	0.627280
C	-0.995538	1.205985	-0.820144
C	2.022630	-1.726048	1.702583
C	1.456890	-0.698043	0.934726
H	-0.860130	2.616883	-2.361923
H	0.259302	1.593923	2.408794
H	3.095504	-1.864967	1.648271
C	0.090011	1.957863	1.396491
C	-0.500626	2.543767	-1.334244
H	-0.575255	2.818794	1.416761
H	-0.917804	3.377834	-0.766587
N	2.340412	0.027227	0.065701
H	1.027020	2.213787	0.911140
H	0.586391	2.608747	-1.350606
O	1.837801	0.814002	-0.734029
O	3.547916	-0.165132	0.137739

(1d) - Imidate
Energy: -817.70502038 a.u.

C	0.615278	-1.188423	2.232004
C	0.302948	-0.264669	1.235128
C	1.333367	0.173809	0.390902
C	2.624887	-0.338126	0.506560
C	2.915974	-1.266446	1.495588
C	1.906379	-1.684396	2.365048
O	-0.981249	0.203281	1.225232
C	-1.844510	0.155177	0.142892
C	-1.728235	-0.971497	-0.866006
N	-0.650808	-0.646645	-1.806501
C	-0.490838	-1.642145	-2.864876
C	-1.515482	-2.339461	-0.214876
N	-2.769690	1.008876	0.060726
C	-2.797467	2.085888	1.042245
H	-0.187204	-1.518038	2.883374
N	1.113496	1.193599	-0.630345
H	3.387330	0.015664	-0.176740
H	-2.705945	-0.980376	-1.372540
H	-0.881178	0.246904	-2.238444
H	-1.826512	2.589740	1.099038
H	3.923455	-1.654347	1.591689
H	-3.565479	2.805383	0.757295
H	-1.441210	-1.908996	-3.354170
H	0.190538	-1.244316	-3.619668
H	-1.778926	-3.132519	-0.918123
H	-3.034344	1.698883	2.039686
H	-2.154328	-2.447526	0.666049
H	-0.045657	-2.553612	-2.458244
H	-0.474081	-2.482258	0.084471
H	2.122673	-2.405902	3.145847
O	0.151191	1.936041	-0.508568

O	1.916111	1.269824	-1.545118

(1d) - TS1
Energy: -817.68751072 a.u.

C	0.718850	-1.455629	1.246865
C	0.365446	-0.296962	0.460831
C	1.484272	0.537546	0.100808
C	2.820288	0.157606	0.347478
C	3.104825	-1.012368	1.004371
C	2.022221	-1.803925	1.473268
O	-0.799382	0.356758	0.917515
C	-1.920632	0.346557	0.146690
C	-1.866134	-0.699140	-0.947704
N	-0.426211	-0.889552	-1.163630
C	0.081523	-2.202816	-1.565085
C	-2.594960	-1.966001	-0.506699
N	-2.920862	1.075725	0.374175
C	-2.836022	2.000028	1.500627
H	-0.097089	-2.038658	1.662494
N	1.238010	1.735183	-0.603042
H	3.604671	0.819260	-0.001823
H	-2.335699	-0.289683	-1.846673
H	-0.102975	-0.175635	-1.816038
H	-1.929359	2.613518	1.446569
H	4.129089	-1.310913	1.190192
H	-3.709006	2.652847	1.492557
H	-0.351002	-2.515444	-2.518771
H	1.166173	-2.123916	-1.664381
H	-2.563409	-2.728924	-1.287311
H	-2.815850	1.457380	2.452355
H	-3.637812	-1.709293	-0.313947
H	-0.146515	-2.940614	-0.795806
H	-2.167023	-2.377576	0.411815
H	2.227772	-2.696922	2.056549
O	0.105763	1.915379	-1.084980
O	2.143134	2.560461	-0.745984

(1d) - Spiro
Energy: -817.69154474 a.u.

C	0.585647	-1.473837	1.112180
C	0.329081	-0.340824	0.185529
C	1.563965	0.411469	-0.132850
C	2.831626	0.075296	0.422118
C	2.979197	-0.983621	1.262000
C	1.811941	-1.749554	1.610519
O	-0.704688	0.517063	0.734931
C	-1.935288	0.294702	0.213856
C	-1.875979	-0.733154	-0.897108
N	-0.398713	-0.823463	-1.133752
C	0.138545	-2.088618	-1.683434
C	-2.556628	-2.044434	-0.530273
N	-2.994013	0.855272	0.600117
C	-2.877487	1.801371	1.706727
H	-0.281502	-2.043682	1.431059
N	1.470905	1.489883	-0.984555
H	3.673352	0.694383	0.134633
H	-2.330304	-0.320810	-1.800834
H	-0.181038	-0.048305	-1.780682
H	-2.177707	2.609103	1.465416
H	3.947161	-1.245284	1.670874
H	-3.857472	2.232755	1.910380
H	-0.327740	-2.272553	-2.651070
H	1.215912	-1.967805	-1.802300
H	-2.520493	-2.753431	-1.359458
H	-2.515129	1.304851	2.613611
H	-3.602790	-1.815230	-0.319458
H	-0.067919	-2.905230	-0.994513
H	-2.124634	-2.505461	0.359956
H	1.909874	-2.573983	2.311197
O	0.376015	1.706958	-1.582795

O	2.447039	2.231828	-1.185605

(1d) - TS2
Energy: -817.67812404 a.u.

C	0.817346	-0.368751	1.283980
C	0.489482	-0.409948	-0.102234
C	1.380501	0.292699	-0.967461
C	2.381797	1.142440	-0.458872
C	2.599728	1.237092	0.893665
C	1.805704	0.456772	1.761741
O	-1.174004	0.500054	-0.289546
C	-2.107596	-0.371680	-0.046849
C	-1.610214	-1.814641	-0.155129
N	-0.166697	-1.669137	-0.593808
C	0.688803	-2.868595	-0.364415
C	-1.838431	-2.647216	1.096451
N	-3.338307	-0.171786	0.251119
C	-3.732622	1.229853	0.328377
H	0.234165	-0.964266	1.975215
N	1.194186	0.284312	-2.383782
H	2.977156	1.705967	-1.166427
H	-2.107887	-2.303401	-0.997337
H	-0.204404	-1.505465	-1.617003
H	-3.644917	1.730630	-0.644744
H	3.380768	1.878509	1.282967
H	-4.773635	1.294183	0.651752
H	0.199347	-3.727385	-0.822910
H	1.656481	-2.690349	-0.832818
H	-1.505358	-3.678857	0.968277
H	-3.111992	1.792165	1.037836
H	-2.916842	-2.654578	1.263414
H	0.816109	-3.024789	0.705474
H	-1.371012	-2.220505	1.985195
H	1.986082	0.488145	2.831880
O	0.335718	-0.467188	-2.881985
O	1.881506	1.011530	-3.085609

(14a) - Imidate
Energy: -857.00123152 a.u.

C	2.505743	-0.834380	-0.095728
C	1.740515	0.436463	0.134224
O	0.612466	0.540125	-0.685599
C	-0.619762	0.703389	-0.145434
N	0.592983	-2.229490	0.489217
C	2.001903	-1.986143	0.788546
C	-1.663826	1.183100	-0.950721
C	-2.944786	1.399433	-0.440915
C	-3.211676	1.110679	0.887224
C	-2.182958	0.623496	1.699178
C	-0.904897	0.425378	1.195631
N	2.129376	1.335556	0.927470
C	1.402607	2.584678	1.081367
C	2.908970	-3.209508	0.629893
N	-1.454127	1.484449	-2.363706
O	-2.119608	2.388391	-2.851101
C	-0.092287	-3.090007	1.444577
O	-0.653932	0.815381	-2.994953
H	2.126196	3.378624	1.274445
H	0.801930	2.853264	0.205193
H	0.738161	2.521470	1.950313
H	3.937630	-2.975492	0.920293
H	-0.112912	0.043982	1.830131
H	2.913484	-3.541913	-0.414718
H	2.044769	-1.646696	1.833986
H	-2.377964	0.392812	2.741455
H	-3.711599	1.781097	-1.104908
H	-4.207252	1.262111	1.287566
H	0.506341	-2.610825	-0.450961
H	-0.076818	-2.610441	2.429689
H	2.564352	-4.038821	1.253249
H	-1.137309	-3.198683	1.143576
H	0.340658	-4.095757	1.549661
H	3.558736	-0.641833	0.121099
H	2.414424	-1.120831	-1.150318

(14a) - TS1
Energy: -856.98202554 a.u.

