

Photoredox Catalysis Leading to Triazolo-Quinoxalinones at room temperature:

Selectivity of the rate determining step

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Electronic Supplementary Information

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Table S2. Summary of the activation energy (in kcal/mol), HOMO and LUMO energies (in a.u.), chemical potential, chemical hardness, electrophilicity and NBO charge on the reactive C and N atoms of species **D** of the different scaffolds at the B3LYP-D3(SMD)/Def2TZVP level of theory in dichloroethane.

B3LYP-D3/Def2SVP Cartesian coordinates of the optimized geometries of the species calculated in this study.

Table S1. Summary of the activation energy (in kcal/mol), HOMO and LUMO energies (in a.u.), chemical potential, chemical hardness, electrophilicity and NBO charge on the radical carbon of species **C** of the different scaffolds at the B3LYP-D3(SMD)/Def2TZVP level of theory in dichloroethane.

Species C	$\Delta G^\ddagger$ (kcal/mol)	HOMO (a.u.)	LUMO (a.u.)	Chemical Potential	Chemical Hardness	Electrophilicity	NBO (C)
Reference	14.3	-0.26646	-0.15599	-0.211	0.110	0.202	0.045
3ib	13.9	-0.26746	-0.15692	-0.212	0.111	0.204	0.045
3ic	13.5	-0.25518	-0.15725	-0.206	0.098	0.217	0.046
3id	12.5	-0.25544	-0.15370	-0.205	0.102	0.206	0.065
COOH	13.2	-0.27140	-0.15969	-0.216	0.112	0.208	0.037
COOtBu	14.6	-0.26364	-0.15267	-0.208	0.111	0.195	0.044
H	14.5	-0.26139	-0.14420	-0.203	0.117	0.175	-0.124
Me	17.3	-0.24009	-0.12904	-0.185	0.111	0.153	0.111
tBu	20.3	-0.23824	-0.12870	-0.183	0.110	0.154	0.125

Table S2. Summary of the activation energy (in kcal/mol), HOMO and LUMO energies (in a.u.), chemical potential, chemical hardness, electrophilicity and NBO charge on the reactive C and N atoms of species **D** of the different scaffolds at the B3LYP-D3(SMD)/Def2TZVP level of theory in dichloroethane.

Species D	$\Delta G^\ddagger$ (kcal/mol)	HOMO (a.u.)	LUMO (a.u.)	Chemical Potential	Chemical Hardness	Electrophilicity	NBO (C)	NBO (N)
Reference	14.3	-0.23262	-0.07771	-0.155	0.155	0.078	0.018	-0.380
3aa	14.5	-0.23090	-0.08170	-0.156	0.149	0.082	0.026	-0.382
3ab	14.7	-0.23209	-0.08266	-0.157	0.149	0.083	0.027	-0.379
3ac	14.7	-0.23196	-0.08320	-0.158	0.149	0.083	0.027	-0.379
3ad	13.0	-0.24228	-0.08412	-0.163	0.158	0.084	0.028	-0.376
3ae	14.0	-0.22168	-0.07821	-0.150	0.143	0.078	0.019	-0.379
3af	15.7	-0.24867	-0.10044	-0.175	0.148	0.103	0.032	-0.372
3ag	14.3	-0.23682	-0.08228	-0.160	0.155	0.082	0.020	-0.377
3ah	14.5	-0.23691	-0.0829	-0.160	0.154	0.083	0.022	-0.377
3ai	15.0	-0.24033	-0.08672	-0.164	0.154	0.087	0.033	-0.380
3aj	13.0	-0.22293	-0.07339	-0.148	0.150	0.073	0.007	-0.380
3ak	14.8	-0.23653	-0.08693	-0.162	0.150	0.087	0.029	-0.377
3al	15.3	-0.24082	-0.08493	-0.163	0.156	0.085	0.027	-0.378

B3LYP-D3/Def2SVP Cartesian coordinates of the optimized geometries of the species calculated in this study.

61			
Ru-bpy-3-2+ SCF Done: -1581.61082747 A.U.			
Ru	-0.000002	-0.000355	0.000331
N	-0.787407	1.621984	1.054779
C	-0.435667	2.851731	0.584165
C	-0.916897	4.017694	1.193440
C	-1.768215	3.923070	2.293549
C	-2.123093	2.656082	2.763428
C	-1.612295	1.534550	2.115071
H	-0.632104	4.997660	0.811713
H	-2.149306	4.825892	2.775314
H	-2.787406	2.531460	3.620242
H	-1.863745	0.527470	2.450271
N	1.797918	-0.129931	1.056085
N	0.806408	1.612368	-1.054463
N	0.994543	-1.504598	-1.054243
C	0.469197	2.846284	-0.584067
C	2.688121	-1.048122	0.585073
C	2.133137	0.627105	2.117623
C	1.629707	1.515069	-2.115164
C	2.231929	-1.828710	-0.583771
C	0.499284	-2.169084	-2.115166
C	0.963704	4.006399	-1.193873
C	3.938404	-1.213641	1.194731
C	3.359557	0.509199	2.766537
H	1.385656	1.347053	2.453320
C	2.153101	2.630405	-2.764134
H	1.869214	0.505032	-2.450236
C	2.990238	-2.836293	-1.193707
C	1.204315	-3.179421	-2.764184
H	-0.495386	-1.872263	-2.450375
C	1.813293	3.901572	-2.294384
H	0.690532	4.989708	-0.812240
C	4.280718	-0.429919	2.295876
H	4.645680	-1.949029	0.812464
H	3.582584	1.145879	3.624365
H	2.815453	2.497843	-3.621274
C	2.475328	-3.519812	-2.294419
H	3.978516	-3.090683	-0.811929
H	0.758786	-3.686977	-3.621426
H	2.204585	4.799761	-2.776630
H	5.253044	-0.550751	2.777953
H	3.058186	-4.307230	-2.776770
N	-1.012221	-1.492805	1.054817
N	-1.799283	-0.108410	-1.055538
C	-2.252876	-1.802953	0.583576
C	-0.524985	-2.163047	2.115803
C	-2.699702	-1.016973	-0.585244
C	-2.126049	0.652996	-2.116575
C	-3.022727	-2.802181	1.192786
C	-1.241523	-3.165773	2.764054
H	0.472688	-1.877332	2.451670
C	-3.951454	-1.168662	-1.195494
C	-3.353415	0.548755	-2.766008

H	-1.370895	1.365311	-2.451450
C	-2.515975	-3.491829	2.293474
H	-4.013646	-3.045349	0.810535
H	-0.802142	-3.678517	3.621381
C	-4.284807	-0.380764	-2.296396
H	-4.666802	-1.896533	-0.813862
H	-3.569292	1.188443	-3.623428
H	-3.107814	-4.272913	2.775191
H	-5.258118	-0.490910	-2.779045
61			
Ru-bpy-3-2rad+ SCF Done: -1581.53203143 A.U.			
Ru	0.000001	-0.000182	0.000032
N	-0.987788	1.511385	1.038858
C	-0.745126	2.783670	0.579871
C	-1.338698	3.885669	1.224891
C	-2.181998	3.682998	2.308629
C	-2.436475	2.370100	2.746104
C	-1.821758	1.318843	2.082326
H	-1.136884	4.897618	0.874680
H	-2.643657	4.534833	2.812296
H	-3.100385	2.167697	3.587583
H	-1.984341	0.284395	2.388833
N	1.802523	0.098940	1.039850
N	0.641488	1.688061	-1.038516
N	1.141763	-1.398760	-1.039075
C	0.132032	2.878800	-0.579322
C	2.783312	-0.746769	0.580359
C	2.052135	0.916249	2.084361
C	1.497032	1.678660	-2.082225
C	2.427590	-1.553087	-0.579553
C	0.706332	-2.134362	-2.083454
C	0.475650	4.082428	-1.224295
C	4.034267	-0.784111	1.225730
C	3.269706	0.922587	2.748521
H	1.237109	1.573487	2.391309
C	1.872231	2.837256	-2.745925
H	1.877035	0.702998	-2.389036
C	3.298489	-2.451909	-1.224895
C	1.522437	-3.038040	-2.747478
H	-0.328537	-1.975698	-2.390584
C	1.342590	4.065140	-2.308195
H	0.061747	5.027614	-0.873990
C	4.279841	0.046496	2.310390
H	4.809960	-1.464374	0.875077
H	3.425932	1.597811	3.590835
H	2.563863	2.781834	-3.587591
C	2.850537	-3.193407	-2.309432
H	4.323907	-2.566140	-0.874346
H	1.128961	-3.608788	-3.589650
H	1.610964	4.996125	-2.811857
H	5.248234	0.020106	2.814324
H	3.522868	-3.890886	-2.813342
N	-0.815756	-1.610840	1.038966
N	-1.781695	-0.289130	-1.039893
C	-2.038734	-2.036827	0.579257
C	-0.232854	-2.236654	2.083035
C	-2.558845	-1.325138	-0.580425

C	-2.200711	0.456227	-2.084066
C	-2.696974	-3.101526	1.224271
C	-0.836543	-3.294305	2.746701
H	0.744142	-1.860366	2.390215
C	-3.772939	-1.629136	-1.225771
C	-3.391527	0.202079	-2.748084
H	-1.545382	1.272780	-2.391031
C	-2.100660	-3.730257	2.308573
H	-3.674118	-3.432560	0.873531
H	-0.329961	-3.767911	3.588662
C	-4.190731	-0.870055	-2.310140
H	-4.384998	-2.459759	-0.875262
H	-3.688777	0.828502	-3.590142
H	-2.608028	-4.555702	2.812206
H	-5.131110	-1.102934	-2.814010
69			
Ru-bpy-3-3+OTf- SCF Done: -2543.35714377 A.U.			
Ru	-0.969619	0.055538	0.011866
N	-1.105472	1.696749	1.300521
C	-0.189462	2.674364	1.058959
C	-0.105797	3.789523	1.902778
C	-0.978788	3.903145	2.983173
C	-1.930714	2.901299	3.199736
C	-1.959069	1.812557	2.334048
H	0.641847	4.560812	1.721932
H	-0.917512	4.766021	3.649966
H	-2.637408	2.955476	4.029418
H	-2.673844	0.998833	2.468301
N	0.301577	-1.027054	1.208591
N	0.444828	1.293776	-0.800900
N	-0.597818	-1.596240	-1.219831
C	0.657947	2.465748	-0.125547
C	0.638493	-2.260607	0.721399
C	0.718515	-0.653074	2.436475
C	1.170543	1.009354	-1.898075
C	0.216591	-2.530008	-0.664028
C	-1.044309	-1.756191	-2.478858
C	1.610265	3.377677	-0.572086
C	1.332212	-3.167630	1.518329
C	1.414542	-1.517245	3.271013
H	0.482476	0.362515	2.746646
C	2.126987	1.889702	-2.392799
H	0.982034	0.057765	-2.384583
C	0.621155	-3.649089	-1.398887
C	-0.683261	-2.850232	-3.258203
H	-1.700504	-0.974886	-2.866954
C	2.358875	3.083805	-1.713726
H	1.786615	4.304794	-0.028915
C	1.714676	-2.799263	2.809070
H	1.599064	-4.149652	1.131233
H	1.741035	-1.173984	4.253105
H	2.705537	1.611537	-3.273588
C	0.172970	-3.809497	-2.708032
H	1.305240	-4.374790	-0.961269
H	-1.060158	-2.939607	-4.278284
H	3.125295	3.779562	-2.060988
H	2.274584	-3.497638	3.433859

