

Prepared April 11, 2000

SUPPORTING INFORMATION

For J. Am. Chem. Soc. article entitled "Quantum Chemical Analysis of Heteroarylnitrenium Ions and Mechanisms for Their Self-destruction" by M. B. Sullivan and C. J. Cramer

CONTENTS: Absolute energies (E_h) and BPW91/cc-pVDZ geometries (as cartesian coordinates in Å) for all stationary points.

syn 1s

N	1.257935	0.418594	0.000000
C	1.224700	-0.894318	0.000000
C	-0.005356	-1.665436	0.000000
C	-1.259171	-1.032257	0.000000
C	-1.262207	0.360870	0.000000
C	0.015610	1.071960	0.000000
N	-0.048508	2.380844	0.000000
H	2.190811	-1.424300	0.000000
H	0.062088	-2.764221	0.000000
H	-2.190826	-1.612793	0.000000
H	-2.182877	0.961777	0.000000
H	0.925079	2.764221	0.000000

BPW91/cc-pVDZ: -302.679 97

syn 1t

N	1.124008	0.370163	0.000000
C	1.212479	-0.943909	0.000000
C	-0.029297	-1.652359	0.000000
C	-1.248596	-0.942413	0.000000
C	-1.260788	0.454742	0.000000
C	0.013718	1.102570	0.000000
N	0.232605	2.440109	0.000000
H	2.194717	-1.438309	0.000000
H	0.003220	-2.751297	0.000000
H	-2.194717	-1.500809	0.000000
H	-2.179840	1.056656	0.000000
H	1.227386	2.751297	0.000000

BPW91/cc-pVDZ: -302.653 53

anti 1s

N	1.245056	0.426498	0.000000
C	1.243362	-0.887085	0.000000
C	0.038010	-1.688339	0.000000
C	-1.233047	-1.082138	0.000000
C	-1.269653	0.307037	0.000000
C	-0.009796	1.059036	0.000000
N	0.051987	2.369919	0.000000
H	2.224106	-1.389847	0.000000
H	0.128357	-2.785660	0.000000
H	-2.150604	-1.685013	0.000000
H	-2.224106	0.855148	0.000000
H	-0.904404	2.785660	0.000000

BPW91/cc-pVDZ: -302.671 21

anti 1t

N	-1.152542	0.285583	0.000000
C	-1.188950	-1.017990	0.000000
C	0.015793	-1.789673	0.000000
C	1.227173	-1.086014	0.000000
C	1.245422	0.302856	0.000000
C	-0.020142	1.064804	0.000000
N	-0.037735	2.370346	0.000000
H	-2.184448	-1.496292	0.000000
H	-0.043320	-2.885269	0.000000
H	2.184448	-1.629333	0.000000
H	2.179367	0.878891	0.000000
H	0.856918	2.885269	0.000000

BPW91/cc-pVDZ: -302.659 26

syn 2s

C	1.256241	0.228088	0.162430
N	1.217819	-1.071915	0.099716
C	0.070847	-1.746048	-0.068619
C	-1.202515	-1.154129	0.200836
C	-1.241043	0.221268	0.118118
C	-0.001800	1.011093	0.013977
N	-0.093307	2.308823	-0.000244
H	2.187851	0.719757	0.491409
H	0.150650	-2.761856	-0.491409
H	-2.110733	-1.768417	0.246170
H	-2.187851	0.775421	0.039459
H	0.835403	2.761841	-0.131622

BPW91/cc-pVDZ: -302.680 48

syn 2t

C	1.238434	0.231125	0.000000
N	1.168594	-1.066895	0.000000
C	0.054153	-1.815170	0.000000
C	-1.201996	-1.162200	0.000000
C	-1.256927	0.220459	0.000000
C	-0.042313	1.007660	0.000000
N	-0.044083	2.307755	0.000000
H	2.211029	0.744080	0.000000
H	0.171158	-2.908249	0.000000
H	-2.117706	-1.768646	0.000000
H	-2.211029	0.763046	0.000000
H	0.794174	2.908264	0.000000

BPW91/cc-pVDZ: -302.668 07

anti 2s

C	-1.261505	0.206207	-0.151749
N	-1.219604	-1.097321	-0.091644
C	-0.063660	-1.756226	0.048447
C	1.207900	-1.143234	-0.203323
C	1.236877	0.229874	-0.098100
C	-0.014832	1.000000	-0.005234
N	-0.151215	2.294815	0.012985
H	-2.192520	0.715698	-0.448868
H	-0.123260	-2.782791	0.448883
H	2.121292	-1.750031	-0.250931
H	2.192505	0.767838	-0.003616
H	0.762817	2.782806	-0.094421

BPW91/cc-pVDZ: -302.680 39

anti 2t

C	-1.235443	0.151779	0.000000
N	-1.155700	-1.144562	0.000000
C	-0.026215	-1.871277	0.000000
C	1.213989	-1.184357	0.000000
C	1.257980	0.195587	0.000000
C	0.023285	0.970459	0.000000
N	-0.116882	2.248459	0.000000
H	-2.209610	0.662109	0.000000
H	-0.113464	-2.966705	0.000000
H	2.140106	-1.776917	0.000000
H	2.209610	0.742874	0.000000
H	0.620941	2.966705	0.000000