C	2.529823	-0.805019	-0.074884
C	1.951258	0.578028	-0.020841
O	0.757448	0.719320	-0.714091
C	-0.371737	0.053503	-0.230804
N	0.297219	-1.719918	-0.424748
C	1.541498	-1.892294	0.353467
C	-1.535921	0.148805	-1.078556
C	-2.843254	0.246900	-0.554199
C	-3.060601	0.294846	0.798066
C	-1.930544	0.298263	1.661478
C	-0.653077	0.219131	1.183625
N	2.539844	1.557876	0.511109
C	1.914854	2.873390	0.486586
C	2.154022	-3.280838	0.192258
N	-1.387917	0.032727	-2.479319
O	-2.332681	0.333043	-3.215456
C	-0.767894	-2.666919	-0.085030
O	-0.320819	-0.401267	-2.939259
H	2.361267	3.462496	-0.321165
H	0.831652	2.838745	0.338536
H	2.140614	3.380504	1.426453
H	3.109002	-3.318848	0.722860
H	0.193046	0.298493	1.860077
H	2.338924	-3.500665	-0.864486
H	1.263018	-1.742742	1.404696
H	-2.077184	0.405919	2.732627
H	-3.664700	0.269299	-1.261089
H	-4.064242	0.357941	1.199612
H	0.492608	-1.740671	-1.429751
H	-0.954843	-2.608493	0.990703
H	1.509792	-4.058070	0.607385
H	-1.674528	-2.385569	-0.623585
H	-0.497571	-3.689365	-0.355583
H	3.417016	-0.839300	0.558723
H	2.841958	-0.999800	-1.110616

(14a) - Spiro
Energy: -856.98760330 a.u.

C	2.627383	-0.494763	0.366916
C	1.640295	-1.596526	0.742426
N	0.347728	-1.359869	0.001934
C	-0.252721	0.077435	0.222347
O	0.798287	0.981422	-0.166819
C	2.023556	0.874355	0.450949
N	2.620791	1.871270	0.942923
C	1.942205	3.162367	0.927278
C	-1.416404	0.296603	-0.680709
C	-2.692644	0.698805	-0.194809
C	-2.932121	0.854458	1.134682
C	-1.849312	0.637805	2.059006
C	-0.613909	0.264787	1.658819
C	-0.668788	-2.407120	0.297400
C	2.206609	-2.974516	0.427163
N	-1.244268	0.113410	-2.030863
O	-0.164796	-0.390671	-2.461194
O	-2.147876	0.414458	-2.834710
H	2.089627	3.647366	-0.043865
H	0.865491	3.072835	1.103145
H	2.385835	3.799895	1.693050
H	3.206175	-3.040335	0.863143
H	0.187410	0.161224	2.384349
H	2.297883	-3.124410	-0.653477
H	1.391189	-1.537640	1.806032

H	-2.023150	0.792405	3.120342
H	-3.471123	0.855711	-0.932313
H	-3.910978	1.142164	1.497556
H	0.528463	-1.353181	-1.018910
H	-0.770786	-2.499459	1.379470
H	1.604890	-3.778341	0.852720
H	-1.618565	-2.105009	-0.141718
H	-0.344666	-3.348800	-0.139791
H	3.499359	-0.550274	1.019513
H	2.962631	-0.654314	-0.666963

(14a) - TS2
Energy: -856.97262772 a.u.

C	2.592824	-0.496186	0.462960
C	1.626332	-1.638825	0.782949
N	0.325662	-1.485844	-0.000823
C	-0.469206	-0.239991	0.286656
O	0.882057	0.915993	-0.354078
C	1.932815	0.860825	0.435548
N	2.399951	1.823045	1.147555
C	1.680311	3.087450	1.041116
C	-1.543754	0.116643	-0.590393
C	-2.599588	0.935043	-0.154629
C	-2.704770	1.308009	1.165411
C	-1.736676	0.837283	2.074352
C	-0.682133	0.054389	1.666081
C	-0.564820	-2.682187	0.157840
C	2.271775	-2.982902	0.463128
N	-1.482758	-0.182847	-1.983200
O	-0.568421	-0.908134	-2.407616
O	-2.337518	0.271373	-2.735214
H	1.875679	3.575100	0.077080
H	0.594092	2.955947	1.123356
H	2.018519	3.759590	1.832939
H	3.271810	-2.983186	0.902217
H	0.036212	-0.283052	2.402048
H	2.381021	-3.121486	-0.617693
H	1.342593	-1.620505	1.836635
H	-1.824923	1.077272	3.129573
H	-3.331360	1.249513	-0.888689
H	-3.529531	1.924247	1.501312
H	0.556172	-1.402967	-1.002733
H	-0.725775	-2.853534	1.222599
H	1.725047	-3.827081	0.884066
H	-1.513132	-2.475315	-0.333773
H	-0.087745	-3.540798	-0.307524
H	3.397274	-0.521637	1.200270
H	3.029558	-0.681262	-0.527447

(14b) - Imidate
Energy: -857.00510603 a.u.

C	-1.583598	0.579508	0.246762
C	-0.900735	1.155135	-0.835534
C	-1.594386	1.354960	-2.027770
C	-2.928086	0.979685	-2.148130
C	-3.591725	0.390615	-1.071399
C	-2.916205	0.189839	0.124497
N	0.271468	-1.874609	0.358514
C	1.440348	-1.833299	-0.521350
C	1.308181	-0.626196	-1.456502
C	1.454212	0.690052	-0.731393
O	0.395100	1.589998	-0.777702
N	2.540254	1.036277	-0.194082
C	2.623375	2.340372	0.450385
C	0.453402	-2.686360	1.557148
C	1.653568	-3.116418	-1.328365
N	-0.956193	0.381068	1.557472
O	0.075415	0.977539	1.810850
O	-1.529081	-0.347508	2.351717
H	-1.055453	1.803041	-2.855984
H	3.519760	2.371365	1.071386
H	2.705258	3.130900	-0.304678
H	1.743191	2.547203	1.065541
H	2.585331	-3.072215	-1.900083
H	0.826343	-3.262271	-2.033042
H	2.313075	-1.659386	0.120551
H	-3.407512	-0.257457	0.979622
H	-3.447349	1.144362	-3.086388
H	-4.630479	0.093263	-1.158898
H	-0.527328	-2.223142	-0.170791
H	1.225145	-2.225427	2.182602
H	1.701617	-3.989515	-0.671941
H	-0.478890	-2.695759	2.126570
H	0.749922	-3.727263	1.358594
H	2.099414	-0.661577	-2.211835
H	0.350367	-0.677982	-1.985429

(14b) - TS1
Energy: -856.97804954 a.u.

C	-0.927389	0.164345	1.359951
C	-0.359555	0.008600	0.035661
C	-1.355101	0.094756	-1.024984
C	-2.695557	0.125896	-0.776207
C	-3.213290	0.152547	0.550478
C	-2.322673	0.197216	1.588645
N	0.268546	-1.750985	-0.166995
C	1.697674	-2.034330	0.133695
C	2.520945	-0.934448	-0.524859
C	2.101343	0.448013	-0.130782
O	0.770742	0.764987	-0.301063
N	2.929417	1.345882	0.187168
C	2.402272	2.662080	0.526271
C	-0.678900	-2.626801	0.541968
C	2.126283	-3.411988	-0.362259
N	-0.073558	0.222480	2.474494
O	1.131831	-0.021744	2.306610
O	-0.528329	0.499501	3.589995
H	-0.968053	0.135769	-2.038903
H	3.206327	3.269639	0.942935
H	2.008029	3.169156	-0.361687
H	1.589279	2.590141	1.257975
H	3.197871	-3.538885	-0.186892
H	1.943298	-3.512384	-1.437648
H	1.798941	-1.972983	1.219586
H	-2.655676	0.260772	2.618269
H	-3.379972	0.165792	-1.618943
H	-4.281213	0.171494	0.728724
H	0.124883	-1.870580	-1.174791
H	-0.514885	-2.522110	1.616567
H	1.606227	-4.215693	0.162276
H	-1.696356	-2.317242	0.295903
H	-0.539308	-3.668599	0.250341
H	3.574619	-1.053950	-0.269895
H	2.426414	-1.023662	-1.616787

(14b) - Spiro
Energy: -856.97807191 a.u.

C	1.466206	1.127652	-1.355617
C	1.534088	2.198361	-0.275133
C	1.146224	1.637121	1.068063
O	0.564365	0.394808	1.036959
C	-0.475148	0.084980	0.108988
C	-0.736252	-1.370214	0.124337
C	-2.039226	-1.910145	0.291786
C	-3.130860	-1.113576	0.467932
C	-2.929513	0.306449	0.542329
C	-1.707693	0.869856	0.397807
N	0.041116	0.634308	-1.347710
C	-0.305238	-0.300716	-2.454518
C	1.860533	1.669516	-2.721224

N	1.423077	2.212750	2.156496
C	0.995858	1.584739	3.401337
N	0.325107	-2.239270	-0.053054
O	1.441747	-1.780283	-0.383106
O	0.161976	-3.467846	0.086383
H	-1.571233	1.944702	0.507554
H	0.964328	2.343894	4.183994
H	0.013803	1.108217	3.315370
H	1.718879	0.818251	3.701607
H	2.847447	2.130070	-2.635330
H	1.158678	2.436902	-3.063982
H	2.073586	0.263360	-1.083157
H	-2.127454	-2.989907	0.258337
H	-3.777485	0.954205	0.746639
H	-4.122449	-1.534769	0.576167
H	-0.545992	1.464078	-1.496240
H	0.391376	-1.137777	-2.436373
H	1.925987	0.881139	-3.472335
H	-1.328448	-0.644393	-2.306123
H	-0.235450	0.237627	-3.398038
H	2.548160	2.596722	-0.202813
H	0.881005	3.041268	-0.538266

(14b) - TS2
Energy: -856.95987155 a.u.

