

Supporting Information

Design of N-N ylide bond based high energy density materials: a theoretical survey

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Table S1. Cartesian coordinates of the optimized structures at the B3LYP/6-311G(2d,d,p) level.

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"if"----"lowest frequency(cm-1)"
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SP2-I-1-CH3 b3lyp/6-311g(2d,d,p) if=133.6028

6  0.485878  -1.281380  -0.000066
6  1.818375  -0.970767  -0.000016
6  2.254226  0.362960  0.000071
6  1.273025  1.341462  -0.000004
6  -0.074977  1.018061  -0.000080
1  0.084431  -2.283136  -0.000186
1  2.527166  -1.790130  -0.000043
1  3.306160  0.613130  0.000136
1  1.534368  2.393376  -0.000101
1  -0.844745  1.768864  -0.000030
7  -0.499935  -0.301226  0.000061
7  -1.742862  -0.729331  0.000074
6  -2.730577  0.318150  -0.000020
1  -2.678371  0.973906  -0.888460
1  -3.706494  -0.166795  -0.000143
1  -2.678640  0.973779  0.888571
#####
SP2-I-1-CN b3lyp/6-311g(2d,d,p) if=94.0628

6  -0.869674  -1.274887  -0.000066
6  -2.167521  -0.820436  0.000063
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6	-2.439201	0.549479	0.000213
6	-1.358140	1.423636	0.000227
6	-0.062088	0.943650	0.000096
1	-0.578478	-2.314303	-0.000186
1	-2.965640	-1.551652	0.000045
1	-3.456582	0.917001	0.000314
1	-1.502516	2.496635	0.000340
1	0.813813	1.576433	0.000101
7	0.186183	-0.403265	-0.000051
7	1.415193	-0.971038	-0.000187
6	2.414796	-0.109019	-0.000169
7	3.338678	0.603067	-0.000161

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SP2-l-1-COOH b3lyp/6-311g(2d,d,p) if=44.5225

6	1.174620	-1.302283	0.000186
6	2.515011	-1.000321	0.000376
6	2.934712	0.331467	0.000107
6	1.955222	1.314006	-0.000329
6	0.608901	0.986691	-0.000435
1	0.769771	-2.302672	0.000321
1	3.225498	-1.816945	0.000650
1	3.986550	0.586306	0.000242
1	2.216306	2.365009	-0.000564
1	-0.196766	1.702895	-0.000526
7	0.211394	-0.326319	-0.000189
7	-1.052378	-0.825008	-0.000448
6	-2.082245	0.057763	0.000107
8	-2.099791	1.287900	0.000768
8	-3.251673	-0.642169	-0.000326
1	-3.940078	0.034909	0.000718

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SP2-l-1-H b3lyp/6-311g(2d,d,p) if=189.7533

6	-0.246967	-1.189496	0.000101
6	1.126749	-1.176780	-0.000030
6	1.843769	0.023033	-0.000176
6	1.099228	1.198834	-0.000185
6	-0.279987	1.170970	-0.000053
1	-0.854385	-2.081492	0.000216
1	1.637771	-2.132133	-0.000016
1	2.924746	0.037127	-0.000279
1	1.583723	2.168175	-0.000296
1	-0.891330	2.062472	-0.000060

7 -0.988416 -0.019713 0.000095
7 -2.296573 -0.128639 0.000233
1 -2.662354 0.824940 0.000205

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SP2-I-1-NH2 b3lyp/6-311g(2d,d,p) if=139.8932

6 -0.084921 1.026894 0.028326
6 1.263797 1.339565 0.017406
6 2.241652 0.355664 -0.015116
6 1.799884 -0.976536 -0.018301
6 0.466558 -1.283196 0.000472
1 -0.871331 1.758308 0.090733
1 1.531606 2.389850 0.032847
1 3.294431 0.600898 -0.038295
1 2.505402 -1.798612 -0.034143
1 0.063596 -2.284555 -0.001244
7 -0.506336 -0.292771 0.020872
7 -1.758890 -0.710377 0.004770
7 -2.645802 0.396446 0.048084
1 -2.717534 0.823786 -0.883572
1 -3.550793 -0.017100 0.240871

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SP2-I-1-NO2 b3lyp/6-311g(2d,d,p) if=57.7327

6 -1.065876 -1.290637 0.122948
6 -2.408683 -1.002893 0.241029
6 -2.850613 0.309318 0.084898
6 -1.909342 1.290835 -0.207296
6 -0.571963 0.966492 -0.338788
1 -0.635501 -2.273924 0.240215
1 -3.093831 -1.808551 0.469644
1 -3.899354 0.558001 0.184962
1 -2.201887 2.322687 -0.352821
1 0.193282 1.685977 -0.569390
7 -0.156250 -0.320145 -0.163757
7 1.121146 -0.807984 -0.390582
7 2.116976 0.027688 0.063219
8 1.868834 1.086260 0.667150
8 3.244047 -0.388735 -0.161089

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SP2-I-1-OH b3lyp/6-311g(2d,d,p) if=153.1243

6 -0.456834 -1.288580 -0.000127
6 -1.788405 -0.975184 -0.000163

6	-2.224922	0.358307	-0.000088
6	-1.243057	1.339402	0.000031
6	0.104885	1.027366	0.000072
1	-0.060319	-2.292484	-0.000184
1	-2.496715	-1.794931	-0.000257
1	-3.276938	0.607054	-0.000121
1	-1.507708	2.390446	0.000097
1	0.893700	1.756544	0.000165
7	0.516205	-0.295722	-0.000009
7	1.762780	-0.710258	0.000036
8	2.585604	0.445255	0.000186
1	3.460255	0.045332	0.000273

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SP2-I-2-CH3 b3lyp/6-311g(2d,d,p) if=135.7076

6	0.057995	1.011884	-0.000438
6	-1.298592	1.288249	-0.000032
6	-1.827411	-0.894623	0.000225
6	-0.511294	-1.266029	-0.000266
1	0.807047	1.783491	-0.000686
1	-1.600954	2.332120	0.000156
1	-2.581421	-1.675473	0.000287
1	-0.150972	-2.283024	-0.000478
7	0.495362	-0.305726	-0.000397
7	1.724354	-0.731804	0.000157
7	-2.271619	0.379784	0.000361
6	2.722380	0.311081	0.000321
1	3.694276	-0.180328	0.000934
1	2.668808	0.961565	-0.888952
1	2.668064	0.962492	0.889032

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SP2-I-2-CN b3lyp/6-311g(2d,d,p) if=102.0333

6	-0.891049	-1.256621	0.000057
6	-2.168125	-0.743897	0.000114
6	-1.393366	1.375044	0.000047
6	-0.079763	0.941901	-0.000011
1	-0.639941	-2.306164	0.000059
1	-3.005758	-1.433025	0.000163
1	-1.584114	2.443291	0.000044
1	0.777650	1.598862	-0.000060
7	0.182084	-0.404165	-0.000008
7	1.395057	-0.967571	-0.000056
7	-2.454441	0.566348	0.000109

6 2.404307 -0.111038 -0.000114
7 3.337320 0.586059 -0.000155

SP2-I-2-COOH b3lyp/6-311g(2d,d,p) if=52.9057

6 -0.621814 0.980630 0.000049
6 -1.980514 1.259589 0.000043
6 -2.519111 -0.925729 -0.000037
6 -1.193157 -1.287448 -0.000004
1 0.158725 1.722433 0.000122
1 -2.285486 2.301245 0.000060
1 -3.273673 -1.704969 -0.000049
1 -0.827289 -2.302456 0.000123
7 -0.209487 -0.329640 -0.000014
7 1.036296 -0.826143 0.000006
7 -2.948689 0.345284 -0.000017
6 2.076832 0.060194 -0.000021
8 2.086098 1.285549 -0.000077
8 3.235380 -0.646226 0.000031
1 3.935656 0.019251 0.000125

SP2-I-2-H b3lyp/6-311g(2d,d,p) if=191.8457

6 -0.222468 -1.180984 -0.000030
6 1.148819 -1.110686 -0.000008
6 1.118381 1.136324 -0.000005
6 -0.259448 1.161281 0.000011
1 -0.797713 -2.093824 -0.000059
1 1.708317 -2.041126 -0.000047
1 1.646846 2.085405 0.000037
1 -0.844038 2.070363 0.000070
7 -0.982646 -0.022413 -0.000036
7 -2.278210 -0.129753 0.000062
7 1.864338 0.026621 -0.000022
1 -2.649489 0.822382 0.000157

SP2-I-2-NH2 b3lyp/6-311g(2d,d,p) if=145.8228

6 0.490127 -1.270549 -0.004834
6 1.805404 -0.902525 0.024484
6 1.288354 1.284860 -0.017110
6 -0.069319 1.021451 -0.038804
1 0.127719 -2.286892 -0.003539
1 2.555628 -1.686740 0.047706

1 1.598098 2.326518 -0.034848
1 -0.827449 1.780063 -0.118979
7 -0.505487 -0.297836 -0.028327
7 -1.741838 -0.708500 -0.011968
7 2.257191 0.371083 0.027396
7 -2.636313 0.379150 -0.045150
1 -3.554610 -0.044890 -0.101975
1 -2.601655 0.905236 0.835555

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SP2-I-2-NO2 b3lyp/6-311g(2d,d,p) if=42.2528

6 -1.131163 -1.276394 0.105672
6 -2.460293 -0.925675 0.132909
6 -1.946907 1.249799 -0.145134
6 -0.586101 0.979344 -0.188844
1 -0.755875 -2.283640 0.201725
1 -3.205006 -1.702956 0.263962
1 -2.263556 2.282059 -0.252279
1 0.169733 1.732762 -0.308013
7 -0.165384 -0.316460 -0.055773
7 1.081326 -0.853696 -0.153016
7 -2.900072 0.335315 0.014757
7 2.144154 0.020629 0.028629
8 1.984875 1.186222 0.415449
8 3.225291 -0.497620 -0.187347

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SP2-I-2-OH b3lyp/6-311g(2d,d,p) if=154.2317

6 0.479614 -1.273396 -0.000045
6 1.794994 -0.900985 -0.000079
6 1.270312 1.285352 -0.000024
6 -0.086117 1.022704 0.000018
1 0.121718 -2.291323 -0.000052
1 2.546573 -1.684299 -0.000122
1 1.578304 2.327385 -0.000011
1 -0.852825 1.775170 0.000061
7 -0.512754 -0.297693 0.000005
7 -1.746951 -0.707501 0.000047
7 2.242505 0.371710 -0.000074
8 -2.572308 0.433908 0.000115
1 -3.447724 0.034145 0.000146

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SP2-I-3-CH3 b3lyp/6-311g(2d,d,p) if=129.4507

6	0.555382	1.278178	-0.000197
6	1.844363	0.842613	0.000240
6	1.152773	-1.283992	-0.000231
1	0.223887	2.304342	-0.000203
1	2.650142	1.569299	0.000497
1	1.353912	-2.351708	0.000414
7	-0.467829	0.329623	-0.000405
7	-1.679265	0.735172	-0.000066
7	-0.151080	-0.999773	-0.000500
7	2.192979	-0.466266	0.000423
6	-2.668752	-0.324103	0.000446
1	-3.645705	0.156861	0.000060
1	-2.574171	-0.973503	-0.878996
1	-2.574294	-0.972748	0.880509

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SP2-I-3-CN b3lyp/6-311g(2d,d,p) if=103.7259

6	0.919908	-1.256063	0.000251
6	2.175986	-0.705946	0.000126
6	1.284924	1.349393	-0.000142
1	0.681750	-2.308029	0.000309
1	3.043448	-1.357011	0.000131
1	1.386368	2.429496	-0.000149
7	-0.156948	-0.401403	0.000325
7	-1.352505	-0.928924	0.000053
7	0.020162	0.934256	0.000041
7	2.395228	0.619513	-0.000022
6	-2.372359	-0.073454	-0.000268
7	-3.357697	0.541123	-0.000409

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SP2-I-3-COOH b3lyp/6-311g(2d,d,p) if=57.1322

6	1.241308	-1.270965	-0.191220
6	2.532665	-0.810068	-0.171788
6	1.788658	1.251957	0.270304
1	0.929893	-2.286939	-0.374905
1	3.349015	-1.501456	-0.352249
1	1.967610	2.303107	0.471495
7	0.220745	-0.375655	0.038490
7	-0.988797	-0.848245	0.074741
7	0.500963	0.921398	0.289027
7	2.846254	0.475150	0.053943
6	-2.040459	0.052544	-0.102133
8	-2.059895	1.067691	-0.753725

8 -3.136594 -0.467371 0.497827
1 -3.861803 0.133389 0.278462

SP2-I-3-H b3lyp/6-311g(2d,d,p) if=163.9171

6 0.198532 1.196211 0.000162
6 -1.163117 1.088674 0.000035
6 -1.010260 -1.141077 -0.000218
1 0.767700 2.112153 0.000206
1 -1.764408 1.992171 0.000025
1 -1.466971 -2.126470 -0.000326
7 0.953395 0.030567 0.000267
7 2.228516 0.099673 -0.000020
7 0.318686 -1.180286 -0.000056
7 -1.820309 -0.088427 -0.000128
1 2.550735 -0.871387 -0.000229

SP2-I-3-NH2 b3lyp/6-311g(2d,d,p) if=129.4649

6 0.527926 1.291929 -0.004467
6 1.812371 0.863260 -0.001844
6 1.147373 -1.279379 -0.001076
1 0.187638 2.315435 -0.006022
1 2.614065 1.594001 -0.002046
1 1.361406 -2.345163 -0.002172
7 -0.484211 0.321270 -0.000901
7 -1.707588 0.694249 -0.006152
7 -0.162328 -1.016576 0.001462
7 2.175865 -0.452427 0.001187
7 -2.590309 -0.336787 0.087193
1 -3.480371 -0.053561 -0.294846
1 -2.228755 -1.233677 -0.230112

SP2-I-3-NO2 b3lyp/6-311g(2d,d,p) if=43.0200

6 1.302791 1.271476 0.000370
6 2.526748 0.662734 0.000272
6 1.550825 -1.351018 -0.000493
1 1.115555 2.333595 0.000807
1 3.422485 1.274576 0.000556
1 1.602211 -2.434905 -0.001072
7 0.180213 0.461221 -0.000167
7 -0.976377 1.039844 -0.000130
7 0.302176 -0.884859 -0.000573

7 2.690215 -0.674150 -0.000239
7 -2.048757 0.031244 0.000188
8 -2.464933 -0.281197 1.088943
8 -2.466908 -0.279492 -1.088285

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SP2-I-3-OH b3lyp/6-311g(2d,d,p) if=131.4706

6 0.498168 1.277642 -0.000081
6 1.796764 0.878530 -0.000299
6 1.167403 -1.269313 -0.000206
1 0.138543 2.294429 -0.000226
1 2.580108 1.629223 -0.000567
1 1.400957 -2.330226 0.000340
7 -0.486074 0.285004 0.000450
7 -1.710605 0.673546 0.000097
7 -0.145716 -1.034041 0.000281
7 2.184255 -0.421019 -0.000254
8 -2.546893 -0.429500 0.000051
1 -3.411497 -0.003023 -0.000462

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SP2-I-4-CH3 b3lyp/6-311g(2d,d,p) if=95.8772

6 1.751639 -0.858358 -0.000076
6 1.153647 1.275625 0.000089
1 2.511601 -1.634222 -0.000374
1 1.382560 2.338056 0.000200
7 -0.445390 -0.334170 0.000268
7 -1.638428 -0.742303 -0.000287
7 -0.144540 1.007743 0.000845
7 2.168444 0.419722 -0.000838
7 0.522160 -1.316823 0.000548
6 -2.641667 0.305861 -0.000433
1 -2.549585 0.953483 -0.880101
1 -3.611556 -0.187762 -0.001068
1 -2.550453 0.952497 0.880099

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SP2-I-4-CN b3lyp/6-311g(2d,d,p) if=96.3637

6 1.288366 1.339544 -0.000092
6 2.081519 -0.732807 -0.000220
1 1.415959 2.417307 -0.000167
1 2.902436 -1.442107 -0.000381
7 -0.137329 -0.404051 0.000575
7 -1.313344 -0.931031 0.000124

7 0.883522 -1.290605 0.000156
7 2.374458 0.571391 -0.000298
7 0.023625 0.941106 0.000278
6 -2.339524 -0.080182 -0.000183
7 -3.331012 0.522544 -0.000333

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SP2-I-4-COOH b3lyp/6-311g(2d,d,p) if=34.9985

6 2.467831 -0.697262 -0.018274
6 1.604920 1.344237 0.005650
1 3.314940 -1.376027 -0.031330
1 1.697751 2.426152 0.014185
7 0.229311 -0.453522 -0.003232
7 -0.911626 -0.993903 0.004882
7 0.355183 0.910676 0.000736
7 2.719082 0.616275 -0.001192
7 1.296632 -1.304248 -0.019751
6 -2.010310 -0.094313 0.116666
8 -2.495862 0.234214 1.160346
8 -2.494978 0.198127 -1.099537
1 -3.280689 0.748233 -0.963687

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SP2-I-4-H b3lyp/6-311g(2d,d,p) if=117.4995

6 1.008071 1.133060 0.000007
6 1.077348 -1.081987 0.000121
1 1.487652 2.107809 0.000003
1 1.623384 -2.020573 0.000199
7 -0.927975 -0.050785 -0.000232
7 -2.186762 -0.130388 0.000088
7 -0.233717 -1.228325 -0.000009
7 1.787122 0.051120 0.000103
7 -0.311595 1.182129 -0.000114
1 -2.513063 0.840059 0.000180

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SP2-I-4-NH2 b3lyp/6-311g(2d,d,p) if=96.1933

6 1.151246 1.271100 0.001556
6 1.715363 -0.882644 -0.000161
1 1.402289 2.328905 0.006591
1 2.469328 -1.664303 0.003075
7 -0.457770 -0.318748 0.005078
7 -1.668799 -0.696319 -0.000639
7 0.488082 -1.330814 0.013945

7 2.150392 0.397389 -0.014373
7 -0.151110 1.032081 0.011137
7 -2.558114 0.311220 -0.081683
1 -3.463711 0.011963 0.244525
1 -2.226326 1.229036 0.203183

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SP2-I-4-NO2 b3lyp/6-311g(2d,d,p) if=60.4319

6 1.550688 1.342545 -0.000260
6 2.429820 -0.694259 0.000046
1 1.632897 2.424883 -0.000498
1 3.281736 -1.366536 0.000171
7 0.197262 -0.458352 0.000070
7 -0.939646 -1.040553 0.000371
7 1.262333 -1.308174 0.000233
7 2.667383 0.622486 -0.000205
7 0.301747 0.896993 -0.000152
7 -2.025271 -0.032369 0.000021
8 -2.440552 0.267611 -1.089726
8 -2.439988 0.268854 1.089632

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SP2-I-4-OH b3lyp/6-311g(2d,d,p) if=98.3086

6 -1.169486 1.260185 -0.000200
6 -1.699268 -0.896021 -0.000268
1 -1.436929 2.313152 -0.000212
1 -2.431915 -1.697488 -0.000404
7 0.460535 -0.284088 0.000132
7 1.671879 -0.679428 0.000255
7 -0.455887 -1.313700 -0.000051
7 -2.156406 0.367946 -0.000354
7 0.137549 1.046082 0.000049
8 2.512816 0.408256 0.000350
1 3.375157 -0.024382 0.000408

#####

SP2-I-5-CH3 b3lyp/6-311g(2d,d,p) if=82.8422

6 -0.000123 1.008926 0.200719
1 -0.705436 1.784132 0.459377
7 -0.450370 -0.297810 0.068052
7 -1.629279 -0.736831 -0.065247
7 1.256317 1.300124 0.002792
7 2.151053 0.350596 -0.230212
7 1.762253 -0.912942 -0.024499

7 0.559338 -1.293934 0.164075
6 -2.664662 0.281628 -0.114488
1 -2.469790 1.040664 -0.885162
1 -3.597403 -0.227382 -0.346377
1 -2.783849 0.794841 0.850055

#####

SP2-I-5-CN b3lyp/6-311g(2d,d,p) if=64.5892

6 0.960626 1.223631 0.000119
1 0.755620 2.287183 0.000173
7 -0.138122 0.385560 -0.000002
7 -1.319447 0.909931 -0.000026
7 2.161324 0.746087 0.000169
7 2.351816 -0.592882 0.000103
7 1.307552 -1.379475 0.000001
7 0.067390 -0.968332 -0.000056
6 -2.351818 0.065733 -0.000122
7 -3.346009 -0.532798 -0.000210