BPW91/cc-pVDZ: -302.662 00

3s

C	-1.277527	-0.183090	0.031036
C	-1.244415	-1.576935	0.040222
N	-0.082077	-2.266937	-0.050018
C	1.119339	-1.631683	0.040329
C	1.231750	-0.247055	0.027206
C	-0.003082	0.537277	0.001343
N	-0.078964	1.849121	-0.001862
H	-2.209915	0.398270	0.002945
H	-2.165771	-2.178162	0.039078
H	2.005112	-2.284027	0.050003
H	2.209915	0.255280	0.003922
H	0.870500	2.284012	0.001800

BPW91/cc-pVDZ: -302.658 94

3t

C	-1.257736	-0.229279	0.000000
C	-1.254868	-1.623138	0.000000
N	-0.061569	-2.237244	0.000000
C	1.124222	-1.665771	0.000000
C	1.218460	-0.255829	0.000000
C	-0.011871	0.491806	0.000000
N	0.018097	1.829391	0.000000
H	-2.207504	0.320343	0.000000
H	-2.163132	-2.241531	0.000000
H	2.031143	-2.294510	0.000000
H	2.207520	0.223328	0.000000
H	0.945435	2.294525	0.000000

BPW91/cc-pVDZ: -302.649 77

syn 4s

N	1.283707	-0.197311	0.047684
C	1.198425	-1.509262	-0.050415
N	0.023422	-2.189865	0.191864
C	-1.141708	-1.559357	0.054703
C	-1.184265	-0.153351	-0.067123
C	0.091385	0.522461	0.067963
N	0.083878	1.841934	0.107483
H	2.109909	-2.108994	-0.191864
H	-2.059235	-2.161209	0.168335
H	-2.109924	0.427078	-0.187119
H	1.069305	2.189865	0.169968

BPW91/cc-pVDZ: -318.689 14

syn **4t**

N	1.168961	-0.167618	0.000000
C	1.237778	-1.493546	0.000000
N	0.057877	-2.140793	0.000000
C	-1.139084	-1.551315	0.000000
C	-1.237762	-0.153000	0.000000
C	0.015457	0.544785	0.000000
N	0.081223	1.899185	0.000000
H	2.192764	-2.034653	0.000000
H	-2.020294	-2.214539	0.000000
H	-2.192749	0.387344	0.000000
H	1.076035	2.214539	0.000000

BPW91/cc-pVDZ: -318.695 86

anti **4s**

N	-1.237686	-0.187759	-0.064819
C	-1.231979	-1.497910	0.037292
N	-0.090698	-2.212234	-0.251114
C	1.097244	-1.632294	-0.092300
C	1.208618	-0.237762	0.067764
C	-0.027603	0.507156	-0.092911
N	-0.141006	1.820251	-0.175812
H	-2.170532	-2.049896	0.192673
H	1.988510	-2.270844	-0.223190
H	2.170532	0.262558	0.251114
H	0.798630	2.270844	-0.132111

BPW91/cc-pVDZ: -318.682 03

anti **4t**

N	-1.210266	-0.333374	0.000000
C	-1.200974	-1.644089	0.000000
N	0.006363	-2.283432	0.000000
C	1.148346	-1.616287	0.000000
C	1.186768	-0.208084	0.000000
C	-0.092346	0.467500	0.000000
N	-0.220093	1.795609	0.000000
H	-2.132385	-2.226303	0.000000
H	2.079666	-2.210297	0.000000
H	2.132370	0.350571	0.000000
H	0.696335	2.283432	0.000000

BPW91/cc-pVDZ: -318.694 30

5s

N	-1.301071	0.347412	0.068024
C	-1.244217	-0.968552	-0.050995
C	0.006744	-1.654617	0.039825
C	1.208755	-0.880371	0.067993
N	1.173386	0.434570	-0.074036
C	-0.086502	1.030350	0.008820
N	-0.188660	2.343903	0.058365
H	-2.197083	-1.519700	-0.103287
H	0.043884	-2.753708	0.087357
H	2.197067	-1.366913	0.103302
H	0.765213	2.753708	-0.074463

BPW91/cc-pVDZ: -318.691 74

5t

N	-1.122849	0.348557	0.000000
C	-1.186066	-0.959427	0.000000
C	0.000290	-1.741745	0.000000
C	1.196014	-0.975525	0.000000
N	1.166016	0.337570	0.000000
C	0.019867	1.117569	0.000000
N	-0.057007	2.431030	0.000000
H	-2.190994	-1.419434	0.000000
H	-0.009277	-2.838638	0.000000
H	2.190979	-1.456497	0.000000
H	0.899124	2.838623	0.000000

BPW91/cc-pVDZ: -318.700 71

6s

C	-1.198212	0.168427	-0.010100
N	-1.139740	-1.130005	-0.037308
C	0.060883	-1.761917	0.134186
N	1.197372	-1.060638	0.112671
C	1.257629	0.231827	-0.024017
C	0.017181	1.050308	0.054321
N	-0.142838	2.328827	0.085373
H	-2.171860	0.653259	0.179138
H	0.082352	-2.848740	0.288895
H	2.171860	0.673325	-0.459137
H	0.676224	2.848740	0.459152

BPW91/cc-pVDZ: -318.708 27

6t

C	-1.231796	0.189377	0.000000
N	-1.181564	-1.118240	0.000000
C	-0.019623	-1.805786	0.000000
N	1.139908	-1.117905	0.000000
C	1.219360	0.186310	0.000000
C	-0.007813	1.013565	0.000000
N	-0.084503	2.304077	0.000000
H	-2.212891	0.691574	0.000000
H	-0.017044	-2.902878	0.000000
H	2.212891	0.663666	0.000000
H	0.756729	2.902893	0.000000