H	0.493147	-4.672045	-3.296421
N	-2.680387	-1.012717	0.699096
N	-2.539448	0.916218	-1.126969
C	-3.852098	-0.694270	0.083994
C	-2.664426	-1.979392	1.635914
C	-3.776351	0.386219	-0.920716
C	-2.385822	1.924490	-2.006705
C	-5.036678	-1.364010	0.413221
C	-3.810693	-2.677188	2.008453
H	-1.704940	-2.195529	2.104623
C	-4.885500	0.870401	-1.624542
C	-3.450923	2.446093	-2.736114
H	-1.376964	2.316528	-2.131539
C	-5.019279	-2.366097	1.383023
H	-5.971878	-1.108722	-0.083580
H	-3.746491	-3.450171	2.776171
C	-4.724580	1.907563	-2.542966
H	-5.874311	0.445076	-1.457301
H	-3.275453	3.260875	-3.440666
H	-5.938330	-2.894355	1.646016
H	-5.584271	2.290892	-3.096988
S	3.363911	-0.361154	0.290153
O	2.756502	0.907797	0.784974
O	3.730689	-1.324120	1.340404
O	2.617773	-0.955375	-0.864050
C	4.988032	0.183811	-0.465371
F	5.766428	0.718614	0.463231
F	4.754888	1.110675	-1.414624
F	5.600782	-0.849047	-1.025997
48			
A SCF Done: -2115.69398910 A.U.			
C	-2.372486	-1.727376	0.247437
C	-0.970358	-1.821585	0.266360
C	-0.347164	-3.047451	0.468203
C	-1.125209	-4.195070	0.663063
C	-2.520633	-4.116471	0.655330
C	-3.143125	-2.887559	0.447125
H	0.742270	-3.119300	0.471273
H	-0.628689	-5.155833	0.819853
H	-3.123603	-5.013945	0.808446
H	-4.230973	-2.800185	0.431588
I	0.238925	-0.001660	-0.050735
C	-3.024220	-0.415509	0.006223
O	-2.403921	0.613530	-0.210579
O	-4.349824	-0.468417	0.044783
C	-5.072747	0.733581	-0.187551
H	-4.832207	1.492102	0.574869
H	-4.812584	1.167889	-1.166466
C	-6.554176	0.394965	-0.142032
O	-7.015089	-0.700299	0.039062
O	-7.260486	1.511928	-0.338548
C	-8.699920	1.386370	-0.333673
H	-9.012636	0.961784	0.634195
H	-8.992786	0.665208	-1.114078
C	-9.283706	2.761468	-0.573529
H	-8.953119	3.163948	-1.543194
H	-10.383157	2.706267	-0.576669

H	-8.973142	3.462341	0.216309
C	2.035454	-1.027499	0.239336
C	2.829956	-1.452537	-0.930208
O	2.447888	-1.378902	-2.070744
N	2.542630	-1.083338	1.445934
N	2.991451	-1.180853	2.475118
O	4.012462	-1.932808	-0.526989
C	5.018926	-2.162053	-1.537095
H	4.903238	-1.403594	-2.325590
H	4.838005	-3.150375	-1.992168
C	6.368928	-2.077080	-0.857568
H	6.456176	-2.826258	-0.055541
H	7.170985	-2.256850	-1.590202
H	6.506262	-1.077162	-0.420241
S	2.727475	2.465314	0.548393
C	4.448927	2.110257	-0.108032
F	4.658598	2.712156	-1.275895
F	5.374581	2.518380	0.758666
F	4.613552	0.780953	-0.288737
O	1.867463	1.901298	-0.566372
O	2.675969	3.918368	0.684144
O	2.642231	1.639567	1.771274
40			
B SCF Done: -1153.91718110 A.U.			
C	0.069466	1.746228	-0.345909
C	-1.313107	1.542325	-0.186104
C	-2.214245	2.043539	-1.128318
C	-1.746083	2.750058	-2.238395
C	-0.377503	2.971030	-2.406818
C	0.519389	2.475977	-1.463491
H	-3.283958	1.870541	-1.008672
H	-2.462262	3.122059	-2.975035
H	-0.007631	3.520053	-3.275628
H	1.594108	2.612320	-1.588450
I	-2.171978	0.511797	1.496446
C	1.110904	1.118359	0.520815
O	1.059564	0.011133	0.996163
O	2.188736	1.928174	0.668308
C	3.343477	1.306673	1.197915
H	4.067916	2.106008	1.409858
H	3.128924	0.759272	2.128019
C	3.940892	0.339581	0.180591
O	3.570796	0.234445	-0.962145
O	4.931079	-0.360945	0.734434
C	5.595759	-1.331356	-0.103660
H	5.973005	-0.822306	-1.005396
H	4.851398	-2.073686	-0.434974
C	6.705845	-1.959996	0.710060
H	6.301373	-2.455427	1.605858
H	7.234603	-2.712677	0.105182
H	7.433627	-1.199981	1.033367
C	-3.269552	-2.802271	-0.784619
C	-2.242906	-1.941495	-1.394940
O	-2.532850	-0.964261	-2.047076
N	-3.932134	-2.559471	0.255266
N	-4.605574	-2.460103	1.195614
O	-1.021322	-2.423591	-1.201362

C	0.081638	-1.685441	-1.785715
H	-0.003455	-0.633001	-1.486078
H	-0.017343	-1.731026	-2.882784
C	1.366821	-2.306657	-1.290376
H	1.441681	-3.361119	-1.598434
H	2.222626	-1.745550	-1.693733
H	1.411394	-2.242696	-0.193712
13			
C SCF Done: -415.454451630 A.U.			
C	1.428820	-0.132864	0.699699
C	0.210980	0.512360	0.185337
O	0.185235	1.675053	-0.143202
O	-0.836291	-0.312529	0.211691
C	-2.105734	0.240312	-0.204320
H	-2.338620	1.106140	0.436543
H	-2.009593	0.615483	-1.236372
C	-3.141762	-0.856155	-0.087918
H	-3.215235	-1.215968	0.949604
H	-4.127398	-0.474075	-0.395454
H	-2.882537	-1.709664	-0.732814
N	3.459967	-0.709051	-0.472537
N	2.458318	-0.405809	0.025937
27			
I_hypervalent SCF Done: -738.452475190 A.U.			
C	-0.772581	0.999631	0.128971
C	-2.114091	0.656205	-0.107177
C	-3.072142	1.653580	-0.315142
C	-2.695210	2.999367	-0.307580
C	-1.364297	3.355929	-0.077983
C	-0.415574	2.361136	0.147668
H	-4.116249	1.383735	-0.481997
H	-3.452739	3.767951	-0.480746
H	-1.065076	4.406459	-0.074149
H	0.632782	2.612164	0.317122
I	-2.822160	-1.378035	-0.084674
C	0.336412	0.006871	0.287106
O	0.512321	-0.976419	-0.382895
O	1.174269	0.384846	1.287248
C	2.412348	-0.294621	1.342494
H	2.854128	-0.083221	2.326866
H	2.292846	-1.382709	1.228394
C	3.344313	0.221430	0.251762
O	3.092041	1.137097	-0.488820
O	4.481155	-0.480333	0.246691
C	5.471939	-0.108786	-0.734373
H	5.746710	0.947422	-0.578200
H	5.018930	-0.180618	-1.736495
C	6.654272	-1.039241	-0.571323
H	6.352228	-2.085848	-0.729522
H	7.434881	-0.787625	-1.305809
H	7.085399	-0.952412	0.437911
33			
D SCF Done: -948.210744416 A.U.			
O	1.598660	-1.411623	-1.497823
N	-0.446994	-0.390054	-1.226420

N	-0.894267	-2.138239	0.931160
C	-1.875591	-1.252449	0.527351
C	-1.675413	-0.366856	-0.568303
C	0.540888	-1.320546	-0.890347
C	-2.715306	0.507147	-0.941113
H	-2.587568	1.199870	-1.770768
C	-3.099997	-1.234104	1.222786
H	-3.208176	-1.927898	2.058594
C	-4.117007	-0.366431	0.848946
H	-5.063545	-0.356610	1.393233
C	-0.174890	0.533038	-2.325273
H	-0.271556	1.573627	-1.982840
H	0.850632	0.355378	-2.664430
H	-0.871152	0.359935	-3.160331
C	-3.916529	0.500534	-0.236918
H	-4.709355	1.189497	-0.537638
C	0.212185	-2.166929	0.275684
H	0.999866	-2.867543	0.575876
C	1.960469	1.440949	0.532444
O	2.488075	0.274664	0.885336
O	2.426353	2.212501	-0.278141
C	3.728908	-0.095705	0.230475
H	3.577544	-0.044435	-0.856584
H	4.491650	0.648388	0.512777
C	4.087851	-1.493829	0.677775
H	3.343298	-2.208890	0.301719
H	5.069719	-1.771589	0.264188
H	4.139785	-1.558947	1.775411
C	0.756746	1.767780	1.318480
N	-0.273791	2.303135	0.825638
N	-1.262054	2.809342	0.495893

33			
TS-DE SCF Done: -948.200789106 A.U.			
O	-1.341825	1.764392	0.079702
N	0.837432	1.285401	-0.468158
N	0.902352	-0.442353	1.763879
C	2.030352	-0.188902	1.043239
C	2.025044	0.662986	-0.110830
C	-0.331655	1.113504	0.283760
C	3.223082	0.856270	-0.825138
H	3.244522	1.489256	-1.710733
C	3.246031	-0.793843	1.449768
H	3.207224	-1.430239	2.335601
C	4.413433	-0.592760	0.736856
H	5.343411	-1.071211	1.050514
C	0.790632	2.201764	-1.603231
H	1.074124	1.674002	-2.526264
H	-0.235761	2.572982	-1.690089
H	1.472438	3.052086	-1.447460
C	4.393078	0.231618	-0.405474
H	5.311366	0.389051	-0.976433
C	-0.236649	0.054294	1.331454
H	-1.135806	-0.065298	1.940713
C	-2.354742	-1.139306	-0.553065
O	-3.052704	-0.573890	0.438691
O	-2.771939	-1.331398	-1.674923
C	-4.282238	0.086287	0.091033