#####

SP2-I-5-COOH b3lyp/6-311g(2d,d,p) if=38.9348

6 -0.665683 0.985472 -0.107807
1 0.064439 1.765447 -0.249480
7 -0.228070 -0.320201 -0.078029
7 0.961830 -0.825772 -0.011151
7 -1.937018 1.259654 0.087503
7 -2.828097 0.303301 0.223327
7 -2.433823 -0.953758 -0.018002
7 -1.212274 -1.303459 -0.175677
6 2.037703 0.060256 0.005670
8 2.038877 1.270202 -0.116745
8 3.155632 -0.661114 0.177829
1 3.889533 -0.030876 0.177838

#####

SP2-I-5-H b3lyp/6-311g(2d,d,p) if=63.7930

6 -0.153090 1.181079 0.000087
1 -0.698621 2.116807 0.000150
7 -0.926783 0.023000 -0.000022
7 -2.189772 0.081975 -0.000066
7 1.135220 1.127396 0.000107
7 1.773283 -0.066478 0.000030
7 1.048195 -1.157470 -0.000050
1 -2.519729 -0.889986 -0.000143

7 -0.249158 -1.196037 -0.000075

SP2-I-5-NH2 b3lyp/6-311g(2d,d,p) if=58.0178

6 -0.567888 1.267915 -0.016419
1 -0.251247 2.305545 -0.042569
7 0.459514 0.315830 -0.006762
7 1.678974 0.680340 0.022643
7 -1.792020 0.914806 0.004467
7 -2.123133 -0.441709 0.035265
7 -1.167964 -1.307742 -0.000078
7 0.113590 -1.047878 -0.042648
7 2.544836 -0.338273 -0.051697
1 3.468624 -0.073401 0.249371
1 2.193382 -1.267248 0.163382

SP2-I-5-NO2 b3lyp/6-311g(2d,d,p) if=38.0455

6 -1.352757 1.238335 0.000347
1 -1.213520 2.312403 0.000743
7 -0.196061 0.462006 0.000196
7 0.940206 1.039744 0.000648
7 -2.517541 0.688108 0.000076
7 -2.639192 -0.661663 -0.000414
7 -1.552345 -1.384232 -0.000447
7 -0.337632 -0.916746 -0.000188
7 2.041316 0.018630 0.000010
8 2.447836 -0.277926 -1.090651
8 2.447015 -0.279992 1.090402

SP2-I-5-OH b3lyp/6-311g(2d,d,p) if=16.2151

6 0.534334 1.252948 0.000012
1 0.198958 2.283805 0.000059
7 -0.467771 0.276325 0.000237
7 -1.681809 0.657724 0.000315
7 1.772164 0.928078 -0.000299
7 2.137183 -0.396878 -0.000407
7 1.197130 -1.293112 -0.000286
7 -0.088699 -1.074594 0.000018
8 -2.512279 -0.433169 0.000320
1 -3.384116 -0.018936 0.000265

SP2-I-6-CH3 b3lyp/6-311g(2d,d,p) if=120.0816

7 0.412139 -0.329798 -0.113308
7 1.563118 -0.734636 0.134301
7 -1.125558 1.304907 -0.043764
7 -2.002812 0.429605 0.392329
7 -1.758599 -0.858672 0.072427
7 -0.612347 -1.291965 -0.255724
7 0.081085 0.984742 -0.402789
6 2.590169 0.299919 0.167507
1 2.320016 1.116715 0.844231
1 3.509489 -0.178601 0.495260
1 2.730301 0.733098 -0.828840

#####

SP2-I-6-CN b3lyp/6-311g(2d,d,p) if=100.1827

7 0.109485 -0.397736 0.118396
7 1.253630 -0.913994 -0.083776
7 -2.086736 -0.731983 -0.093687
7 -2.221731 0.566524 -0.379104
7 -1.267243 1.364871 0.059318
7 -0.091486 0.933810 0.387914
7 -0.959691 -1.263204 0.207772
6 2.297285 -0.079583 -0.092107
7 3.294671 0.509927 -0.137884

#####

SP2-I-6-COOH b3lyp/6-311g(2d,d,p) if=48.5062

7 0.245738 0.475762 -0.039811
7 -0.860383 0.946719 0.289465
7 1.559222 -1.309103 -0.390547
7 2.541169 -0.675968 0.221699
7 2.460104 0.660584 0.237746
7 1.370317 1.300381 0.053293
7 0.410632 -0.768079 -0.629299
6 -2.000536 0.106065 0.020197
8 -2.709345 0.278369 -0.922352
8 -2.177998 -0.752285 1.026817
1 -2.985636 -1.257131 0.845276

#####

SP2-I-6-H b3lyp/6-311g(2d,d,p) if=154.2863

7 -0.891056 -0.047269 -0.039474
7 -2.096944 -0.132298 0.262562
7 1.084147 -1.099802 -0.010825

7 1.663911 0.056262 0.321287
7 1.006308 1.155006 -0.016148
1 -2.446762 0.833533 0.313124
7 -0.251486 1.162914 -0.293720
7 -0.165342 -1.213890 -0.268415

#####

SP2-I-6-NH2 b3lyp/6-311g(2d,d,p) if=119.0994

7 -0.422407 -0.312694 -0.085299
7 -1.604521 -0.683509 0.132674
7 1.723704 -0.887291 0.049787
7 1.994544 0.406442 0.382665
7 1.122694 1.303448 -0.030492
7 -0.087074 1.013537 -0.376563
7 0.580200 -1.309246 -0.266427
7 -2.492743 0.299362 0.190589
1 -2.255396 1.213260 -0.179628
1 -3.445389 -0.023608 0.201085

#####

SP2-I-6-NO2 b3lyp/6-311g(2d,d,p) if=62.9458

7 -0.218297 0.480420 -0.051140
7 0.867689 1.010933 0.270985
7 -2.441718 0.661962 0.162868
7 -2.507745 -0.674894 0.252035
7 -1.504715 -1.338352 -0.282802
7 -0.353130 -0.808641 -0.537009
7 -1.364187 1.304633 -0.048866
7 2.011338 0.001108 0.095253
8 2.596197 0.113039 -0.941546
8 2.225722 -0.670561 1.062887

#####

SP2-I-6-OH b3lyp/6-311g(2d,d,p) if=125.3617

7 0.433468 -0.285463 0.120309
7 1.600743 -0.668684 -0.135230
7 -1.699730 -0.895917 -0.071568
7 -1.984118 0.371884 -0.414834
7 -1.141288 1.286732 0.037858
7 0.065613 1.031829 0.408275
7 -0.546887 -1.291486 0.284580
8 2.451497 0.396975 -0.152902
1 3.293418 -0.018064 -0.382515

#####

SP2-II-1-CH3 b3lyp/6-311g(2d,d,p) if=121.5221

6	-1.649992	-0.982869	0.184038
6	-2.035878	0.484852	-0.104211
6	-0.733183	1.189544	0.079611
6	-0.161853	-1.046662	-0.160959
1	-1.791331	-1.200452	1.245063
1	-2.235103	-1.703661	-0.389750
1	-2.818750	0.846898	0.568918
1	-2.429865	0.592901	-1.127651
1	-0.554968	2.251061	0.147605
1	0.027856	-1.334929	-1.198371
1	0.416243	-1.697469	0.491455
7	0.312164	0.376859	-0.000723
7	1.561409	0.760669	-0.024372
6	2.538991	-0.306974	0.043298
1	2.470253	-1.048961	-0.769909
1	3.518125	0.166353	-0.040666
1	2.534023	-0.861786	0.998306

#####

SP2-II-1-CN b3lyp/6-311g(2d,d,p) if=98.5001

6	2.320716	-0.224268	-0.203336
6	1.751584	1.186228	0.096318
6	0.274838	0.969771	0.010291
6	1.160732	-1.172578	0.120352
1	2.580674	-0.300198	-1.260790
1	3.213177	-0.452379	0.378978
1	2.103368	1.941638	-0.611060
1	2.033882	1.537520	1.097643
1	-0.505705	1.716799	-0.016689
1	1.184187	-1.568238	1.138045
1	1.029943	-2.001676	-0.572400
7	-0.037550	-0.299598	0.020132
7	-1.213718	-0.938290	0.001387
6	-2.254272	-0.117035	-0.021935
7	-3.200319	0.562719	-0.044929

#####

SP2-II-1-COOH b3lyp/6-311g(2d,d,p) if=49.8045

6	2.318874	0.967435	0.035470
6	2.703043	-0.529670	0.066418
6	1.378111	-1.195548	0.219699
6	0.855516	0.975635	-0.410884

1 2.401568 1.391138 1.038413
1 2.953116 1.553532 -0.629984
1 3.393066 -0.781122 0.875734
1 3.184257 -0.848954 -0.868523
1 1.180296 -2.234130 0.442586
1 0.727646 1.052767 -1.493903
1 0.215997 1.704574 0.072944
7 0.372340 -0.409930 -0.034207
7 -0.882468 -0.870108 -0.137281
6 -1.868392 0.046485 0.062370
8 -1.813807 1.217309 0.425781
8 -3.071929 -0.543430 -0.185403
1 -3.722073 0.145404 0.001687

#####

SP2-II-1-H b3lyp/6-311g(2d,d,p) if=161.5469

6 1.413104 -0.714519 -0.192734
6 1.405982 0.804574 0.108167
6 -0.045157 1.145210 -0.031664
6 -0.008459 -1.160714 0.152033
1 1.608387 -0.878500 -1.254821
1 2.167713 -1.259145 0.376616
1 2.045515 1.362998 -0.582611
1 1.785574 1.010438 1.120374
1 -0.484729 2.130525 -0.087768
1 -0.123737 -1.484783 1.188731
1 -0.433014 -1.921404 -0.500098
7 -0.827334 0.076664 -0.005171
7 -2.117920 -0.109371 -0.048552
1 -2.541749 0.821511 -0.099177

#####

SP2-II-1-NH2 b3lyp/6-311g(2d,d,p) if=132.9155

6 1.983748 -0.403560 -0.256330
6 1.610757 1.050129 0.121493
6 0.115374 1.032644 0.018082
6 0.744087 -1.210599 0.138581
1 2.146453 -0.475258 -1.334268
1 2.883510 -0.760933 0.246592
1 2.078770 1.779342 -0.547303
1 1.956680 1.291433 1.138398
1 -0.558454 1.866010 0.114850
1 0.776927 -1.561555 1.173004
1 0.510774 -2.051826 -0.511503

7 -0.355060 -0.217735 0.045346
7 -1.561363 -0.700292 0.010809
7 -2.482392 0.374961 0.014519
1 -2.334426 0.962703 -0.818298
1 -3.392324 -0.060137 -0.087149

#####

SP2-II-1-NO2 b3lyp/6-311g(2d,d,p) if=66.5547

6 -2.670389 -0.446767 0.206262
6 -2.274249 1.016075 -0.092207
6 -0.780921 0.993580 -0.007549
6 -1.406612 -1.240414 -0.131039
1 -2.912610 -0.558656 1.264826
1 -3.530595 -0.781520 -0.372892
1 -2.709810 1.731828 0.609525
1 -2.586694 1.332828 -1.096086
1 -0.113347 1.834861 0.024124
1 -1.383238 -1.618444 -1.154844
1 -1.174855 -2.058057 0.547438
7 -0.311097 -0.227000 -0.019720
7 0.895789 -0.836192 -0.002996
7 1.982186 0.014812 0.014836
8 3.059983 -0.559577 0.021211
8 1.844521 1.249699 0.026322

#####

SP2-II-1-OH b3lyp/6-311g(2d,d,p) if=138.3640

6 1.977977 -0.412575 -0.230166
6 1.603736 1.050810 0.108401
6 0.109292 1.034554 0.002348
6 0.727680 -1.209026 0.155501
1 2.162642 -0.508200 -1.302385
1 2.864614 -0.764445 0.299253
1 2.071287 1.761336 -0.580473
1 1.948259 1.322768 1.117767
1 -0.570643 1.866656 -0.024025
1 0.738275 -1.545163 1.194799
1 0.502731 -2.057855 -0.488259
7 -0.360068 -0.207660 0.019334
7 -1.564943 -0.698453 -0.011771
8 -2.432565 0.434546 -0.049310
1 -3.293683 0.008740 -0.091640

#####

SP2-II-2-CH3 b3lyp/6-311g(2d,d,p) if=103.2104

6	-1.674814	-0.915925	0.191137
6	-0.744484	1.163147	0.085470
6	-0.201328	-1.049815	-0.212055
1	-1.797729	-1.180261	1.245473
1	-2.340055	-1.544440	-0.401490
1	-0.617531	2.225945	0.201925
1	-0.040332	-1.326975	-1.258384
1	0.359075	-1.727097	0.427705
7	0.301452	0.360355	-0.038388
7	1.558486	0.746763	-0.095371
7	-1.996847	0.515866	0.022994
1	-2.482111	0.687539	-0.856787
6	2.522444	-0.317148	0.096156
1	3.509220	0.141565	0.017410
1	2.471204	-0.795333	1.092391
1	2.485714	-1.123389	-0.657138

#####

SP2-II-2-CN b3lyp/6-311g(2d,d,p) if=90.5093

6	2.313529	0.128173	-0.162757
6	0.292689	-0.945238	0.031343
6	1.196142	1.149938	0.105142
1	3.190615	0.289726	0.462772
1	2.616677	0.150101	-1.215488
1	-0.449297	-1.729039	0.036407
1	1.144459	1.966654	-0.611855
1	1.221803	1.560845	1.117076
7	-0.020854	0.322238	-0.013090
7	-1.215185	0.978385	-0.014771
7	1.650497	-1.153512	0.168699
1	2.022219	-1.985931	-0.269208
6	-2.234328	0.137443	-0.022391
7	-3.150839	-0.586289	-0.030514

#####

SP2-II-2-COOH b3lyp/6-311g(2d,d,p) if=35.9555

6	-2.399186	0.827765	0.281827
6	-1.368825	-1.154024	-0.239903
6	-0.873210	1.030422	0.215557
1	-2.939319	1.587112	-0.283189
1	-2.762345	0.829330	1.315747
1	-1.229063	-2.206383	-0.431763
1	-0.441430	1.469706	1.111855

1 -0.536633 1.601346 -0.645314
7 -0.372388 -0.378615 0.065398
7 0.889972 -0.853863 0.286125
7 -2.572631 -0.508061 -0.327759
1 -3.402970 -1.035486 -0.099407
6 1.851595 0.031749 -0.048405
8 1.760508 1.158621 -0.539047
8 3.081302 -0.492662 0.244157
1 3.700361 0.195000 -0.029616

#####

SP2-II-2-H b3lyp/6-311g(2d,d,p) if=165.0953

6 1.427262 -0.630425 -0.207214
6 -0.027889 1.126469 -0.015109
6 0.038279 -1.153741 0.176132
1 1.623106 -0.815157 -1.267038
1 2.233166 -1.077805 0.374836
1 -0.422035 2.125157 -0.118148
1 -0.055910 -1.479752 1.215237
1 -0.355422 -1.928107 -0.477974
7 -0.809502 0.060921 0.015162
7 -2.105799 -0.145837 -0.061269
7 1.358667 0.834379 0.011417
1 1.786504 1.094225 0.898612
1 -2.538881 0.781374 -0.105555

#####

SP2-II-2-NH2 b3lyp/6-311g(2d,d,p) if=142.0149

6 1.977773 0.326547 0.238629
6 0.133767 -1.022334 -0.014231
6 0.781223 1.184636 -0.197583
1 2.162421 0.457995 1.308668
1 2.894643 0.562920 -0.301901
1 -0.502838 -1.867162 0.177601
1 0.814021 1.496015 -1.245149
1 0.589326 2.052286 0.430025
7 -0.333683 0.224056 -0.030819
7 -1.543201 0.726001 0.031917
7 1.554875 -1.071544 -0.000245
1 1.931774 -1.422578 -0.878346
7 -2.453367 -0.361872 0.127347
1 -3.368085 0.067979 0.203826
1 -2.450208 -0.897031 -0.753011

#####

SP2-II-2-NO2 b3lyp/6-311g(2d,d,p) if=69.3914

6	2.668642	0.360397	-0.180111
6	0.799969	-0.967910	0.070397
6	1.430483	1.231244	0.083961
1	3.516739	0.636541	0.445475
1	2.970583	0.406423	-1.232190
1	0.173134	-1.839943	0.094129
1	1.266132	2.018599	-0.647771
1	1.419097	1.665086	1.085958
7	0.320109	0.251641	0.003134
7	-0.913461	0.864455	0.024392
7	2.163374	-0.981296	0.161736
1	2.650895	-1.795708	-0.182269
7	-1.955995	-0.002780	-0.017878
8	-3.064556	0.521331	-0.004052
8	-1.771610	-1.241022	-0.072011

#####

SP2-II-2-OH b3lyp/6-311g(2d,d,p) if=139.5209

6	-1.966905	0.323768	-0.241386
6	-0.126155	-1.020394	0.007133
6	-0.768526	1.189542	0.179740
1	-2.153225	0.440489	-1.312587
1	-2.881521	0.569515	0.298383
1	0.515598	-1.877004	-0.072392
1	-0.795827	1.516881	1.222409
1	-0.583013	2.047040	-0.463890
7	0.341333	0.220226	0.032213
7	1.549340	0.725295	-0.028610
7	-1.545859	-1.069907	0.016210
1	-1.909688	-1.404609	0.906939
8	2.412059	-0.420944	-0.025598
1	3.267031	-0.011548	-0.185688

#####

SP2-II-3-CH3 b3lyp/6-311g(2d,d,p) if=163.0066

7	0.268092	-0.410473	-0.015895
7	1.492859	-0.762642	-0.049121
7	-0.720795	-1.227230	-0.114463
6	-1.935694	-0.465257	0.136137
1	-2.745163	-0.832138	-0.496371
1	-2.246132	-0.578104	1.185044
6	-1.554230	0.992602	-0.160765

1 -2.102726 1.710796 0.449183
1 -1.690510 1.230788 -1.222602
7 -0.141156 0.980177 0.225600
1 0.444745 1.572209 -0.353581
6 2.459179 0.317053 0.024136
1 3.443067 -0.147580 0.071343
1 2.455896 0.969497 -0.866148
1 2.332290 0.949321 0.913236

#####

SP2-II-3-CN b3lyp/6-311g(2d,d,p) if=109.6014

7 0.051662 -0.484631 -0.011242
7 -1.148573 -1.005399 0.032891
7 1.101741 -1.184176 0.085879
6 2.233487 -0.271827 -0.087991
1 3.034056 -0.547339 0.597618
1 2.608355 -0.368625 -1.114121
6 1.650235 1.128481 0.169356
1 2.112268 1.902177 -0.441937
1 1.711071 1.405992 1.227966
7 0.269510 0.902273 -0.263012
1 -0.463435 1.446141 0.185027
6 -2.139031 -0.122322 0.011025
7 -3.055835 0.594171 0.011356

#####

SP2-II-3-COOH b3lyp/6-311g(2d,d,p) if=89.1844

7 0.417508 -0.463882 -0.038328
7 -0.821800 -0.904850 -0.049994
7 1.386669 -1.246275 0.192779
6 2.611251 -0.464684 0.003245
1 3.343967 -0.749351 0.757280
1 3.023386 -0.698635 -0.986451
6 2.151488 0.998491 0.089584
1 2.719899 1.664713 -0.558066
1 2.177165 1.375982 1.119572
7 0.785974 0.853164 -0.407250
1 0.040139 1.481790 -0.089091
6 -1.802984 0.043864 0.035773
8 -1.717843 1.258574 0.216677
8 -3.005393 -0.553984 -0.079409
1 -3.655649 0.155658 0.006551

#####

SP2-II-3-H b3lyp/6-311g(2d,d,p) if=195.6243

7 -0.782574 -0.145537 -0.000957
7 -2.059173 -0.138191 0.045898
7 -0.043489 -1.182493 0.094273
6 1.336837 -0.759633 -0.106197
1 1.998472 -1.305545 0.568115
1 1.647563 -0.979425 -1.136381
6 1.334394 0.757308 0.156849
1 2.053656 1.294718 -0.461338
1 1.522995 0.975762 1.214416
7 -0.034171 1.095060 -0.245630
1 -0.462710 1.798349 0.349168
1 -2.351521 0.828219 -0.092980

#####

SP2-II-3-NH2 b3lyp/6-311g(2d,d,p) if=149.5890

7 0.263467 -0.403499 0.009541
7 1.505480 -0.763614 -0.031029
7 -0.714731 -1.228315 -0.088317
6 -1.931076 -0.443050 0.116436
1 -2.723665 -0.813054 -0.534811
1 -2.272951 -0.532565 1.157568
6 -1.511441 1.000883 -0.198013
1 -2.067943 1.745808 0.370813
1 -1.592498 1.217873 -1.270691
7 -0.122278 0.956980 0.258527
1 0.570798 1.536777 -0.211098
7 2.340176 0.410047 -0.050214
1 2.693651 0.560252 0.896059
1 3.142920 0.136726 -0.607942