BPW91/cc-pVDZ: -318.708 72

7s

N	1.268387	-0.219452	0.215424
N	-1.127441	-0.226822	-0.093018
C	-1.152252	-1.538361	0.067810
N	-0.001205	-2.184189	-0.268860
C	1.159500	-1.520309	-0.055405
C	0.084045	0.447968	-0.036255
N	-0.003143	1.758789	-0.204453
H	-2.083481	-2.089172	0.268845
H	2.083466	-2.125351	-0.122772
H	0.933273	2.184204	-0.009232

BPW91/cc-pVDZ: -334.705 26

7t

N	1.196136	-0.204407	0.000000
C	1.133300	-1.527634	0.000000
N	0.018326	-2.288788	0.000000
C	-1.123734	-1.547745	0.000000
N	-1.087433	-0.231842	0.000000
C	0.034912	0.552322	0.000000
N	-0.050171	1.876007	0.000000
H	2.102127	-2.065552	0.000000
H	-2.102127	-2.058075	0.000000
H	0.905960	2.288788	0.000000

BPW91/cc-pVDZ: -334.719 17

syn 1tsa

N	0.942856	0.307968	-0.062622
C	-1.174591	0.167175	-0.045380
C	-1.196426	-1.177643	0.466721
C	0.002411	-1.825546	0.581268
C	1.115967	-0.941711	0.255280
C	-0.208572	1.167800	0.337372
N	-0.199768	2.358841	0.718582
H	-1.760529	0.398651	-0.959030
H	-2.167419	-1.671127	0.636978
H	0.139160	-2.845474	0.959015
H	2.167404	-1.269943	0.370682
H	0.711670	2.845474	0.652039

BPW91/cc-pVDZ: -302.636 31

syn 1int

N	0.584305	0.035980	-0.585342
C	-0.898575	0.008224	-0.354843
C	-1.163437	-1.189926	0.428070
C	0.046616	-1.842102	0.645264
C	1.080429	-1.017670	0.136444
C	-0.043457	1.152328	0.183548
N	0.019608	2.220413	0.770630
H	-1.543869	0.325287	-1.192581
H	-2.159943	-1.525330	0.739853
H	0.195450	-2.779510	1.192581
H	2.159927	-1.088989	0.326904
H	0.880417	2.779510	0.859512

BPW91/cc-pVDZ: -302.671 00

syn 1tsb

N	0.067474	-0.097000	-0.670242
C	-1.219177	-0.637482	-0.346146
C	-0.957886	-1.841705	0.383972
C	0.439758	-1.999634	0.501495
C	1.050964	-0.882721	-0.059631
C	-0.515198	0.913406	0.062073
N	-0.792374	1.939209	0.634796
H	-2.082214	-0.410980	-0.986572
H	-1.725052	-2.550964	0.714371
H	0.960342	-2.831955	0.986588
H	2.082214	-0.517883	-0.007339
H	-0.281723	2.831970	0.661865

BPW91/cc-pVDZ: -302.666 09

1rcp (same product from either syn or anti reactants)

C	1.177841	-0.985626	0.189331
C	0.728378	-2.269913	0.188889
C	-0.728210	-2.269974	0.188934
C	-1.177811	-0.985733	0.189331
N	0.000000	-0.147751	0.195557
C	-0.000259	1.143005	0.148544
N	-0.000504	2.322433	0.300858
H	2.169312	-0.528442	0.194138
H	1.371552	-3.155060	0.194290
H	-1.371323	-3.155167	0.194443
H	-2.169312	-0.528580	0.194200
H	-0.000671	3.155182	-0.300873

BPW91/cc-pVDZ: -302.703 88

anti **1tsa**

N	0.340698	0.884537	0.015854
C	0.167816	-1.206009	0.029404
C	-1.200241	-1.198914	-0.405167
C	-1.840271	0.009918	-0.488144
C	-0.914444	1.102875	-0.235550
C	1.190231	-0.230209	-0.348419
N	2.419876	-0.108170	-0.583572
H	2.873123	-0.973389	-0.924057
H	-1.716766	-2.161514	-0.554459
H	-1.209274	2.161530	-0.371658
H	0.426895	-1.809586	0.924072
H	-2.873138	0.165237	-0.820389

BPW91/cc-pVDZ: -302.632 56

anti **1int**

N	0.120773	0.422684	0.567383
C	-0.097855	-1.040421	0.382538
C	-1.330353	-1.168762	-0.339508
C	-1.832733	0.117432	-0.596603
C	-0.885818	1.051147	-0.151215
C	1.163361	-0.183243	-0.168762
N	2.260620	-0.020660	-0.684418
H	2.760529	-0.770782	-1.181870
H	-1.816025	-2.120956	-0.583984
H	-0.798492	2.120956	-0.379135
H	0.237808	-1.719620	1.181870
H	-2.760513	0.359863	-1.126083

BPW91/cc-pVDZ: -302.672 69

anti **1tsb**

N	-0.077515	-0.170670	0.720398
C	0.209213	1.199066	0.399521
C	1.457077	1.171982	-0.315689
C	1.879654	-0.167328	-0.423950
C	0.884125	-0.979797	0.118515
C	-1.164795	0.242828	-0.018234
N	-2.279526	0.051300	-0.468445
H	-2.802155	0.706802	-1.064178
H	2.012772	2.060257	-0.637161
H	0.716507	-2.060257	0.047241
H	-0.148392	1.998352	1.064178
H	2.802139	-0.521622	-0.895813