C	1.129415	0.092313	-1.286604
C	1.113604	1.168775	-0.210723
C	0.762736	0.590244	1.145396
O	0.180357	-0.579604	1.109054
C	-1.061782	-0.982334	-0.286877
C	-1.197581	-2.388226	-0.079671
C	-2.324308	-2.925872	0.564580
C	-3.385810	-2.129691	0.931323
C	-3.322177	-0.754517	0.637515
C	-2.224423	-0.211045	0.012808
N	-0.316248	-0.388832	-1.476132
C	-0.544620	-1.198142	-2.726551
C	1.672704	0.621611	-2.606263
N	1.063648	1.254158	2.207097
C	0.656486	0.634380	3.461672
N	-0.108815	-3.279506	-0.332182
O	0.934752	-2.818515	-0.797065
O	-0.238706	-4.474547	-0.078588
H	-2.208507	0.852406	-0.213390
H	0.851341	1.325552	4.285091
H	-0.410117	0.373113	3.467835
H	1.212798	-0.292296	3.657874
H	2.660463	1.044211	-2.410384
H	1.044075	1.420864	-3.013374
H	1.685030	-0.780665	-0.952060
H	-2.328098	-3.990927	0.761430
H	-4.158252	-0.107003	0.882246
H	-4.254800	-2.556608	1.416552
H	-0.833158	0.480970	-1.647115
H	0.182285	-2.004650	-2.764551
H	1.792166	-0.160509	-3.356952
H	-1.560914	-1.586464	-2.693583
H	-0.433681	-0.536790	-3.582222
H	2.099371	1.636493	-0.160044
H	0.407612	1.967402	-0.480870

(2) - Imidate
Energy: -817.71292573 a.u.

O	-1.381919	1.293423	0.520309
C	-0.118292	0.840551	0.238525
N	-1.733045	-1.494365	0.865384
C	-2.343365	-0.834321	-0.289329
C	-2.507079	0.638262	0.048007
C	0.718535	0.526576	1.309638
C	2.024108	0.131319	1.063370
C	2.461354	0.061406	-0.258381
C	1.643024	0.384641	-1.334868
C	0.337912	0.787563	-1.078955
C	-0.874180	-2.618929	0.512304
N	3.835469	-0.363314	-0.524683
O	4.546775	-0.643912	0.427918
C	-3.651316	-1.465741	-0.754304
N	-3.607778	1.251961	-0.001856
C	-3.629678	2.659970	0.375956
O	4.206164	-0.418159	-1.687425
H	-1.358987	-3.368105	-0.131861
H	0.011863	-2.239286	-0.010478
H	-0.537593	-3.114863	1.425265
H	-3.479868	-2.522049	-0.979398
H	2.024348	0.330695	-2.347122
H	-1.618607	-0.904841	-1.109911
H	-0.323485	1.067182	-1.892828
H	-2.464169	-1.792833	1.505680
H	-4.034196	-0.975145	-1.651777
H	-4.411229	-1.387785	0.027916
H	2.694075	-0.128828	1.873567
H	0.326927	0.576869	2.318720
H	-2.848121	3.232230	-0.135204
H	-4.604140	3.079872	0.125150
H	-3.470907	2.771755	1.454514

(2) - TS1
Energy: -817.69306419 a.u.

O	-1.579332	0.953959	0.429584
C	-0.448329	0.118733	0.271303
N	-1.469794	-1.425211	0.334116
C	-2.674831	-1.006111	-0.390715
C	-2.758103	0.476091	-0.070948
C	0.425633	0.085938	1.419735
C	1.762695	-0.158564	1.270329
C	2.326483	-0.281960	-0.018167
C	1.525149	-0.074246	-1.159224
C	0.184005	0.165250	-1.027512
C	-0.753210	-2.592389	-0.182957
N	3.706043	-0.535999	-0.163035
O	4.403307	-0.679297	0.850130
C	-3.936252	-1.774817	-0.030459
N	-3.790460	1.181000	-0.210909
C	-3.689478	2.598703	0.122125
O	4.188889	-0.617375	-1.300394
H	-1.368035	-3.492137	-0.112856
H	-0.489495	-2.404209	-1.225230
H	0.158162	-2.723074	0.404959
H	-3.824572	-2.830752	-0.286319
H	1.988543	-0.071994	-2.139425
H	-2.457872	-1.121351	-1.459653
H	-0.430020	0.375610	-1.898024
H	-1.675782	-1.548655	1.328998
H	-4.779244	-1.365228	-0.588987
H	-4.151630	-1.680879	1.037386
H	2.406348	-0.232231	2.139510
H	-0.016785	0.221138	2.401268
H	-2.828207	3.069074	-0.363936
H	-4.600671	3.104904	-0.196372
H	-3.577532	2.731552	1.203988

(2) - Spiro
Energy: -817.69504024 a.u.

H	-1.418750	-3.321373	0.007869
H	-0.540459	-2.386192	-1.244477
H	0.187618	-2.623877	0.371048
C	-0.744211	-2.486642	-0.179416
H	-3.781168	-2.618271	-0.308614
H	2.104577	0.042101	-2.136411
H	-2.395149	-0.936814	-1.498198

H	-0.327015	0.304366	-1.938302
N	-1.379294	-1.237632	0.298968
C	1.629382	-0.011175	-1.163159
O	4.330802	-0.362605	-1.275246
C	0.281521	0.124630	-1.056674
C	-3.858715	-1.563976	-0.036419
N	3.816389	-0.342720	-0.139597
H	-1.613748	-1.356461	1.292504
C	2.441548	-0.187824	-0.012279
C	-2.605367	-0.807580	-0.430984
H	-4.704035	-1.127681	-0.570754
C	-0.402352	0.044938	0.248232
H	-4.047794	-1.473549	1.036429
O	4.519720	-0.466301	0.882618
C	1.841314	-0.128538	1.272384
C	0.497088	0.015897	1.412591
H	2.475319	-0.179197	2.150541
H	0.039449	0.104278	2.393437
C	-2.631766	0.670181	-0.096340
O	-1.422468	1.060001	0.394901
N	-3.632793	1.418811	-0.230213
C	-3.467104	2.826361	0.122677
H	-2.588619	3.264442	-0.362645
H	-4.356735	3.376075	-0.184114
H	-3.343502	2.938445	1.205503

(2) - TS2
Energy: -817.68323523 a.u.

H	-1.894240	-3.351889	0.162368
H	-0.827847	-2.741303	-1.143285
H	-0.164030	-3.038476	0.490649
C	-1.039198	-2.721497	-0.074823
H	-3.882622	-2.412407	-0.467143
H	2.237546	0.144840	-2.150207
H	-2.287745	-0.847262	-1.503208
H	-0.152631	-0.387708	-1.958738
N	-1.362976	-1.316935	0.315141
C	1.788396	0.004396	-1.174183
O	4.440397	0.600381	-1.270262
C	0.452419	-0.299493	-1.062907
C	-3.838743	-1.383959	-0.104080
N	3.972989	0.412639	-0.147071
H	-1.631078	-1.321637	1.306691
C	2.581246	0.109432	-0.022590
C	-2.519360	-0.718636	-0.441001
H	-4.627059	-0.809038	-0.591526
C	-0.151031	-0.416063	0.224307
H	-4.026546	-1.365661	0.973631
O	4.658914	0.477896	0.872982
C	2.035023	-0.133704	1.244715
C	0.699251	-0.436179	1.367079
H	2.672734	-0.100906	2.120110
H	0.270529	-0.632645	2.345234
C	-2.428799	0.759287	-0.065116
O	-1.258308	1.057238	0.433932
N	-3.431770	1.527121	-0.265488
C	-3.216939	2.924769	0.091841
H	-2.360007	3.355427	-0.441828
H	-4.108701	3.502170	-0.159002
H	-3.020464	3.041188	1.165449

(3) - Imidate
Energy: -857.00825787 a.u.

C	-3.061006	-0.801555	0.660621
C	-2.271410	-1.547107	1.544126
C	-0.931006	-1.241008	1.751273
C	-0.335537	-0.170858	1.088718
C	-1.125930	0.581916	0.213018
C	-2.463359	0.264026	-0.008611
O	0.972507	0.120524	1.378287
C	1.995314	-0.123291	0.475550
C	1.699109	-1.092412	-0.651443
N	0.921809	-0.360812	-1.656205
C	0.033102	-1.203381	-2.447312
N	-0.580203	1.723982	-0.521666
O	-1.149034	2.059096	-1.548112
N	3.109001	0.444854	0.633546
C	3.234502	1.412770	1.717250
C	2.963533	-1.749030	-1.196093
O	0.392792	2.300421	-0.066130
H	4.199885	1.913484	1.636096
H	2.432685	2.157837	1.677484
H	3.182530	0.915795	2.692624
H	3.480410	-2.319393	-0.420090
H	-0.317701	-1.826897	2.428058
H	3.649141	-0.987753	-1.576434
H	1.037821	-1.869143	-0.245662
H	-2.711152	-2.385643	2.077279
H	-3.029353	0.867912	-0.709271
C	-4.510848	-1.147911	0.443163
H	1.557210	0.159510	-2.256879
H	-0.748759	-1.603959	-1.790901
H	2.699514	-2.429683	-2.010077
H	-0.452327	-0.591250	-3.210985
H	0.534051	-2.048136	-2.942687
H	-4.979101	-0.461380	-0.264506
H	-4.610138	-2.164721	0.052238
H	-5.064440	-1.101044	1.385274

(3) - TS1
Energy: -856.98855274 a.u.