#####

SP2-II-3-NO2 b3lyp/6-311g(2d,d,p) if=80.2036

7 -0.372170 -0.443623 0.021874
7 0.867092 -0.935785 0.076579
7 -1.324249 -1.221220 -0.272209
6 -2.562619 -0.478021 -0.025242
1 -3.293109 -0.729351 -0.792659
1 -2.960081 -0.787523 0.949213
6 -2.125820 0.993533 -0.016109
1 -2.701315 1.606797 0.675221
1 -2.154678 1.437179 -1.018336
7 -0.754181 0.841340 0.473698
1 -0.035595 1.494411 0.153643

7 1.882077 0.016348 -0.034813
8 2.986579 -0.434213 0.177950
8 1.661601 1.194961 -0.374811

SP2-II-3-OH b3lyp/6-311g(2d,d,p) if=153.1324

7 -0.281396 -0.396958 -0.009603
7 -1.517202 -0.753142 0.006772
7 0.693296 -1.230739 0.131883
6 1.907083 -0.458861 -0.125286
1 2.717184 -0.826524 0.504787
1 2.216261 -0.554056 -1.176648
6 1.504231 0.990717 0.184585
1 2.061280 1.726944 -0.394432
1 1.594369 1.212155 1.255396
7 0.109902 0.959755 -0.262394
1 -0.547573 1.570601 0.210215
8 -2.294600 0.443240 0.015867
1 -3.184794 0.081408 0.051348

SP2-II-4-CH3 b3lyp/6-311g(2d,d,p) if=148.5692

7 0.297348 0.219543 -0.047355
7 1.468668 0.730691 0.007765
7 -1.495653 -1.054862 -0.020618
1 -1.780509 -1.328915 -0.961268
7 -1.981720 0.286445 0.208516
1 -2.128379 0.353226 1.211423
6 -0.893813 1.138886 -0.183997
1 -0.935251 1.429975 -1.236867
1 -0.756611 2.010085 0.450193
7 -0.056494 -1.027846 -0.013277
6 2.503208 -0.285899 0.071282
1 2.489159 -0.938575 -0.813170
1 3.465013 0.220513 0.137685
1 2.365158 -0.942027 0.943072

SP2-II-4-CN b3lyp/6-311g(2d,d,p) if=103.5615

7 0.047768 -0.469540 0.011713
7 -1.147107 -1.010900 -0.076973
7 2.205598 -0.293337 -0.026983
1 2.739772 -0.433109 0.829550
7 1.745231 1.070363 -0.129750

1 1.857834 1.321297 -1.107480
6 0.353777 1.021263 0.212291
1 0.141054 1.222813 1.265689
1 -0.279770 1.629809 -0.427959
7 1.109655 -1.166024 -0.009350
6 -2.141190 -0.132850 -0.030347
7 -3.066062 0.573541 -0.004581

#####

SP2-II-4-COOH b3lyp/6-311g(2d,d,p) if=38.3836

7 0.391364 0.222188 0.046614
7 -0.791719 0.783307 0.014845
7 2.179531 -0.999339 -0.048508
1 2.529454 -1.434233 0.803834
7 2.674641 0.353442 -0.170884
1 2.883733 0.470035 -1.157874
6 1.557697 1.179258 0.194830
1 1.553769 1.485137 1.244494
1 1.409079 2.037086 -0.454152
7 0.773051 -0.992962 0.017845
6 -1.878892 -0.075687 -0.011244
8 -1.908996 -1.285807 0.014413
8 -3.003824 0.685837 -0.073486
1 -3.734376 0.053865 -0.084613

#####

SP2-II-4-H b3lyp/6-311g(2d,d,p) if=198.9350

7 -0.774565 -0.128994 -0.003119
7 -2.060332 -0.134154 -0.075497
7 1.330668 -0.763517 0.021789
1 1.660312 -0.981052 0.962720
7 1.391422 0.670055 -0.149823
1 1.557456 0.817476 -1.140861
6 0.082087 1.127184 0.200047
1 -0.022231 1.385097 1.257945
1 -0.285396 1.931117 -0.434562
7 -0.038099 -1.180540 -0.049620
1 -2.346314 0.844313 -0.051640

#####

SP2-II-4-NH2 b3lyp/6-311g(2d,d,p) if=126.9115

7 -0.269524 -0.392584 0.000085
7 -1.508153 -0.763131 -0.110335
7 1.924615 -0.458564 0.021472

1 2.310837 -0.572353 0.959237
7 1.603801 0.932389 -0.165593
1 1.717721 1.107448 -1.159649
6 0.222585 1.054170 0.194611
1 0.069503 1.285506 1.251437
1 -0.352459 1.731121 -0.426138
7 0.710450 -1.223184 -0.020392
7 -2.345013 0.405531 -0.009658
1 -3.079660 0.257790 -0.696793
1 -2.814683 0.362269 0.895183

#####

SP2-II-4-NO2 b3lyp/6-311g(2d,d,p) if=69.3712

7 -0.344286 0.424233 0.030069
7 0.879416 0.935940 0.157992
7 -2.486398 0.470125 -0.227654
1 -3.122780 0.907253 0.435861
7 -2.218562 -0.907634 0.079341
1 -2.263559 -1.396311 -0.810715
6 -0.868714 -0.920075 0.570133
1 -0.786148 -0.821352 1.656632
1 -0.275691 -1.742878 0.195348
7 -1.308980 1.183683 -0.293559
7 1.878192 -0.018400 -0.066161
8 1.617670 -1.115822 -0.578456
8 2.990429 0.360587 0.246189

#####

SP2-II-4-OH b3lyp/6-311g(2d,d,p) if=140.2163

7 -0.284407 -0.398723 0.002056
7 -1.516692 -0.760926 -0.024755
7 1.909638 -0.454813 0.051859
1 2.207093 -0.555124 1.023872
7 1.581335 0.930369 -0.152824
1 1.706068 1.099754 -1.146699
6 0.195938 1.045996 0.190884
1 0.020573 1.280159 1.243620
1 -0.368000 1.717779 -0.448229
7 0.705867 -1.230723 -0.105856
8 -2.291098 0.438168 -0.017936
1 -3.182772 0.079829 -0.067751

#####

SP2-II-5-CH3 b3lyp/6-311g(2d,d,p) if=142.7243

7 -0.292776 -0.217847 -0.000484
7 -1.450748 -0.729467 0.026724
7 1.517135 1.017267 -0.076848
1 1.721927 1.227336 -1.056094
7 0.087389 1.022203 0.063578
7 0.845317 -1.161997 -0.094721
1 0.854653 -1.422883 -1.082000
1 2.081806 -0.377654 1.189647
7 1.947510 -0.329202 0.182865
6 -2.491591 0.286259 0.025504
1 -2.400893 0.962705 -0.835538
1 -3.451736 -0.225761 -0.003071
1 -2.433002 0.912009 0.926240

#####

SP2-II-5-CN b3lyp/6-311g(2d,d,p) if=98.9389

7 -0.058791 0.471357 0.010067
7 1.135340 0.974382 -0.029189
7 -2.214360 0.252869 0.011946
1 -2.642489 0.353719 0.934142
7 -1.128809 1.153624 -0.063389
7 -0.320019 -1.000456 0.148099
1 -0.167531 -1.175105 1.144737
1 -1.741640 -1.260814 -1.155274
7 -1.686082 -1.075939 -0.156601
6 2.135633 0.097069 -0.034249
7 3.092416 -0.561583 -0.023519

#####

SP2-II-5-COOH b3lyp/6-311g(2d,d,p) if=31.5807

7 -0.389745 -0.226326 -0.025202
7 0.776279 -0.787902 -0.055798
7 -2.202860 0.967621 -0.027495
1 -2.434727 1.363388 0.885234
7 -0.790509 0.976432 -0.143512
7 -1.503847 -1.185721 0.178297
1 -1.448958 -1.395350 1.177152
1 -2.835098 -0.558128 -1.091732
7 -2.633923 -0.404516 -0.106871
6 1.867069 0.077425 0.002891
8 1.888117 1.279129 0.129747
8 2.987573 -0.678788 -0.090595
1 3.723077 -0.054304 -0.037150

#####

SP2-II-5-H b3lyp/6-311g(2d,d,p) if=211.3764

7	-0.772980	-0.134063	-0.015015
7	-2.042268	-0.095466	-0.032015
7	1.331221	-0.732018	0.079216
1	1.581236	-0.881984	1.059163
7	-0.020468	-1.169479	-0.094784
7	0.052811	1.146127	0.114367
1	-0.004711	1.329727	1.119471
1	1.461235	0.776884	-1.178816
1	-2.292937	0.885518	-0.151881
7	1.345281	0.683450	-0.172902

#####

SP2-II-5-NH2 b3lyp/6-311g(2d,d,p) if=179.6183

7	-0.275041	-0.404111	-0.000467
7	-1.494895	-0.731534	0.044837
7	1.903122	-0.434174	0.118672
1	2.065839	-0.505433	1.127067
7	0.736831	-1.206125	-0.207908
7	0.166617	1.048799	0.096406
1	0.014433	1.267964	1.083989
1	1.664163	1.049729	-1.148309
7	1.551960	0.934358	-0.143793
7	-2.358806	0.376714	0.055223
1	-2.079816	1.088134	-0.621708
1	-3.273136	0.012114	-0.181831

#####

SP2-II-5-NO2 b3lyp/6-311g(2d,d,p) if=94.5274

7	0.332760	0.419546	-0.009025
7	-0.850908	0.925001	0.282471
7	2.474227	0.450514	-0.166369
1	2.990936	0.391513	-1.043816
7	1.301998	1.142160	-0.370196
7	0.787544	-1.022402	0.282866
1	0.555583	-1.491159	-0.592304
1	2.342210	-0.711518	1.413816
7	2.163327	-0.843382	0.421001
7	-1.858064	-0.004251	-0.031697
8	-2.951773	0.276476	0.408996
8	-1.591342	-0.983869	-0.739128

#####

SP2-II-5-OH b3lyp/6-311g(2d,d,p) if=172.0029

7	-0.278805	-0.375832	-0.017417
7	-1.501729	-0.718876	0.067518
7	1.892338	-0.446072	0.121759
1	2.065317	-0.531298	1.126973
7	0.711719	-1.201799	-0.193416
7	0.166578	1.048983	0.076860
1	-0.014605	1.296703	1.051511
1	1.685457	1.043713	-1.140113
7	1.556705	0.921976	-0.138471
8	-2.297881	0.441611	-0.056053
1	-3.180770	0.059340	-0.007789

#####

SP3-1-CH3 b3lyp/6-311g(2d,d,p) if=72.5092

7	-0.586565	0.400990	0.027881
7	-2.050241	0.240379	0.014892
6	-0.441531	1.880532	0.134263
1	-0.966782	2.305333	-0.717321
1	-0.958972	2.178746	1.042447
1	0.603916	2.185094	0.151562
6	-2.449741	-1.143216	-0.080328
1	-2.167512	-1.695205	-1.005475
1	-3.543277	-1.109858	-0.083735
1	-2.176766	-1.814657	0.765161
6	1.597704	-0.000951	-1.263148
1	1.924226	1.043905	-1.287706
1	1.954121	-0.454060	-2.194013
6	0.069415	-0.088463	-1.249901
1	-0.399774	0.482144	-2.050715
1	-0.241610	-1.127972	-1.357519
6	2.208754	-0.713303	-0.049907
1	3.295237	-0.589801	-0.040570
1	2.013678	-1.790024	-0.126520
6	1.596220	-0.180071	1.251181
1	1.921963	0.850928	1.424064
1	1.951727	-0.760360	2.108942
6	0.068027	-0.265862	1.223529
1	-0.242744	-1.310266	1.181031
1	-0.402880	0.184474	2.096824

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SP3-l-1-CN b3lyp/6-311g(2d,d,p) if=95.6148

7	-0.314488	0.643129	-0.000128
7	-1.791486	0.751621	-0.000087
6	0.124490	2.067843	-0.000740
1	-0.300218	2.535433	-0.885541
1	-0.299440	2.536032	0.884118
1	1.209712	2.139670	-0.001220
6	1.681984	-0.327278	-1.260109
1	2.230220	0.615187	-1.362617
1	1.908725	-0.911247	-2.156958
6	0.174504	-0.077556	-1.244514
1	-0.167912	0.524154	-2.085831
1	-0.375487	-1.020224	-1.258563
6	2.139410	-1.071812	0.000270
1	3.226197	-1.188205	0.000183
1	1.711236	-2.080646	0.000763
6	1.682286	-0.326213	1.260126
1	2.230457	0.616396	1.361642
1	1.909316	-0.909371	2.157432
6	0.174782	-0.076627	1.244658
1	-0.375071	-1.019364	1.259456
1	-0.167545	0.525613	2.085635
6	-2.328756	-0.452351	0.000647
7	-2.841510	-1.506102	0.000139

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SP3-I-1-COOH b3lyp/6-311g(2d,d,p) if=108.6595

7	0.046448	0.675847	0.000153
7	-1.409118	0.845087	0.000150
6	0.529460	2.090377	0.000403
1	0.119234	2.572568	-0.883111
1	0.119979	2.572119	0.884514
1	1.616276	2.129594	0.000005
6	2.040966	-0.301633	-1.260325
1	2.603000	0.633261	-1.359062
1	2.265592	-0.887831	-2.156581
6	0.534745	-0.043145	-1.252968
1	0.207789	0.577173	-2.087329
1	-0.020663	-0.978792	-1.265220
6	2.485883	-1.054648	-0.000235
1	3.571089	-1.188137	-0.000244
1	2.039282	-2.055010	-0.000485
6	2.040897	-0.302290	1.260234
1	2.602890	0.632580	1.359388
1	2.265617	-0.888873	2.156221

6 0.534663 -0.043762 1.252943
1 -0.020733 -0.979409 1.264689
1 0.207642 0.576103 2.087614
6 -2.074524 -0.318278 -0.000109
8 -1.672574 -1.493681 -0.000106
8 -3.424352 -0.076647 -0.000140
1 -3.815428 -0.958987 -0.000202

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SP3-I-1-H b3lyp/6-311g(2d,d,p) if=161.3612

7 -0.943010 -0.000005 -0.074107
7 -2.227388 0.000020 -0.735713
6 -1.296984 -0.000016 1.374811
1 -1.908378 0.882770 1.543776
1 -1.907996 -0.883042 1.543911
1 -0.414395 0.000211 2.013756
6 1.286534 1.263047 0.183108
1 1.235120 1.371287 1.271718
1 1.796840 2.157576 -0.188306
6 -0.123162 1.233429 -0.416225
1 -0.741906 2.079038 -0.119182
1 -0.075806 1.230050 -1.507286
6 2.076245 -0.000015 -0.185663
1 3.050985 -0.000026 0.310044
1 2.271424 -0.000023 -1.265139
6 1.286498 -1.263057 0.183112
1 1.235039 -1.371271 1.271722
1 1.796795 -2.157602 -0.188270
6 -0.123175 -1.233404 -0.416270
1 -0.075749 -1.229968 -1.507329
1 -0.741930 -2.079035 -0.119310
1 -1.962992 0.000031 -1.728597

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SP3-I-1-NH2 b3lyp/6-311g(2d,d,p) if=136.4450

7 -0.560488 -0.421319 -0.000856
7 -2.112944 -0.158256 -0.000321
6 -0.523006 -1.897659 -0.003785
1 -1.064328 -2.234153 0.878137
1 -1.064566 -2.230716 -0.886863
1 0.498794 -2.276771 -0.004639
6 1.595614 0.075695 1.258992
1 1.923507 -0.966023 1.351191
1 1.948884 0.589263 2.159050

6 0.066104 0.156035 1.230430
1 -0.398420 -0.355699 2.073787
1 -0.266299 1.196746 1.239468
6 2.207222 0.705662 0.001439
1 3.294416 0.585608 0.001193
1 2.005934 1.783709 0.003672
6 1.595627 0.080906 -1.258726
1 1.923557 -0.960402 -1.355265
1 1.948853 0.598227 -2.156650
6 0.066108 0.161067 -1.229789
1 -0.266262 1.201810 -1.234521
1 -0.398422 -0.347139 -2.075264
7 -2.269838 1.235660 0.002442
1 -2.764644 1.567961 -0.823115
1 -2.764121 1.564749 0.829590

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SP3-I-1-NO2 b3lyp/6-311g(2d,d,p) if=106.3678

7 0.008139 0.646740 0.000099
7 -1.473845 0.821036 0.000062
6 0.436948 2.081092 0.000512
1 0.015940 2.551376 -0.884315
1 0.015839 2.550887 0.885552
1 1.521266 2.150605 0.000592
6 2.024966 -0.267011 -1.259849
1 2.565742 0.681082 -1.350738
1 2.267397 -0.843162 -2.157627
6 0.512959 -0.043363 -1.262624
1 0.180912 0.585269 -2.088601
1 -0.019402 -0.989943 -1.298357
6 2.479820 -1.014330 -0.000199
1 3.566768 -1.129971 -0.000165
1 2.050175 -2.022132 -0.000506
6 2.024807 -0.267705 1.259807
1 2.565576 0.680334 1.351293
1 2.267116 -0.844355 2.157297
6 0.512803 -0.044048 1.262510
1 -0.019579 -0.990639 1.297656
1 0.180651 0.584140 2.088783
7 -2.156132 -0.346583 -0.000095
8 -3.375766 -0.212038 -0.000148
8 -1.594155 -1.472919 -0.000137

#####

SP3-I-1-OH b3lyp/6-311g(2d,d,p) if=132.5646

7	0.603422	-0.388425	0.112516
7	2.095564	-0.126017	-0.003217
6	0.588766	-1.806229	0.543288
1	1.173635	-2.361493	-0.187328
1	1.089508	-1.861445	1.507619
1	-0.427037	-2.191981	0.608972
6	-1.581071	-0.316921	-1.212405
1	-1.893045	-1.345362	-0.996438
1	-1.949967	-0.090513	-2.217706
6	-0.054383	-0.209021	-1.234349
1	0.415174	-0.943159	-1.888047
1	0.267821	0.780636	-1.559134
6	-2.195512	0.638875	-0.182708
1	-3.280390	0.508926	-0.137163
1	-2.011907	1.674176	-0.493883
6	-1.569121	0.406632	1.197388
1	-1.873757	-0.571635	1.586187
1	-1.930564	1.148419	1.916888
6	-0.043033	0.507702	1.135976
1	0.258425	1.514811	0.843476
1	0.436100	0.269194	2.085817
8	2.186476	1.250192	-0.455347
1	2.467421	1.742756	0.325282

#####

SP3-I-2-CH3 b3lyp/6-311g(2d,d,p) if=89.0821

7	-0.541664	-0.221133	0.056246
7	-1.765033	-0.490589	-0.710376
6	-0.727346	-0.464656	1.526023
1	-1.448625	0.256671	1.903751
1	-1.138805	-1.466795	1.623513
1	0.206262	-0.369962	2.082791
6	-2.837475	0.399098	-0.326698
1	-3.216635	0.316218	0.716492
1	-3.676585	0.110889	-0.966395
1	-2.681608	1.485619	-0.508398
6	1.476947	1.343741	0.249353
1	1.553150	1.319157	1.342356
1	1.818380	2.335862	-0.059654
6	0.019764	1.169636	-0.193797
1	-0.639207	1.881402	0.303745
1	-0.090515	1.298215	-1.272199
6	1.874406	-1.014483	-0.051516

1 1.985402 -1.232014 1.016743
1 2.507188 -1.735236 -0.575993
6 0.429681 -1.223794 -0.508897
1 0.320789 -1.106552 -1.587642
1 0.032690 -2.204628 -0.247488
7 2.387351 0.336395 -0.294805
1 2.487684 0.481193 -1.295879

#####

SP3-I-2-CN b3lyp/6-311g(2d,d,p) if=82.4118

7 -0.295638 -0.341547 0.034672
7 -1.493497 -0.735403 -0.741352
6 -0.524969 -0.574273 1.498660
1 -1.379329 0.030927 1.797368
1 -0.767359 -1.627261 1.622745
1 0.353978 -0.307848 2.084012
6 1.491210 1.453575 0.243661
1 1.531063 1.463121 1.338230
1 1.720813 2.471854 -0.079501
6 0.082626 1.101157 -0.246582
1 -0.694662 1.722528 0.199476
1 0.008452 1.191019 -1.331289
6 2.181955 -0.849615 0.000736
1 2.279121 -1.042809 1.074607
1 2.913489 -1.493886 -0.492783
6 0.788084 -1.243192 -0.497261
1 0.706431 -1.155618 -1.580953
1 0.504352 -2.259298 -0.223032
7 2.528863 0.548536 -0.248405
1 2.670582 0.695967 -1.243353
6 -2.520245 0.005423 -0.367611
7 -3.430999 0.664535 -0.038508