H	-4.156362	0.580843	-0.884500
H	-5.072789	-0.675015	-0.022114
C	-4.587304	1.079980	1.192116
H	-3.766304	1.808222	1.265336
H	-5.524850	1.614203	0.972144
H	-4.697704	0.570534	2.162187
C	-1.023470	-1.530261	-0.088123
N	-0.042209	-1.828066	-0.840339
N	0.935949	-2.105274	-1.379789
33			
E SCF Done: -948.242840708 A.U.			
O	-0.814924	-2.120931	0.342318
N	1.376545	-1.470585	0.407152
N	0.716653	0.808170	-1.213667
C	1.969746	0.541373	-0.861335
C	2.359391	-0.571320	-0.014349
C	0.037865	-1.300990	0.069472
C	3.706762	-0.733135	0.328642
H	4.017423	-1.555476	0.971474
C	3.005691	1.409432	-1.344128
H	2.684743	2.230362	-1.988010
C	4.328024	1.223648	-0.995463
H	5.097890	1.903524	-1.366957
C	1.745822	-2.659080	1.168990
H	2.200843	-2.376521	2.131189
H	0.833157	-3.235547	1.352403
H	2.460616	-3.276552	0.602808
C	4.679038	0.152641	-0.150066
H	5.722311	0.001500	0.136759
C	-0.330788	0.016982	-0.628319
H	-1.057204	-0.259978	-1.408755
C	-2.608852	0.867031	0.474926
O	-3.168794	0.100888	-0.477625
O	-3.229639	1.474249	1.319552
C	-4.595718	-0.056885	-0.425953
H	-4.883651	-0.367400	0.591492
H	-5.072045	0.920480	-0.611986
C	-4.975049	-1.088927	-1.466803
H	-4.469877	-2.044824	-1.260189
H	-6.063363	-1.255728	-1.456745
H	-4.683839	-0.754761	-2.474721
C	-1.145001	0.865421	0.348264
N	-0.493359	1.610526	1.205706
N	0.094199	2.257620	1.927098
33			
TS-12H-2 SCF Done: -948.175531911 A.U.			
O	-0.949833	-1.505743	0.932275
N	1.285515	-1.392974	0.434502
N	0.955693	1.320511	-0.442294
C	2.204173	0.729145	-0.372710
C	2.397973	-0.615953	0.062658
C	-0.012497	-0.873203	0.477849
C	3.704045	-1.129268	0.106429
H	3.883084	-2.151485	0.435524
C	3.320270	1.502469	-0.750764
H	3.130884	2.526670	-1.078014

C	4.607361	0.978778	-0.699856
H	5.461833	1.592543	-0.992993
C	1.481715	-2.756653	0.906483
H	2.114663	-2.774048	1.808763
H	0.499612	-3.173819	1.151027
H	1.959797	-3.370162	0.126357
C	4.795508	-0.340429	-0.270467
H	5.800456	-0.766497	-0.226017
C	-0.173951	0.496871	-0.077752
H	0.208127	0.734068	-1.279432
C	-2.778681	0.728658	-0.164317
O	-2.690031	-0.271145	-1.058212
O	-3.811723	1.185924	0.270258
C	-3.885989	-1.028957	-1.314911
H	-4.734252	-0.337280	-1.434952
H	-3.694056	-1.529027	-2.275360
C	-4.141390	-2.032155	-0.201943
H	-4.375994	-1.509067	0.736515
H	-4.994018	-2.679110	-0.463728
H	-3.249223	-2.652630	-0.033819
C	-1.430253	1.208051	0.190471
N	-1.371879	2.362216	0.821941
N	-1.287602	3.369309	1.332216

33			
E-NH SCF Done: -948.262177922 A.U.			
O	0.982142	-1.277299	-1.307124
N	-1.232193	-1.234254	-0.679692
N	-0.861749	1.288978	0.376431
C	-2.138265	0.758855	0.388244
C	-2.328350	-0.542493	-0.150007
C	0.064843	-0.675469	-0.759611
C	-3.624110	-1.084451	-0.124482
H	-3.805544	-2.079595	-0.526775
C	-3.219358	1.470933	0.926963
H	-3.044191	2.470342	1.334867
C	-4.497203	0.912276	0.943180
H	-5.331629	1.475590	1.366049
C	-1.425636	-2.560949	-1.241958
H	-2.144479	-2.534585	-2.077872
H	-0.456930	-2.911078	-1.613058
H	-1.800941	-3.259310	-0.475870
C	-4.695927	-0.365707	0.415976
H	-5.691218	-0.815313	0.421999
C	0.231115	0.632301	-0.151458
H	-0.706622	2.169899	0.854275
C	2.823650	0.674991	0.176650
O	2.618841	-0.424201	0.913843
O	3.902962	1.119603	-0.140915
C	3.710201	-1.342569	1.091880
H	4.484289	-1.131585	0.339016
H	4.153012	-1.160533	2.086131
C	3.154364	-2.748016	0.964571
H	2.686011	-2.872987	-0.022773
H	3.959967	-3.489619	1.085678
H	2.389139	-2.936674	1.733856
C	1.525511	1.293359	-0.181657
N	1.599915	2.520160	-0.666506

N	1.607251	3.595438	-1.033334
41			
F SCF Done: -1910.00647755 A.U.			
O	1.856383	0.566344	1.984302
N	-0.036134	1.680688	1.313107
N	0.863644	1.499502	-1.400916
C	-0.265465	2.037479	-1.093102
C	-0.780241	2.143742	0.297847
C	1.193634	0.974015	1.073308
C	-2.044486	2.759463	0.505173
H	-2.473694	2.801521	1.501678
C	-1.085049	2.569367	-2.174595
H	-0.681393	2.448562	-3.180535
C	-2.277831	3.161640	-1.919364
H	-2.897399	3.551649	-2.728704
C	-0.538020	1.681927	2.695023
H	-1.449529	1.066367	2.729358
H	0.239395	1.244933	3.327309
H	-0.742976	2.714068	3.011555
C	-2.748752	3.250019	-0.565709
H	-3.723989	3.707574	-0.380340
C	1.653129	0.876285	-0.382036
H	2.634785	1.387699	-0.384254
C	3.342713	-1.124088	-0.647880
O	4.212524	-0.212797	-0.162067
O	3.630714	-2.267349	-0.918400
C	5.541007	-0.680329	0.127019
H	5.471063	-1.578301	0.761581
H	6.025544	-0.986647	-0.815129
C	6.281034	0.447750	0.813773
H	5.764363	0.737543	1.741664
H	7.304387	0.130478	1.067060
H	6.344595	1.331974	0.160361
C	2.009662	-0.532464	-0.794659
N	1.082821	-1.313320	-1.311493
N	0.307207	-1.985637	-1.773361
C	-2.884945	-2.324375	0.150070
F	-2.982921	-2.977683	1.307822
F	-2.225223	-3.089555	-0.719164
F	-4.112601	-2.101090	-0.321896
S	-1.992199	-0.699888	0.407359
O	-2.840162	0.022615	1.385574
O	-1.957727	-0.089084	-0.953410
O	-0.646028	-1.076661	0.910155
41			
TS-12H SCF Done: -1909.96384273 A.U.			
O	2.050167	0.379331	1.673527
N	0.253342	1.734132	1.197777
N	0.470743	1.030938	-1.526039
C	-0.373405	2.017597	-1.132624
C	-0.552725	2.327826	0.253390
C	1.269010	0.821584	0.869068
C	-1.577699	3.234218	0.598238
H	-1.783222	3.462521	1.640869
C	-1.177380	2.630866	-2.127612
H	-1.014076	2.329152	-3.162943

C	-2.152283	3.530588	-1.764708
H	-2.790473	3.995139	-2.518096
C	-0.138308	1.786243	2.610633
H	-1.151579	1.362467	2.690217
H	0.572689	1.180419	3.179135
H	-0.110723	2.820666	2.981437
C	-2.346003	3.819975	-0.393124
H	-3.136120	4.515834	-0.100811
C	1.272359	0.410171	-0.588572
H	1.756082	1.283498	-1.407437
C	3.228869	-1.296599	-0.654757
O	3.965021	-0.205473	-0.380807
O	3.632175	-2.433062	-0.679447
C	5.253944	-0.399243	0.234236
H	5.234408	-1.335521	0.811941
H	6.005428	-0.516819	-0.564590
C	5.527912	0.807212	1.108639
H	4.744996	0.898712	1.875998
H	6.506028	0.702111	1.603340
H	5.541540	1.731996	0.510528
C	1.851467	-0.872385	-0.955684
N	1.022017	-1.763812	-1.480824
N	0.285716	-2.504502	-1.890672
C	-2.855834	-2.280220	0.505795
F	-2.911753	-2.543252	1.812823
F	-2.245395	-3.298251	-0.107896
F	-4.101187	-2.185571	0.036703
S	-1.918460	-0.694452	0.193293
O	-2.657739	0.340678	0.948505
O	-1.921286	-0.553978	-1.281680
O	-0.562947	-0.999943	0.746634
41			
F-NH SCF Done: -1910.07386311 A.U.			
O	-3.460780	-0.461795	-1.155979
N	-2.871364	1.651994	-0.489342
N	-0.357292	0.700158	0.096760
C	-0.583122	2.062134	0.181097
C	-1.882415	2.553940	-0.094947
C	-2.634224	0.291576	-0.678510
C	-2.115897	3.936371	0.026424
H	-3.100771	4.353272	-0.175359
C	0.461396	2.927578	0.558394
H	1.458895	2.525640	0.744755
C	0.208886	4.287860	0.664959
H	1.015564	4.965545	0.949946
C	-4.203135	2.148505	-0.834809
H	-4.141708	2.863014	-1.669722
H	-4.816875	1.294014	-1.135352
H	-4.657067	2.645612	0.035206
C	-1.077831	4.784964	0.403158
H	-1.274926	5.855982	0.489752
C	-1.262143	-0.172203	-0.282690
H	0.655692	0.329474	0.430812
C	-1.878719	-2.704648	-0.128580
O	-2.807267	-2.318984	0.749900
O	-1.756822	-3.815023	-0.582732
C	-3.918151	-3.212635	0.961345

H	-4.243327	-3.607909	-0.013614
H	-3.572410	-4.066810	1.566548
C	-5.009440	-2.421584	1.649873
H	-5.327280	-1.581858	1.013520
H	-5.880034	-3.067279	1.842611
H	-4.655949	-2.019485	2.611939
C	-0.954227	-1.573301	-0.425492
N	0.250891	-1.947755	-0.847752
N	1.237772	-2.323401	-1.230309
S	2.993159	0.314560	-0.104692
C	4.326433	-0.942486	0.272009
F	4.747820	-0.807056	1.527368
F	3.857153	-2.180418	0.106765
F	5.354884	-0.758683	-0.553143
O	3.582079	1.619341	0.218655
O	1.904285	-0.110423	0.880794
O	2.579309	0.065614	-1.496110
32			
G SCF Done: -947.678013037 A.U.			
O	-0.977477	-1.279203	-1.275254
O	-2.626701	-0.428308	0.766097
O	-3.849217	1.166522	-0.274484
N	1.213672	-1.288036	-0.597172
N	0.873187	1.355973	0.258411
C	2.116530	0.770517	0.285043
C	2.311402	-0.580895	-0.113947
C	-0.148097	0.677366	-0.163238
C	-0.050401	-0.707856	-0.725380
C	-2.785728	0.697311	0.058745
C	-1.468592	1.318300	-0.213206
C	3.598704	-1.145690	-0.023039
H	3.774253	-2.179316	-0.317614
C	3.214366	1.521804	0.751390
H	3.021960	2.554388	1.048869
C	4.479923	0.957495	0.831336
H	5.324817	1.546110	1.194950
C	-3.755862	-1.309930	0.877824
H	-4.354864	-1.243640	-0.043484
H	-4.392978	-0.965157	1.710161
C	-3.217682	-2.707368	1.108383
H	-4.047801	-3.424499	1.205736
H	-2.613965	-2.747768	2.028530
H	-2.582129	-3.005331	0.261208
C	1.381451	-2.653266	-1.084893
H	1.731272	-3.309297	-0.273184
H	0.410092	-3.002156	-1.449526
H	2.110471	-2.683290	-1.909565
C	4.664194	-0.379947	0.444560
H	5.656347	-0.833582	0.507704
N	-1.495255	2.615283	-0.438772
N	-1.513257	3.727409	-0.636197
8			
AcONa SCF Done: -390.974623231 A.U.			
C	2.043823	-0.001642	-0.000355
H	2.448424	-1.021990	0.005126
H	2.403076	0.553871	0.880033