BPW91/cc-pVDZ: -302.670 95

syn **4tsa**

N	-0.228546	0.940826	-0.102203
C	-0.354446	-1.200623	-0.035904
C	-1.706085	-1.133652	-0.549728
N	-2.342300	-0.006073	-0.720474
C	-1.495163	1.059464	-0.371658
C	0.627060	-0.207855	-0.424789
N	1.836319	-0.237610	-0.770400
H	2.342300	0.664841	-0.698517
H	-2.211929	-2.082825	-0.817490
H	-1.910538	2.082840	-0.425919
H	-0.102509	-1.861694	0.817490

BPW91/cc-pVDZ: -318.663 33

syn **4int**

N	-0.442047	0.488464	0.439758
C	-0.541077	-0.991791	0.205627
C	-1.765137	-1.124786	-0.591965
N	-2.332504	0.059402	-0.813324
C	-1.483810	0.986649	-0.298508
C	0.647598	-0.222855	-0.327484
N	1.706421	-0.207184	-0.927231
H	2.332504	0.602432	-1.039597
H	-2.216553	-2.064423	-0.940750
H	-1.584457	2.064423	-0.489365
H	-0.292313	-1.671921	1.039612

BPW91/cc-pVDZ: -318.701 11

syn **4tsb**

N	-0.448715	0.188126	0.566100
C	-0.695114	-1.199081	0.235260
C	-1.910858	-1.149033	-0.527115
N	-2.349136	0.126526	-0.681793
C	-1.442337	0.912460	-0.123535
C	0.656677	-0.229645	-0.156769
N	1.711884	-0.297546	-0.738464
H	2.489090	0.372894	-0.802750
H	-2.489090	-2.004913	-0.897781
H	-1.385193	2.004929	-0.207825
H	-0.344360	-2.003098	0.897797

BPW91/cc-pVDZ: -318.697 97

4rcp

C	-1.012833	-1.156464	-0.108749
C	-2.272522	-0.632600	-0.105362
N	-2.255768	0.771683	-0.101181
C	-1.034607	1.163071	-0.099365
N	-0.144669	-0.017960	-0.108307
C	1.149872	-0.002136	-0.093658
N	2.320145	0.088654	-0.246658
H	3.217529	0.130219	0.246674
H	-3.217514	-1.184479	-0.108551
H	-0.611404	2.172668	-0.099930
H	-0.612183	-2.172668	-0.115707

BPW91/cc-pVDZ: -318.742 76

5tsa

N	0.265198	0.967194	0.230865
N	0.154922	-1.124420	0.172836
C	-1.130524	-1.155396	-0.081528
C	-1.899017	0.016296	-0.081161
C	-1.017105	1.113968	0.118881
C	1.155380	-0.184845	0.056168
N	2.390045	-0.281204	-0.112686
H	2.980500	0.549347	0.024551
H	-1.582504	-2.166946	-0.130051
H	-1.367111	2.166962	0.076416
H	-2.980484	0.077774	-0.230881

BPW91/cc-pVDZ: -318.668 41

5int

N	0.034210	0.555756	0.719833
N	-0.056915	-0.891998	0.529526
C	-1.217209	-1.147583	-0.163589
C	-1.929138	0.047821	-0.297485
C	-1.083557	1.084030	0.142731
C	1.142776	-0.265793	0.109589
N	2.263153	-0.424835	-0.339096
H	2.932617	0.340469	-0.493088
H	-1.464264	-2.170456	-0.470062
H	-1.229721	2.170456	0.123322
H	-2.932617	0.162430	-0.719833

BPW91/cc-pVDZ: -318.699 64

5tsb

N	-0.039429	0.450943	0.640823
N	-0.168259	-0.952408	0.553635
C	-1.370956	-1.155258	-0.052353
C	-2.030884	0.080490	-0.263382
C	-1.132294	1.085297	0.068710
C	1.140182	-0.026718	0.118622
N	2.245667	-0.190430	-0.315948
H	3.048950	0.436768	-0.430800
H	-1.714630	-2.176590	-0.250824
H	-1.185165	2.176605	0.004608
H	-3.048935	0.218643	-0.640823

BPW91/cc-pVDZ: -318.693 79

5rcp

N	-0.811829	-1.493561	-0.132080
C	-2.074539	-1.117340	-0.101715
C	-2.266815	0.318542	-0.049713
C	-1.020523	0.870500	-0.047119
N	-0.129944	-0.239426	-0.104431
C	1.167587	-0.247803	-0.092651
N	2.338333	-0.261673	-0.264954
H	3.216888	-0.310913	0.264969
H	-2.846100	-1.897079	-0.119827
H	-0.645767	1.897079	-0.021271
H	-3.216873	0.859451	-0.022766

BPW91/cc-pVDZ: -318.731 21

7tsa

N	-0.273727	1.127487	-0.114304
N	-0.331512	-1.069870	0.079651
C	-1.630844	-1.101395	0.012985
N	-2.396332	0.025879	0.090881
C	-1.570328	1.081635	0.024414
C	0.588730	-0.039169	0.003433
N	1.849548	-0.093475	-0.076874
H	2.396347	0.760666	0.114288
H	-2.123291	-2.093918	0.014633
H	-2.044449	2.093903	0.011246

BPW91/cc-pVDZ: -334.696 25

7tsb

N	-0.557602	0.493561	0.546722
N	-0.666367	-0.922394	0.466415
C	-1.869324	-1.106293	-0.151123
N	-2.531860	0.054474	-0.378311
C	-1.694412	1.028503	-0.064377
C	0.633759	-0.030289	0.066071
N	1.734711	-0.193192	-0.379471
H	2.531876	0.430038	-0.546707
H	-2.262711	-2.108276	-0.359344
H	-1.855148	2.108276	-0.164658