#####

SP3-I-2-COOH b3lyp/6-311g(2d,d,p) if=106.5777

7 0.057142 -0.287008 0.183861
7 -1.196456 -0.794228 -0.378640
6 -0.022066 -0.186539 1.683755
1 -0.784759 0.551629 1.913863
1 -0.322495 -1.166717 2.048139
1 0.941366 0.097405 2.103692
6 1.935323 1.394590 -0.162363
1 2.072107 1.642028 0.895697
1 2.175565 2.303248 -0.720444

6 0.475518 1.034493 -0.449380
1 -0.234860 1.778723 -0.096667
1 0.314140 0.878360 -1.517682
6 2.510051 -0.936937 0.065687
1 2.700083 -0.895516 1.143386
1 3.163101 -1.719598 -0.328565
6 1.061418 -1.342536 -0.218196
1 0.887449 -1.492441 -1.283713
1 0.765917 -2.257232 0.295738
7 2.894544 0.348141 -0.517918
1 2.942831 0.261249 -1.529119
6 -2.228509 0.032110 -0.151107
8 -2.285872 1.121386 0.440548
8 -3.370211 -0.493833 -0.697963
1 -4.048797 0.159031 -0.486507

#####

SP3-I-2-H b3lyp/6-311g(2d,d,p) if=166.4437

7 -0.927608 0.001394 -0.077847
7 -2.096535 -0.111032 -0.921458
6 -1.305587 0.010640 1.376417
1 -1.904044 0.904725 1.545723
1 -1.928079 -0.865946 1.534898
1 -0.441474 0.011290 2.048936
6 1.324624 1.207887 0.173567
1 1.291554 1.319460 1.263376
1 1.877732 2.070499 -0.208516
6 -0.092440 1.226673 -0.415894
1 -0.671236 2.091840 -0.084571
1 -0.080472 1.227010 -1.506282
6 1.291140 -1.206566 0.199726
1 1.250913 -1.286439 1.292137
1 1.827810 -2.091603 -0.151740
6 -0.116672 -1.225198 -0.400334
1 -0.095298 -1.241030 -1.490641
1 -0.714855 -2.075592 -0.072252
7 2.069081 -0.012325 -0.138774
1 2.292106 -0.026092 -1.130232
1 -2.625611 0.735006 -0.675176

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SP3-I-2-NH2 b3lyp/6-311g(2d,d,p) if=135.5356

7 -0.512677 -0.219290 0.065531
7 -1.812039 -0.470526 -0.751060

6	-0.767603	-0.445857	1.511620
1	-1.593560	0.210734	1.782730
1	-1.074286	-1.483434	1.630286
1	0.106654	-0.232064	2.131593
6	1.474098	1.343264	0.260838
1	1.544157	1.319152	1.354076
1	1.821156	2.333124	-0.048664
6	0.021739	1.160137	-0.194969
1	-0.668312	1.857634	0.281258
1	-0.066863	1.280264	-1.277020
6	1.870531	-1.022148	-0.045299
1	1.968665	-1.241412	1.024018
1	2.510332	-1.739261	-0.566270
6	0.424597	-1.227492	-0.505603
1	0.320539	-1.113887	-1.586822
1	0.029334	-2.208931	-0.241688
7	2.385636	0.330658	-0.278785
1	2.492229	0.478149	-1.278878
7	-2.758937	0.447441	-0.250810
1	-3.061542	1.104640	-0.967129
1	-3.582549	-0.030112	0.108856

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SP3-l-2-NO2 b3lyp/6-311g(2d,d,p) if=102.4057

7	0.022331	-0.264453	0.188880
7	-1.231063	-0.796480	-0.416856
6	-0.066227	-0.206002	1.689665
1	-0.814387	0.536177	1.946076
1	-0.382084	-1.191560	2.025615
1	0.902649	0.047774	2.115229
6	1.926398	1.385762	-0.135662
1	2.063168	1.615960	0.926263
1	2.179960	2.298882	-0.679835
6	0.459656	1.057447	-0.429770
1	-0.230345	1.814196	-0.068474
1	0.296102	0.919206	-1.500258
6	2.463828	-0.955124	0.059413
1	2.652499	-0.934746	1.137747
1	3.102405	-1.743506	-0.346510
6	1.009733	-1.334236	-0.233209
1	0.839397	-1.463644	-1.301941
1	0.701658	-2.252395	0.266376
7	2.868795	0.330797	-0.503937
1	2.927581	0.260073	-1.515614

7 -2.298117 0.008985 -0.207725
8 -3.343873 -0.408639 -0.694678
8 -2.222697 1.090459 0.428449

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SP3-I-2-OH b3lyp/6-311g(2d,d,p) if=134.3020

7 -0.536924 -0.226810 0.044301
7 -1.774640 -0.485895 -0.782963
6 -0.809141 -0.423653 1.497868
1 -1.619161 0.254803 1.757750
1 -1.136762 -1.453190 1.628787
1 0.063710 -0.215732 2.120348
6 1.444956 1.349877 0.247565
1 1.495588 1.347854 1.342322
1 1.795009 2.334443 -0.074186
6 0.004563 1.157602 -0.234545
1 -0.699583 1.860741 0.208398
1 -0.069847 1.249651 -1.319307
6 1.857674 -1.018303 0.000709
1 1.938072 -1.213419 1.076184
1 2.508328 -1.745196 -0.492224
6 0.421880 -1.247315 -0.480986
1 0.337717 -1.161136 -1.566410
1 0.030511 -2.224046 -0.194605
7 2.369392 0.329809 -0.254498
1 2.496536 0.456854 -1.254846
8 -2.713231 0.529901 -0.331891
1 -3.358656 0.040183 0.191371

#####

SP3-I-3-CH3 b3lyp/6-311g(2d,d,p) if=53.3019

7 -0.559548 0.417053 -0.004108
6 0.120554 -0.174753 1.242732
1 -0.220935 -1.208101 1.281975
1 -0.296040 0.365845 2.090674
6 2.112207 -0.729287 0.007557
1 1.899111 -1.803387 0.022136
1 3.195099 -0.602343 0.004170
6 0.116600 -0.209637 -1.235525
1 -0.303559 0.305661 -2.097434
1 -0.223001 -1.244362 -1.243934
6 -2.440536 -1.109956 0.012225
1 -2.170568 -1.723377 0.899411
1 -3.532859 -1.053509 0.021253

1 -2.185623 -1.731751 -0.873477
6 -0.371738 1.888763 -0.025178
1 -0.873842 2.259236 -0.916053
1 -0.884587 2.284321 0.848630
1 0.684542 2.161632 -0.022701
7 1.562151 -0.152346 1.234208
1 1.924628 0.780541 1.397359
7 1.558095 -0.185274 -1.232298
1 1.919037 0.743464 -1.420495
7 -2.011259 0.274188 0.001858

#####

SP3-I-3-CN b3lyp/6-311g(2d,d,p) if=94.4150

7 -0.280323 0.658246 0.000015
6 0.223720 -0.110391 1.247949
1 -0.368347 -1.026605 1.247992
1 -0.057888 0.498157 2.105380
6 2.029991 -1.093863 -0.000038
1 1.571047 -2.087134 -0.000146
1 3.112195 -1.220550 -0.000001
6 0.223829 -0.110172 -1.248008
1 -0.057704 0.498525 -2.105358
1 -0.368232 -1.026389 -1.248268
6 0.218703 2.054244 0.000160
1 -0.178468 2.546705 -0.884903
1 -0.178545 2.546551 0.885274
1 1.307937 2.072715 0.000210
7 1.620684 -0.415352 1.229389
1 2.201564 0.388601 1.437324
7 1.620793 -0.415136 -1.229382
1 2.201689 0.388855 -1.437123
7 -1.735352 0.792922 -0.000021
6 -2.311035 -0.396180 -0.000049
7 -2.868159 -1.426574 -0.000068

#####

SP3-I-3-COOH b3lyp/6-311g(2d,d,p) if=103.9872

7 -0.068448 0.677992 0.000021
6 -0.580248 -0.087461 -1.255051
1 -0.001225 -1.008006 -1.245346
1 -0.299370 0.528879 -2.107455
6 -2.393166 -1.048852 -0.000001
1 -1.934261 -2.041550 -0.000043
1 -3.476142 -1.172634 -0.000013

6	-0.580154	-0.087694	1.254928
1	-0.299064	0.528410	2.107434
1	-0.001238	-1.008299	1.244961
6	-0.595527	2.067554	0.000109
1	-0.208251	2.568490	0.884557
1	-0.206864	2.568940	-0.883465
1	-1.684681	2.067255	-0.000668
7	-1.983888	-0.369684	-1.229771
1	-2.553064	0.447935	-1.417312
7	-1.983841	-0.369804	1.229797
1	-2.552937	0.447864	1.417363
7	1.371204	0.863698	0.000076
6	2.057697	-0.288976	0.000010
8	1.674738	-1.470953	-0.000060
8	3.401681	-0.025281	-0.000033
1	3.808940	-0.900245	-0.000112

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SP3-I-3-H b3lyp/6-311g(2d,d,p) if=177.3448

7	0.922526	0.000011	-0.067140
6	0.061739	1.233687	-0.403967
1	0.023071	1.224064	-1.495092
1	0.644577	2.095752	-0.084679
6	-1.993529	-0.000089	-0.177542
1	-2.195530	-0.000184	-1.254145
1	-2.951536	-0.000104	0.342857
6	0.061857	-1.233628	-0.403944
1	0.644776	-2.095692	-0.084795
1	0.022987	-1.223987	-1.495064
6	1.278043	0.000071	1.373436
1	1.887229	-0.883774	1.549790
1	1.888488	0.883162	1.549197
1	0.391261	0.000877	2.009694
7	-1.273678	1.234825	0.134548
1	-1.281847	1.433650	1.128727
7	-1.273539	-1.234896	0.134704
1	-1.281512	-1.433428	1.128950
7	2.176785	0.000038	-0.756269
1	1.894720	-0.000427	-1.744229

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SP3-I-3-NH2 b3lyp/6-311g(2d,d,p) if=131.1048

7	-0.552415	0.431000	-0.000178
6	0.109233	-0.172576	1.232807

1 -0.248657 -1.202253 1.235216
1 -0.304559 0.356537 2.090059
6 2.104058 -0.716011 0.000341
1 1.885570 -1.788620 0.001021
1 3.187627 -0.591883 0.000186
6 0.109059 -0.174086 -1.232520
1 -0.304846 0.353985 -2.090357
1 -0.248867 -1.203755 -1.233618
6 -0.456416 1.902293 -0.001077
1 -0.980810 2.261822 -0.884515
1 -0.980637 2.262885 0.882029
1 0.582787 2.234100 -0.001380
7 1.553760 -0.152469 1.233537
1 1.913812 0.781916 1.398388
7 1.553589 -0.154000 -1.233477
1 1.913638 0.780170 -1.399553
7 -2.050857 0.197509 0.000044
7 -2.230301 -1.218595 0.000641
1 -2.763762 -1.503028 0.819550
1 -2.763334 -1.503704 -0.818307

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SP3-I-3-NO2 b3lyp/6-311g(2d,d,p) if=103.3115

7 -0.024676 0.646668 -0.000113
6 -0.561419 -0.092559 -1.265986
1 -0.009206 -1.027434 -1.275217
1 -0.271594 0.529200 -2.111325
6 -2.394676 -1.003364 0.000217
1 -1.958975 -2.006454 0.000311
1 -3.479916 -1.102238 0.000254
6 -0.561255 -0.092374 1.265867
1 -0.271134 0.529440 2.111055
1 -0.009152 -1.027321 1.275057
6 -0.501968 2.056316 -0.000254
1 -0.103972 2.547284 0.884954
1 -0.102591 2.547411 -0.884764
1 -1.589703 2.084179 -0.001045
7 -1.970472 -0.331978 -1.228571
1 -2.519361 0.498955 -1.416973
7 -1.970352 -0.331727 1.228824
1 -2.519123 0.499349 1.416982
7 1.437620 0.843494 0.000187
7 2.142385 -0.313223 -0.000004
8 1.597756 -1.449032 -0.000211

8 3.358381 -0.160110 0.000136

SP3-I-3-OH b3lyp/6-311g(2d,d,p) if=140.1849

7 -0.585636 0.417857 0.032518
6 0.088589 -0.277632 1.216378
1 -0.243009 -1.311352 1.126651
1 -0.341700 0.165206 2.113760
6 2.096349 -0.674481 -0.048577
1 1.895857 -1.746574 -0.142001
1 3.177433 -0.533456 -0.029007
6 0.102609 -0.062552 -1.253141
1 -0.316436 0.539737 -2.056908
1 -0.244640 -1.088914 -1.358673
6 -0.520003 1.887362 0.160545
1 -1.102698 2.304249 -0.659336
1 -0.990490 2.164769 1.102152
1 0.511441 2.238277 0.124508
7 1.529368 -0.228407 1.225573
1 1.870298 0.694530 1.473454
7 1.543076 -0.014831 -1.229986
1 1.891673 0.933586 -1.319296
7 -2.052163 0.159078 -0.028571
8 -2.155527 -1.292757 -0.185326
1 -2.511302 -1.590067 0.659337

SP3-I-4-CH3 b3lyp/6-311g(2d,d,p) if=68.0721

7 -0.650970 -0.409375 -0.001623
6 -2.357849 1.188523 0.004996
1 -2.017389 1.744668 -0.879272
1 -3.449993 1.199157 0.009656
1 -2.009682 1.740322 0.888916
6 -0.429427 -1.892567 -0.007865
1 -0.921809 -2.289816 0.875909
1 -0.920272 -2.282401 -0.895824
1 0.629918 -2.136877 -0.008023
7 -1.970867 -0.218266 0.000142
7 0.091122 0.262561 -1.197212
1 -0.341710 -0.198628 -1.996315
6 1.555865 0.116159 -1.182563
1 1.905904 -0.925904 -1.229503
1 1.926587 0.624997 -2.077419
1 -0.338946 -0.217255 1.995153

7 2.131297 0.720900 0.002162
1 1.886900 1.708547 0.006553
1 1.908144 -0.936456 1.219963
7 0.093016 0.251948 1.200320
6 1.557656 0.105928 1.182505
1 1.929693 0.607009 2.081235

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SP3-I-4-CN b3lyp/6-311g(2d,d,p) if=84.1465

7 0.286097 0.618110 0.000002
6 -0.224791 2.035476 0.000005
1 0.178888 2.517563 0.886309
1 0.178892 2.517569 -0.886294
1 -1.310989 2.052818 0.000003
7 1.685340 0.757955 -0.000001
7 -0.189180 -0.163920 -1.167390
1 0.168622 0.345516 -1.972460
6 -1.647921 -0.386670 -1.182989
1 -2.238821 0.537603 -1.251011
1 -1.849509 -0.978033 -2.078000
1 0.168631 0.345499 1.972461
7 -2.068153 -1.107210 -0.000001
1 -1.620749 -2.020778 -0.000005
1 -2.238817 0.537595 1.251020
7 -0.189176 -0.163925 1.167386
6 -1.647916 -0.386678 1.182989
1 -1.849501 -0.978046 2.077998
6 2.316160 -0.416434 -0.000001
7 2.995095 -1.362649 -0.000004

#####

SP3-I-4-COOH b3lyp/6-311g(2d,d,p) if=82.2563

7 0.062085 0.664108 -0.000207
6 0.587979 2.078704 -0.000615
1 0.188224 2.566058 -0.885703
1 0.188111 2.566621 0.884092
1 1.674999 2.084013 -0.000617
7 -1.332244 0.832768 0.000167
7 0.541633 -0.096659 1.179437
1 0.209732 0.445339 1.973316
6 1.991007 -0.354848 1.179831
1 2.613627 0.550873 1.226782
1 2.187172 -0.940673 2.080111
1 0.209917 0.444351 -1.973682

7 2.375685 -1.101736 0.000324
1 1.863677 -1.981662 0.000656
1 2.613510 0.549972 -1.227247
7 0.541421 -0.097303 -1.179390
6 1.990954 -0.355719 -1.179614
1 2.186883 -0.942170 -2.079529
6 -2.039654 -0.337758 0.000058
8 -1.700887 -1.507343 -0.000042
8 -3.375857 -0.002164 0.000208
1 -3.823678 -0.857183 0.000218

#####

SP3-I-4-H b3lyp/6-311g(2d,d,p) if=167.2976

7 0.963635 0.000033 -0.115932
6 1.293959 -0.000377 1.348266
1 1.895317 -0.886380 1.534197
1 1.894859 0.885806 1.534874
1 0.398326 -0.000826 1.964626
7 2.127115 -0.000099 -0.781280
7 0.050302 1.180908 -0.491072
1 0.633244 1.983285 -0.256779
6 -1.258380 1.186488 0.188674
1 -1.194651 1.245868 1.285017
1 -1.785778 2.079600 -0.157130
1 0.632559 -1.983411 -0.256902
7 -2.022630 0.000328 -0.149835
1 -2.177016 0.000472 -1.155392
1 -1.195276 -1.245971 1.284740
7 0.049704 -1.181014 -0.491374
6 -1.258918 -1.186292 0.188404
1 -1.786776 -2.079061 -0.157614
1 1.848336 0.000612 -1.765239

#####

SP3-I-4-NH2 b3lyp/6-311g(2d,d,p) if=123.2795

7 0.609168 0.375964 -0.000127
6 0.447521 1.868975 -0.000681
1 0.952149 2.245915 0.884556
1 0.951906 2.245280 -0.886329
1 -0.603143 2.145897 -0.000646
7 1.989258 0.193834 -0.000078
7 -0.090162 -0.259612 -1.179480
1 0.368542 0.177300 -1.976240
6 -1.554567 -0.103328 -1.181174

1 -1.900364 0.940523 -1.227808
1 -1.916695 -0.610038 -2.079582
1 0.368447 0.178768 1.976160
7 -2.138277 -0.709151 0.000232
1 -1.891092 -1.696512 0.000618
1 -1.900460 0.941462 1.227030
7 -0.090245 -0.258715 1.179710
6 -1.554636 -0.102420 1.181210
1 -1.916815 -0.608451 2.079982
7 2.262211 -1.213776 0.000500
1 2.831697 -1.420104 -0.815189
1 2.832250 -1.419213 0.816012

#####

SP3-I-4-NO2 b3lyp/6-311g(2d,d,p) if=82.7284

7 0.029425 0.650034 -0.000043
6 0.503966 2.084720 -0.000210
1 0.093704 2.561854 -0.886144
1 0.093664 2.562137 0.885557
1 1.589808 2.115546 -0.000173
7 -1.399560 0.830430 0.000093
7 0.508302 -0.087944 1.180589
1 0.172855 0.455532 1.971848
6 1.962398 -0.332237 1.179214
1 2.572171 0.581921 1.225615
1 2.163718 -0.915016 2.079802
1 0.171676 0.454137 -1.971913
7 2.354196 -1.072458 -0.000071
1 1.866259 -1.965491 0.000159
1 2.571886 0.581472 -1.226425
7 0.508062 -0.088213 -1.180319
6 1.961935 -0.332571 -1.179498
1 2.162957 -0.915652 -2.079959
7 -2.111022 -0.363106 0.000123
8 -1.582541 -1.471922 0.000471
8 -3.324248 -0.167718 -0.000220

#####

SP3-I-4-OH b3lyp/6-311g(2d,d,p) if=120.2717

7 0.640226 0.363317 -0.035791
6 0.529524 1.851267 -0.201862
1 1.149962 2.297194 0.570858
1 0.931039 2.104283 -1.179651
1 -0.503531 2.174092 -0.111090

7 2.010091 0.141329 0.043493
7 -0.041999 -0.399385 -1.116492
1 0.478578 -0.157399 -1.955736
6 -1.492124 -0.183415 -1.190263
1 -1.791109 0.863202 -1.351840
1 -1.844892 -0.762678 -2.046814
1 0.315185 0.454995 1.953422
7 -2.138172 -0.646257 0.023994
1 -1.941488 -1.639254 0.126338
1 -1.895614 1.101742 1.104442
7 -0.108604 -0.120473 1.226392
6 -1.575996 0.050664 1.162455
1 -1.978831 -0.363441 2.090781
8 2.216275 -1.274177 0.030932
1 2.051287 -1.560138 0.938686