H	2.401697	0.542980	-0.888163
C	0.520169	-0.010230	0.000386
O	-0.081209	-1.124307	0.000471
O	-0.069889	1.111686	0.000491
Na	-1.948034	0.008849	-0.000443

8			
AcOH SCF Done: -229.199995950 A.U.			
C	1.390818	-0.169898	-0.000088
H	1.605915	-1.245559	-0.006800
H	1.839073	0.298159	0.889420
H	1.841766	0.310390	-0.881590
C	-0.091566	0.117888	-0.000202
O	-0.833965	-1.009710	0.000050
H	-1.766451	-0.730591	-0.000027
O	-0.580511	1.219667	0.000042

9			
NaOTf SCF Done: -1124.17450114 A.U.			
S	0.322169	0.745104	0.000007
C	-1.147521	-0.414647	-0.000043
F	-1.897895	-0.248978	1.082592
F	-1.898318	-0.248762	-1.082360
F	-0.678017	-1.684534	-0.000325
O	1.072466	0.284810	1.220946
O	-0.209304	2.098748	0.000015
O	1.072829	0.285100	-1.220853
Na	2.410050	-1.012960	0.000011

32			
TS-GH SCF Done: -947.659144312 A.U.			
O	-1.081302	-1.540997	-0.815421
O	-3.012236	-0.138807	0.497082
O	-3.655388	1.721211	-0.607101
N	1.135560	-1.495470	-0.234344
N	0.961926	1.241868	-0.002314
N	0.072834	3.135143	0.049262
N	-0.981133	2.649946	-0.059927
C	2.198639	0.656189	0.073823
C	2.301215	-0.758504	-0.008508
C	-0.147890	0.563298	-0.141311
C	-0.120530	-0.907784	-0.425075
C	-2.791119	1.017433	-0.138069
C	-1.353556	1.355169	-0.142252
C	3.570898	-1.353965	0.109938
H	3.683943	-2.435490	0.052737
C	3.351545	1.440761	0.255933
H	3.227463	2.523582	0.313056
C	4.598126	0.837385	0.368020
H	5.491609	1.448286	0.512798
C	-4.317576	-0.722029	0.373829
H	-4.653268	-0.631431	-0.671899
H	-5.028380	-0.148300	0.992749
C	-4.205679	-2.167458	0.813299
H	-5.179979	-2.672117	0.719839
H	-3.879653	-2.232155	1.863161
H	-3.465933	-2.690823	0.189562
C	1.225482	-2.941853	-0.411899

H	1.645914	-3.410254	0.490819
H	0.216795	-3.326081	-0.592109
H	1.863956	-3.188426	-1.274787
C	4.701445	-0.560018	0.297546
H	5.678650	-1.040204	0.387221
32			
H SCF Done: -947.697624383 A.U.			
O	1.087870	1.790006	-0.513721
O	3.136992	-0.000499	0.429293
O	3.514872	-1.848499	-0.810712
N	-1.176830	1.552349	-0.200337
N	-0.858162	-1.171313	0.028218
N	-0.530257	-2.473200	0.111199
N	0.761717	-2.555831	0.025058
C	-2.164765	-0.668895	0.083226
C	-2.302870	0.734952	-0.025340
C	0.252997	-0.390921	-0.105966
C	0.139069	1.064270	-0.289892
C	2.770308	-1.111251	-0.216108
C	1.298377	-1.314586	-0.100298
C	-3.608537	1.261604	0.039328
H	-3.771819	2.334685	-0.038222
C	-3.266399	-1.514108	0.244486
H	-3.090534	-2.587063	0.321638
C	-4.544725	-0.967154	0.303952
H	-5.411152	-1.619093	0.430362
C	4.488132	0.456867	0.255434
H	4.751234	0.390879	-0.812770
H	5.168633	-0.220190	0.799213
C	4.547228	1.878823	0.773665
H	5.557124	2.294654	0.633413
H	4.301369	1.913971	1.846312
H	3.819745	2.503497	0.234353
C	-1.356479	2.993591	-0.346831
H	-1.828889	3.418307	0.552407
H	-0.367435	3.441922	-0.484175
H	-1.982145	3.221179	-1.224029
C	-4.707637	0.419778	0.201859
H	-5.707479	0.857328	0.248543
20			
D-aa SCF Done: -632.026493998 A.U.			
O	3.584415	-0.256767	0.000593
N	1.473307	0.667587	0.000265
N	0.462899	-1.961546	0.000006
C	-0.393456	-0.875053	-0.000097
C	0.096824	0.461829	0.000028
C	2.373611	-0.404790	0.000386
C	-0.827313	1.526138	-0.000082
H	-0.485101	2.559812	0.000018
C	-1.780143	-1.116165	-0.000340
H	-2.139072	-2.145582	-0.000433
C	-2.659145	-0.047960	-0.000452
C	2.022064	2.018177	0.000402
H	1.697412	2.569081	0.896956
H	3.114043	1.931488	0.000573
H	1.697696	2.569145	-0.896216

C	-2.195736	1.271845	-0.000318
H	-2.920388	2.088106	-0.000402
C	1.730041	-1.738418	0.000226
H	2.431442	-2.581884	0.000314
F	-3.980586	-0.272436	-0.000664

33			
TS-DE-aa SCF Done: -1047.47996525 A.U.			
O	1.718587	1.714931	-0.342536
N	-0.452081	1.427317	0.352941
N	-0.699938	-0.580438	-1.617813
C	-1.781473	-0.171750	-0.897544
C	-1.682942	0.826223	0.128806
C	0.671655	1.095217	-0.413396
C	-2.837674	1.177547	0.855456
H	-2.791074	1.922759	1.647490
C	-3.038481	-0.761400	-1.178060
H	-3.101249	-1.515435	-1.962582
C	-4.144447	-0.389814	-0.445512
C	-0.311883	2.484776	1.349121
H	-0.578596	2.102047	2.345804
H	0.733839	2.809317	1.345883
H	-0.958176	3.341705	1.103644
C	-4.056196	0.571972	0.574324
H	-4.956681	0.831485	1.133819
C	0.479156	-0.091769	-1.299142
H	1.344092	-0.343029	-1.917871
C	2.617328	-1.116922	0.665208
O	3.299162	-0.732937	-0.419358
O	3.069479	-1.173232	1.788316
C	4.573811	-0.098950	-0.211394
H	4.512459	0.534674	0.686859
H	5.328846	-0.879432	-0.016644
C	4.882686	0.710274	-1.453288
H	4.096985	1.465182	-1.603296
H	5.853870	1.217646	-1.343462
H	4.928088	0.063209	-2.343198
C	1.250465	-1.498348	0.304665
N	0.286766	-1.631006	1.124106
N	-0.683235	-1.772749	1.727084
F	-5.333649	-0.949381	-0.696389

20			
D-ab SCF Done: -992.374040552 A.U.			
O	3.963873	-0.342720	0.000349
N	1.882154	0.645684	0.000412
N	0.792389	-1.951633	0.000053
C	-0.029346	-0.838559	0.000031
C	0.501878	0.481760	0.000150
C	2.749689	-0.454952	0.000704
C	-0.391399	1.571997	-0.000001
H	-0.020065	2.595726	0.000076
C	-1.422316	-1.037142	-0.000199
H	-1.796336	-2.060968	-0.000299
C	-2.281436	0.052897	-0.000306
C	2.472859	1.978845	0.000421
H	2.165337	2.539373	0.896927
H	3.561599	1.858217	0.000666

H	2.165710	2.539228	-0.896303
C	-1.766016	1.359123	-0.000225
H	-2.452362	2.207312	-0.000332
C	2.065808	-1.768363	0.000222
H	2.740924	-2.632968	0.000173
Cl	-4.011524	-0.190362	-0.000691
33			
TS-DE-ab SCF Done: -1407.82714343 A.U.			
O	2.094589	1.643246	-0.534572
N	-0.066379	1.536256	0.238270
N	-0.459979	-0.656178	-1.498339
C	-1.500300	-0.120431	-0.800309
C	-1.327361	0.974485	0.108829
C	1.019718	1.070164	-0.514347
C	-2.445298	1.453607	0.819004
H	-2.344957	2.275840	1.525441
C	-2.789709	-0.676280	-0.985271
H	-2.891156	-1.504426	-1.686427
C	-3.868604	-0.183752	-0.275249
C	0.150078	2.685063	1.112559
H	-0.104679	2.422252	2.150303
H	1.208777	2.957179	1.049662
H	-0.464000	3.541032	0.792651
C	-3.696566	0.879993	0.633740
H	-4.557824	1.251680	1.190919
C	0.748847	-0.193938	-1.262355
H	1.583333	-0.550437	-1.871102
C	2.894384	-1.111335	0.745747
O	3.559710	-0.873898	-0.389800
O	3.377700	-1.075825	1.856652
C	4.869184	-0.287774	-0.281084
H	4.865443	0.437504	0.547226
H	5.591229	-1.081465	-0.024534
C	5.179040	0.372037	-1.608154
H	4.426130	1.146157	-1.817038
H	6.176152	0.838305	-1.576178
H	5.166900	-0.365052	-2.426222
C	1.500572	-1.458527	0.462600
N	0.557258	-1.458115	1.315888
N	-0.398628	-1.488744	1.956004
Cl	-5.455362	-0.874656	-0.489998
20			
D-ac SCF Done: -3106.32945704 A.U.			
O	4.614748	-0.399439	0.001211
N	2.553311	0.630812	0.000107
N	1.411810	-1.944386	0.000202
C	0.612982	-0.814947	-0.000056
C	1.170716	0.494534	0.000058
C	3.398804	-0.487512	-0.000248
C	0.299727	1.602288	0.000080
H	0.691452	2.618502	0.000180
C	-0.784036	-0.985416	-0.000193
H	-1.172217	-2.004099	-0.000214
C	-1.620617	0.122230	-0.000242
C	3.170331	1.952181	0.000479
H	2.874038	2.518217	0.897289