BPW91/cc-pVDZ: -334.727 52

7rcp

N	-1.034714	-1.585114	-0.097778
C	-2.262329	-1.102280	-0.105652
N	-2.387924	0.288712	-0.104233
C	-1.178741	0.741500	-0.092377
N	-0.282852	-0.393738	-0.091858
C	1.019791	-0.446487	-0.075165
N	2.188248	-0.436081	-0.203247
H	3.128006	-0.466232	0.203262
H	-3.127991	-1.774841	-0.114044
H	-0.814728	1.774841	-0.089844

BPW91/cc-pVDZ: -334.770 54

8 s

C	-1.026550	-0.728928	0.999985
C	-1.204773	-2.072845	0.716888
C	-0.224640	-2.754089	-0.045578
C	0.939438	-2.099213	-0.543579
C	1.132645	-0.755615	-0.293564
C	0.136490	-0.023300	0.478271
N	0.167725	1.278458	0.706284
C	1.235489	2.157150	0.474518
O	2.074326	2.038315	1.372467
C	1.171280	3.179733	-0.602127
H	-1.744781	-0.149811	1.595062
H	-2.085297	-2.612686	1.087082
H	-0.359177	-3.825302	-0.254730
H	1.676468	-2.671356	-1.121445
H	2.030502	-0.233200	-0.648941
H	2.085281	3.799042	-0.583664
H	0.285690	3.825302	-0.430710
H	1.044754	2.705627	-1.595062

BPW91/cc-pVDZ: -439.306 20

8 tsc

C	-1.416611	-1.418442	-0.117264
C	-0.934250	-2.670074	-0.420517
C	0.477158	-2.918747	-0.401093
C	1.420532	-1.930145	-0.056885
C	0.973740	-0.657242	0.287933
C	-0.454132	-0.330658	0.083160
N	-0.910446	0.871475	-0.187317
C	0.121048	1.849930	-0.365631
O	1.251633	1.522186	-0.740540
C	-0.316010	3.261673	-0.094955
H	-2.480240	-1.153824	-0.171600
H	-1.622162	-3.485626	-0.679321
H	0.831161	-3.943619	-0.587082
H	2.480255	-2.195023	0.047913
H	1.625488	0.024902	0.848877
H	0.547470	3.943634	-0.130310
H	-0.844100	3.327972	0.875092
H	-1.057327	3.533691	-0.875076

BPW91/cc-pVDZ: -439.296 83

8bzo

C	-1.469727	-1.538010	-0.183197
C	-0.705902	-2.679306	-0.403030
C	0.738449	-2.668472	-0.532532
C	1.470032	-1.522202	-0.380371
C	0.717972	-0.340439	0.125351
C	-0.757126	-0.319580	-0.094391
N	-1.183655	0.944534	-0.288544
C	-0.059479	1.683853	-0.339325
O	1.102936	1.019974	-0.182098
C	-0.006897	3.145447	-0.526657
H	-2.565414	-1.548676	-0.227692
H	-1.223114	-3.636765	-0.559830
H	1.246400	-3.609238	-0.781479
H	2.565414	-1.492844	-0.449432
H	0.859300	-0.426880	1.239471
H	0.990800	3.477356	-0.856628
H	-0.245926	3.636749	0.441055
H	-0.794159	3.451309	-1.239471

BPW91/cc-pVDZ: -439.335 75

8t

C	-1.188065	-0.893021	-0.000015
C	-1.295517	-2.272873	-0.000015
C	-0.132660	-3.081955	-0.000046
C	1.159058	-2.489960	-0.000107
C	1.308044	-1.116058	-0.000107
C	0.127274	-0.273331	-0.000046
N	0.127487	1.061615	-0.000015
C	1.110367	2.074722	-0.000031
O	2.269928	1.656265	0.000107
C	0.653839	3.486923	-0.000168
H	-2.070633	-0.242432	0.000031
H	-2.289261	-2.739456	0.000015
H	-0.228287	-4.175919	-0.000061
H	2.051682	-3.129898	-0.000153
H	2.289246	-0.627335	-0.000183
H	1.514435	4.175903	-0.000549
H	0.020294	3.661728	0.892944
H	0.019700	3.661392	-0.892944

BPW91/cc-pVDZ: -439.292 66

9s

N	-1.594177	-1.697189	0.179031
C	-2.861389	-1.326600	0.131302
N	-3.291290	0.043030	0.149872
C	-2.340118	1.080521	0.196167
C	-0.996231	0.725937	0.219315
C	-0.647385	-0.682907	0.200500
N	0.605194	-1.125565	0.147003
H	-3.610641	-2.132980	0.093979
H	-2.651154	2.132996	0.213272
C	1.784821	-0.420090	0.346710
O	1.930908	-0.268936	1.568634
C	2.745422	-0.133545	-0.745667
H	3.610657	0.425369	-0.347366
H	2.262039	0.427826	-1.568634
H	3.096832	-1.098572	-1.166336
H	-0.205521	1.487381	0.262833

BPW91/cc-pVDZ: -471.347 44

9tsc

N	1.583130	-1.618210	-0.443497
C	2.850937	-1.250107	-0.593400
N	3.251343	-0.004349	-0.221863
C	2.373550	0.992386	-0.087372
C	0.989594	0.733429	-0.095917
C	0.622375	-0.660843	-0.255615
N	-0.618271	-1.152283	-0.435410
H	3.608810	-1.990524	-0.885864
H	2.769684	1.990540	0.158829
C	-1.655426	-0.208832	-0.529724
O	-1.595551	0.887268	-1.078690
C	-2.921341	-0.745468	0.149200
H	-3.608826	0.097931	0.322479
H	-2.687057	-1.292038	1.078690
H	-3.352737	-1.474075	-0.569473
H	0.260757	1.537231	0.055237