#####

SP3-I-5-CN b3lyp/6-311g(2d,d,p) if=90.1735

7 0.237104 0.817279 0.094091
6 -0.110779 2.220723 0.434736
1 0.346448 2.461857 1.393144
1 0.318755 2.855058 -0.337195
1 -1.193993 2.340703 0.492957
7 -1.871060 -0.008486 -0.814452
1 -2.301836 0.686532 -0.194231
7 1.617392 0.816095 -0.192889
7 -0.563945 0.317516 -1.131047
1 -0.521808 1.073537 -1.809594
6 -0.236156 -0.174147 1.246124
1 -1.004952 0.358329 1.808817
1 0.652041 -0.318683 1.856467
7 -0.715658 -1.408419 0.746947
1 0.022750 -1.923670 0.277412
7 -1.824133 -1.310036 -0.157360
1 -2.682163 -1.371602 0.386049
6 2.082477 -0.422873 -0.268289
7 2.541943 -1.495990 -0.309468

#####

SP3-I-5-COOH b3lyp/6-311g(2d,d,p) if=98.8116

7 -0.102788 0.808843 0.170123
6 -0.521207 2.190813 0.539641
1 -0.131778 2.403791 1.533746
1 -0.064955 2.870011 -0.175806

1 -1.609275 2.277813 0.538715
7 -2.124815 0.093377 -0.966684
1 -2.582417 0.800544 -0.381015
7 1.291793 0.906278 -0.022243
7 -0.774352 0.359488 -1.131538
1 -0.627036 1.126381 -1.782644
6 -0.694779 -0.224222 1.246864
1 -1.471097 0.332603 1.774291
1 0.138356 -0.447243 1.905032
7 -1.200308 -1.408108 0.660290
1 -0.419730 -1.890911 0.218959
7 -2.219605 -1.219872 -0.327026
1 -3.123117 -1.222913 0.141317
6 1.920085 -0.284305 -0.088716
8 1.504722 -1.433720 0.092481
8 3.239859 -0.085223 -0.375865
1 3.620335 -0.972297 -0.372734

#####

SP3-I-5-NO2 b3lyp/6-311g(2d,d,p) if=92.7407

7 0.039942 0.774252 -0.179352
6 0.397053 2.176443 -0.547840
1 0.013380 2.370754 -1.547693
1 -0.090710 2.840944 0.160685
1 1.479726 2.305424 -0.533255
7 2.067562 0.173903 0.988464
1 2.496134 0.921252 0.432379
7 -1.379695 0.870018 -0.002723
7 0.700744 0.351860 1.127499
1 0.492218 1.097479 1.786680
6 0.686245 -0.232167 -1.256475
1 1.421817 0.375434 -1.785493
1 -0.131544 -0.512226 -1.911299
7 1.276941 -1.371766 -0.666171
1 0.545217 -1.923258 -0.230000
7 2.269766 -1.117359 0.331600
1 3.176319 -1.048231 -0.125169
7 -1.998221 -0.339600 0.118617
8 -3.185678 -0.264270 0.402003
8 -1.407025 -1.421027 -0.082812

#####

SP3-I-6-CN b3lyp/6-311g(2d,d,p) if=66.8292

7 -0.941730 -0.249771 0.000212

6 -2.422567 -0.323731 -0.000320
1 -2.708460 -0.867609 -0.895974
1 -2.709114 -0.868540 0.894554
1 -2.845219 0.682504 -0.000003
7 -0.473314 -1.551485 0.000248
7 -0.533788 0.560681 1.261265
1 -1.121230 1.395643 1.215275
7 -0.533321 0.560593 -1.261404
1 -1.120692 1.395632 -1.215412
7 1.219805 1.615723 0.000000
1 0.907854 2.581804 -0.000251
7 0.797324 0.994890 1.201387
1 1.409517 0.210460 1.402330
7 0.797595 0.994461 -1.201383
1 1.409870 0.209991 -1.401916
6 0.840698 -1.676290 0.000182
7 1.991528 -1.887915 -0.000008

#####

SP3-I-6-COOH b3lyp/6-311g(2d,d,p) if=84.3179

7 0.164674 0.701066 -0.147312
6 -0.356147 2.099974 -0.135568
1 -0.640257 2.328178 -1.160068
1 -1.211388 2.111923 0.532608
1 0.439331 2.769813 0.199676
7 -0.661468 -0.319560 -0.631098
7 0.652357 0.364423 1.277595
1 1.330719 1.093942 1.503647
7 1.342694 0.685563 -1.083138
1 1.986154 1.378723 -0.698706
7 2.314870 -1.047381 0.257684
1 3.173666 -0.600199 0.562301
7 1.329712 -0.862183 1.271507
1 0.628818 -1.587569 1.165210
7 1.992883 -0.561681 -1.041739
1 1.346821 -1.217232 -1.472172
6 -1.894597 -0.345801 -0.068483
8 -2.431975 0.405245 0.739951
8 -2.574652 -1.425191 -0.562507
1 -3.446437 -1.364774 -0.152226

#####

SP3-I-6-NO2 b3lyp/6-311g(2d,d,p) if=100.1433

7 0.088426 0.923438 0.000254

6	0.264216	2.407252	-0.000565
1	-0.225744	2.785744	-0.892750
1	-0.226043	2.786755	0.891007
1	1.328946	2.647703	-0.000479
7	-1.344095	0.824977	0.000322
7	0.789276	0.421460	1.272943
1	1.563006	1.075531	1.377046
7	0.789770	0.420228	-1.273414
1	1.563600	1.074365	-1.376924
7	2.049441	-1.183048	0.000232
1	2.956902	-0.727770	-0.000084
7	1.358828	-0.863335	1.196047
1	0.592390	-1.522473	1.283847
7	1.358497	-0.864045	-1.195922
1	0.592163	-1.523253	-1.283247
7	-1.813990	-0.436829	0.000098
8	-1.051326	-1.439597	0.000549
8	-3.031622	-0.527908	-0.000416

#####

SP3-II-1-CH3 b3lyp/6-311g(2d,d,p) if=103.3505

7	0.710190	0.000002	-0.077632
6	1.036792	-0.000029	1.379397
1	1.641908	-0.884181	1.562038
1	1.641920	0.884108	1.562071
1	0.135239	-0.000033	1.994392
7	1.980085	0.000018	-0.727665
6	-0.207937	1.180732	-0.394122
1	-0.135673	1.296653	-1.475334
1	0.208136	2.069706	0.075373
6	-1.617889	0.781673	0.053479
1	-2.372138	1.187243	-0.622828
1	-1.843603	1.167992	1.049372
6	-1.617877	-0.781683	0.053472
1	-2.372145	-1.187264	-0.622806
1	-1.843543	-1.168013	1.049372
6	-0.207933	-1.180710	-0.394177
1	0.208150	-2.069713	0.075254
1	-0.135691	-1.296565	-1.475399
1	1.724580	0.000031	-1.722719

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SP3-II-1-CN b3lyp/6-311g(2d,d,p) if=83.4297

7	0.000190	0.576078	0.000001
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6	0.694945	1.895565	0.000005
1	0.367463	2.434001	-0.885822
1	0.367457	2.433999	0.885830
1	1.775729	1.757342	0.000008
7	-1.423328	0.927393	0.000000
6	0.442959	-0.265014	1.186534
1	-0.337698	-1.015409	1.312319
1	0.468610	0.371782	2.068432
6	1.781679	-0.889773	0.779865
1	1.867872	-1.898122	1.185977
1	2.625232	-0.315649	1.167309
6	1.781685	-0.889760	-0.779868
1	1.867893	-1.898101	-1.185998
1	2.625233	-0.315619	-1.167296
6	0.442961	-0.265009	-1.186534
1	0.468606	0.371788	-2.068431
1	-0.337692	-1.015409	-1.312319
6	-2.151033	-0.171373	-0.000001
7	-2.822274	-1.131815	-0.000003

#####

SP3-II-1-COOH b3lyp/6-311g(2d,d,p) if=82.7426

7	0.328418	0.581693	-0.000309
6	0.971287	1.931043	-0.001117
1	0.622765	2.457340	-0.885969
1	0.623890	2.457982	0.883793
1	2.056844	1.835187	-0.001820
7	-1.091273	0.893688	-0.000041
6	0.828566	-0.224682	1.193358
1	0.106014	-1.027104	1.313115
1	0.822908	0.425977	2.065857
6	2.206224	-0.756254	0.780083
1	2.359223	-1.757163	1.185305
1	3.012488	-0.128642	1.164954
6	2.205258	-0.759237	-0.779204
1	2.354750	-1.762266	-1.180467
1	3.012896	-0.135577	-1.167533
6	0.828378	-0.225767	-1.193337
1	0.824267	0.424619	-2.066051
1	0.104942	-1.027311	-1.313493
6	-1.862096	-0.201431	0.000204
8	-1.562628	-1.407223	0.000351
8	-3.184074	0.158720	0.000168
1	-3.653089	-0.684725	0.000675

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SP3-II-1-H b3lyp/6-311g(2d,d,p) if=103.3505

7	0.710190	0.000002	-0.077632
6	1.036792	-0.000029	1.379397
1	1.641908	-0.884181	1.562038
1	1.641920	0.884108	1.562071
1	0.135239	-0.000033	1.994392
7	1.980085	0.000018	-0.727665
6	-0.207937	1.180732	-0.394122
1	-0.135673	1.296653	-1.475334
1	0.208136	2.069706	0.075373
6	-1.617889	0.781673	0.053479
1	-2.372138	1.187243	-0.622828
1	-1.843603	1.167992	1.049372
6	-1.617877	-0.781683	0.053472
1	-2.372145	-1.187264	-0.622806
1	-1.843543	-1.168013	1.049372
6	-0.207933	-1.180710	-0.394177
1	0.208150	-2.069713	0.075254
1	-0.135691	-1.296565	-1.475399
1	1.724580	0.000031	-1.722719

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SP3-II-1-NH2 b3lyp/6-311g(2d,d,p) if=92.8233

7	0.302752	0.409126	-0.000011
6	0.049877	1.868096	-0.000618
1	0.534032	2.277536	0.883197
1	0.534363	2.276872	-0.884561
1	-1.019490	2.083432	-0.000903
7	1.815535	0.340351	0.000192
6	-0.358050	-0.265451	-1.176653
1	0.188560	-1.202419	-1.286633
1	-0.206158	0.349717	-2.061894
6	-1.821278	-0.502464	-0.779915
1	-2.187611	-1.446557	-1.187654
1	-2.472287	0.285190	-1.165489
6	-1.821523	-0.501864	0.779925
1	-2.187958	-1.445656	1.188268
1	-2.472686	0.286062	1.164680
6	-0.358422	-0.264515	1.176955
1	-0.206833	0.351386	2.061739
1	0.188185	-1.201373	1.287863
7	2.136494	-1.042858	0.000194

1 2.690565 -1.281634 -0.820039
1 2.690231 -1.281698 0.820634

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SP3-II-1-NO2 b3lyp/6-311g(2d,d,p) if=42.0441

7 -0.284327 0.567360 -0.000414
6 -0.874735 1.943235 -0.001064
1 -0.514793 2.459488 0.885065
1 -0.513659 2.458921 -0.887056
1 -1.961667 1.877079 -0.001743
7 1.159018 0.881905 -0.000618
6 -0.806750 -0.209095 -1.204266
1 -0.097963 -1.014830 -1.363537
1 -0.813903 0.464798 -2.058753
6 -2.184562 -0.733619 -0.778765
1 -2.341739 -1.735771 -1.178490
1 -2.988717 -0.105139 -1.165806
6 -2.185418 -0.730252 0.779924
1 -2.346291 -1.730054 1.184040
1 -2.987973 -0.097457 1.163304
6 -0.806609 -0.207863 1.204234
1 -0.811915 0.466301 2.058521
1 -0.098859 -1.014595 1.362974
7 1.940805 -0.220609 0.000127
8 1.469983 -1.388563 0.000373
8 3.144699 0.013092 0.000556

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SP3-II-1-OH b3lyp/6-311g(2d,d,p) if=87.3949

7 0.339358 0.404929 -0.005588
6 0.116913 1.871589 -0.036853
1 0.641801 2.288026 0.820258
1 0.568673 2.254109 -0.949473
1 -0.947397 2.104050 0.001393
7 1.818931 0.302785 0.032509
6 -0.338259 -0.276101 -1.177380
1 0.180961 -1.229196 -1.270427
1 -0.168101 0.319715 -2.072279
6 -1.804969 -0.467860 -0.779789
1 -2.201873 -1.399448 -1.187038
1 -2.429106 0.340164 -1.167306
6 -1.807614 -0.466159 0.780937
1 -2.172783 -1.411721 1.185058
1 -2.464347 0.318027 1.163194

6 -0.348265 -0.228894 1.190136
1 -0.202606 0.421525 2.050146
1 0.196392 -1.157761 1.348144
8 2.070313 -1.130982 0.099882
1 2.421025 -1.349077 -0.771485

#####

SP3-II-2-CH3 b3lyp/6-311g(2d,d,p) if=74.7850

7 -0.420788 -0.495483 -0.005532
6 -0.850849 -1.910041 -0.172434
1 -1.491966 -2.146877 0.672543
1 -1.438058 -1.966314 -1.086203
1 0.016605 -2.572175 -0.216313
7 -1.667979 0.225970 0.157275
6 0.459442 -0.067085 -1.225287
1 -0.195722 0.437602 -1.929670
1 0.865773 -0.980908 -1.667930
6 0.562450 -0.358385 1.176978
1 0.639980 -1.317732 1.685697
1 0.110867 0.366178 1.849324
7 1.516758 0.755906 -0.721033
1 1.170496 1.695963 -0.560462
1 2.566362 -0.697420 0.369643
6 1.882070 0.135734 0.563149
1 2.399230 0.853032 1.202056
6 -1.445992 1.645909 0.174183
1 -1.087304 2.114012 -0.773799
1 -2.424207 2.095306 0.365572
1 -0.770709 2.037789 0.975041

#####

SP3-II-2-CN b3lyp/6-311g(2d,d,p) if=55.6476

7 0.727671 -0.407284 0.018317
6 2.049904 -1.081792 0.093132
1 2.047542 -1.731107 0.965191
1 2.156920 -1.690415 -0.802034
1 2.842468 -0.336017 0.159315
7 -0.235573 -1.505089 -0.144356
6 0.653497 0.594979 -1.170340
1 0.442395 0.018507 -2.066674
1 1.634971 1.079261 -1.230488
6 0.458271 0.497785 1.215246
1 1.407633 0.712854 1.705314
1 -0.188688 -0.053526 1.892225

7 -0.364977 1.524522 -0.824405
1 -1.281026 1.120758 -0.997119
1 0.446696 2.639935 0.771911
6 -0.200288 1.772018 0.616114
1 -1.169847 1.974231 1.068257
6 -1.473241 -1.077929 -0.009845
7 -2.593968 -0.749982 0.103053

#####

SP3-II-2-COOH b3lyp/6-311g(2d,d,p) if=95.3844

7 0.428598 -0.733473 -0.020238
6 1.008871 -2.102331 -0.136969
1 0.609270 -2.702156 0.676331
1 0.679530 -2.523604 -1.084547
1 2.097516 -2.047394 -0.092898
7 -1.005090 -0.977860 0.017161
6 0.951826 0.161192 -1.222460
1 0.120171 0.312636 -1.901807
1 1.743344 -0.424993 -1.694140
6 0.994180 -0.016541 1.207365
1 1.396975 -0.759642 1.893645
1 0.166905 0.514561 1.665926
7 1.458168 1.372041 -0.667557
1 0.646510 1.960976 -0.487062
1 2.994584 0.494934 0.474291
6 2.019814 0.970823 0.627705
1 2.166131 1.836766 1.273720
6 -1.705184 0.159549 0.034324
8 -1.322869 1.344225 0.005455
8 -3.046117 -0.105524 0.096965
1 -3.457826 0.767192 0.091831

#####

SP3-II-2-H b3lyp/6-311g(2d,d,p) if=118.1295

7 0.648813 0.010280 0.072838
6 1.965463 0.156194 -0.592571
1 2.484482 0.989197 -0.124740
1 2.520576 -0.757593 -0.391503
1 1.841407 0.316032 -1.666447
7 0.923278 -0.350318 1.441672
6 -0.238665 -1.040483 -0.640242
1 0.167849 -2.017341 -0.397025
1 -0.225947 -0.846142 -1.719917
6 -0.228255 1.236522 -0.077693

1 -0.023835 1.721331 -1.035927
1 0.029899 1.905427 0.738959
7 -1.545426 -0.814529 -0.098484
1 -1.533479 -1.182456 0.849260
1 -2.245621 1.019732 -0.894101
6 -1.673309 0.661812 -0.034543
1 -2.212643 0.950901 0.867295
1 0.059246 -0.101391 1.932258

#####

SP3-II-2-NH2 b3lyp/6-311g(2d,d,p) if=82.1328

7 -0.459651 -0.472898 -0.000153
6 -1.155171 -1.772710 -0.128613
1 -1.811069 -1.878902 0.732343
1 -1.764001 -1.733563 -1.029425
1 -0.431365 -2.588094 -0.178507
7 -1.607202 0.498936 0.138833
6 0.439691 -0.191279 -1.221807
1 -0.176672 0.323892 -1.953672
1 0.789809 -1.151966 -1.616385
6 0.524317 -0.445629 1.164570
1 0.538233 -1.418087 1.656838
1 0.143734 0.303900 1.852765
7 1.542109 0.592636 -0.744141
1 1.152604 1.511192 -0.531830
1 2.502695 -0.920758 0.354672
6 1.875975 -0.042022 0.540301
1 2.438806 0.646090 1.172532
7 -1.020771 1.805179 0.173237
1 -1.384984 2.367570 -0.593800
1 -1.288053 2.281602 1.033329

#####

SP3-II-2-NO2 b3lyp/6-311g(2d,d,p) if=110.9140

7 0.350322 -0.712850 -0.024723
6 0.861615 -2.110861 -0.156813
1 0.441998 -2.701585 0.653176
1 0.514391 -2.508239 -1.108128
1 1.950648 -2.101164 -0.114993
7 -1.103725 -0.939593 0.014601
6 0.911283 0.163423 -1.225914
1 0.081409 0.412281 -1.877898
1 1.627765 -0.486315 -1.731767
6 0.947824 -0.044476 1.210932

1 1.283565 -0.819651 1.897481
1 0.163256 0.552171 1.663573
7 1.547833 1.304926 -0.659972
1 0.823504 1.996921 -0.491039
1 2.989065 0.289125 0.491542
6 2.060063 0.850241 0.638318
1 2.279982 1.697888 1.287192
7 -1.793720 0.215267 0.043505
8 -3.012202 0.091771 0.104768
8 -1.218457 1.338773 0.009962

#####

SP3-II-2-OH b3lyp/6-311g(2d,d,p) if=64.2396

7 -0.535373 -0.389331 0.005019
6 -1.336834 -1.632515 -0.105834
1 -2.004220 -1.672797 0.752164
1 -1.930254 -1.559493 -1.014698
1 -0.679487 -2.501961 -0.134460
7 -1.566912 0.660157 0.085291
6 0.407050 -0.218776 -1.225401
1 -0.138685 0.383237 -1.945245
1 0.617910 -1.219140 -1.618104
6 0.444672 -0.421403 1.183121
1 0.307285 -1.344230 1.745062
1 0.180494 0.429820 1.804052
7 1.605808 0.397312 -0.745580
1 1.384874 1.375656 -0.575347
1 2.308784 -1.232683 0.375367
6 1.838650 -0.258954 0.550066
1 2.513739 0.334505 1.168087
8 -0.782004 1.905149 0.082891
1 -0.950292 2.278820 0.955165

#####

SP3-II-3-CH3 b3lyp/6-311g(2d,d,p) if=81.7116

7 0.348006 0.515941 -0.028357
6 0.510715 1.983090 -0.220526
1 1.108804 2.343607 0.612146
1 1.064277 2.134988 -1.144250
1 -0.464361 2.474627 -0.258587
7 1.697020 0.032366 0.151623
6 1.728634 -1.406956 0.166881
1 1.138489 -1.916681 0.965447
1 2.771902 -1.677703 0.348653

1 1.448069 -1.922986 -0.782049
6 -0.471704 -0.080625 -1.206501
1 0.216192 -0.606557 -1.862910
1 -0.946409 0.748508 -1.735103
6 -0.607708 0.225571 1.168766
1 -0.779558 1.140590 1.732753
1 -0.071210 -0.496300 1.778526
7 -1.476290 -0.938578 -0.627698
1 -1.095887 -1.856437 -0.420772
7 -1.830608 -0.335098 0.631004
1 -2.516818 0.385442 0.428417