C	-3.114960	-0.456651	0.493206
C	-2.303491	-1.472836	1.083743
C	-0.939377	-1.413370	1.103161
C	-0.216541	-0.335102	0.469071
C	-1.054387	0.728303	-0.018848
C	-2.466826	0.633540	-0.026850
O	0.953887	0.030403	1.167875
C	2.170546	-0.169783	0.592510
C	2.103662	-1.122422	-0.582756
N	0.713400	-1.038567	-1.029614
C	0.102844	-2.267809	-1.538160
N	-0.445583	1.853216	-0.599249
O	-1.120875	2.853161	-0.865525
N	3.233387	0.333094	1.041606
C	3.120397	1.200971	2.209719
C	3.116892	-0.805952	-1.671421
O	0.772805	1.801136	-0.858727
H	4.088034	1.663164	2.405963
H	2.372800	1.986595	2.051703
H	2.821084	0.628822	3.095026
H	4.125971	-0.864745	-1.261031
H	-0.348705	-2.173841	1.605425
H	2.955100	0.207908	-2.049328
H	2.258409	-2.136388	-0.193289
H	-2.793019	-2.317021	1.565116
H	-3.019938	1.458365	-0.464032
C	-4.614936	-0.591509	0.482960
H	0.625652	-0.284282	-1.712007
H	0.140314	-3.033978	-0.762232
H	3.026879	-1.519164	-2.494174
H	-0.940303	-2.061741	-1.786280
H	0.628520	-2.621202	-2.428817
H	-5.081764	0.287974	0.033329
H	-4.931236	-1.471169	-0.087323
H	-5.009099	-0.703169	1.498478

(3) - Spiro
Energy: -856.99409086 a.u.

C	-3.100517	-0.481284	0.592637

C	-2.176379	-1.508158	1.029973
C	-0.851446	-1.468641	0.780499
C	-0.207726	-0.334918	0.063872
C	-1.192645	0.664457	-0.408805
C	-2.586427	0.566688	-0.100977
O	0.808976	0.265289	0.917543
C	2.059675	-0.186846	0.646448
C	2.013331	-1.185163	-0.490118
N	0.696921	-0.847043	-1.103472
C	0.074748	-1.897119	-1.939909
N	-0.738963	1.731337	-1.132958
O	-1.504343	2.655816	-1.469973
N	3.105195	0.169670	1.248684
C	2.947058	1.125917	2.341389
C	3.169052	-1.080906	-1.465223
O	0.485224	1.769221	-1.485858
H	3.932466	1.414441	2.706795
H	2.411572	2.023177	2.012198
H	2.381781	0.682600	3.168596
H	4.097258	-1.251874	-0.917978
H	-0.190012	-2.244671	1.156486
H	3.210481	-0.082601	-1.909759
H	1.932150	-2.199092	-0.081739
H	-2.571573	-2.348917	1.596403
H	-3.222132	1.369773	-0.457456
C	-4.561939	-0.615017	0.922458
H	0.833658	0.024510	-1.656334
H	-0.024810	-2.810675	-1.354686
H	3.086501	-1.831079	-2.253965
H	-0.907632	-1.544159	-2.255744
H	0.707338	-2.067365	-2.810036
H	-5.131289	0.225158	0.518422
H	-4.978657	-1.540167	0.509380
H	-4.721713	-0.644875	2.005992

(3) - TS2

Energy: -856.98145180 a.u.

C	-3.093737	-0.459458	0.729211
C	-2.182948	-1.513088	1.010455
C	-0.907110	-1.535014	0.513311
C	-0.392897	-0.445738	-0.255906
C	-1.351699	0.530892	-0.649543
C	-2.656694	0.539345	-0.104619
O	0.818821	0.460547	0.866828
C	1.980963	-0.113288	0.727056
C	1.975424	-1.145726	-0.400576
N	0.740233	-0.788381	-1.179500
C	0.339709	-1.799302	-2.199593
N	-0.982850	1.623494	-1.480532
O	-1.786760	2.523018	-1.691119
N	3.052004	0.075816	1.402782
C	2.930367	1.049659	2.481829
C	3.216611	-1.130420	-1.271315
O	0.156146	1.649337	-1.988238
H	3.882096	1.121874	3.011959
H	2.669731	2.045559	2.100701
H	2.151271	0.765720	3.201162
H	4.077556	-1.256278	-0.613598
H	-0.249809	-2.365170	0.749012
H	3.322296	-0.170826	-1.786370
H	1.812398	-2.146163	0.013585
H	-2.512712	-2.343317	1.630224
H	-3.310231	1.359795	-0.378272
C	-4.481998	-0.475012	1.312194
H	0.922630	0.107606	-1.668759
H	0.181825	-2.758122	-1.706784
H	3.215404	-1.940403	-2.003169
H	-0.582383	-1.462462	-2.672448
H	1.134958	-1.873996	-2.939020
H	-5.068860	0.370131	0.946239
H	-5.008665	-1.397335	1.047766
H	-4.448799	-0.418894	2.404854

(4) - Imidate

Energy: -857.01550931 a.u.

C	-0.234016	-0.797653	-1.208117
C	0.228519	-0.784213	0.106197
C	-0.623970	-0.566302	1.199613
C	-1.966944	-0.328309	0.930439
C	-2.417386	-0.319494	-0.388674
C	-1.576413	-0.551950	-1.469550
N	1.512476	1.722051	0.646482
C	2.236331	1.125886	-0.475128
C	2.577787	-0.307637	-0.102050
O	1.540475	-1.087805	0.376415
C	0.509770	2.704127	0.252785
C	3.465961	1.911692	-0.917787
N	3.746484	-0.781344	-0.140034
C	3.937523	-2.170844	0.259174
C	-0.069865	-0.562646	2.593215
N	-3.833403	-0.058929	-0.645102
O	-4.213792	-0.031587	-1.806131
O	-4.570686	0.120756	0.312688
H	0.898764	3.513075	-0.384265
H	-0.292300	2.192291	-0.292337
H	0.073391	3.150333	1.149378
H	3.165125	2.931706	-1.173044
H	-1.964180	-0.550837	-2.480489
H	1.533791	1.085508	-1.316660
H	0.457229	-1.005931	-2.018653
H	2.177454	2.132203	1.297069
H	3.937947	1.456085	-1.790830
H	4.204160	1.949556	-0.112079
H	-2.664864	-0.140308	1.738432
H	3.257859	-2.843431	-0.275375
H	4.966940	-2.462307	0.048405
H	3.752256	-2.297022	1.331799
H	-0.855110	-0.357494	3.322691
H	0.390966	-1.525295	2.832622
H	0.706150	0.205957	2.664386

(4) - TS1

Energy: -856.99194018 a.u.

C	-0.173631	-0.119328	-1.132428
C	0.444677	0.044500	0.167800
C	-0.430799	-0.019175	1.332786
C	-1.781440	0.079033	1.147346
C	-2.353736	0.120326	-0.147788
C	-1.530030	-0.033142	-1.280638
N	1.250389	1.667258	0.195417
C	2.507697	1.394249	-0.517177
C	2.776602	-0.057383	-0.163034
O	1.660694	-0.665372	0.336072
C	0.394240	2.726793	-0.349086
C	3.650658	2.328889	-0.157634
N	3.890648	-0.628819	-0.281961
C	3.966171	-2.039949	0.085429
C	0.189726	-0.162605	2.696878
N	-3.745033	0.223824	-0.298462
O	-4.236143	0.218510	-1.438683
O	-4.459977	0.325720	0.711277
H	0.891359	3.695995	-0.277433
H	0.174940	2.495895	-1.392254
H	-0.534290	2.743984	0.225815
H	3.405158	3.356906	-0.432689
H	-1.982721	-0.115320	-2.262313
H	2.285814	1.460145	-1.588915
H	0.470479	-0.287596	-1.990356
H	1.445304	1.855655	1.181635
H	4.546834	2.024450	-0.700268

H	3.863465	2.280618	0.913897
H	-2.441034	0.088967	2.008798
H	3.200340	-2.631945	-0.427058
H	4.950888	-2.424043	-0.180716
H	3.821381	-2.166018	1.164191
H	-0.584007	-0.130594	3.466353
H	0.728183	-1.110817	2.786706
H	0.911710	0.632183	2.920251

(4) - Spiro
Energy: -856.99292565 a.u.