H	4.256460	1.810147	0.000373
H	2.873957	2.518735	-0.895975
C	-1.079544	1.417626	-0.000085
H	-1.742621	2.284278	-0.000075
C	2.688635	-1.786997	0.000432
H	3.346232	-2.665015	0.000790
Br	-3.512661	-0.107833	-0.000445

33			
TS-DE-ac SCF Done: -3521.78246334 A.U.			
O	2.747627	1.557496	-0.686116
N	0.604483	1.628631	0.138888
N	0.058650	-0.680850	-1.392890
C	-0.935299	-0.034118	-0.721905
C	-0.685462	1.123885	0.085063
C	1.646717	1.044364	-0.593602
C	-1.759938	1.718884	0.774201
H	-1.601327	2.592374	1.404401
C	-2.255484	-0.536812	-0.830808
H	-2.408790	-1.415477	-1.457376
C	-3.289999	0.069697	-0.143562
C	0.900088	2.835342	0.905500
H	0.658293	2.676193	1.967124
H	1.969245	3.045361	0.797626
H	0.322074	3.691577	0.524911
C	-3.042994	1.196859	0.665992
H	-3.865947	1.663697	1.209443
C	1.294619	-0.263378	-1.223481
H	2.094602	-0.713130	-1.816575
C	3.442373	-1.116422	0.809738
O	4.088999	-1.011643	-0.356133
O	3.955457	-1.011796	1.902771
C	5.429272	-0.489101	-0.326555
H	5.484284	0.303186	0.435941
H	6.115953	-1.295525	-0.017937
C	5.738309	0.037717	-1.711987
H	5.021464	0.830669	-1.971050
H	6.758716	0.450683	-1.741692
H	5.666884	-0.764627	-2.462863
C	2.025987	-1.413417	0.587978
N	1.106373	-1.290879	1.458244
N	0.167356	-1.216913	2.119374
Br	-5.061694	-0.613096	-0.276597

23			
D-ad SCF Done: -869.944114513 A.U.			
O	4.551746	-0.401085	0.000342
N	2.494118	0.636178	0.000151
N	1.346962	-1.938056	-0.000349
C	0.551584	-0.805548	-0.000336
C	1.113047	0.504771	-0.000184
C	3.336634	-0.486435	0.000516
C	0.247485	1.617041	-0.000415
H	0.645178	2.630556	-0.000401
C	-0.842317	-0.964790	-0.000700
H	-1.233724	-1.983485	-0.001037
C	-1.683785	0.143143	-0.000810
C	3.117344	1.955418	0.000199

H	2.823275	2.522476	0.896876
H	4.202782	1.808746	0.000435
H	2.823626	2.522379	-0.896652
C	-1.131114	1.432679	-0.000705
H	-1.792047	2.300472	-0.000966
C	2.623603	-1.784956	-0.000062
H	3.279172	-2.664400	-0.000099
C	-3.175656	-0.071072	0.000106
F	-3.573378	-0.761115	1.085772
F	-3.571990	-0.779609	-1.074037
F	-3.853603	1.090011	-0.010087
36			
TS-DE-ad SCF Done: -1285.39696382 A.U.			
O	2.677411	1.593589	-0.643956
N	0.531188	1.620461	0.176006
N	0.018128	-0.657816	-1.412935
C	-0.984278	-0.038255	-0.728660
C	-0.750922	1.102543	0.106562
C	1.583401	1.065166	-0.568049
C	-1.833088	1.669282	0.811386
H	-1.681741	2.527063	1.464143
C	-2.298507	-0.550381	-0.848998
H	-2.444189	-1.415544	-1.495732
C	-3.345218	0.022163	-0.151670
C	0.812456	2.811984	0.972436
H	0.573236	2.623845	2.029778
H	1.878899	3.037524	0.869626
H	0.224063	3.669901	0.612597
C	-3.105336	1.131855	0.686206
H	-3.933028	1.573206	1.245240
C	1.248995	-0.230864	-1.230791
H	2.055282	-0.655820	-1.833552
C	3.398737	-1.120283	0.783353
O	4.047347	-0.968847	-0.375640
O	3.906331	-1.049707	1.881501
C	5.385179	-0.440532	-0.323441
H	5.432523	0.327135	0.464366
H	6.074337	-1.253058	-0.037479
C	5.697338	0.131524	-1.689998
H	4.977160	0.928086	-1.927912
H	6.715340	0.551169	-1.701551
H	5.634446	-0.647169	-2.466071
C	1.985558	-1.422581	0.547879
N	1.060350	-1.339854	1.416757
N	0.117277	-1.299208	2.074918
C	-4.752721	-0.502803	-0.276884
F	-4.809214	-1.642190	-0.981759
F	-5.552431	0.392872	-0.888761
F	-5.293156	-0.740083	0.932977
30			
D-ae SCF Done: -763.900902142 A.U.			
O	5.134517	-0.483364	-0.080198
N	3.103091	0.592732	0.083437
N	1.887209	-1.919108	-0.293816
C	1.120082	-0.780735	-0.116880
C	1.716860	0.496728	0.071558

C	3.915706	-0.536316	-0.087083
C	0.874272	1.613350	0.239981
H	1.293594	2.605985	0.398662
C	-0.279649	-0.903567	-0.133382
H	-0.680189	-1.904094	-0.304022
C	-1.120243	0.199788	0.031013
C	3.757332	1.881574	0.273697
H	3.480039	2.317507	1.246118
H	4.839034	1.711292	0.244396
H	3.473249	2.582368	-0.526736
C	-0.506987	1.459178	0.218743
H	-1.132999	2.340122	0.376673
C	3.168359	-1.799830	-0.277986
H	3.800665	-2.685775	-0.414950
C	-2.598833	0.056965	0.013389
C	-3.416060	1.044502	-0.568664
C	-3.222624	-1.072294	0.576982
C	-4.805793	0.908728	-0.585800
H	-2.956469	1.917882	-1.037587
C	-4.611999	-1.209114	0.558755
H	-2.612427	-1.841424	1.056276
C	-5.410598	-0.218931	-0.022148
H	-5.419349	1.684652	-1.050980
H	-5.074194	-2.091358	1.009142
H	-6.498137	-0.325760	-0.035809
43			
TS-DE-ae SCF Done: -1179.35501383 A.U.			
O	3.234396	1.163575	-1.139875
N	1.111461	1.635295	-0.398615
N	0.396136	-1.001985	-1.112091
C	-0.546141	-0.110630	-0.693167
C	-0.208490	1.224331	-0.295719
C	2.103250	0.780371	-0.896399
C	-1.235216	2.072178	0.160301
H	-1.015959	3.092893	0.469524
C	-1.895981	-0.529751	-0.639573
H	-2.094125	-1.560699	-0.935975
C	-2.910740	0.306932	-0.187117
C	1.494006	3.001200	-0.055169
H	1.256637	3.205064	0.999807
H	2.572788	3.096280	-0.216714
H	0.965927	3.726999	-0.692759
C	-2.545790	1.617305	0.215386
H	-3.322402	2.304655	0.557334
C	1.658663	-0.633778	-1.075819
H	2.420449	-1.301218	-1.485983
C	3.770564	-0.921628	1.145041
O	4.410065	-1.244163	0.014520
O	4.303760	-0.498069	2.148016
C	5.778043	-0.820610	-0.116577
H	5.888847	0.171446	0.347848
H	6.420897	-1.522230	0.441865
C	6.100894	-0.790273	-1.595710
H	5.428690	-0.082464	-2.102577
H	7.143540	-0.471161	-1.750147
H	5.972667	-1.786731	-2.046714
C	2.336816	-1.184379	1.017612

N	1.437437	-0.732279	1.794848
N	0.513535	-0.391040	2.390457
C	-4.322900	-0.148344	-0.123346
C	-5.165102	0.250458	0.931650
C	-4.853484	-0.994696	-1.115152
C	-6.491175	-0.182669	0.993277
H	-4.769941	0.884205	1.729180
C	-6.179264	-1.427672	-1.053493
H	-4.226170	-1.298140	-1.956562
C	-7.004345	-1.023358	0.000821
H	-7.124482	0.131302	1.826941
H	-6.572551	-2.078636	-1.838481
H	-8.042204	-1.362174	0.048840
22			
D-af SCF Done: -737.342068951 A.U.			
O	-4.204025	-0.352021	-0.000113
N	-2.127622	0.647407	0.000018
N	-1.029931	-1.948803	0.000096
C	-0.214797	-0.830963	0.000048
C	-0.752803	0.490922	0.000006
C	-2.992197	-0.462298	-0.000010
C	0.131818	1.593050	-0.000032
H	-0.251274	2.611986	-0.000049
C	1.175310	-1.018322	0.000021
H	1.577222	-2.030401	0.000032
C	2.014400	0.086078	-0.000015
C	-2.729867	1.977676	0.000008
H	-2.426930	2.539028	-0.896997
H	-3.817429	1.848317	-0.000269
H	-2.427386	2.538834	0.897310
C	1.504552	1.391647	-0.000022
H	2.199260	2.231133	-0.000039
C	-2.303470	-1.773594	0.000047
H	-2.974331	-2.641310	0.000197
N	3.475187	-0.116551	0.000006
O	3.885550	-1.265562	-0.000186
O	4.180944	0.880442	0.000134
35			
TS-DE-af SCF Done: -1152.79336278 A.U.			
O	2.324102	1.552704	-0.769365
N	0.166630	1.601328	0.019650
N	-0.268972	-0.821328	-1.369373
C	-1.295478	-0.167963	-0.753571
C	-1.100381	1.050016	-0.018380
C	1.243138	1.006308	-0.659993
C	-2.203811	1.654046	0.621315
H	-2.079225	2.570955	1.194205
C	-2.591664	-0.721030	-0.843861
H	-2.736083	-1.641244	-1.407816
C	-3.645972	-0.097893	-0.204176
C	0.411299	2.865744	0.710290
H	0.161570	2.766737	1.777137
H	1.473895	3.105388	0.600478
H	-0.190087	3.674328	0.267652
C	-3.464740	1.083500	0.534311
H	-4.324982	1.535578	1.027115