#####

SP3-II-3-CN b3lyp/6-311g(2d,d,p) if=75.3778

7 0.316918 -0.680479 0.020829
6 1.214415 -1.856547 0.169621
1 0.943939 -2.372196 1.088704
1 1.032110 -2.515920 -0.675318
1 2.253979 -1.527297 0.199066
7 -1.024937 -1.250314 -0.135894
1 2.224270 1.426541 -0.416079
1 -0.384401 1.982401 0.441890
6 0.466546 0.303758 1.212455
1 1.399451 0.049938 1.720659
1 -0.387832 0.174427 1.871417
1 -0.190038 0.394869 -1.724287
6 0.733029 0.227773 -1.173667
1 1.467803 -0.283515 -1.793244
7 0.545763 1.622614 0.642927
7 1.227818 1.459712 -0.608293
6 -1.908238 -0.271461 -0.116814
7 -2.693245 0.598412 -0.099910

#####

SP3-II-3-COOH b3lyp/6-311g(2d,d,p) if=108.9522

7 0.433574 -0.712234 0.048655
6 1.051028 -2.061763 0.190905
1 0.733988 -2.479052 1.144326
1 0.670835 -2.684743 -0.614243
1 2.138116 -1.975033 0.148924
7 -0.990132 -0.988743 -0.020814
1 2.893171 0.543340 -0.562915
1 0.708045 2.022723 0.372194
6 0.931140 0.220359 1.197806

1 1.703985 -0.335808 1.730938
1 0.092765 0.452429 1.845529
1 0.163474 0.533676 -1.639994
6 1.009019 0.017545 -1.197124
1 1.433669 -0.713135 -1.883279
7 1.485276 1.397317 0.574993
7 1.978986 0.961917 -0.704292
6 -1.710792 0.138014 -0.029253
8 -1.343608 1.324954 0.037100
8 -3.044183 -0.146858 -0.123761
1 -3.472021 0.718109 -0.111976

#####

SP3-II-3-H b3lyp/6-311g(2d,d,p) if=56.5608

7 0.650646 -0.031610 -0.068977
6 1.796667 0.417174 0.763266
1 2.381747 -0.466357 1.008478
1 2.402346 1.076446 0.146531
1 1.446004 0.923134 1.665149
7 1.231910 -0.672842 -1.213933
1 -1.967678 1.122587 0.785225
1 -1.675111 -1.185525 -0.744088
6 -0.302031 -0.936352 0.733978
1 -0.316844 -0.616751 1.782680
1 0.068613 -1.950125 0.619096
1 -0.162759 1.258262 -1.500140
6 -0.311654 1.141981 -0.429138
1 -0.039148 2.058357 0.097618
7 -1.601478 -0.718208 0.155894
7 -1.659327 0.701775 -0.084853
1 0.412680 -0.910659 -1.786103

#####

SP3-II-3-NH2 b3lyp/6-311g(2d,d,p) if=90.9309

7 -0.360090 -0.515156 0.024919
6 -0.691698 -1.947599 0.199119
1 -1.257828 -2.051276 1.122182
1 -1.327228 -2.233232 -0.635919
1 0.219346 -2.548649 0.228964
7 -1.701479 0.127822 -0.158100
1 2.489261 -0.514916 -0.377730
1 1.049771 1.753106 0.382431
6 0.459690 0.024215 1.203194
1 0.914827 -0.822691 1.725002

1 -0.217742 0.563735 1.858812
1 0.107354 0.481825 -1.756474
6 0.602945 -0.274179 -1.153969
1 0.742306 -1.190212 -1.727362
7 1.487077 0.871105 0.640058
7 1.845738 0.237271 -0.605722
7 -1.442637 1.538125 -0.166410
1 -1.780273 1.946299 -1.036486
1 -1.965682 1.987223 0.583296

#####

SP3-II-3-NO2 b3lyp/6-311g(2d,d,p) if=113.3765

7 0.362325 0.693744 -0.049242
6 0.911904 2.075413 -0.192430
1 0.581533 2.477134 -1.147777
1 0.506318 2.683059 0.612215
1 2.000430 2.033937 -0.147194
7 -1.083754 0.954620 0.013873
1 2.892871 -0.384768 0.580990
1 0.874297 -2.050517 -0.398637
6 0.898313 -0.210753 -1.203277
1 1.608822 0.403980 -1.757746
1 0.068907 -0.518022 -1.830883
1 0.160678 -0.575329 1.638748
6 0.968421 0.000647 1.200015
1 1.339536 0.758015 1.887850
7 1.564763 -1.328581 -0.581557
7 2.007407 -0.865688 0.703725
7 -1.798976 -0.188365 0.041407
8 -1.245908 -1.321002 -0.013571
8 -3.012540 -0.038928 0.118465

#####

SP3-II-3-OH b3lyp/6-311g(2d,d,p) if=84.1292

7 -0.466615 -0.438651 0.016177
6 -1.006842 -1.810458 0.184128
1 -1.583792 -1.831681 1.105828
1 -1.670919 -2.003642 -0.655697
1 -0.191045 -2.533865 0.215302
7 -1.667233 0.385744 -0.130662
1 2.357539 -0.885947 -0.392425
1 1.329057 1.580327 0.418995
6 0.431185 -0.034361 1.208866
1 0.732487 -0.948568 1.727244

1 -0.158993 0.612334 1.850462
1 0.166831 0.498073 -1.753007
6 0.534535 -0.336922 -1.162854
1 0.525655 -1.255470 -1.748155
7 1.586262 0.625110 0.651217
7 1.837343 -0.039725 -0.603622
8 -1.120478 1.753498 -0.089706
1 -1.324565 2.103559 -0.963505

#####

SP3-II-4-CN b3lyp/6-311g(2d,d,p) if=60.0505

7 -0.212174 -0.703160 0.045981
6 -1.070000 -1.912948 0.143028
1 -0.851007 -2.530505 -0.722995
1 -0.807655 -2.425891 1.064829
1 -2.109564 -1.596186 0.159302
7 1.115200 -1.127317 -0.066865
7 -0.548212 0.204181 1.204182
1 0.316078 0.210943 1.742150
6 -0.803158 1.535385 0.597396
1 0.116903 2.105003 0.441944
1 -1.498669 2.096250 1.222065
7 -0.717122 0.124752 -1.199249
1 0.180359 0.458543 -1.555824
7 -1.407700 1.221054 -0.687907
1 -2.382771 0.958214 -0.579434
6 1.946217 -0.093762 -0.089663
7 2.712575 0.787858 -0.107086

#####

SP3-II-4-COOH b3lyp/6-311g(2d,d,p) if=47.8623

7 -0.361190 0.658303 -0.059237
6 -1.066377 1.964052 -0.131766
1 -0.754158 2.542442 0.732445
1 -0.755999 2.438592 -1.057469
1 -2.141341 1.791640 -0.133250
7 1.015597 0.950699 -0.041806
7 -0.834098 -0.193723 -1.193964
1 -0.006789 -0.761402 -1.370598
6 -1.853434 -1.110477 -0.620135
1 -1.496226 -2.139647 -0.702817
1 -2.808933 -1.010644 -1.137427
7 -0.877637 -0.074704 1.218669
1 -0.143805 -0.783769 1.303403

7 -2.027619 -0.735443 0.793400
1 -2.816417 -0.109996 0.912296
6 1.766521 -0.160095 0.020817
8 1.400303 -1.351238 0.047440
8 3.087418 0.144416 0.044024
1 3.536267 -0.709433 0.088767

#####

SP3-II-4-H b3lyp/6-311g(2d,d,p) if=105.7273

7 0.725410 0.087771 -0.086193
6 1.662811 -0.593757 0.839439
1 2.286409 -1.248831 0.237574
1 2.268940 0.170424 1.322147
1 1.089727 -1.154731 1.571970
7 1.382092 0.717147 -1.051493
7 -0.278745 0.898546 0.792951
1 0.055310 1.842461 0.613156
6 -1.581171 0.663124 0.157423
1 -1.710657 1.197342 -0.795109
1 -2.388347 0.939407 0.837224
7 -0.338889 -1.109695 -0.601521
1 -0.305714 -0.835683 -1.586371
7 -1.595352 -0.771861 -0.101662
1 -1.720562 -1.272964 0.773447
1 0.673438 1.193012 -1.619776

#####

SP3-II-4-NO2 b3lyp/6-311g(2d,d,p) if=83.6657

7 0.324923 0.669121 0.060532
6 0.955342 2.016700 0.121913
1 0.609405 2.577127 -0.741326
1 0.637653 2.479688 1.051375
1 2.035519 1.889697 0.111399
7 -1.076690 0.942359 0.041507
7 0.844657 -0.134033 1.211502
1 0.008773 -0.608196 1.544811
6 1.725218 -1.175043 0.604110
1 1.208367 -2.136366 0.580528
1 2.656157 -1.256643 1.165311
7 0.891531 -0.031947 -1.218955
1 0.158734 -0.732112 -1.359917
7 2.007234 -0.723153 -0.756029
1 2.809813 -0.103719 -0.788083
7 -1.820191 -0.191613 -0.035954

8 -3.026492 -0.026362 -0.048705
8 -1.274511 -1.332959 -0.081102

#####

SP3-II-5-CN b3lyp/6-311g(2d,d,p) if=70.3259

7 0.356448 0.683715 -0.004287
6 1.393595 1.735016 0.128071
1 1.279092 2.411146 -0.714845
1 1.213409 2.257222 1.064782
1 2.369172 1.257729 0.130404
7 -0.893461 1.287185 -0.089174
7 0.613838 -0.352170 1.217071
1 -0.184977 -0.160884 1.827404
7 1.069862 -1.489758 -0.633514
1 2.068645 -1.466983 -0.445435
7 0.703976 -0.226653 -1.170132
1 -0.204474 -0.346178 -1.618328
7 0.421035 -1.617625 0.619091
1 -0.567929 -1.790978 0.419505
6 -1.858541 0.377886 -0.081067
7 -2.726450 -0.404479 -0.074128

#####

SP3-II-5-COOH b3lyp/6-311g(2d,d,p) if=52.0517

7 0.426321 0.736403 0.024769
6 1.123795 2.023459 0.263417
1 0.800487 2.716886 -0.508089
1 0.827205 2.376554 1.247889
1 2.196679 1.852895 0.228353
7 -0.937554 0.995769 -0.048138
7 1.050836 -0.273172 1.206521
1 0.200808 -0.524522 1.719787
7 1.916040 -0.917425 -0.750387
1 2.807784 -0.469148 -0.558024
7 1.009782 0.083921 -1.190286
1 0.208596 -0.405479 -1.584837
7 1.415010 -1.417932 0.479927
1 0.564525 -1.936260 0.237306
6 -1.695507 -0.115948 -0.017645
8 -1.351049 -1.300289 0.136160
8 -3.007467 0.193155 -0.162880
1 -3.470734 -0.651867 -0.100102

#####

SP3-II-5-NO2 b3lyp/6-311g(2d,d,p) if=74.2834

7	-0.342593	0.723216	-0.013694
6	-0.986377	2.043736	-0.230676
1	-0.624022	2.720775	0.538256
1	-0.699715	2.389124	-1.220440
1	-2.063619	1.914516	-0.173376
7	1.037316	0.976495	0.023685
7	-1.046063	-0.249049	-1.226800
1	-0.214405	-0.566840	-1.735444
7	-1.936836	-0.819620	0.746152
1	-2.787188	-0.288691	0.579639
7	-0.931201	0.081763	1.190615
1	-0.171515	-0.498475	1.543019
7	-1.503806	-1.344266	-0.500398
1	-0.727738	-1.970954	-0.278119
7	1.782438	-0.162406	0.028876
8	1.238061	-1.298323	-0.068453
8	2.985898	-0.002278	0.117386

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SP3-III-1-CH3 b3lyp/6-311g(2d,d,p) if=69.7868

6	-1.290488	0.858755	-1.194016
6	-1.290381	0.860269	1.194605
1	-1.394270	1.947125	1.147812
6	0.204901	0.442597	1.280633
1	0.413619	-0.274754	2.072908
6	0.249129	0.634116	-1.169702
1	0.801697	1.563839	-1.044665
7	0.623410	-0.260928	-0.000524
7	1.992517	-0.739549	-0.000102
7	-1.928713	0.289138	0.000111
1	-1.734835	0.388684	-2.074480
1	-1.526365	1.924637	-1.240366
1	0.633312	0.122629	-2.051409
1	-1.833619	0.519538	2.079265
1	0.872498	1.293300	1.405391
6	2.934603	0.355479	0.001917
1	2.906264	1.044807	0.876375
1	3.918797	-0.120278	0.035020
1	2.947021	1.010582	-0.897450
6	-1.713048	-1.165864	0.000393
1	-2.138682	-1.571714	0.921275
1	-2.269824	-1.601098	-0.832806
6	-0.203511	-1.510414	-0.113697

1 0.167884 -2.164141 0.673304
1 0.078775 -1.953419 -1.067367

#####

SP3-III-1-CN b3lyp/6-311g(2d,d,p) if=31.7233

6 -1.329832 -0.976835 1.194915
6 -1.330053 -0.976234 -1.195294
1 -1.334356 -2.067892 -1.188918
6 0.128094 -0.432269 -1.233494
1 0.326032 0.226345 -2.077984
6 0.128012 -0.432113 1.233605
1 0.887281 -1.213329 1.224790
7 0.372769 0.411344 0.000012
7 1.696541 1.038184 0.000003
7 -2.038290 -0.501468 -0.000007
1 -1.882348 -0.652483 2.079096
1 -1.333558 -2.068490 1.187591
1 0.325239 0.226806 2.078024
1 -1.882394 -0.650823 -2.079197
1 0.886957 -1.213873 -1.224163
6 -2.053217 0.966802 0.000368
1 -2.602979 1.307562 -0.879256
1 -2.602244 1.307067 0.880643
6 -0.609254 1.546754 -0.000100
1 -0.372349 2.141592 -0.880570
1 -0.371962 2.142108 0.879914
6 2.627703 0.101038 -0.000004
7 3.481546 -0.700554 0.000001

#####

SP3-III-1-COOH b3lyp/6-311g(2d,d,p) if=41.3822

6 -1.761325 -0.885045 1.194526
6 -1.761888 -0.882495 -1.196305
1 -1.846498 -1.971054 -1.187234
6 -0.267455 -0.453229 -1.241917
1 -0.032815 0.203119 -2.079164
6 -0.267687 -0.453431 1.242078
1 0.430964 -1.285467 1.236784
7 0.049985 0.362207 0.000121
7 1.395197 0.913136 0.000059
7 -2.433755 -0.358543 -0.000201
1 -2.293865 -0.526181 2.078225
1 -1.844134 -1.973717 1.181905
1 -0.035271 0.203643 2.079461

1 -2.293632 -0.519951 -2.078997
1 0.429588 -1.286575 -1.235441
6 -2.334052 1.105560 0.001410
1 -2.856433 1.489462 -0.877542
1 -2.854532 1.487206 0.882460
6 -0.849915 1.569736 0.000271
1 -0.569293 2.146433 -0.879277
1 -0.568191 2.147184 0.878985
6 2.334405 -0.044479 -0.000020
8 2.235302 -1.282121 0.000216
8 3.579877 0.526804 -0.000248
1 4.180197 -0.228866 -0.000019

#####

SP3-III-1-H b3lyp/6-311g(2d,d,p) if=39.2627

6 -1.117299 0.684523 -1.196571
6 -1.117243 0.682411 1.197772
1 -1.526705 1.695323 1.198987
6 0.440998 0.708658 1.223855
1 0.883718 0.188166 2.071092
6 0.440931 0.709581 -1.223351
1 0.852185 1.719181 -1.193678
7 1.000708 0.005819 0.000007
7 2.427934 -0.114394 -0.000106
7 -1.606252 -0.014349 0.000003
1 -1.511550 0.174785 -2.078762
1 -1.525904 1.697789 -1.195267
1 0.882882 0.189038 -2.070954
1 -1.510643 0.170387 2.079052
1 0.851379 1.718617 1.194365
6 -1.081377 -1.387358 -0.001182
1 -1.473095 -1.904897 0.877600
1 -1.472364 -1.903025 -0.881392
6 0.472809 -1.400148 -0.000532
1 0.913022 -1.868811 0.877931
1 0.913733 -1.868348 -0.878885
1 2.733698 0.866263 0.000631

#####

SP3-III-1-NH2 b3lyp/6-311g(2d,d,p) if=44.0824

6 -1.274182 -0.872812 1.192826
6 -1.274454 -0.871848 -1.193366
1 -1.429812 -1.953334 -1.181899
6 0.242634 -0.523164 -1.225365

1 0.523712 0.107623 -2.068234
6 0.242730 -0.523434 1.225174
1 0.895111 -1.395272 1.213451
7 0.605203 0.271545 -0.000022
7 2.036961 0.737794 0.000000
7 -1.918370 -0.302280 0.000032
1 -1.779404 -0.481566 2.079294
1 -1.429031 -1.954358 1.180159
1 0.523316 0.107413 2.068164
1 -1.779519 -0.479383 -2.079385
1 0.894603 -1.395307 -1.213574
6 -1.715239 1.155444 0.000602
1 -2.213233 1.570283 -0.878915
1 -2.212498 1.569446 0.880929
6 -0.201851 1.524077 0.000125
1 0.115610 2.082971 -0.879436
1 0.116163 2.083110 0.879399
7 2.820404 -0.455149 0.000037
1 3.423648 -0.477477 -0.819344
1 3.424107 -0.477094 0.819084

#####

SP3-III-1-NO2 b3lyp/6-311g(2d,d,p) if=17.5946

6 1.747537 0.875084 1.194418
6 1.747972 0.872166 -1.196485
1 1.845426 1.959304 -1.183330
6 0.247258 0.463283 -1.250378
1 0.012407 -0.201571 -2.080839
6 0.248070 0.462230 1.251284
1 -0.436956 1.303236 1.268415
7 -0.082956 -0.333749 0.000276
7 -1.437715 -0.920301 0.000266
7 2.408579 0.336019 -0.000305
1 2.277326 0.514001 2.078562
1 1.842094 1.962414 1.176707
1 0.017043 -0.204436 2.081375
1 2.276105 0.506113 -2.079585
1 -0.435777 1.305975 -1.264573
6 2.284092 -1.125088 0.001584
1 2.798692 -1.519408 -0.877021
1 2.795541 -1.516532 0.883312
6 0.792028 -1.564729 -0.000556
1 0.504625 -2.135442 -0.881671
1 0.502738 -2.138119 0.878192

7 -2.411244 0.019870 -0.000003
8 -2.167232 1.254132 0.000265
8 -3.549974 -0.434893 -0.000312

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SP3-III-1-OH b3lyp/6-311g(2d,d,p) if=63.4059

6 1.259596 -0.872456 -1.191877
6 1.236681 -0.880386 1.196195
1 1.335960 -1.967528 1.151635
6 -0.256531 -0.452542 1.256602
1 -0.477988 0.246491 2.061692
6 -0.269454 -0.580733 -1.197059
1 -0.881233 -1.476258 -1.104316
7 -0.620812 0.285443 -0.010397
7 -2.025663 0.761830 0.002516
7 1.895451 -0.312260 0.008925
1 1.738926 -0.434141 -2.070485
1 1.453169 -1.947320 -1.216879
1 -0.602031 -0.019696 -2.070067
1 1.769946 -0.541094 2.087347
1 -0.957273 -1.281867 1.324431
6 1.707086 1.146679 0.012570
1 2.147860 1.543188 0.930067
1 2.264267 1.571083 -0.825688
6 0.201044 1.529491 -0.086062
1 -0.149216 2.165002 0.726516
1 -0.065535 2.010957 -1.026361
8 -2.801391 -0.471165 0.106921
1 -3.179089 -0.584905 -0.772771

#####

SP3-III-2-CH3 b3lyp/6-311g(2d,d,p) if=109.5203

6 -1.311613 1.052537 -1.016752
6 -1.301150 0.564183 1.334964
1 -1.631914 1.563463 1.626780
6 0.241935 0.485870 1.237686
1 0.704962 -0.092086 2.036641
6 -0.207548 -1.490655 -0.080237
1 0.205687 -2.089594 -0.889790
6 0.166242 0.629849 -1.218854
1 0.853086 1.473077 -1.263203
7 0.611984 -0.238580 -0.047035
7 1.976090 -0.716966 -0.134094
7 -1.919783 0.226867 0.036759

1 -1.879856 0.912611 -1.936230
1 -0.015424 -1.997454 0.869548
1 -1.395822 2.099805 -0.715185
1 0.315941 0.008950 -2.099296
1 -1.687250 -0.136987 2.077996
1 0.712126 1.467171 1.198500
6 2.916887 0.361030 0.063535
1 2.927655 0.838256 1.068157
1 3.902502 -0.096154 -0.059631
1 2.880709 1.198314 -0.669429
7 -1.621380 -1.132397 -0.333851
1 -2.249298 -1.738715 0.180639