O	1.529873	-0.869444	0.213862
C	0.384724	-0.002854	0.105935
N	1.184803	1.411508	0.167758
C	2.451468	1.158633	-0.572263
C	2.672945	-0.310965	-0.273719
C	-0.493118	-0.112915	1.295975
C	-1.842463	-0.046072	1.138791
C	-2.455652	0.022167	-0.144011
C	-1.645756	-0.090851	-1.301962
C	-0.292307	-0.142725	-1.195649
C	0.379053	2.564670	-0.292123
N	-3.834365	0.100594	-0.258028
O	-4.537854	0.157736	0.772564
C	3.596262	2.060553	-0.153336
N	3.760491	-0.920878	-0.432173
C	3.779271	-2.346333	-0.113480
O	-4.361630	0.119845	-1.390428
H	0.932888	3.483710	-0.103942
H	0.178260	2.446022	-1.355714
H	-0.557091	2.567540	0.268567
H	3.384311	3.102205	-0.401876
H	-2.121294	-0.166540	-2.273401
H	2.225081	1.284707	-1.636638
H	0.331449	-0.278591	-2.074396
H	1.412524	1.553999	1.157699
H	4.494288	1.749399	-0.689326
H	3.788563	1.970754	0.919278
H	-2.482649	-0.079442	2.014421
C	0.158544	-0.293796	2.642600
H	3.001756	-2.889402	-0.661255
H	4.753365	-2.756733	-0.378613
H	3.610321	-2.506938	0.957000
H	-0.601683	-0.289390	3.426091
H	0.701766	-1.242212	2.693669
H	0.879825	0.496222	2.888589

(4) - TS2
Energy: -856.98221018 a.u.

O	1.384227	-1.050219	0.370727
C	0.119481	0.265890	0.261906
N	1.214636	1.307962	0.408281
C	2.417296	0.912304	-0.404651
C	2.485736	-0.596027	-0.172184
C	-0.715431	0.094001	1.419046
C	-2.005522	-0.346759	1.239487
C	-2.535438	-0.541428	-0.046784
C	-1.767521	-0.256315	-1.181514
C	-0.474857	0.185950	-1.032814
C	0.709263	2.684734	0.138485
N	-3.881683	-0.984888	-0.196498
O	-4.553154	-1.202749	0.814061
C	3.665017	1.669817	0.005703
N	3.533804	-1.243890	-0.509841
C	3.473956	-2.683190	-0.279451
O	-4.334817	-1.138829	-1.332590
H	1.489744	3.399002	0.394617
H	0.451372	2.756354	-0.917147
H	-0.175607	2.850963	0.752674
H	3.596770	2.731626	-0.237783
H	-2.199331	-0.366533	-2.169070
H	2.168181	1.121690	-1.449395
H	0.115943	0.414464	-1.913519
H	1.507363	1.268107	1.391453
H	4.503428	1.239743	-0.543688
H	3.865307	1.550769	1.074908
H	-2.634325	-0.534544	2.103307
C	-0.140511	0.313820	2.794962
H	2.603927	-3.139119	-0.768765
H	4.379397	-3.148669	-0.673087
H	3.403594	-2.916621	0.790666
H	-0.828099	-0.061015	3.554734
H	0.810243	-0.218473	2.913889
H	0.027104	1.375478	3.016843

(5) - Imidate
Energy: -932.19191874 a.u.

H	4.580202	0.632382	2.362277
H	3.325167	-0.480553	2.941506
C	3.548827	0.309880	2.216000
H	2.873704	1.148571	2.417659
N	3.392526	-0.178366	0.850569
H	-4.997873	-1.873868	1.108902
O	-0.505937	2.675631	-0.801745
C	2.229603	-0.468013	0.458511
C	-4.940903	-1.635414	0.041955
O	-4.147644	-0.475047	-0.176038
H	-5.933432	-1.391484	-0.332293
H	-2.776767	-2.535078	0.995859
C	-2.849467	-0.518785	0.204383
C	-2.231332	-1.620431	0.799963
C	-2.108056	0.642193	-0.034932
C	-0.882083	-1.549944	1.147282
H	-2.577230	1.498803	-0.503782
H	-0.386856	-2.403436	1.598701
C	-0.132233	-0.403582	0.926837
C	-0.775525	0.694694	0.336410
O	1.173710	-0.384069	1.349593
N	-0.063463	1.948802	0.072106
H	3.502778	-2.391454	-1.123550
H	1.128097	-1.686376	-0.880670
O	0.911486	2.215847	0.752135
C	1.910965	-0.919982	-0.952479
H	-4.539301	-2.491248	-0.510215
C	3.126387	-1.514598	-1.656514
H	3.929522	-0.775475	-1.710734
H	2.850254	-1.816128	-2.670467
N	1.314992	0.226278	-1.644964
H	2.057129	0.840078	-1.973746
H	-0.460706	-0.638409	-2.318342
C	0.420394	-0.137469	-2.737174
H	0.871305	-0.802470	-3.488445
H	0.081948	0.772408	-3.238132

(5) - TS1
Energy: -932.16713272 a.u.

H	4.352841	0.320013	2.962776
H	2.940412	-0.722344	3.220564
C	3.358681	0.070909	2.590881
H	2.710239	0.949307	2.684087
N	3.464991	-0.366777	1.202482
H	-4.872055	-1.642198	1.232945
O	-0.500195	3.175962	0.164109
C	2.391409	-0.549945	0.571949
C	-5.010535	-1.182339	0.248016
O	-4.217422	-0.015954	0.108091
H	-6.044792	-0.856809	0.144665
H	-2.782933	-2.316911	0.535902
C	-2.856640	-0.158263	0.204457
C	-2.203980	-1.410008	0.399333

C	-2.092129	0.974347	0.128002
C	-0.841673	-1.501054	0.463388
H	-2.556287	1.946801	0.013528
H	-0.364333	-2.453933	0.670233
C	0.026563	-0.357910	0.279455
C	-0.680774	0.896763	0.193631
O	1.160700	-0.394135	1.128725
N	0.063997	2.078391	0.082350
H	4.397739	-0.884225	-1.322324
H	2.280828	-2.128948	-0.842462
O	1.291732	1.990065	-0.128462
C	2.308024	-1.032386	-0.860355
H	-4.782488	-1.914675	-0.534841
C	3.448745	-0.537198	-1.733421
H	3.460744	0.556693	-1.752350
H	3.343897	-0.917228	-2.752017
N	0.985179	-0.574770	-1.294738
H	1.064061	0.384967	-1.636039
H	0.147445	-2.411232	-1.855921
C	0.277191	-1.409748	-2.268774
H	0.839259	-1.466680	-3.203738
H	-0.703140	-0.968259	-2.457940

(5) - Spiro
Energy: -932.17272058 a.u.

H	3.749242	-0.444558	3.386666
H	2.067271	-0.997581	3.227155
C	2.839132	-0.351712	2.794478
H	2.482074	0.682345	2.852842
N	3.128573	-0.730949	1.413771
H	-4.509934	-0.132597	1.933048
O	-1.001039	3.111916	-0.463340
C	2.177843	-0.669287	0.592834
C	-4.756626	-0.925407	1.218287
O	-4.259923	-0.593643	-0.077323
H	-5.838863	-1.018978	1.126986
H	-2.578196	-2.631957	-0.030691
C	-2.888790	-0.473088	-0.123996
C	-2.079668	-1.669449	-0.109493
C	-2.293067	0.737003	-0.233894
C	-0.735311	-1.622197	-0.196491
H	-2.880224	1.647283	-0.254472
H	-0.145222	-2.533713	-0.159711
C	0.019114	-0.338608	-0.257709
C	-0.871437	0.842887	-0.349535
O	0.918454	-0.250918	0.884590
N	-0.305743	2.078794	-0.489528
H	4.391422	-1.100790	-1.032979
H	2.109358	-2.127498	-0.978405
O	0.953167	2.171682	-0.667717
C	2.270741	-1.049233	-0.869436
H	-4.337866	-1.875239	1.570015
C	3.557333	-0.621422	-1.547603
H	3.687693	0.462119	-1.480041
H	3.570619	-0.928420	-2.595055
N	1.064802	-0.361472	-1.414390
H	1.298460	0.652279	-1.496994
H	0.327334	-1.942488	-2.597018
C	0.544728	-0.879626	-2.699924
H	1.299570	-0.717157	-3.468173
H	-0.364640	-0.330929	-2.947721

(5) - TS2
Energy: -932.15992320 a.u.

H	3.628799	-0.724066	3.510102
H	1.882153	-0.982553	3.309314
C	2.761829	-0.471604	2.896559
H	2.578521	0.607043	2.983147
N	3.017300	-0.867066	1.516178
H	-4.196762	-0.171532	2.247149
O	-1.265026	3.117828	-0.733592
C	2.056734	-0.633496	0.702960
C	-4.555477	-0.961733	1.578836
O	-4.275430	-0.624502	0.219850
H	-5.638174	-1.054653	1.661443
H	-2.571728	-2.636551	-0.037124
C	-2.933650	-0.502218	-0.051139
C	-2.121750	-1.656484	-0.165573
C	-2.385997	0.729468	-0.289648
C	-0.791240	-1.555516	-0.470701
H	-2.995924	1.622937	-0.238540
H	-0.192842	-2.454884	-0.565861
C	-0.150655	-0.282866	-0.604215
C	-1.020364	0.844920	-0.633778
O	0.903988	-0.073095	0.943771
N	-0.514633	2.157812	-0.848761
H	4.300580	-1.248760	-0.749206
H	1.947514	-2.114732	-0.869033
O	0.684187	2.308962	-1.153471
C	2.193646	-1.053512	-0.760683
H	-4.085429	-1.912564	1.852177
C	3.550055	-0.761874	-1.372880
H	3.756988	0.312511	-1.375175
H	3.634752	-1.153396	-2.388342
N	1.095242	-0.281570	-1.439991
H	1.371467	0.717285	-1.452492
H	0.558401	-1.761466	-2.849782
C	0.822339	-0.704315	-2.843962
H	1.719167	-0.529691	-3.435371
H	-0.003133	-0.106275	-3.229055

(6) - Imidate
Energy: -932.19542724 a.u.