C	0.948663	-0.351517	-1.209452
H	1.772927	-0.807522	-1.763268
C	3.092486	-1.021739	0.893959
O	3.749007	-0.949470	-0.267162
O	3.586290	-0.860701	1.988551
C	5.083145	-0.407611	-0.244755
H	5.118874	0.415338	0.485778
H	5.775491	-1.192140	0.104271
C	5.400922	0.065346	-1.647332
H	4.676141	0.835585	-1.949435
H	6.415291	0.492289	-1.682034
H	5.351277	-0.768873	-2.364357
C	1.685533	-1.362973	0.672173
N	0.748472	-1.224693	1.521055
N	-0.203416	-1.145696	2.162604
N	-4.997224	-0.687240	-0.295420
O	-5.901180	-0.107301	0.285386
O	-5.122263	-1.711287	-0.945224
20			
D-ag SCF Done: -992.374699645 A.U.			
O	3.768567	-0.830347	0.000335
N	1.464409	-0.860966	0.000034
N	1.556754	1.953722	0.000100
C	0.347750	1.285158	-0.000026
C	0.279322	-0.137507	-0.000001
C	2.713182	-0.220253	-0.000203
C	-0.980434	-0.766936	-0.000040
H	-1.076789	-1.850143	-0.000048
C	-0.843810	2.033775	-0.000080
H	-0.750694	3.121417	-0.000073
C	-2.085829	1.416087	-0.000132
H	-3.010415	1.993679	-0.000177
C	1.445478	-2.319207	0.000223
H	0.932104	-2.700054	-0.896300
H	2.485193	-2.663792	0.000357
H	0.931909	-2.699810	0.896733
C	-2.135149	0.012623	-0.000112
C	2.639602	1.257837	0.000148
H	3.613345	1.762636	0.000335
Cl	-3.688353	-0.784701	-0.000183
33			
TS-DE-ag SCF Done: -1407.82844437 A.U.			
O	-1.888193	1.749657	0.307580
N	0.312310	1.260394	-0.134335
N	0.139623	-0.764463	1.826467
C	1.327814	-0.460975	1.236994
C	1.444756	0.544479	0.220438
C	-0.920368	1.034104	0.495044
C	2.697482	0.790052	-0.368008
H	2.824181	1.536830	-1.148069
C	2.489069	-1.166317	1.639460
H	2.364785	-1.920285	2.418595
C	3.718028	-0.922744	1.058538
H	4.610465	-1.472158	1.359147
C	0.388072	2.326218	-1.128897
H	0.729720	1.919152	-2.092464

H	-0.615332	2.749605	-1.241507
H	1.081188	3.116680	-0.801992
C	3.806056	0.057595	0.049612
C	-0.944489	-0.162735	1.386424
H	-1.893374	-0.328125	1.902216
C	-2.939898	-0.992512	-0.810321
O	-3.698172	-0.537622	0.193536
O	-3.266724	-1.008076	-1.977395
C	-4.872811	0.217142	-0.152952
H	-4.647784	0.840199	-1.032324
H	-5.672938	-0.486099	-0.440076
C	-5.242009	1.055038	1.052945
H	-4.409154	1.730069	1.298757
H	-6.140234	1.654638	0.837634
H	-5.451714	0.417244	1.925843
C	-1.667327	-1.506441	-0.302131
N	-0.632896	-1.736900	-1.004451
N	0.382468	-1.976124	-1.491333
Cl	5.348713	0.367813	-0.694874

20			
D-ah SCF Done: -3106.33001787 A.U.			
O	4.294775	-1.075678	0.000357
N	1.996904	-0.901790	0.000072
N	2.339441	1.894015	0.000135
C	1.075600	1.335355	0.000010
C	0.880932	-0.075314	0.000034
C	3.297557	-0.374649	-0.000158
C	-0.430511	-0.590298	-0.000011
H	-0.615493	-1.662014	-0.000021
C	-0.044227	2.187099	-0.000045
H	0.145056	3.262234	-0.000037
C	-1.336965	1.682710	-0.000100
H	-2.202017	2.346291	-0.000145
C	1.848755	-2.352711	0.000259
H	1.303852	-2.686633	-0.896340
H	2.853896	-2.787931	0.000399
H	1.303665	-2.686374	0.896835
C	-1.510522	0.289437	-0.000084
C	3.355782	1.104344	0.000183
H	4.370654	1.520356	0.000364
Br	-3.276875	-0.425198	-0.000168

33			
TS-DE-ah SCF Done: -3521.78345739 A.U.			
O	-2.437832	1.716806	0.476736
N	-0.232560	1.221206	0.066613
N	-0.524044	-0.990663	1.798383
C	0.692567	-0.657085	1.287893
C	0.870110	0.444687	0.387008
C	-1.493178	0.961913	0.623489
C	2.150695	0.719492	-0.125585
H	2.316062	1.541742	-0.817588
C	1.822024	-1.428307	1.657575
H	1.651900	-2.255743	2.348595
C	3.078513	-1.156150	1.151706
H	3.942652	-1.759502	1.431002
C	-0.096184	2.382303	-0.807715

H	0.275593	2.069461	-1.795013
H	-1.085894	2.838459	-0.913230
H	0.598348	3.118317	-0.374109
C	3.226183	-0.079039	0.254973
C	-1.577174	-0.319992	1.383662
H	-2.548801	-0.514073	1.844183
C	-3.500811	-0.867208	-0.960751
O	-4.288314	-0.497672	0.055426
O	-3.780714	-0.754785	-2.134671
C	-5.430659	0.319674	-0.255428
H	-5.154657	1.026290	-1.053348
H	-6.232637	-0.328219	-0.648130
C	-5.833064	1.034487	1.017200
H	-4.997674	1.658761	1.366726
H	-6.708726	1.675835	0.831294
H	-6.092802	0.313478	1.808011
C	-2.261392	-1.463681	-0.460684
N	-1.204848	-1.647651	-1.143793
N	-0.176242	-1.862074	-1.613930
Br	4.947703	0.300232	-0.453694

23			
D-ai SCF Done: -869.943403678 A.U.			
O	4.265001	-1.007556	0.012544
N	1.964227	-0.878601	-0.006336
N	2.253860	1.924662	0.010482
C	0.999454	1.341108	-0.003087
C	0.833690	-0.072226	-0.010780
C	3.253741	-0.327926	0.007605
C	-0.468924	-0.607545	-0.025079
H	-0.633879	-1.682415	-0.036487
C	-0.134467	2.174968	-0.012379
H	0.038139	3.252590	-0.010186
C	-1.413688	1.641124	-0.027774
H	-2.291401	2.288903	-0.042928
C	1.842004	-2.332448	-0.015088
H	1.311198	-2.671093	-0.918193
H	2.854669	-2.749774	-0.008322
H	1.295337	-2.680540	0.874872
C	-1.569479	0.244351	-0.031797
C	3.283292	1.153387	0.015746
H	4.290479	1.587916	0.026918
C	-2.965075	-0.332210	0.003774
F	-3.788402	0.324263	-0.831921
F	-2.987838	-1.632214	-0.339900
F	-3.498699	-0.236834	1.236056

36			
TS-DE-ai SCF Done: -1285.39585577 A.U.			
O	2.389483	1.739954	-0.398387
N	0.187186	1.227861	0.008944
N	0.455603	-0.889987	-1.842118
C	-0.756711	-0.579678	-1.302707
C	-0.919677	0.471637	-0.343377
C	1.441136	0.996397	-0.572663
C	-2.196496	0.718328	0.195296
H	-2.352062	1.500391	0.934234
C	-1.890916	-1.329267	-1.703678

H	-1.727009	-2.118761	-2.438776
C	-3.137556	-1.077397	-1.167590
H	-4.005534	-1.666489	-1.468068
C	0.060127	2.343223	0.943181
H	-0.303396	1.980556	1.916272
H	1.051305	2.792554	1.063057
H	-0.637055	3.100997	0.553970
C	-3.280541	-0.049776	-0.211810
C	1.513942	-0.246538	-1.398987
H	2.481333	-0.418871	-1.877096
C	3.456007	-0.927083	0.891886
O	4.232618	-0.501783	-0.109346
O	3.750694	-0.893530	2.066792
C	5.391365	0.279648	0.235095
H	5.137722	0.934713	1.082859
H	6.190257	-0.403312	0.570133
C	5.782201	1.071798	-0.994482
H	4.948882	1.726198	-1.289554
H	6.667848	1.690339	-0.780957
H	6.021825	0.401368	-1.834564
C	2.203387	-1.480777	0.373064
N	1.153882	-1.694965	1.059352
N	0.130346	-1.928359	1.530414
C	-4.657425	0.221962	0.347541
F	-5.216346	-0.901822	0.827345
F	-4.636927	1.124752	1.342245
F	-5.479911	0.693345	-0.607895
26			
D-aj SCF Done: -611.417470917 A.U.			
O	3.906594	0.140790	0.000216
N	1.678218	0.729282	-0.000059
N	1.080657	-2.021057	-0.000100
C	0.071263	-1.077252	-0.000053
C	0.350431	0.314546	-0.000025
C	2.732522	-0.194069	0.000097
C	-0.728256	1.219189	0.000077
H	-0.540279	2.292465	0.000247
C	-1.268197	-1.508741	-0.000015
H	-1.434952	-2.588306	-0.000036
C	-2.335499	-0.618109	0.000023
C	2.014421	2.147138	-0.000189
H	1.609184	2.642504	0.896009
H	3.106886	2.228150	-0.000689
H	1.608279	2.642507	-0.895961
C	-2.052087	0.775176	0.000071
C	2.300849	-1.608746	-0.000059
H	3.122561	-2.335440	0.000010
C	-3.759852	-1.112982	0.000020
C	-3.181381	1.773502	0.000041
H	-3.829196	1.644537	-0.883491
H	-3.830190	1.643746	0.882688
H	-2.812264	2.809092	0.000674
H	-4.314382	-0.754575	0.883979
H	-3.801600	-2.211556	0.000237
H	-4.314216	-0.754941	-0.884204
39			

TS-DE-aj SCF Done: -1026.87334368 A.U.

O	1.992633	1.618263	-0.672499
N	-0.200632	1.414424	-0.019318
N	-0.321821	-0.957220	-1.546024
C	-1.437652	-0.443753	-0.960859
C	-1.405287	0.740709	-0.159024
C	0.962239	0.965895	-0.658577
C	-2.597175	1.187265	0.437406
H	-2.593683	2.080155	1.061162
C	-2.675541	-1.107101	-1.145076
H	-2.656168	-2.003668	-1.768166
C	-3.847649	-0.667121	-0.555386
C	-0.126017	2.654677	0.745231
H	-0.422461	2.473076	1.789348
H	0.910534	3.005864	0.710958
H	-0.784704	3.422286	0.310240
C	-3.801083	0.505183	0.259228
C	0.832852	-0.378003	-1.293460
H	1.728371	-0.722554	-1.816077
C	2.901041	-0.923119	0.924912
O	3.625618	-0.750025	-0.187884
O	3.303321	-0.724897	2.051455
C	4.866360	-0.034871	-0.064432
H	4.740328	0.770914	0.675130
H	5.635960	-0.723979	0.323465
C	5.212289	0.507876	-1.435195
H	4.411973	1.182254	-1.773445
H	6.161070	1.065612	-1.394657
H	5.320904	-0.309053	-2.165723
C	1.565054	-1.418394	0.595269
N	0.567743	-1.421320	1.383056
N	-0.425769	-1.476027	1.962866
C	-5.144545	-1.408098	-0.755783
C	-5.054230	1.004799	0.926920
H	-5.839093	1.231268	0.185649
H	-5.475247	0.240634	1.601894
H	-4.870034	1.913820	1.516638
H	-5.557595	-1.764459	0.202925
H	-5.008650	-2.281521	-1.408974
H	-5.914654	-0.762049	-1.210054

20

D-ak SCF Done: -1451.99653502 A.U.