#####

SP3-III-2-CN b3lyp/6-311g(2d,d,p) if=76.5606

6 1.315654 -1.134140 -1.059675
6 1.389106 -0.737687 1.310436
1 1.539884 -1.792886 1.545425
6 -0.119140 -0.387622 1.248487
1 -0.452285 0.261968 2.056281
6 0.615426 1.522316 -0.063728
1 0.305318 2.168642 -0.883718
6 -0.098451 -0.513535 -1.217063
1 -0.906181 -1.244469 -1.228717
7 -0.363854 0.390457 -0.027802
7 -1.680675 1.025154 -0.073067
7 2.038946 -0.447461 0.017760
1 1.884540 -1.024925 -1.982010
1 0.492704 2.059571 0.881139
1 1.259373 -2.195575 -0.809209
1 -0.189580 0.125492 -2.093386
1 1.898651 -0.153938 2.079456
1 -0.775157 -1.256367 1.210964
7 1.959933 0.953365 -0.299748
1 2.665420 1.438708 0.241250
6 -2.616642 0.094720 -0.003920
7 -3.474121 -0.700162 0.053613

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SP3-III-2-COOH b3lyp/6-311g(2d,d,p) if=104.0597

6 -1.742444 1.030315 -1.078960
6 -1.812217 0.654384 1.294243
1 -2.051933 1.695317 1.520053
6 -0.280217 0.437042 1.248686

1 0.095453 -0.173856 2.068596
6 -0.855700 -1.546819 -0.033489
1 -0.488070 -2.190565 -0.830947
6 -0.292283 0.504776 -1.234506
1 0.460956 1.286619 -1.268825
7 0.042457 -0.344112 -0.014767
7 1.380363 -0.906021 -0.036176
7 -2.427433 0.304183 -0.001363
1 -2.301619 0.886264 -2.003051
1 -0.706364 -2.050724 0.926008
1 -1.752972 2.093390 -0.828596
1 -0.174826 -0.162072 -2.087014
1 -2.281517 0.036206 2.062627
1 0.305420 1.350159 1.191879
7 -2.235447 -1.089976 -0.300548
1 -2.907958 -1.621564 0.239217
6 2.321966 0.049264 0.003601
8 2.219586 1.284867 0.048014
8 3.565535 -0.522639 -0.014135
1 4.168254 0.230701 0.011561

#####

SP3-III-2-H b3lyp/6-311g(2d,d,p) if=101.0503

6 1.152030 1.347813 -0.171307
6 1.118302 -0.906106 -1.017504
1 1.659834 -0.639971 -1.928066
6 -0.414253 -0.761210 -1.198759
1 -0.959822 -1.702896 -1.194172
6 -0.476343 -0.636326 1.217374
1 -1.020590 -0.170752 2.037343
6 -0.398418 1.424162 -0.086040
1 -0.862558 1.896818 -0.951719
7 -0.982798 0.020007 -0.027679
7 -2.409513 -0.022787 0.078674
7 1.588062 -0.032577 0.077437
1 1.614615 1.990965 0.576881
1 -0.774857 -1.685339 1.143311
1 1.516305 1.646972 -1.157227
1 -0.763270 1.918311 0.811675
1 1.391420 -1.932610 -0.763462
1 -0.693389 -0.203547 -2.094026
7 0.983511 -0.402042 1.330152
1 1.461138 -1.228014 1.670675
1 -2.711577 0.361859 -0.823890

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SP3-III-2-NH2 b3lyp/6-311g(2d,d,p) if=106.9339

6	1.274530	-1.178201	-0.896632
6	1.313964	-0.418623	1.380719
1	1.610470	-1.399266	1.760168
6	-0.227558	-0.273789	1.309180
1	-0.629537	0.455665	2.011620
6	0.208251	1.471434	-0.297278
1	-0.197674	1.930194	-1.198687
6	-0.215433	-0.786028	-1.088864
1	-0.915888	-1.607741	-0.947757
7	-0.593941	0.245665	-0.056513
7	-2.022330	0.706443	-0.169588
7	1.911474	-0.241308	0.040746
1	1.811313	-1.132213	-1.844023
1	0.022563	2.135119	0.551791
1	1.378445	-2.186649	-0.488481
1	-0.408364	-0.314761	-2.051173
1	1.752035	0.332941	2.041455
1	-0.769817	-1.209496	1.432467
7	1.625707	1.072020	-0.482072
1	2.250472	1.725120	-0.024556
7	-2.807339	-0.450672	0.107441
1	-3.404561	-0.288022	0.915708
1	-3.416980	-0.654690	-0.681380

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SP3-III-2-NO2 b3lyp/6-311g(2d,d,p) if=106.9627

6	1.725500	1.031715	1.068465
6	1.797389	0.624873	-1.300904
1	2.065225	1.654105	-1.546323
6	0.258560	0.456374	-1.251827
1	-0.139539	-0.141361	-2.070992
6	0.800688	-1.540406	0.024483
1	0.417512	-2.192949	0.807450
6	0.276245	0.511254	1.245692
1	-0.469782	1.296012	1.314038
7	-0.075596	-0.315100	0.015824
7	-1.421668	-0.913612	0.043331
7	2.400976	0.280545	0.001452
1	2.287403	0.906588	1.993497
1	0.655547	-2.024639	-0.945746
1	1.735623	2.089080	0.795526

1 0.177338 -0.171517 2.087688
1 2.247826 -0.020377 -2.057831
1 -0.291776 1.389133 -1.196883
7 2.179671 -1.104966 0.317138
1 2.854686 -1.658996 -0.196518
7 -2.397595 0.023317 -0.002752
8 -2.150954 1.255093 -0.050367
8 -3.535404 -0.432497 0.009829

#####

SP3-III-2-OH b3lyp/6-311g(2d,d,p) if=107.0360

6 1.250544 -1.170476 -0.914222
6 1.286670 -0.441839 1.375725
1 1.583075 -1.424872 1.748237
6 -0.253430 -0.299931 1.300951
1 -0.669271 0.407666 2.016319
6 0.208032 1.485776 -0.263912
1 -0.190929 1.979448 -1.150353
6 -0.231106 -0.755300 -1.115272
1 -0.938193 -1.575051 -1.001803
7 -0.610149 0.259559 -0.058368
7 -2.010562 0.735835 -0.146468
7 1.889007 -0.251634 0.039172
1 1.795509 -1.121038 -1.856612
1 0.032545 2.121752 0.607811
1 1.336873 -2.184494 -0.516531
1 -0.406946 -0.258503 -2.067790
1 1.721748 0.304435 2.044121
1 -0.795744 -1.237754 1.395243
7 1.616533 1.069759 -0.467819
1 2.253594 1.711416 -0.010877
8 -2.787926 -0.450651 0.196259
1 -3.176919 -0.721815 -0.643067

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SP3-III-3-CH3 b3lyp/6-311g(2d,d,p) if=125.5235

6 -0.148584 0.364466 -1.311526
1 -0.182058 -0.440760 -2.046123
6 -0.228595 0.691920 1.113575
1 -0.712931 1.635767 0.862345
7 -0.605895 -0.286389 0.000819
7 -1.965235 -0.763976 -0.007568
1 -0.673698 0.296937 2.025923
1 -0.885034 1.119081 -1.579152

6 -2.905516 0.335498 0.020821
1 -2.837968 1.076096 -0.809297
1 -3.891377 -0.127049 -0.077881
1 -2.946330 0.936211 0.955327
6 0.248081 -1.510222 0.171933
1 -0.178233 -2.242928 -0.509618
1 0.067303 -1.858769 1.187815
6 1.725908 -1.164126 -0.112293
1 2.038449 -1.503960 -1.102780
1 2.376390 -1.646563 0.620813
6 1.869044 0.364633 -0.018608
1 2.914645 0.676297 -0.018585
7 1.182129 0.948287 -1.167857
1 1.127781 1.953611 -1.043738
7 1.223456 0.857435 1.221543
1 1.579850 0.345523 2.022979

#####

SP3-III-3-CN b3lyp/6-311g(2d,d,p) if=71.3027

6 -0.082518 -0.217770 1.286400
1 -0.103366 0.619185 1.990727
6 0.641024 1.489544 -0.282133
1 0.499649 1.814814 -1.313430
6 -0.097983 -0.667791 -1.134984
1 -0.750834 -1.507982 -0.905696
7 -0.353370 0.381457 -0.066676
7 -1.664582 1.015194 -0.144096
7 2.021600 -0.464109 0.110536
1 0.360657 2.300677 0.388693
1 -0.422540 -0.213463 -2.069423
1 -0.902861 -0.900786 1.508705
7 1.994183 0.973181 -0.038732
1 2.412469 1.368387 0.794278
7 1.203986 -0.935391 1.200105
1 1.739963 -0.845523 2.055343
6 1.412870 -1.026384 -1.103314
1 1.944363 -0.609653 -1.958326
1 1.554774 -2.104870 -1.079180
6 -2.608372 0.096569 -0.017030
7 -3.476445 -0.679733 0.095246

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SP3-III-3-COOH b3lyp/6-311g(2d,d,p) if=102.3903

6 0.301127 0.362087 -1.263546

1 0.255284 -0.414340 -2.034192
6 0.879425 -1.534295 0.135019
1 0.719251 -1.937077 1.135772
6 0.303051 0.574959 1.203484
1 -0.271879 1.482892 1.053193
7 -0.035706 -0.338536 0.030109
7 -1.367893 -0.905412 0.055127
7 2.409817 0.328433 -0.063283
1 0.534604 -2.261993 -0.597739
1 -0.067493 0.052866 2.084311
1 -0.464115 1.115235 -1.430985
7 2.266190 -1.111148 -0.080925
1 2.632577 -1.435335 -0.967394
7 1.629385 0.981576 -1.083952
1 2.164556 0.964175 -1.944404
6 1.839972 0.789349 1.212052
1 2.327100 0.225206 2.007461
1 2.078705 1.845572 1.320502
6 -2.313912 0.047916 0.000055
8 -2.210570 1.279564 -0.080867
8 -3.554153 -0.527430 0.038663
1 -4.161335 0.221233 -0.010816

#####

SP3-III-3-H b3lyp/6-311g(2d,d,p) if=100.4469

6 -0.413662 -0.829082 -1.124888
1 -0.735404 -1.848273 -0.897050
6 -0.444634 -0.523515 1.277113
1 -0.757536 0.187436 2.041406
6 -0.377666 1.419580 -0.167010
1 -0.668400 1.762367 -1.160165
7 -0.969554 0.025863 -0.015963
7 -2.394091 -0.033958 0.088620
7 1.581358 -0.066181 0.019780
1 -0.963226 -1.467615 1.439777
1 -0.893324 2.020967 0.578977
1 -0.902326 -0.499665 -2.042677
7 1.020991 -0.664219 1.210555
1 1.309827 -1.634851 1.212787
7 1.052985 -0.628898 -1.199145
1 1.542592 -1.500487 -1.366789
6 1.163670 1.343509 0.020625
1 1.474511 1.772835 0.972827
1 1.687901 1.846421 -0.790290

1 -2.702680 0.469663 -0.750763

SP3-III-3-NH2 b3lyp/6-311g(2d,d,p) if=94.4512

6 -0.208312 0.096214 1.319061
1 -0.341576 1.093846 1.747732
6 0.233148 1.319794 -0.710646
1 0.020757 1.314904 -1.779914
6 -0.205324 -1.051736 -0.840841
1 -0.755174 -1.850808 -0.348985
7 -0.582019 0.222236 -0.121667
7 -2.006389 0.661618 -0.309512
7 1.895384 -0.228681 0.161310
1 -0.137353 2.251685 -0.282818
1 -0.587189 -0.930081 -1.853754
1 -0.922098 -0.595808 1.764517
7 1.660750 1.073124 -0.428277
1 2.041265 1.756129 0.215265
7 1.174067 -0.431247 1.396307
1 1.703079 0.021368 2.132954
6 1.338729 -1.217996 -0.774306
1 1.804022 -1.045073 -1.744747
1 1.616451 -2.206282 -0.411714
7 -2.797498 -0.414054 0.190186
1 -3.410159 -0.079817 0.930341
1 -3.391542 -0.788692 -0.546925

SP3-III-3-NO2 b3lyp/6-311g(2d,d,p) if=105.7363

6 0.285806 0.361487 -1.275993
1 0.261597 -0.435754 -2.026776
6 0.828890 -1.527148 0.146854
1 0.679925 -1.902089 1.159743
6 0.281621 0.595631 1.204220
1 -0.254952 1.524318 1.052470
7 -0.070718 -0.310351 0.028205
7 -1.408135 -0.915199 0.052691
7 2.383757 0.307380 -0.063651
1 0.465691 -2.267517 -0.563839
1 -0.111141 0.088661 2.084441
1 -0.472615 1.108841 -1.487808
7 2.212998 -1.129084 -0.101379
1 2.553686 -1.449117 -0.999564
7 1.604052 0.986090 -1.069967

1 2.143317 1.006353 -1.927913
6 1.825566 0.758535 1.220804
1 2.293240 0.164246 2.005823
1 2.094271 1.804702 1.352617
7 -2.389007 0.021476 0.002256
8 -2.139691 1.248414 -0.085984
8 -3.524677 -0.435395 0.040785

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SP3-III-3-OH b3lyp/6-311g(2d,d,p) if=118.9129

6 -0.220007 0.043091 1.326271
1 -0.315719 1.027758 1.791989
6 0.236333 1.357637 -0.651273
1 0.048292 1.386300 -1.724850
6 -0.233415 -1.002217 -0.893067
1 -0.762379 -1.827325 -0.422524
7 -0.598515 0.243642 -0.110972
7 -1.996243 0.711933 -0.248181
7 1.872746 -0.250593 0.147464
1 -0.135984 2.277544 -0.199723
1 -0.634306 -0.840462 -1.893170
1 -0.957148 -0.634847 1.752151
7 1.653101 1.093106 -0.346597
1 2.015520 1.726713 0.355362
7 1.140392 -0.536747 1.359601
1 1.680889 -0.173850 2.136505
6 1.311583 -1.162961 -0.860888
1 1.763617 -0.906820 -1.819193
1 1.597587 -2.176877 -0.586718
8 -2.777562 -0.410486 0.251925
1 -3.147212 -0.816934 -0.540694

#####

SP3-III-4-CH3 b3lyp/6-311g(2d,d,p) if=109.1329

7 -0.641217 0.281843 -0.034045
7 -1.892554 0.715025 -0.036675
7 1.849791 -0.267202 0.024952
7 0.220677 1.461641 -0.181682
1 -0.269503 2.179762 0.346106
7 -0.244219 -0.569005 1.215498
1 -0.326396 0.130449 1.950546
7 -0.212258 -0.674911 -1.166674
1 -0.627735 -0.190476 -1.961193
6 1.148784 -1.034995 1.060990

1 1.151815 -2.085732 0.766145
1 1.669587 -0.938442 2.018046
6 1.598657 1.150238 0.263737
1 1.779202 1.354787 1.327023
1 2.282165 1.766023 -0.325863
6 1.282485 -0.640426 -1.268568
1 1.636101 0.069079 -2.022273
1 1.622737 -1.643410 -1.536462
6 -2.866967 -0.366667 0.033153
1 -2.758001 -0.998209 0.925027
1 -3.847995 0.110958 0.067930
1 -2.851279 -1.035422 -0.840513

#####

SP3-III-4-CN b3lyp/6-311g(2d,d,p) if=69.1200

7 0.359988 0.347771 0.031341
7 1.615408 0.950288 0.041636
7 -2.004392 -0.436531 -0.032025
7 -0.586888 1.471972 0.098734
1 -0.164300 2.192087 -0.482509
7 0.148100 -0.535090 -1.137046
1 0.243208 0.095289 -1.929725
7 0.072099 -0.530761 1.185603
1 0.445316 0.012060 1.962340
6 -1.203669 -1.147146 -1.029656
1 -1.100591 -2.187394 -0.719646
1 -1.689112 -1.112061 -2.007160
6 -1.929732 0.993394 -0.316496
1 -2.139472 1.144942 -1.381838
1 -2.672516 1.540810 0.266821
6 -1.420431 -0.692905 1.281289
1 -1.866611 -0.008886 2.007686
1 -1.619979 -1.722544 1.580664
6 2.610021 0.065138 -0.001531
7 3.570959 -0.591247 -0.030852

#####

SP3-III-4-COOH b3lyp/6-311g(2d,d,p) if=68.0708

7 0.039060 -0.296243 -0.060683
7 1.316192 -0.841889 -0.111852
7 -2.385924 0.300938 0.066603
7 -0.841807 -1.456145 -0.336947
1 -0.362783 -2.234957 0.109069
7 -0.263323 0.347820 1.237588

1 -0.181208 -0.420272 1.899149
7 -0.305504 0.735497 -1.058703
1 0.144538 0.389234 -1.902781
6 -1.635837 0.907292 1.171423
1 -1.575042 1.982767 1.003667
1 -2.137483 0.720477 2.123486
6 -2.208364 -1.148003 0.143470
1 -2.401275 -1.464849 1.175841
1 -2.915437 -1.658642 -0.513808
6 -1.799064 0.775340 -1.185059
1 -2.172531 0.157029 -2.006065
1 -2.081452 1.815520 -1.355433
6 2.321575 0.077882 -0.007477
8 2.308275 1.293908 0.027338
8 3.507238 -0.615056 0.035563
1 4.177846 0.077962 0.077474

#####

SP3-III-4-H b3lyp/6-311g(2d,d,p) if=177.2364

7 -1.000084 0.026316 -0.024949
7 -2.329604 0.009470 0.066699
7 1.536265 -0.043446 0.051434
7 -0.468957 -0.193922 1.330518
1 -1.115334 -0.870508 1.728668
7 -0.434492 -0.945742 -1.045170
1 -0.718733 -1.841604 -0.654256
7 -0.353887 1.342209 -0.501500
1 -0.897330 2.001480 0.053246
6 1.042889 -0.798451 -1.102788
1 1.315742 -0.257292 -2.009986
1 1.504181 -1.789331 -1.130855
6 0.948117 -0.618411 1.256665
1 1.082407 -1.707127 1.215875
1 1.456466 -0.241619 2.147346
6 1.084815 1.341965 -0.085022
1 1.253353 1.857722 0.864845
1 1.665110 1.836169 -0.867615
1 -2.645472 0.097293 -0.899613

#####

SP3-III-4-NH2 b3lyp/6-311g(2d,d,p) if=110.9358

7 0.618500 0.221287 0.056165
7 1.921571 0.688151 0.100532
7 -1.857490 -0.239197 -0.050010

7 -0.189128 1.401926 0.378621
1 0.327968 2.167096 -0.049494
7 0.235776 -0.397981 -1.265556
1 0.344067 0.388956 -1.901754
7 0.207913 -0.849783 1.030542
1 0.680304 -0.535006 1.875125
6 -1.168701 -0.864261 -1.185720
1 -1.184587 -1.945896 -1.045233
1 -1.680948 -0.621176 -2.120398
6 -1.576113 1.194479 -0.092777
1 -1.759337 1.548912 -1.115575
1 -2.240571 1.736708 0.584027
6 -1.281180 -0.792231 1.176626
1 -1.603932 -0.176946 2.021874
1 -1.641806 -1.813550 1.318561
7 2.796886 -0.432674 -0.057306
1 3.261299 -0.372591 -0.960779
1 3.515308 -0.346534 0.653955

#####

SP3-III-4-NO2 b3lyp/6-311g(2d,d,p) if=80.4507

7 -0.061451 -0.285649 0.073184
7 -1.360062 -0.881184 0.145871
7 2.348597 0.299702 -0.086557
7 0.804177 -1.462178 0.322308
1 0.325334 -2.231967 -0.140513
7 0.206422 0.357296 -1.217580
1 0.109768 -0.402617 -1.886274
7 0.289728 0.718240 1.082198
1 -0.144062 0.355754 1.928096
6 1.581457 0.917743 -1.172520
1 1.524086 1.991699 -0.995588
1 2.062431 0.736941 -2.135846
6 2.168679 -1.147763 -0.170681
1 2.348370 -1.460433 -1.205986
1 2.879951 -1.663051 0.477647
6 1.787393 0.764532 1.179345
1 2.177044 0.142717 1.989723
1 2.067263 1.804850 1.350325
7 -2.387072 0.040378 0.003926
8 -2.197166 1.253925 -0.015776
8 -3.485051 -0.502326 -0.066962