BPW91/cc-pVDZ: -471.337 27

9bzo

N	1.534653	-1.916504	0.120651
C	2.573273	-1.205231	-0.224915
N	2.529100	0.154251	-0.654556
C	1.488464	0.835129	-0.328873
C	0.349854	0.203415	0.524948
C	0.366760	-1.247177	0.198029
N	-0.829269	-1.673660	-0.223404
H	3.571716	-1.667984	-0.224609
H	1.440414	1.916519	-0.546631
C	-1.615540	-0.577271	-0.162872
O	-1.015656	0.561279	0.235840
C	-3.046875	-0.536469	-0.499588
H	-3.489365	0.450684	-0.294159
H	-3.571716	-1.335892	0.060760
H	-3.166321	-0.792831	-1.573532
H	0.560059	0.514679	1.573547

BPW91/cc-pVDZ: -471.402 23

9t

N	-1.638611	-1.349640	0.185104
C	-2.949814	-1.169830	0.294373
N	-3.407990	0.047394	0.638229
C	-2.601730	1.036926	1.033173
C	-1.211502	0.889800	0.996902
C	-0.743149	-0.375793	0.505417
N	0.541565	-0.797302	0.348312
H	-3.650162	-1.981125	0.056641
H	-3.081284	1.981140	1.337631
C	1.691711	-0.022629	0.495392
O	1.651871	0.831955	1.392181
C	2.877411	-0.366928	-0.339432
H	3.650162	0.415436	-0.256073
H	2.565430	-0.510147	-1.392181
H	3.283981	-1.333893	0.022247
H	-0.533203	1.675644	1.345612

BPW91/cc-pVDZ: -471.354 99

10s

C	-1.271561	-1.355545	0.114410
N	-2.538177	-1.015060	0.039429
C	-2.910812	0.267349	0.168762
C	-1.980530	1.350845	0.159225
C	-0.647064	1.045303	0.339569
C	-0.223800	-0.347382	0.342712
N	1.009918	-0.802368	0.336075
H	-0.974136	-2.386734	-0.130875
H	-3.979523	0.449127	0.367889
H	-2.342728	2.386749	0.179000
C	2.194214	-0.046982	0.433884
O	2.381485	0.298218	1.602020
C	3.109940	0.086258	-0.728790
H	3.979507	0.707932	-0.453003
H	2.583618	0.518723	-1.602036
H	3.459717	-0.924835	-1.022263
H	0.089340	1.829056	0.565400

BPW91/cc-pVDZ: -455.335 09

10tsc

C	-0.638824	1.470886	-0.083755
N	-1.877884	1.427246	-0.466492
C	-2.610016	0.278870	-0.410156
C	-2.069870	-0.991394	-0.165894
C	-0.760406	-1.023376	0.343155
C	0.050980	0.192978	0.246414
N	1.335068	0.197052	-0.010498
C	1.798691	-1.134537	-0.279968
O	0.983673	-2.042007	-0.516449
C	3.280563	-1.319061	-0.267822
H	-0.023087	2.367691	-0.252380
H	-3.702423	0.407776	-0.473740
H	-2.724228	-1.871414	-0.130676
H	-0.497589	-1.801300	1.077377
H	3.550430	-2.375229	-0.419052
H	3.700439	-0.925919	0.678513
H	3.701813	-0.686768	-1.077377

BPW91/cc-pVDZ: -455.330 40

10bzo

C	-1.433090	-1.602783	-0.059174
N	-0.747681	-2.678589	-0.383484
C	0.642212	-2.650391	-0.495956
C	1.437012	-1.554108	-0.289047
C	0.733337	-0.364960	0.269058
C	-0.737091	-0.346115	0.070145
N	-1.178345	0.888900	-0.189102
C	-0.051758	1.648819	-0.247162
O	1.104218	1.002594	-0.060791
C	-0.028336	3.101578	-0.477768
H	-2.532791	-1.651581	-0.048080
H	1.089828	-3.606064	-0.804764
H	2.532791	-1.587448	-0.351532
H	0.930222	-0.442749	1.375244
H	0.997513	3.486252	-0.586639
H	-0.540314	3.606079	0.368759
H	-0.638306	3.328674	-1.375229

BPW91/cc-pVDZ: -455.351 82

10t

C	-1.037048	1.210068	-0.175674
N	-2.349014	1.175797	-0.154663
C	-3.030624	0.015625	-0.097565
C	-2.359116	-1.236450	-0.076553
C	-0.979218	-1.272415	-0.090820
C	-0.235077	-0.035477	-0.136261
N	1.069931	0.144394	-0.155823
C	2.134079	-0.818527	-0.146835
O	1.826431	-2.001633	-0.249359
C	3.507736	-0.258377	-0.027344
H	-0.521332	2.178802	-0.234604
H	-4.127991	0.083420	-0.062698
H	-2.951126	-2.160721	-0.038132
H	-0.405228	-2.209457	-0.072037
H	4.260818	-1.061996	-0.000870
H	3.565109	0.364182	0.888290
H	3.689590	0.416962	-0.888275