O	-4.408970	0.175577	0.000387
N	-2.170818	0.723154	0.000076
N	-1.630017	-2.043375	0.000129
C	-0.602829	-1.118824	-0.000001
C	-0.855074	0.281240	0.000030
C	-3.243792	-0.181063	-0.000156
C	0.235323	1.168757	-0.000012
H	0.089865	2.246561	-0.000013
C	0.722486	-1.584599	-0.000064
H	0.886819	-2.662267	-0.000062
C	1.797859	-0.705079	-0.000119
C	-2.476639	2.149173	0.000268
H	-2.061011	2.634436	-0.896473
H	-3.566950	2.254127	0.000409
H	-2.060756	2.634240	0.896993

C	1.543297	0.684876	-0.000094
C	-2.840453	-1.606315	0.000188
H	-3.676485	-2.316223	0.000379
Cl	3.420792	-1.331059	-0.000193
Cl	2.848916	1.832063	-0.000160
33			
TS-DE-ak SCF Done: -1867.44942623 A.U.			
O	2.488491	1.391435	-1.058571
N	0.292020	1.377945	-0.386667
N	0.162163	-1.309410	-1.251706
C	-0.952876	-0.654311	-0.826961
C	-0.915649	0.699443	-0.359156
C	1.455115	0.771706	-0.882766
C	-2.102643	1.299641	0.089509
H	-2.116139	2.321202	0.461683
C	-2.189223	-1.340336	-0.847494
H	-2.193038	-2.367426	-1.212251
C	-3.354727	-0.742081	-0.403304
C	0.370679	2.773670	0.033727
H	0.063282	2.868242	1.086104
H	1.410546	3.097753	-0.077927
H	-0.276132	3.407151	-0.592764
C	-3.304019	0.593154	0.075180
C	1.319130	-0.691499	-1.150581
H	2.213716	-1.164258	-1.562960
C	3.388104	-0.670648	1.134079
O	4.108482	-0.784029	0.013289
O	3.792439	-0.208448	2.178853
C	5.365027	-0.084717	-0.040765
H	5.255527	0.881383	0.475757
H	6.119780	-0.672009	0.509183
C	5.719454	0.092794	-1.501977
H	4.932925	0.676874	-2.001992
H	6.678750	0.625010	-1.597379
H	5.812186	-0.882157	-2.005486
C	2.044227	-1.218214	0.939691
N	1.044991	-1.002514	1.696042
N	0.048423	-0.891909	2.261319
Cl	-4.847519	-1.630600	-0.434617
Cl	-4.735155	1.385081	0.649997
19			
D-al SCF Done: -548.796133208 A.U.			
O	-3.189009	-0.078842	0.000152
N	-1.021265	0.703458	0.000062
N	-0.190212	-1.996348	-0.000010
C	0.729919	-0.965660	-0.000057
C	0.329925	0.401302	-0.000029
C	-1.992512	-0.307031	0.000008
C	2.106294	-1.236856	-0.000118
H	2.424618	-2.281576	-0.000148
C	3.009487	-0.178896	-0.000147
H	4.087558	-0.349362	-0.000206
C	-1.447305	2.102066	0.000145
H	-1.054788	2.615842	-0.888519
H	-2.542348	2.113163	0.000477
H	-1.054199	2.615902	0.888507

C	2.497554	1.128047	-0.000090
H	3.181566	1.984645	-0.000123
C	-1.439455	-1.684963	0.000046
H	-2.198003	-2.477300	0.000116
N	1.197795	1.415942	-0.000034
32			
TS-DE-al SCF Done: -964.248243004 A.U.			
O	-1.321656	1.773700	0.059896
N	0.850471	1.266270	-0.487723
N	0.909032	-0.418626	1.788099
C	2.031411	-0.183349	1.054909
C	2.027996	0.646153	-0.115143
C	-0.316985	1.119957	0.271835
C	3.266049	-0.759948	1.427534
H	3.286402	-1.389188	2.319573
C	4.388172	-0.525415	0.649943
H	5.356368	-0.963055	0.899636
C	0.841764	2.158956	-1.647398
H	1.508457	3.015814	-1.474658
H	1.205066	1.615381	-2.529399
H	-0.186930	2.503889	-1.793325
C	4.254104	0.295425	-0.486602
H	5.123480	0.494441	-1.123461
C	-0.226079	0.079769	1.345529
H	-1.126027	-0.020057	1.957232
C	-2.344996	-1.157355	-0.525345
O	-3.042663	-0.541848	0.434802
O	-2.753951	-1.396139	-1.640756
C	-4.265378	0.112279	0.049832
H	-4.121616	0.579875	-0.936526
H	-5.055725	-0.650120	-0.055758
C	-4.584513	1.135732	1.118880
H	-3.762206	1.862903	1.186957
H	-5.515999	1.667097	0.868656
H	-4.713691	0.652398	2.099916
C	-1.022190	-1.543716	-0.032134
N	-0.028578	-1.875164	-0.752453
N	0.963069	-2.176936	-1.252979
N	3.113499	0.872169	-0.855147
10			
Crad-ib SCF Done: -376.116962359 A.U.			
C	-0.942944	-0.163754	-0.687078
C	0.368229	0.275595	-0.189054
O	0.614459	1.431651	0.060591
O	1.241557	-0.733087	-0.133801
C	2.572644	-0.390790	0.275669
H	3.012897	0.343606	-0.415680
H	2.571682	0.036909	1.289934
N	-3.064624	-0.244583	0.462975
N	-2.015957	-0.179544	-0.026100
H	3.143779	-1.326451	0.256081
30			
TS-DE-ib SCF Done: -908.863514400 A.U.			
O	1.490381	1.723064	-0.816651
N	-0.630069	1.374501	-0.001252

N	-0.725057	-0.977987	-1.560701
C	-1.819079	-0.552861	-0.869460
C	-1.796786	0.625533	-0.051469
C	0.502392	1.013783	-0.742442
C	-2.959329	0.991628	0.653779
H	-2.966705	1.875616	1.289288
C	-3.016787	-1.305031	-0.965036
H	-2.992183	-2.191028	-1.601917
C	-4.149003	-0.931167	-0.265200
H	-5.064439	-1.522011	-0.336145
C	-0.567449	2.601964	0.786015
H	-0.763506	2.380676	1.845966
H	0.439657	3.017251	0.675831
H	-1.305084	3.335526	0.425614
C	-4.111205	0.218817	0.547926
H	-5.001330	0.515976	1.107764
C	0.404681	-0.322581	-1.401135
H	1.267473	-0.590091	-2.016190
C	2.716691	-0.712946	0.541236
O	3.328022	-0.555834	-0.642173
O	3.200682	-0.417351	1.611864
C	4.510052	0.245184	-0.638669
H	4.252770	1.284335	-0.382402
H	5.246034	-0.139409	0.082833
C	1.401150	-1.330626	0.364806
N	0.500332	-1.385061	1.262538
N	-0.412116	-1.499351	1.953930
H	4.911037	0.199227	-1.658678
20			
Crad-ic SCF Done: -607.267364508 A.U.			
C	-3.052982	-0.585603	-0.453654
C	-2.086803	0.521209	-0.399261
O	-2.402835	1.671054	-0.592523
O	-0.843079	0.080275	-0.196790
C	0.203405	1.074565	-0.220065
N	-4.834028	-1.131650	1.082835
N	-3.962455	-0.811661	0.389530
H	0.022927	1.813741	0.576489
H	0.141731	1.615304	-1.180248
C	1.534557	0.391341	-0.052964
C	1.796727	-0.836093	-0.679914
C	2.546556	1.003153	0.699060
C	3.051134	-1.437409	-0.557153
H	1.005963	-1.323970	-1.253848
C	3.805647	0.405998	0.814242
H	2.349347	1.954529	1.201783
C	4.060469	-0.816593	0.187042
H	3.242466	-2.396488	-1.045309
H	4.586001	0.893970	1.403670
H	5.042001	-1.287949	0.281407
40			
TS-DE-ic SCF Done: -1140.01661217 A.U.			
O	-0.327803	-0.552106	1.495221
N	1.955963	-0.497899	1.264719
N	1.579878	-0.898447	-1.504328
C	2.830439	-0.886663	-0.963542

C	3.056340	-0.662470	0.434746
C	0.651018	-0.562723	0.766097
C	4.377819	-0.636302	0.919837
H	4.577940	-0.457511	1.974966
C	3.941105	-1.099258	-1.817725
H	3.724678	-1.270805	-2.873628
C	5.232591	-1.070576	-1.324606
H	6.083551	-1.225116	-1.991026
C	2.130855	-0.306082	2.701432
H	2.717884	0.605146	2.890860
H	1.136456	-0.204313	3.148127
H	2.644964	-1.169732	3.150464
C	5.443769	-0.833283	0.047882
H	6.462464	-0.803563	0.442073
C	0.560732	-0.617764	-0.721840
H	-0.454634	-0.706479	-1.116863
C	-0.859256	2.056210	-0.178692
O	-1.849772	1.191159	-0.433236
O	-0.978389	3.067674	0.478629
C	-3.078512	1.388186	0.293504
H	-2.829608	1.510217	1.360169
H	-3.555252	2.321205	-0.045709
C	0.375956	1.644415	-0.844503
N	1.536427	2.098121	-0.592873
N	2.641398	2.397537	-0.472167
C	-3.959708	0.190346	0.064538
C	-5.214174	0.323013	-0.543399
C	-3.523203	-1.082567	0.469030
C	-6.030281	-0.796453	-0.740649
H	-5.556818	1.310020	-0.867310
C	-4.334436	-2.200021	0.264412
H	-2.540915	-1.181236	0.937553
C	-5.590662	-2.060101	-0.338664
H	-7.008321	-0.680217	-1.214749
H	-3.987585	-3.187494	0.580515
H	-6.225106	-2.936548	-0.494951
16			
Crad-id SCF Done: -492.675901343 A.U.			
C	-1.964484	-0.316804	-0.532805
C	-0.923358	0.698219	-0.273830
O	-1.256155	1.871353	-0.249382
N	-4.011489	-0.801767	0.652314
N	-3.018399	-0.519714	0.124088
C	0.480473	0.228694	-0.133396
C	1.472410	1.173704	0.180076
C	0.826984	-1.123176	-0.288456
C	2.795329	0.766807	0.342137
H	1.179162	2.219574	0.292627
C	2.152970	-1.528016	-0.124373
H	0.056150	-1.852830	-0.551662
C	3.136342	-0.583974	0.191101
H	3.566623	1.501102	0.586985
H	2.421869	-2.579717	-0.248102
H	4.174656	-0.901304	0.317673
36			
TS-DE-id SCF Done: -1025.42310877 A.U.			