O	1.578823	1.036173	0.552718
C	0.850650	0.100249	-0.133076
N	-1.166280	1.586476	1.162545
C	-0.362541	2.571414	0.441082
C	1.096613	2.314388	0.776011
C	0.367665	-1.016187	0.584565
C	-0.332205	-2.002351	-0.100666
C	-0.511567	-1.857095	-1.478025
C	-0.022020	-0.784523	-2.202756
C	0.677512	0.199899	-1.504710
C	-2.384167	1.185600	0.470166
N	-1.252942	-2.902801	-2.187085
O	-1.657871	-3.859610	-1.544513
C	-0.763926	4.019486	0.700797
N	1.862629	3.181895	1.278165
C	3.237762	2.794648	1.570611
O	-1.432710	-2.768657	-3.387781
H	-3.029654	2.025425	0.171095
H	-2.110383	0.624282	-0.431442
H	-2.961655	0.520221	1.116028
H	-1.821329	4.146832	0.452599
H	-0.174565	-0.721183	-3.272091
H	-0.493907	2.363054	-0.628313
H	1.090811	1.057440	-2.025472
H	-1.378138	1.937207	2.092599
H	-0.174827	4.711636	0.095421
H	-0.611928	4.272778	1.753537
H	-0.740893	-2.869613	0.399678
O	0.622885	-1.033426	1.903765
H	3.271742	1.981077	2.303703
H	3.755320	2.448414	0.669047
H	3.771146	3.655138	1.975490
C	0.065704	-2.095929	2.668271
H	0.354391	-1.902676	3.699539
H	-1.026127	-2.099795	2.584447
H	0.468623	-3.061843	2.347805

(6) - TS1
Energy: -932.17511236 a.u.

O	1.560560	0.539017	0.174002
C	0.508971	-0.224540	-0.380311
N	-0.797303	0.924937	0.258855
C	-0.131219	2.223933	0.132113
C	1.330534	1.874085	0.340600
C	0.236036	-1.467475	0.325310
C	-0.207085	-2.574036	-0.336664
C	-0.329807	-2.544560	-1.752294
C	0.024877	-1.398163	-2.474255
C	0.469354	-0.277121	-1.813589
C	-2.063604	0.753150	-0.452713
N	-0.772580	-3.694957	-2.429946
O	-1.039961	-4.714446	-1.776174
C	-0.640466	3.292233	1.086085
N	2.227644	2.699291	0.651672
C	3.590429	2.193313	0.787168
O	-0.890115	-3.667805	-3.664248
H	-2.816605	1.454156	-0.086428
H	-1.886201	0.920391	-1.517217
H	-2.410163	-0.271416	-0.300106
H	-1.693754	3.505088	0.890890
H	-0.015726	-1.415820	-3.557142
H	-0.266194	2.549222	-0.906945
H	0.802100	0.597276	-2.364139
H	-0.890580	0.661761	1.243742
H	-0.064373	4.207788	0.944314
H	-0.522720	2.967246	2.123488
H	-0.461394	-3.483538	0.191548
O	0.366576	-1.336615	1.675049
H	3.667851	1.514951	1.644086
H	3.906527	1.642487	-0.105232
H	4.267189	3.032931	0.945411
C	0.052835	-2.473921	2.465604
H	0.225492	-2.179836	3.499439
H	-0.995400	-2.762170	2.331216
H	0.703083	-3.316237	2.206704

(6) - Spiro
Energy: -932.17809571 a.u.

O	1.341162	1.049928	0.468981
C	0.121241	0.413578	0.007051
N	-0.916438	1.445924	0.621660
C	-0.258730	2.778880	0.504228
C	1.197868	2.390631	0.652305
C	-0.084263	-0.886063	0.690353
C	-0.314597	-2.038314	0.019860
C	-0.359131	-2.040396	-1.410182
C	-0.165395	-0.829908	-2.116304
C	0.054308	0.342281	-1.461089
C	-2.275765	1.340115	0.042705
N	-0.578815	-3.220303	-2.089680
O	-0.727221	-4.285361	-1.447751
C	-0.747102	3.789777	1.522660
N	2.131003	3.189761	0.918588
C	3.481410	2.638823	0.997795
O	-0.629578	-3.220926	-3.341116
H	-2.943409	1.998208	0.597169
H	-2.230470	1.628263	-1.006710
H	-2.604537	0.304092	0.132815
H	-1.798439	4.034298	1.359913
H	-0.177863	-0.849534	-3.200082
H	-0.442058	3.132659	-0.516398
H	0.240592	1.258813	-2.013194
H	-0.960864	1.188664	1.618184
H	-0.156447	4.700258	1.411223
H	-0.610050	3.413086	2.539732
H	-0.470428	-2.972114	0.544967
O	-0.059528	-0.720987	2.047753
H	3.577397	1.977470	1.865976
H	3.733471	2.058302	0.103969
H	4.192751	3.457643	1.103841
C	-0.310067	-1.872363	2.840127
H	-0.265483	-1.543024	3.876679
H	-1.301228	-2.283520	2.619743
H	0.454328	-2.635197	2.659483

(6) - TS2
Energy: -932.16761979 a.u.

O	1.405596	1.018928	0.525138
C	-0.209686	0.344177	-0.005614
N	-0.912956	1.470747	0.711474
C	-0.171315	2.758457	0.488299
C	1.285767	2.319219	0.617227
C	-0.319628	-0.918157	0.675882
C	-0.237062	-2.099302	-0.009886
C	-0.132136	-2.065175	-1.417664
C	-0.163582	-0.858254	-2.115458
C	-0.259825	0.332368	-1.422915
C	-2.365847	1.519599	0.380433
N	-0.053949	-3.293722	-2.134512
O	-0.062363	-4.351864	-1.501140
C	-0.594245	3.846948	1.453932
N	2.203416	3.193198	0.780059
C	3.559964	2.661066	0.847402
O	0.020427	-3.264669	-3.364897
H	-2.845424	2.244604	1.035823
H	-2.474786	1.809564	-0.663813
H	-2.784309	0.526776	0.543240
H	-1.612894	4.189957	1.263384
H	-0.137809	-0.862256	-3.198364
H	-0.378215	3.058356	-0.544434
H	-0.302206	1.270715	-1.964917
H	-0.827067	1.230146	1.709508
H	0.088319	4.686843	1.317637
H	-0.508941	3.507136	2.490312
H	-0.270571	-3.054193	0.498222
O	-0.468776	-0.782393	2.024418
H	3.682714	1.971550	1.692215
H	3.825304	2.108526	-0.062950
H	4.264495	3.485678	0.969873
C	-0.651849	-1.969871	2.784936
H	-0.794941	-1.648779	3.814719
H	-1.534372	-2.515594	2.435337
H	0.233537	-2.609507	2.715779

(7) - Imidate
Energy: -895.08251673 a.u.

C	0.667646	-0.494009	-2.142798
C	1.205156	-0.529736	-0.863099
C	0.362593	-0.631721	0.242618
C	-1.033312	-0.731019	0.110586
C	-1.565578	-0.690011	-1.177727
C	-0.714690	-0.576089	-2.270915
O	0.901863	-0.739593	1.500219
C	1.637892	0.291384	2.060909
N	2.395707	0.052479	3.040028
C	2.515186	-1.326985	3.497728
C	-1.882682	-0.832867	1.310995
N	-1.299421	-0.525153	-3.612083
O	-2.514140	-0.599316	-3.715289
C	1.398670	1.680574	1.494269
C	2.211172	2.745443	2.223292
N	-0.044457	1.917663	1.492839
C	-0.507986	2.745944	0.386487
O	-0.543460	-0.411221	-4.564830
H	0.012860	3.711541	0.299406
H	-0.368809	2.194383	-0.551145
H	-1.576404	2.939696	0.506065

H	1.996126	3.722663	1.781961
H	1.298065	-0.410616	-3.019076
H	1.716740	1.665779	0.444152
H	2.279403	-0.487289	-0.714091
H	-0.321881	2.321958	2.383362
H	3.283039	2.551714	2.144196
H	1.946200	2.766371	3.283846
H	-2.637670	-0.720293	-1.332894
H	2.732626	-2.012405	2.671612
H	3.316276	-1.388329	4.234863
H	1.583014	-1.659149	3.968367
C	-3.098176	-1.386138	1.332037
H	-1.450820	-0.417079	2.216730
H	-3.678997	-1.412022	2.247728
H	-3.545867	-1.838204	0.450793

(7) - TS1

Energy: -895.06210141 a.u.