BPW91/cc-pVDZ: -455.330 24

11s

C	-0.600845	-0.094162	-0.563309
C	-2.053177	-0.103592	-0.573761
C	-4.885620	-0.114900	-0.588135
C	-2.790588	-1.121918	0.111450
C	-2.791626	0.907593	-1.268295
C	-4.183685	0.891342	-1.283508
C	-4.183060	-1.116150	0.113281
C	2.269943	-0.090271	-0.531815
C	0.141556	1.090958	-0.907715
C	0.146805	-1.282639	-0.214478
C	1.517883	-1.296265	-0.205078
C	1.515121	1.098328	-0.901962
N	3.579697	0.023804	-0.482590
C	4.495804	-1.031479	-0.319077
O	4.620407	-1.753906	-1.308762
C	5.328598	-1.055130	0.923386
H	-5.983887	-0.119263	-0.593903
H	-2.265579	-1.896637	0.682281
H	-2.266266	1.684448	-1.835648
H	-4.733582	1.660782	-1.839783
H	-4.732544	-1.890793	0.662766
H	-0.392746	2.015656	-1.151657
H	-0.391312	-2.210983	0.007095
H	2.065109	-2.220932	0.018707
H	2.088608	2.000870	-1.149094
H	5.988037	-1.940247	0.911880
H	4.692734	-1.058777	1.830215
H	5.947723	-0.136551	0.962036

BPW91/cc-pVDZ: -670.377 03

11tsc

C	1.510330	1.457611	0.657303
C	0.163345	1.379318	0.430878
C	-0.553253	0.102463	0.292694
C	0.162704	-1.094391	0.464249
C	1.543335	-1.060455	0.742386
C	2.267258	0.225662	0.576218
N	3.501907	0.234222	0.112411
C	-2.006561	0.120636	0.111298
C	3.831436	-1.060852	-0.311630
O	2.922791	-1.928986	-0.431793
C	5.257584	-1.354187	-0.638870
C	-4.806595	0.142441	-0.326614
C	-2.656372	1.265488	-0.439804
C	-2.810822	-1.007843	0.447632
C	-4.188600	-0.992020	0.237564
C	-4.033707	1.265700	-0.669846
H	2.049179	2.412369	0.690536
H	-0.407486	2.312119	0.351639
H	-0.360916	-2.055847	0.510712
H	1.946579	-1.806671	1.447067
H	5.391281	-2.401031	-0.951294
H	5.893494	-1.116700	0.236404
H	5.573181	-0.663696	-1.447052
H	-5.892014	0.150421	-0.492493
H	-2.074448	2.142975	-0.745834
H	-2.358582	-1.888229	0.919800
H	-4.793182	-1.862564	0.522156
H	-4.509415	2.145752	-1.120926

BPW91/cc-pVDZ: -670.361 46

11bzo

C	1.617294	1.360306	1.048904
C	0.243240	1.189529	0.926636
C	-0.415237	-0.013443	0.419083
C	0.359543	-1.107193	0.081848
C	1.792984	-1.063065	0.469025
C	2.423508	0.272415	0.649902
N	3.721237	0.236481	0.279114
C	-1.890717	-0.024689	0.256485
C	3.892242	-0.988968	-0.247238
O	2.813049	-1.798004	-0.252090
C	5.159637	-1.518997	-0.786621
C	-4.690613	-0.063965	-0.096848
C	-2.573929	1.129318	-0.194626
C	-2.633774	-1.195862	0.533859
C	-4.023500	-1.212402	0.360275
C	-3.962906	1.104553	-0.375488
H	2.061478	2.326828	1.316010
H	-0.405900	2.037613	1.185898
H	-0.070800	-2.040710	-0.302856
H	1.789749	-1.530914	1.493698
H	4.982742	-2.346176	-1.493698
H	5.774734	-1.901962	0.055817
H	5.730743	-0.698578	-1.255981
H	-5.780167	-0.077911	-0.231308
H	-2.018463	2.043610	-0.445984
H	-2.127441	-2.089081	0.925323
H	-4.589737	-2.123276	0.593948
H	-4.478577	2.002075	-0.740875

BPW91/cc-pVDZ: -670.382 98

11t

C	-1.682022	1.826889	0.431030
C	-1.661911	0.416504	0.517624
C	-0.511490	-0.334656	0.126160
C	0.704910	0.392639	-0.175980
C	0.837753	1.774048	0.350479
C	-0.479385	2.500305	0.173248
N	-0.258759	3.727432	-0.367310
C	-0.546707	-1.784149	-0.026871
C	1.040161	3.758057	-0.666245
O	1.758194	2.640747	-0.375839
C	1.753418	4.876404	-1.320694
C	-0.585373	-4.607086	-0.291107
C	-1.782013	-2.506790	-0.037308
C	0.666977	-2.531952	-0.158051
C	0.645477	-3.919235	-0.280212
C	-1.797241	-3.891769	-0.171967
H	-2.623276	2.386429	0.508789
H	-2.584641	-0.102875	0.795654
H	1.494278	-0.022827	-0.814117
H	1.169128	1.784378	1.420532
H	2.577866	5.232300	-0.671478
H	2.218246	4.530304	-2.265121
H	1.051743	5.699875	-1.525970
H	-0.602432	-5.699875	-0.398254
H	-2.736023	-1.970963	0.026443
H	1.635361	-2.017731	-0.129303
H	1.587097	-4.475937	-0.366928
H	-2.754547	-4.427704	-0.194260