O	-1.375860	3.123046	-0.078205
N	-2.604946	1.262624	0.490218
N	-1.376554	-0.065872	-1.679432
C	-2.347939	-0.680746	-0.938033
C	-2.976457	-0.037124	0.176221
C	-1.645426	1.953140	-0.266432
C	-3.954324	-0.739613	0.906613
H	-4.444704	-0.277867	1.762119
C	-2.729537	-1.998276	-1.283636
H	-2.224669	-2.448747	-2.140187
C	-3.692638	-2.675452	-0.555076
H	-3.977283	-3.694441	-0.824832
C	-3.243505	1.973374	1.592120
H	-3.071755	1.441700	2.540538
H	-2.798875	2.973023	1.643420
H	-4.327474	2.065599	1.421634
C	-4.299270	-2.038208	0.542826
H	-5.057366	-2.567087	1.125802
C	-0.976235	1.124417	-1.306971
H	-0.239467	1.649583	-1.922799
C	1.987364	0.491950	-0.805544
O	1.959425	0.882348	-1.960216
C	0.782621	0.477146	0.034820
N	0.331122	-0.397508	0.823531
N	-0.209577	-1.122027	1.548176
C	3.273174	0.043436	-0.161953
C	3.432730	-0.130520	1.222878
C	4.365057	-0.193265	-1.015379
C	4.660114	-0.548501	1.742386
H	2.609851	0.078743	1.908737
C	5.586730	-0.617456	-0.494809
H	4.227661	-0.037478	-2.086888
C	5.736681	-0.797265	0.885510
H	4.777184	-0.674758	2.821445
H	6.427820	-0.807183	-1.166366
H	6.695390	-1.126977	1.294075
7			
Crad-H SCF Done: -336.799941775 A.U.			
C	0.405605	-0.262674	0.627010
C	-0.903176	0.100891	0.073650
O	-1.253498	1.248083	-0.064373
O	-1.668942	-0.970263	-0.171384
N	2.605734	0.005542	-0.329604
N	1.522273	-0.092360	0.067825
H	-2.531099	-0.644126	-0.485448
27			
TS-DE-H SCF Done: -869.547164836 A.U.			
O	1.627605	1.841192	-0.978045
N	-0.436249	1.400300	-0.063143
N	-0.463295	-0.993826	-1.560277
C	-1.548221	-0.614877	-0.826573
C	-1.557546	0.585114	-0.040954
C	0.682792	1.085208	-0.847803
C	-2.706209	0.901482	0.710494
H	-2.736997	1.800871	1.323240
C	-2.699882	-1.440014	-0.843697

H	-2.651433	-2.340783	-1.458110
C	-3.818903	-1.114192	-0.099648
H	-4.699099	-1.760128	-0.110593
C	-0.407417	2.647438	0.694384
H	-0.538495	2.440645	1.767299
H	0.567223	3.116955	0.524808
H	-1.203193	3.328827	0.355986
C	-3.812600	0.059147	0.680210
H	-4.691918	0.318998	1.274655
C	0.626053	-0.265467	-1.478849
H	1.478062	-0.504117	-2.120917
C	3.104764	-0.618392	0.353676
O	3.627645	-0.451328	-0.873579
O	3.702342	-0.379138	1.380328
C	1.762169	-1.183353	0.294748
N	0.923803	-1.211537	1.248934
N	0.058684	-1.299461	2.002798
H	4.484518	-0.007978	-0.760113

19			
Crad-tBu SCF Done: -494.123755328 A.U.			
C	-1.978515	-0.017217	-0.757539
C	-0.695334	0.469397	-0.218443
O	-0.580888	1.596305	0.206862
O	0.253921	-0.451676	-0.344904
C	1.657505	-0.195341	0.042963
N	-3.995594	-0.618823	0.426907
N	-2.996234	-0.314444	-0.077349
C	2.219627	0.943182	-0.810470
H	1.718354	1.893153	-0.585603
H	3.295964	1.054281	-0.607746
H	2.091301	0.717081	-1.880062
C	1.728780	0.109065	1.540735
H	1.254200	-0.699575	2.117769
H	2.782995	0.178930	1.849834
H	1.228166	1.056456	1.777916
C	2.342088	-1.520373	-0.283721
H	2.237065	-1.754824	-1.353440
H	3.413185	-1.461860	-0.038702
H	1.892394	-2.340078	0.296318

39			
TS-DE-tBu SCF Done: -1026.86992020 A.U.			
O	-0.754214	1.866018	0.342362
N	1.383129	1.342808	-0.321625
N	1.416319	-0.602062	1.724048
C	2.541894	-0.321733	1.007489
C	2.549711	0.638417	-0.057238
C	0.224354	1.145808	0.440180
C	3.740119	0.851516	-0.778716
H	3.770740	1.566098	-1.599587
C	3.737908	-1.012025	1.324321
H	3.689518	-1.730579	2.144417
C	4.898785	-0.789523	0.606519
H	5.813473	-1.333784	0.850029
C	1.358930	2.377689	-1.350180
H	1.595427	1.940616	-2.332055
H	0.352220	2.807618	-1.369475

H	2.086926	3.171716	-1.122606
C	4.890683	0.142000	-0.449973
H	5.803007	0.316768	-1.025438
C	0.292882	-0.020399	1.368075
H	-0.603988	-0.173446	1.973040
C	-1.930001	-1.100215	-0.572673
O	-2.547096	-0.490264	0.438832
O	-2.414150	-1.392349	-1.647373
C	-3.862608	0.148734	0.292419
C	-4.020653	0.880340	1.624350
H	-3.202828	1.605522	1.745783
H	-4.983728	1.411935	1.654987
H	-3.986899	0.166441	2.461599
C	-0.558023	-1.445829	-0.199860
N	0.397492	-1.708138	-0.992108
N	1.359050	-1.952895	-1.577878
C	-4.927297	-0.934248	0.109700
H	-5.927087	-0.472844	0.096122
H	-4.772568	-1.475187	-0.833180
H	-4.888699	-1.653184	0.942680
C	-3.837582	1.145398	-0.870075
H	-2.989565	1.833807	-0.746737
H	-3.746108	0.631085	-1.835286
H	-4.772707	1.726613	-0.867940
4			
Crad-H SCF Done: -148.137918623 A.U.			
C	1.193186	-0.166588	0.000041
N	-1.222211	0.014807	-0.000031
N	-0.062399	0.024342	-0.000009
H	1.833156	0.725490	0.000035
24			
TS-DE-H SCF Done: -680.881502788 A.U.			
O	2.834035	1.131522	-0.627602
N	0.633775	1.250720	0.033346
N	0.181908	-1.121998	-1.432180
C	-0.843933	-0.479960	-0.809314
C	-0.647016	0.715241	-0.040717
C	1.719780	0.639273	-0.603198
C	-1.753712	1.321517	0.583516
H	-1.628292	2.225553	1.177573
C	-2.155691	-1.003138	-0.940239
H	-2.265749	-1.909095	-1.538836
C	-3.231334	-0.396296	-0.318380
H	-4.235034	-0.815086	-0.416401
C	0.872195	2.512574	0.725150
H	0.605254	2.422394	1.789443
H	1.937750	2.747381	0.631071
H	0.278307	3.322518	0.273994
C	-3.022991	0.766532	0.448370
H	-3.868353	1.248001	0.945898
C	1.409871	-0.688531	-1.213113
H	2.224993	-1.104287	-1.812179
C	2.143185	-1.683939	0.585054
N	1.123030	-1.832572	1.338958
N	0.115510	-2.064301	1.853002
H	2.957167	-1.032141	0.915598

7			
Crad-Me SCF Done: -187.479363899 A.U.			
C	0.405138	-0.583099	0.000080
N	-1.878581	0.221170	0.000020
N	-0.752800	-0.081484	-0.000051
C	1.667087	0.206373	0.000053
H	2.549861	-0.446751	0.002420
H	1.719210	0.862492	-0.889378
H	1.717247	0.866807	0.886377
27			
TS-DE-Me SCF Done: -720.218576380 A.U.			
O	2.330408	1.615464	-0.870367
N	0.225907	1.390310	0.026190
N	-0.056187	-0.951434	-1.529279
C	-1.097953	-0.468972	-0.798121
C	-0.983363	0.698941	0.026470
C	1.309215	0.959974	-0.744306
C	-2.096769	1.132327	0.769627
H	-2.028509	2.012340	1.407758
C	-2.348386	-1.135416	-0.865264
H	-2.400777	-2.016412	-1.507281
C	-3.433762	-0.696155	-0.129130
H	-4.386738	-1.227046	-0.180893
C	0.359840	2.649227	0.749408
H	0.198849	2.491008	1.827009
H	1.373984	3.025772	0.578720
H	-0.369469	3.389273	0.384434
C	-3.301610	0.437985	0.694530
H	-4.153823	0.786314	1.282995
C	1.130496	-0.383744	-1.370215
H	1.929815	-0.652478	-2.066930
C	2.114902	-1.373059	0.273640
N	1.150869	-1.846932	0.954269
N	0.177536	-2.317064	1.370374
C	3.312336	-0.676359	0.825858
H	3.859744	-0.174397	0.017968
H	3.072802	0.077732	1.596337
H	3.984313	-1.428468	1.276963
16			
Crad-tBu SCF Done: -305.476589913 A.U.			
C	-0.580224	0.001678	-0.833728
N	-2.848206	-0.000272	0.018046
N	-1.730483	0.000655	-0.315864
C	0.700799	-0.000052	-0.028503
C	0.732753	1.264309	0.861788
H	-0.108094	1.275144	1.573155
H	1.671515	1.288526	1.438461
H	0.683299	2.180189	0.252732
C	0.731428	-1.265651	0.860014
H	0.680875	-2.180630	0.249686
H	1.670181	-1.291847	1.436616
H	-0.109394	-1.276552	1.571418
C	1.904458	0.000079	-0.985109
H	1.889769	0.890308	-1.632264
H	2.849130	-0.001453	-0.417415

H	1.888254	-0.888546	-1.634439
36			
TS-DE-tBu SCF Done: -838.214121756 A.U.			
O	-1.120722	2.193471	0.983730
N	0.777745	1.456841	-0.077090
N	0.781117	-0.728806	1.709837
C	1.821442	-0.522848	0.858078
C	1.836491	0.551818	-0.092114
C	-0.277013	1.323738	0.826725
C	2.927753	0.684026	-0.969889
H	2.950573	1.483211	-1.709454
C	2.937976	-1.396160	0.916385
H	2.898215	-2.195172	1.658779
C	4.005343	-1.249734	0.049598
H	4.851649	-1.938532	0.095245
C	0.808963	2.643088	-0.924929
H	0.801456	2.353515	-1.986954
H	-0.079534	3.241482	-0.698431
H	1.710063	3.242649	-0.722788
C	3.992250	-0.210666	-0.901051
H	4.828818	-0.096508	-1.594560
C	-0.298888	0.028147	1.569772
H	-1.062055	-0.020382	2.350984
C	-1.579326	-0.958218	0.137036
N	-0.757343	-1.473829	-0.681375
N	0.099533	-1.982097	-1.274657
C	-2.949124	-0.422503	-0.241296
C	-2.871768	0.658020	-1.342174
H	-2.343940	0.276734	-2.231417
H	-3.887246	0.954793	-1.651670
H	-2.356374	1.556098	-0.976992
C	-3.741264	-1.641716	-0.780368
H	-3.814851	-2.435075	-0.021611
H	-4.760815	-1.322991	-1.051710
H	-3.266534	-2.065111	-1.679901
C	-3.659106	0.130640	1.006141
H	-3.131006	1.008714	1.401469
H	-4.685770	0.434663	0.746415
H	-3.716607	-0.636417	1.794252