C	-0.187795	-0.120623	-1.140303
C	0.409278	0.040743	0.079450
C	-0.365441	-0.003611	1.296900
C	-1.740131	-0.471390	1.204307
C	-2.306545	-0.627604	-0.039444
C	-1.562467	-0.422394	-1.215449
O	0.336871	-0.468302	2.432442
C	1.103280	0.447396	3.097901
N	1.927272	0.137884	3.996055
C	2.103557	-1.281699	4.288475
C	-2.490994	-0.675082	2.455264
N	-2.175056	-0.605802	-2.475667
O	-3.372510	-0.913411	-2.525344
C	0.810394	1.867043	2.645030
C	0.817563	2.877022	3.781390
N	-0.476148	1.727755	1.956097
C	-0.785434	2.699439	0.905702
O	-1.501275	-0.445683	-3.501166
H	-0.899835	3.702850	1.321041
H	0.024591	2.690970	0.174335
H	-1.715794	2.394126	0.420599
H	0.616352	3.880270	3.399611
H	0.395699	-0.059356	-2.051846
H	1.549603	2.149769	1.885589
H	1.477280	0.220671	0.155565
H	-1.242460	1.685429	2.634040
H	1.797217	2.872269	4.261711
H	0.064443	2.617156	4.530453
H	-3.337627	-0.954125	-0.123469
H	2.352053	-1.849658	3.385511
H	2.907607	-1.398686	5.014801
H	1.186112	-1.707773	4.709609
C	-3.815805	-0.540327	2.593173
H	-1.896869	-0.946527	3.326321
H	-4.298153	-0.734041	3.545175
H	-4.452867	-0.235208	1.767017

(7) - Spiro

Energy: -895.06420903 a.u.

C	0.522320	-0.264560	-2.163690
C	1.083136	0.032083	-0.964140
C	0.305966	-0.006224	0.288901
C	-1.068756	-0.552714	0.169213
C	-1.586884	-0.836592	-1.063559
C	-0.835539	-0.670158	-2.250322
O	1.042393	-0.646234	1.357115
C	1.824316	0.222178	2.058646
N	2.661420	-0.107481	2.936180
C	2.839947	-1.535001	3.188353
C	-1.835444	-0.712709	1.416430
N	-1.395475	-0.981609	-3.485562
O	-2.574626	-1.380428	-3.544740
C	1.520572	1.647193	1.641621
C	1.471027	2.640555	2.785525
N	0.217377	1.462025	0.943895
C	-0.164044	2.519711	-0.019544
O	-0.711878	-0.848447	-4.519287
H	-0.320152	3.451593	0.522402
H	0.634741	2.627847	-0.751835
H	-1.087504	2.210915	-0.512097
H	1.259202	3.647254	2.420551
H	1.118016	-0.224361	-3.068703
H	2.241265	1.965430	0.880519
H	2.134439	0.295832	-0.895354
H	-0.526271	1.393547	1.651707
H	2.445305	2.645838	3.276589
H	0.717339	2.350431	3.522513
H	-2.593431	-1.234998	-1.138418
H	3.026273	-2.088328	2.261830
H	3.684267	-1.673246	3.863313
H	1.944278	-1.957198	3.657227
C	-3.162034	-0.570276	1.533384
H	-1.257107	-0.967793	2.304831
H	-3.659378	-0.744404	2.481511
H	-3.783941	-0.283101	0.689271

(7) - TS2

Energy: -895.05111226 a.u.

C	1.403359	-1.076007	0.373989
C	0.410041	-0.058915	0.315988
C	0.813513	1.312133	0.420353
C	2.161831	1.614610	0.395285
C	3.120331	0.597377	0.348963
C	2.738791	-0.749534	0.348186
N	-0.907161	-0.394113	0.983342
C	-0.727674	-0.669954	2.439619
C	-0.213888	2.372331	0.469255
N	4.511581	0.939007	0.329304
O	5.341384	0.031832	0.293551
C	-1.625725	-1.479500	0.227913
C	-3.084972	-1.587879	0.624571
C	-1.391125	-1.084623	-1.230865
N	-2.090451	-1.632246	-2.151442
C	-1.755067	-1.215668	-3.508518
O	-0.442568	-0.194989	-1.345321
O	4.829664	2.126903	0.350508
H	-1.711053	-0.757826	2.898169
H	-0.165216	-1.596199	2.548700
H	-0.176408	0.162226	2.876745
H	-3.207525	-1.958755	1.643823
H	3.494628	-1.525656	0.347901
H	-1.098385	-2.412078	0.452219
H	1.107873	-2.119350	0.393156
H	-1.483715	0.453099	0.904960
H	-3.555925	-2.292454	-0.062041
H	-3.594169	-0.624818	0.519953
H	2.479607	2.651297	0.404582
H	-0.712281	-1.449650	-3.759016
H	-2.405086	-1.734124	-4.215846
H	-1.885421	-0.134665	-3.646272
C	-0.135050	3.463748	1.236356
H	-1.072212	2.247306	-0.193843
H	-0.897555	4.234152	1.195377
H	0.696994	3.615477	1.919561

(8) - Imidate

Energy: -934.37582499 a.u.

C	0.604644	-1.601126	0.299157
C	0.027006	-0.654807	-0.544480
C	0.766469	0.404342	-1.096749
C	2.094969	0.534158	-0.716660
C	2.650866	-0.385235	0.173015

C	1.933456	-1.460986	0.680115
N	-1.358184	0.820015	1.375008
C	-2.169983	-0.386763	1.289887
C	-2.375638	-0.727038	-0.176893
O	-1.261592	-0.806086	-0.988102
C	-0.666390	0.989687	2.644656
C	-3.497853	-0.318882	2.041550
N	-3.513255	-0.929292	-0.686183
C	-3.576809	-1.260049	-2.104150
C	0.114924	1.371368	-2.058248
C	-0.836723	2.321784	-1.375775
C	-2.116537	2.476548	-1.712432
N	4.049429	-0.227011	0.563507
O	4.527901	-1.039992	1.340962
O	4.677541	0.711851	0.096536
H	-1.324300	0.984720	3.526578
H	0.064216	0.180545	2.759251
H	-0.121311	1.936413	2.629864
H	-3.307848	-0.070723	3.089071
H	2.407042	-2.173666	1.343974
H	-1.568989	-1.194979	1.727783
H	0.018984	-2.444729	0.647648
H	-1.925027	1.633982	1.151993
H	-4.028025	-1.272591	2.000046
H	-4.140950	0.450066	1.604565
H	2.703955	1.341656	-1.107603
H	-3.091584	-0.492995	-2.718360
H	-3.072783	-2.211110	-2.310154
H	-4.621836	-1.344916	-2.403737
H	0.907386	1.946368	-2.550367
H	-0.423202	0.815326	-2.833180
H	-0.415272	2.909433	-0.560093
H	-2.755835	3.187710	-1.197835
H	-2.564027	1.894123	-2.514845

(8) - TS1
Energy: -934.35756601 a.u.

C	0.492433	-1.288318	0.688600
C	-0.224093	-0.195188	0.070645
C	0.574545	0.825797	-0.596150
C	1.911887	0.902698	-0.313924
C	2.550450	-0.060908	0.500710
C	1.832655	-1.189137	0.944021
N	-1.189497	0.637970	1.407084
C	-2.407196	-0.178372	1.456977
C	-2.555547	-0.637549	0.019725
O	-1.374216	-0.571797	-0.659918
C	-0.427054	0.777218	2.649240
C	-3.630706	0.550014	1.988260
N	-3.633794	-1.016780	-0.506882
C	-3.582460	-1.441283	-1.902826
C	-0.095192	1.751268	-1.590792
C	-1.099467	2.693051	-0.972690
C	-2.418594	2.622424	-1.166645
N	3.926123	0.051301	0.774877
O	4.486078	-0.832610	1.439998
O	4.549665	1.035827	0.352135
H	-1.017886	1.293193	3.409275
H	-0.150077	-0.216250	3.005638
H	0.476852	1.352074	2.434418
H	-3.473494	0.852904	3.025775
H	2.356334	-1.987537	1.457126
H	-2.183405	-1.053477	2.079789
H	-0.068463	-2.171026	0.979987
H	-1.413161	1.558411	1.018635
H	-4.495515	-0.113512	1.941168
H	-3.841295	1.434824	1.380050
H	2.511928	1.687109	-0.763772
H	-3.156589	-0.660035	-2.543472
H	-2.963164	-2.337780	-2.017272
H	-4.592644	-1.666778	-2.244141
H	0.687614	2.335639	-2.085410
H	-0.597579	1.154090	-2.360276
H	-0.692382	3.465327	-0.317230
H	-3.102154	3.321865	-0.694571
H	-2.850656	1.861911	-1.814993

(8) - Spiro
Energy: -934.35925533 a.u.