BPW91/cc-pVDZ: -670.357 90

12s

C	-0.828934	-0.348679	-0.126816
C	-2.260239	-0.347412	-0.080826
C	-4.989456	0.190872	-0.153137
C	-3.172226	-1.390137	0.238785
C	-2.727737	0.966217	-0.436295
C	-4.096359	1.231949	-0.472763
C	-4.533936	-1.106628	0.199142
C	1.935928	0.156723	-0.359711
C	-0.369339	0.966736	-0.513321
C	0.096832	-1.414154	0.133469
C	1.442413	-1.170929	0.020233
C	0.972382	1.218216	-0.644318
C	-1.559113	1.875610	-0.727249
N	3.207306	0.481888	-0.432663
C	4.295181	-0.410126	-0.365067
O	4.451172	-1.114594	-1.362137
C	5.227905	-0.282410	0.799454
H	-6.070190	0.386444	-0.176559
H	-2.816055	-2.392181	0.509094
H	-4.477386	2.225296	-0.742371
H	-5.266541	-1.887177	0.439835
H	-0.267914	-2.410110	0.414719
H	2.173859	-1.970779	0.191711
H	1.375015	2.194855	-0.943161
H	-1.592010	2.280945	-1.759735
H	-1.535690	2.754500	-0.050200
H	6.014648	-1.053589	0.730637
H	4.683243	-0.370743	1.759720
H	5.696533	0.721848	0.780579

BPW91/cc-pVDZ: -708.504 95

12tsc

C	0.954636	1.589767	0.381714
C	-0.317734	1.119934	0.196793
C	-0.617966	-0.326050	0.200729
C	0.364059	-1.284164	0.479141
C	1.671951	-0.825119	0.724777
C	2.008377	0.595795	0.412521
N	3.207886	0.898926	-0.048584
C	-2.042557	-0.479660	0.025253
C	3.902542	-0.282211	-0.334076
O	3.283752	-1.381454	-0.371490
C	5.365723	-0.185852	-0.618805
C	-4.791794	-0.247162	-0.359528
C	-2.639389	0.811081	-0.125900
C	-2.831070	-1.657333	-0.019333
C	-4.205536	-1.527908	-0.213943
C	-4.016891	0.927826	-0.316910
C	-1.588654	1.898041	-0.056335
H	1.229324	2.648727	0.298981
H	0.100494	-2.330856	0.672700
H	2.268158	-1.344208	1.492615
H	5.801132	-1.176727	-0.819016
H	5.876648	0.306366	0.231689
H	5.503708	0.482346	-1.492600
H	-5.876648	-0.169769	-0.513107
H	-2.374542	-2.648743	0.095703
H	-4.841354	-2.421234	-0.254333
H	-4.493042	1.909439	-0.437714
H	-1.784592	2.632889	0.751419
H	-1.527679	2.481064	-0.998734

BPW91/cc-pVDZ: -708.490 82

12bzoX

C	1.026169	1.618744	-0.042313
C	-0.266663	1.101837	-0.058304
C	-0.573486	-0.340210	-0.049454
C	0.421860	-1.285034	0.043594
C	1.777832	-0.753235	0.346237
C	2.065170	0.668915	-0.014572
N	3.360474	0.805481	-0.383148
C	-2.028015	-0.483582	-0.180893
C	3.841461	-0.446243	-0.421371
O	2.983627	-1.434570	-0.096298
C	5.229400	-0.819977	-0.762421
C	-4.790207	-0.210449	-0.465637
C	-2.612625	0.805618	-0.267410
C	-2.826202	-1.642807	-0.233246
C	-4.211105	-1.493347	-0.376907
C	-3.996292	0.948746	-0.412018
C	-1.547760	1.878754	-0.182571
H	1.240219	2.683838	-0.194916
H	0.233276	-2.364639	0.092819
H	1.842896	-0.799300	1.468246
H	5.280563	-1.843750	-1.169495
H	5.847580	-0.783600	0.159958
H	5.647827	-0.081970	-1.468231
H	-5.878250	-0.115555	-0.577469
H	-2.382721	-2.644852	-0.163834
H	-4.852829	-2.382568	-0.420288
H	-4.458771	1.942032	-0.482803
H	-1.675797	2.552612	0.692917
H	-1.522690	2.549393	-1.068192

BPW91/cc-pVDZ: -708.512 01

12t

C	-1.083130	-0.486603	-0.513580
C	-2.520126	-0.471146	-0.602554
C	-5.243179	0.119308	-0.690689
C	-3.444519	-1.527847	-0.812698
C	-2.971863	0.882874	-0.437088
C	-4.333115	1.176407	-0.481400
C	-4.802307	-1.219009	-0.854584
H	-3.101654	-2.562607	-0.939285
H	-1.731293	2.589676	-1.012360
H	-4.698654	2.203979	-0.357285
H	-5.541946	-2.013489	-1.015411
H	-6.319275	0.335815	-0.727936
C	1.678650	0.036407	-0.263367
C	-0.613708	0.855865	-0.291351
C	-0.155365	-1.561584	-0.608826
C	1.197662	-1.312347	-0.487244
C	0.732391	1.124969	-0.167358
C	-1.791200	1.805328	-0.229950
H	-0.501358	-2.589676	-0.778168
H	1.944122	-2.111404	-0.554428
H	1.115097	2.138550	0.002228
N	2.973251	0.376800	-0.132416
C	4.186066	-0.294022	-0.151688
O	4.111435	-1.520325	-0.332428
C	5.436371	0.493225	0.039902
H	6.319290	-0.166245	0.003006
H	5.393127	1.016617	1.015427
H	5.506256	1.266434	-0.750504
H	-1.842606	2.338150	0.741882

BPW91/cc-pVDZ: -708.483 17