O	-1.237543	-0.769211	-0.800236
C	-0.189672	-0.254115	0.039709
N	-1.123335	0.495978	1.133535
C	-2.334911	-0.360130	1.247835
C	-2.434186	-0.899537	-0.163064
C	0.634013	0.743913	-0.693236
C	1.967266	0.826537	-0.434120
C	2.628695	-0.090671	0.428953
C	1.911751	-1.213708	0.918187
C	0.577562	-1.331873	0.694937
C	-0.423813	0.815391	2.396740
N	3.985030	0.041928	0.682691
O	4.611884	1.008710	0.201504
C	-3.565841	0.390612	1.717611
N	-3.472725	-1.379081	-0.684923
C	-3.361651	-1.862150	-2.058918
O	4.565575	-0.802227	1.396880
H	-1.074202	1.433702	3.014672
H	-0.178788	-0.114681	2.907204
H	0.488706	1.360784	2.149675
H	-3.438551	0.748901	2.740956
H	2.449803	-1.994823	1.443522
H	-2.085259	-1.177669	1.933383
H	0.029804	-2.211442	1.020007
H	-1.407555	1.375569	0.681252
H	-4.419384	-0.288275	1.688598
H	-3.776992	1.235969	1.056029
H	2.562873	1.581636	-0.937334
C	-0.039591	1.599133	-1.748181
H	-2.979011	-1.081502	-2.726606
H	-2.678503	-2.716387	-2.118164
H	-4.345778	-2.174866	-2.407085
C	-1.092996	2.536014	-1.208780
H	0.739154	2.185743	-2.246242
H	-0.498048	0.950899	-2.503811
C	-2.405517	2.392855	-1.413787
H	-0.731407	3.366903	-0.600161
H	-3.125729	3.093002	-1.000910
H	-2.793455	1.572571	-2.015930

(8) - TS2
Energy: -934.34637958 a.u.

O	-1.096238	-1.074175	-0.876592
C	-0.052849	-0.076652	0.281484
N	-1.311430	0.494572	0.906313
C	-2.376588	-0.561025	1.022579
C	-2.235933	-1.326960	-0.290500
C	0.681567	0.811173	-0.575749
C	2.040153	0.629456	-0.704696
C	2.716590	-0.346175	0.041370
C	2.024220	-1.149530	0.954582
C	0.667549	-0.989873	1.105354
C	-1.017811	1.210358	2.182640
N	4.127976	-0.500498	-0.109580
O	4.724888	0.229401	-0.901984
C	-3.749114	0.037042	1.261898
N	-3.174569	-2.106955	-0.672925
C	-2.912639	-2.821052	-1.917604
O	4.704536	-1.361372	0.556548
H	-1.903792	1.772283	2.474738
H	-0.758051	0.474036	2.942087

H	-0.182246	1.888086	2.010543
H	-3.826086	0.508587	2.243478
H	2.561470	-1.877324	1.550930
H	-2.084852	-1.203239	1.859429
H	0.133338	-1.605547	1.821297
H	-1.661960	1.204808	0.250138
H	-4.475044	-0.775144	1.206921
H	-3.999710	0.765592	0.484407
H	2.602823	1.253250	-1.391356
C	-0.043787	1.850783	-1.407185
H	-2.749768	-2.130636	-2.755192
H	-2.018713	-3.453594	-1.842064
H	-3.767522	-3.456794	-2.155523
C	-0.459871	3.074536	-0.625245
H	0.629542	2.162255	-2.213013
H	-0.921903	1.398638	-1.887642
C	-1.707674	3.545235	-0.568496
H	0.334873	3.582324	-0.078522
H	-1.953642	4.430367	0.009051
H	-2.519562	3.066559	-1.114614

(15) - Imidate
Energy: -1277.27750007 a.u.

O	1.488108	-1.118912	0.051894
C	0.196663	-0.751965	-0.177097
N	1.476137	1.646704	0.501663
C	2.250560	1.136935	-0.625753
C	2.553897	-0.329205	-0.363235
C	-0.671419	-0.605880	0.914103
C	-2.008070	-0.306207	0.711386
C	-2.459343	-0.166429	-0.598284
C	-1.629405	-0.323590	-1.700229
C	-0.292575	-0.628354	-1.477301
C	0.546093	2.713681	0.155585
N	-3.871523	0.153380	-0.814555
O	-4.588896	0.276579	0.165398
C	3.516111	1.930057	-0.937357
Cl	-0.063612	-0.778954	2.523408
N	3.703725	-0.837425	-0.438450
C	3.852765	-2.259661	-0.152776
O	-4.259639	0.280547	-1.964703
H	1.010520	3.565835	-0.363343
H	-0.238374	2.304191	-0.492376
H	0.070534	3.082292	1.067133
H	3.249823	2.975760	-1.113379
H	-2.022536	-0.221539	-2.703816
H	1.593527	1.181694	-1.504128
H	0.384636	-0.781840	-2.311151
H	2.104917	1.941871	1.243718
H	4.020216	1.542023	-1.824789
H	4.214086	1.877012	-0.097339
H	-2.684581	-0.178860	1.547553
H	3.139178	-2.864940	-0.721699
H	4.867300	-2.568130	-0.406023
H	3.683664	-2.458156	0.911445

(15) - TS1
Energy: -1277.25961374 a.u.

O	1.519061	-0.964117	0.285245
C	0.331203	-0.214421	0.197728
N	1.219085	1.410444	0.365242
C	2.458892	1.136629	-0.368320
C	2.668483	-0.347231	-0.130825
C	-0.546861	-0.317678	1.341860
C	-1.904479	-0.214269	1.232334
C	-2.491633	-0.103920	-0.041762
C	-1.690470	-0.148716	-1.196512
C	-0.328553	-0.241130	-1.085876
C	0.398756	2.531144	-0.098581
N	-3.899797	-0.006849	-0.154708
O	-4.584940	0.000336	0.873160
C	3.646017	1.988970	0.050492
Cl	0.207438	-0.461861	2.910849
N	3.762808	-0.949516	-0.268569
C	3.776868	-2.388571	-0.020629
O	-4.404319	0.072207	-1.279314
H	0.930655	3.477684	0.017691
H	0.151217	2.371158	-1.149604
H	-0.520378	2.552435	0.491558
H	3.441565	3.044462	-0.141278
H	-2.161260	-0.146574	-2.172767
H	2.239532	1.291434	-1.431837
H	0.293366	-0.331067	-1.971225
H	1.413435	1.503062	1.365920
H	4.524541	1.691156	-0.523691
H	3.863862	1.848301	1.112793
H	-2.529006	-0.234907	2.117834
H	3.042228	-2.907510	-0.645536
H	4.770362	-2.778306	-0.240951
H	3.537820	-2.604759	1.026467

(15) - Spiro
Energy: -1277.26192110 a.u.

O	1.458002	-0.937172	-0.068909
C	0.356849	-0.007330	-0.140234
N	1.199825	1.348506	0.012718
C	2.473205	1.091915	-0.719349
C	2.635531	-0.397805	-0.495580
C	-0.562342	-0.153062	1.003301
C	-1.911704	-0.221975	0.878196
C	-2.510842	-0.199216	-0.402934
C	-1.686151	-0.145480	-1.553439
C	-0.334478	-0.065251	-1.443552
C	0.446534	2.558486	-0.389385
N	-3.897437	-0.273691	-0.522495
O	-4.597138	-0.343958	0.503985
C	3.640629	1.927348	-0.231045
Cl	0.192648	-0.188261	2.584394
N	3.703407	-1.038086	-0.660981
C	3.665839	-2.478194	-0.418640
O	-4.412986	-0.266117	-1.654396
H	1.043337	3.439075	-0.155618
H	0.241669	2.501785	-1.457423
H	-0.488803	2.577261	0.171867
H	3.468249	2.988846	-0.417919
H	-2.147689	-0.191302	-2.533217
H	2.270924	1.284393	-1.778523
H	0.290697	-0.069050	-2.331608
H	1.414648	1.418774	1.016342
H	4.533114	1.617752	-0.776920
H	3.818340	1.764292	0.835299
H	-2.535876	-0.304860	1.760614
H	2.874643	-2.961903	-1.001234
H	4.627214	-2.909913	-0.695509
H	3.478923	-2.686447	0.640461

(15) - TS2
Energy: -1277.24890176 a.u.

O	1.421663	-0.938542	0.064806
C	0.143181	0.422659	-0.100465
N	1.242441	1.436894	0.052941
C	2.463306	1.015836	-0.725114
C	2.530196	-0.488853	-0.457301
C	-0.732348	0.254358	1.011754
C	-2.013500	-0.216768	0.859061
C	-2.502374	-0.443555	-0.430492
C	-1.719485	-0.167539	-1.555777
C	-0.437316	0.303752	-1.394410
C	0.765239	2.820631	-0.245431
N	-3.845698	-0.924779	-0.592452

O	-4.521154	-1.131323	0.412405	H	-2.131268	-0.307588	-2.547812
C	3.700174	1.784171	-0.301485	H	2.238193	1.202639	-1.779854
Cl	-0.106069	0.548753	2.614673	H	0.163857	0.526910	-2.269122
N	3.592849	-1.134109	-0.758250	H	1.505893	1.405717	1.046770
C	3.534441	-2.568104	-0.497047	H	4.551140	1.335693	-0.815658
O	-4.266866	-1.113413	-1.730351	H	3.870712	1.693840	0.775901
H	1.557383	3.520741	0.012678	H	-2.641042	-0.396477	1.723855
H	0.524619	2.882536	-1.305825	H	2.694519	-3.043939	-1.019361
H	-0.122563	3.013724	0.356082	H	4.462443	-3.033798	-0.834119
H	3.644160	2.838574	-0.577647	H	3.411116	-2.779002	0.572910