#####

SP3-III-4-OH b3lyp/6-311g(2d,d,p) if=120.1416

7 0.623097 0.232737 0.043754
7 1.941335 0.710075 0.077132
7 -1.837560 -0.251859 -0.063208
7 -0.179443 1.462346 0.101009
1 0.333295 2.108669 -0.495285
7 0.313888 -0.640099 -1.107956
1 0.541867 -0.057088 -1.907990
7 0.179478 -0.597334 1.229906
1 0.547078 -0.021771 1.985737
6 -1.107203 -1.054911 -1.046368
1 -1.167606 -2.102546 -0.745255
1 -1.559070 -0.947004 -2.035682
6 -1.564733 1.156094 -0.333851
1 -1.737146 1.338375 -1.401633
1 -2.242432 1.791859 0.240185
6 -1.325161 -0.596688 1.260982
1 -1.720618 0.116960 1.989016
1 -1.660344 -1.601454 1.525094
8 2.794233 -0.415089 -0.142821
1 3.008131 -0.743320 0.739345

#####

SP3-III-5-CN b3lyp/6-311g(2d,d,p) if=75.4073

6 -2.054435 0.912700 -0.021979
6 -0.650965 1.526871 0.180760
1 -0.481045 1.926042 1.178185
7 0.360339 0.427129 0.018264
7 1.619955 1.015035 -0.041633
7 -1.963908 -0.558980 -0.016864
1 -2.497782 1.201259 -0.974625
1 -2.733686 1.214639 0.775502
1 -0.378894 2.279863 -0.555143
7 -1.272798 -0.959646 -1.184633
1 -1.128018 -1.960514 -1.078271
7 0.075843 -0.371322 -1.238328
1 0.069327 0.348768 -1.960469
7 -1.219752 -1.030380 1.123815
1 -1.680923 -0.640934 1.942949
7 0.158429 -0.508990 1.148763
1 0.768537 -1.288808 0.899347
6 2.588507 0.101582 -0.009462
7 3.493869 -0.631022 0.030131

#####

SP3-III-5-COOH b3lyp/6-311g(2d,d,p) if=91.8211

6	2.340038	-1.022333	0.068762
6	0.908290	-1.523438	0.368898
1	0.737090	-1.777909	1.412598
7	-0.041395	-0.395667	0.073786
7	-1.334883	-0.927097	0.066080
7	2.335856	0.443930	-0.092370
1	2.741847	-1.444947	-0.852369
1	3.021935	-1.272553	0.881890
1	0.581247	-2.351321	-0.255804
7	1.635798	0.749128	-1.289727
1	1.514461	1.758603	-1.273503
7	0.289854	0.185488	-1.289884
1	0.305741	-0.646080	-1.879261
7	1.628978	1.075121	0.996274
1	2.077344	0.741999	1.846915
7	0.225408	0.651222	1.079616
1	-0.378817	1.411360	0.749336
6	-2.281751	0.042416	0.019806
8	-2.170025	1.268699	0.075653
8	-3.511399	-0.529762	-0.088428
1	-4.126231	0.214604	-0.078810

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SP3-III-5-H b3lyp/6-311g(2d,d,p) if=97.3740

6	-1.039678	1.348301	-0.257279
6	0.475521	1.413194	0.037530
1	0.706615	1.811085	1.024027
7	1.040898	0.026649	0.034385
7	2.356371	0.058883	-0.005309
7	-1.558855	-0.012680	-0.037755
1	-1.268914	1.608631	-1.291165
1	-1.589189	2.032936	0.390517
1	1.045690	1.963192	-0.707502
7	-1.063551	-0.839234	-1.082376
1	-1.311623	-1.784850	-0.805155
7	0.400709	-0.803718	-1.155101
1	0.645241	-0.208709	-1.947270
7	-1.079809	-0.546454	1.219355
1	-1.340247	0.134669	1.928521
7	0.370967	-0.677560	1.267919
1	0.566313	-1.650681	1.031800
1	2.663937	-0.916455	0.006897

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SP3-III-5-NO2 b3lyp/6-311g(2d,d,p) if=98.0607

6	2.291762	-1.043130	-0.022930
6	0.864215	-1.531495	0.314680
1	0.724712	-1.808451	1.357211
7	-0.069731	-0.371865	0.077511
7	-1.373568	-0.943411	0.083941
7	2.310523	0.430229	-0.099556
1	2.643241	-1.420335	-0.983394
1	3.001616	-1.354475	0.743521
1	0.505017	-2.338481	-0.319686
7	1.576205	0.813447	-1.254924
1	1.461091	1.820990	-1.180336
7	0.237599	0.246448	-1.263964
1	0.247509	-0.562064	-1.884468
7	1.642646	1.003153	1.046004
1	2.095938	0.603382	1.864803
7	0.229813	0.622049	1.122042
1	-0.346365	1.413327	0.828605
7	-2.354290	0.016526	0.010995
8	-2.102195	1.236863	0.067668
8	-3.480679	-0.439635	-0.096557

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SP3-III-6-CN b3lyp/6-311g(2d,d,p) if=75.0556

6	-1.947575	0.982316	-0.115533
7	0.358969	0.395739	0.054921
7	1.590190	1.002985	-0.012285
7	-1.983967	-0.480649	-0.026473
1	-2.198556	1.247632	-1.147186
1	-2.686825	1.413658	0.559815
1	-0.229036	2.260714	-0.108727
7	-1.273049	-0.975252	-1.156423
1	-1.146723	-1.970292	-0.990054
7	0.049834	-0.382935	-1.244818
1	0.017623	0.365223	-1.937815
7	-1.279986	-0.930509	1.167241
1	-1.670312	-0.403121	1.944552
7	0.132088	-0.620366	1.124550
1	0.618751	-1.439323	0.758941
7	-0.606368	1.425222	0.330754
6	2.583811	0.118367	-0.006725
7	3.509098	-0.588320	-0.001178

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SP3-III-6-COOH b3lyp/6-311g(2d,d,p) if=106.8502

6	2.229158	-1.094110	0.001124
7	-0.039479	-0.358594	0.105470
7	-1.306138	-0.913665	0.093277
7	2.345540	0.365299	-0.093109
1	2.458288	-1.499758	-0.989521
1	2.952437	-1.475698	0.722377
1	0.440333	-2.261072	0.156300
7	1.637232	0.753630	-1.270223
1	1.540383	1.764033	-1.209795
7	0.305299	0.196961	-1.287653
1	0.325611	-0.653066	-1.850701
7	1.675735	0.992516	1.039497
1	2.051733	0.540122	1.869487
7	0.251176	0.748326	1.046466
1	-0.255860	1.529538	0.624231
7	0.870284	-1.407564	0.503397
6	-2.272932	0.036657	0.019635
8	-2.174437	1.261845	0.039291
8	-3.489036	-0.562558	-0.077990
1	-4.120032	0.167976	-0.097207

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SP3-III-6-NO2 b3lyp/6-311g(2d,d,p) if=99.1298

6	-2.180930	1.110570	-0.056111
7	0.063229	0.333327	0.110292
7	1.347947	0.931145	0.117457
7	-2.318730	-0.349005	-0.108903
1	-2.379260	1.491479	-1.062692
1	-2.911350	1.526291	0.638106
1	-0.380867	2.254625	0.113283
7	-1.586016	-0.782514	-1.254865
1	-1.505440	-1.792526	-1.169316
7	-0.249443	-0.238786	-1.261961
1	-0.246017	0.592631	-1.852100
7	-1.685546	-0.946659	1.060704
1	-2.066127	-0.457914	1.867785
7	-0.256762	-0.735667	1.080403
1	0.228065	-1.541163	0.685375
7	-0.827651	1.413322	0.469760
7	2.343799	-0.007901	0.011181
8	3.460770	0.471731	-0.091093

8 2.105580 -1.228940 0.034562

SP3-III-7-CN b3lyp/6-311g(2d,d,p) if=72.5485

7 0.362459 0.388000 0.032646
7 1.586397 0.989037 -0.060979
7 -1.991071 -0.439660 -0.016381
1 -2.588765 1.391039 0.364310
1 -0.265642 2.199283 -0.301073
7 -1.278535 -1.027669 -1.109224
1 -1.138054 -2.001675 -0.851932
7 0.005321 -0.408836 -1.259033
1 -0.092805 0.337897 -1.946713
7 -1.290498 -0.841824 1.201579
1 -1.660168 -0.263853 1.952426
7 0.123781 -0.589904 1.128799
1 0.586293 -1.433807 0.788968
7 -0.595226 1.444290 0.302550
7 -1.899136 0.966803 -0.250625
6 2.580775 0.106307 -0.009389
7 3.501435 -0.604054 0.037860

SP3-III-7-COOH b3lyp/6-311g(2d,d,p) if=107.6357

7 0.042453 -0.359916 -0.092217
7 1.301703 -0.912822 -0.069803
7 -2.344605 0.332493 0.092361
1 -2.861559 -1.459875 -0.515765
1 -0.485051 -2.229571 0.034080
7 -1.625320 0.810689 1.238791
1 -1.507970 1.809696 1.087658
7 -0.332687 0.212408 1.299539
1 -0.418210 -0.636647 1.857234
7 -1.686214 0.913613 -1.074873
1 -2.051476 0.413340 -1.881701
7 -0.263034 0.713576 -1.060620
1 0.231455 1.517240 -0.666384
7 -0.865339 -1.431557 -0.477266
7 -2.183633 -1.088528 0.144335
6 2.265015 0.044162 -0.021706
8 2.151817 1.267212 -0.067875
8 3.484149 -0.542271 0.083714
1 4.111721 0.191613 0.086668

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SP3-III-7-NO2 b3lyp/6-311g(2d,d,p) if=99.4195

7	0.066950	-0.335460	-0.096240
7	1.342228	-0.931367	-0.088475
7	-2.316510	0.316536	0.108560
1	-2.818528	-1.509449	-0.415044
1	-0.423241	-2.221639	0.076763
7	-1.573544	0.844819	1.217903
1	-1.473533	1.840541	1.035732
7	-0.275857	0.259448	1.272736
1	-0.339783	-0.570470	1.861094
7	-1.695648	0.861018	-1.096275
1	-2.065011	0.322676	-1.876299
7	-0.268889	0.695717	-1.097840
1	0.202293	1.524415	-0.735142
7	-0.823763	-1.437081	-0.440916
7	-2.128736	-1.099025	0.209119
7	2.334604	0.016378	-0.013407
8	2.081352	1.233906	-0.066910
8	3.455144	-0.449275	0.095253

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SP3-IV-1-CH3 b3lyp/6-311g(2d,d,p) if=89.9621

6	-1.261643	0.872152	-1.254659
6	-1.256383	0.895667	1.243185
1	-1.289335	1.988228	1.190595
6	0.203096	0.388713	1.307952
1	0.357059	-0.384345	2.059044
6	-0.193741	-1.512287	-0.172565
1	0.061328	-1.883166	-1.163938
6	0.269050	0.679148	-1.140644
1	0.784483	1.616950	-0.940279
7	0.625340	-0.261942	-0.001357
7	1.996568	-0.737831	-0.000886
1	-1.644766	0.369266	-2.147269
1	0.221853	-2.211277	0.550189
1	-1.501325	1.933860	-1.359141
1	0.719340	0.228058	-2.023835
1	-1.791834	0.604440	2.150918
1	0.914968	1.189024	1.499271
6	2.936023	0.358882	0.003347
1	2.896095	1.056209	0.871957
1	3.921619	-0.112830	0.051840
1	2.956469	1.007776	-0.900456

6 -1.933283 0.289968 0.000895
1 -3.002603 0.514565 -0.000320
6 -1.700954 -1.231168 0.013739
1 -2.059706 -1.654138 0.956627
1 -2.269990 -1.710650 -0.787006

#####

SP3-IV-1-CN b3lyp/6-311g(2d,d,p) if=57.0613

6 -1.331380 -0.914385 1.295497
6 -1.268251 -1.073808 -1.196884
1 -1.188527 -2.159867 -1.103477
6 0.137330 -0.431129 -1.237705
1 0.275002 0.252246 -2.074494
6 -0.597552 1.557443 0.001562
1 -0.395401 2.106162 0.919902
6 0.137069 -0.430838 1.238515
1 0.858207 -1.245591 1.187740
7 0.375354 0.410869 0.000221
7 1.701798 1.033885 -0.001294
1 -1.839919 -0.479665 2.159879
1 -0.297895 2.190069 -0.831501
1 -1.364709 -1.999836 1.415484
1 0.414779 0.210285 2.073335
1 -1.797953 -0.869806 -2.130566
1 0.945240 -1.161062 -1.263040
6 -2.047685 -0.500037 -0.001158
1 -3.072327 -0.877828 -0.002311
6 -2.049295 1.035870 -0.100411
1 -2.498900 1.347296 -1.046738
1 -2.656774 1.466623 0.698995
6 2.632217 0.096931 0.002795
7 3.486343 -0.704655 -0.001281

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SP3-IV-1-COOH b3lyp/6-311g(2d,d,p) if=60.6410

6 1.766156 0.797740 1.307797
6 1.702540 1.006686 -1.180460
1 1.684513 2.092564 -1.054227
6 0.262402 0.450845 -1.248596
1 0.112238 -0.242209 -2.075804
6 0.838816 -1.577767 0.004175
1 0.611731 -2.097902 0.933324
6 0.258818 0.458003 1.243562
1 -0.384956 1.330767 1.181649

7	-0.052291	-0.361032	-0.000718
7	-1.398713	-0.909279	-0.001333
1	2.236304	0.296586	2.158502
1	0.480854	-2.200432	-0.812800
1	1.897645	1.872477	1.456192
1	-0.076103	-0.161968	2.073909
1	2.224830	0.801127	-2.118453
1	-0.496398	1.226534	-1.291947
6	2.443658	0.356567	-0.000336
1	3.494459	0.655129	-0.001001
6	2.323531	-1.171885	-0.126265
1	2.725239	-1.499039	-1.089086
1	2.913129	-1.665685	0.650017
6	-2.338870	0.046254	0.000347
8	-2.243654	1.284305	-0.001705
8	-3.584332	-0.527146	0.001934
1	-4.184864	0.228293	0.000917

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SP3-IV-1-H b3lyp/6-311g(2d,d,p) if=40.5878

6	1.093064	0.625513	1.300635
6	1.095187	0.802824	-1.198361
1	1.440219	1.838020	-1.123743
6	-0.453482	0.740875	-1.210276
1	-0.867554	0.208976	-2.064694
6	-0.484367	-1.406012	-0.033127
1	-0.894540	-1.873913	0.859940
6	-0.454781	0.679726	1.245296
1	-0.838840	1.699855	1.209960
7	-1.003613	0.004830	-0.000418
7	-2.432075	-0.113927	-0.006382
1	1.423012	0.036784	2.161218
1	-0.976788	-1.860965	-0.890306
1	1.509064	1.629392	1.422805
1	-0.947694	0.167976	2.069303
1	1.498389	0.398456	-2.130788
1	-0.916704	1.727036	-1.178953
6	1.612366	-0.012338	-0.000021
1	2.705059	-0.029690	-0.000025
6	1.059745	-1.444410	-0.102805
1	1.388661	-1.901650	-1.040142
1	1.458604	-2.059506	0.708192
1	-2.737461	0.865840	0.036779

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SP3-IV-1-NH2 b3lyp/6-311g(2d,d,p) if=27.2694

6	-1.264180	-0.840644	1.277520
6	-1.233718	-0.951849	-1.213672
1	-1.321754	-2.040446	-1.149321
6	0.253614	-0.519730	-1.230494
1	0.497371	0.138451	-2.063936
6	-0.186646	1.532891	0.008304
1	0.104588	2.056426	0.917887
6	0.252820	-0.528704	1.228946
1	0.878015	-1.418830	1.183547
7	0.607863	0.270134	0.001723
7	2.039566	0.733352	0.000896
1	-1.719207	-0.377498	2.157746
1	0.187648	2.114171	-0.833124
1	-1.433929	-1.918001	1.359582
1	0.592844	0.080824	2.065343
1	-1.725210	-0.645455	-2.141206
1	0.949635	-1.356774	-1.242987
6	-1.922860	-0.298771	-0.002925
1	-2.992164	-0.525679	-0.005043
6	-1.702215	1.225051	-0.069254
1	-2.125004	1.619899	-0.997462
1	-2.228957	1.716335	0.753256
7	2.823793	-0.459521	-0.002263
1	3.433260	-0.472955	-0.817425
1	3.423414	-0.487698	0.820103

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SP3-IV-1-NO2 b3lyp/6-311g(2d,d,p) if=76.1898

6	1.759478	0.746152	1.325780
6	1.673166	1.031581	-1.154396
1	1.633025	2.109119	-0.974408
6	0.246017	0.451641	-1.261372
1	0.142153	-0.267749	-2.073140
6	0.784945	-1.569999	0.015709
1	0.582369	-2.057905	0.967746
6	0.238165	0.479863	1.245497
1	-0.358583	1.382507	1.173658
7	-0.085801	-0.332733	-0.000738
7	-1.439926	-0.918420	-0.002769
1	2.205177	0.186076	2.152382
1	0.397876	-2.212465	-0.771962
1	1.934504	1.805998	1.524882

1 -0.136997 -0.117567 2.075266
1 2.200158 0.882583 -2.100027
1 -0.520477 1.212936 -1.357654
6 2.418329 0.335862 -0.002212
1 3.473426 0.617210 -0.004811
6 2.268211 -1.185924 -0.170538
1 2.620739 -1.489953 -1.159740
1 2.879146 -1.715969 0.563782
7 -2.414222 0.019731 0.000865
8 -2.171815 1.254451 -0.002995
8 -3.553528 -0.435692 0.004459

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SP3-IV-1-OH b3lyp/6-311g(2d,d,p) if=80.1689

6 -1.199140 -0.944929 1.223747
6 -1.242240 -0.854710 -1.269468
1 -1.441812 -1.924884 -1.371391
6 0.281793 -0.592875 -1.194290
1 0.670347 -0.057511 -2.059980
6 -0.187814 1.536207 -0.103457
1 0.211546 2.195125 0.666437
6 0.262537 -0.441271 1.266187
1 1.000743 -1.233915 1.362874
7 0.623314 0.284021 -0.010812
7 2.028591 0.758500 0.004172
1 -1.714785 -0.674120 2.148955
1 0.053835 1.976082 -1.070351
1 -1.235402 -2.035613 1.145602
1 0.444249 0.285367 2.056588
1 -1.670202 -0.364311 -2.148456
1 0.865814 -1.501924 -1.063962
6 -1.901179 -0.309451 0.010158
1 -2.967988 -0.545673 0.017479
6 -1.692402 1.216978 0.063682
1 -2.266707 1.706687 -0.726880
1 -2.063844 1.606987 1.015493
8 2.805356 -0.474704 0.108416
1 3.178695 -0.592005 -0.772607

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SP3-IV-2-CH3 b3lyp/6-311g(2d,d,p) if=117.7002

6 -1.272866 1.042241 -1.091391
6 -1.293482 0.612439 1.371746
1 -1.336751 1.698112 1.507771

6	0.165093	0.099705	1.368776
1	0.295859	-0.826881	1.925357
6	-0.212308	-1.398577	-0.535647
1	0.005448	-1.462604	-1.602317
6	0.262851	0.941261	-0.944968
1	0.696908	1.833462	-0.496099
7	0.622597	-0.233518	-0.044101
7	1.979957	-0.714515	-0.129667
1	-1.597935	0.656718	-2.060131
1	0.200954	-2.278093	-0.047256
1	-1.597531	2.082982	-1.023744
1	0.774217	0.743404	-1.885687
1	-1.846663	0.165022	2.202604
1	0.871198	0.829141	1.760321
6	2.926616	0.353206	0.094663
1	2.883490	0.861686	1.085224
1	3.911343	-0.120085	0.049131
1	2.946475	1.168359	-0.661413
7	-1.631463	-1.208660	-0.259476
1	-1.910203	-1.772727	0.535904
6	-1.923934	0.210396	0.022643
1	-3.006279	0.354334	0.028113

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SP3-IV-2-CN b3lyp/6-311g(2d,d,p) if=75.0138

6	1.381728	-0.769286	-1.346680
6	1.281695	-1.122238	1.127088
1	1.181994	-2.192324	0.923309
6	-0.102609	-0.444868	1.239502
1	-0.172933	0.252852	2.073094
6	0.620326	1.527396	-0.050629
1	0.479501	1.973551	-1.036667
6	-0.129716	-0.465653	-1.230973
1	-0.748337	-1.355255	-1.119157
7	-0.375657	0.385121	0.001966
7	-1.688389	1.018590	0.021876
1	1.837035	-0.176307	-2.142263
1	0.303232	2.244865	0.703416
1	1.540147	-1.822723	-1.584445
1	-0.517790	0.116664	-2.064337
1	1.820684	-1.024423	2.072958
1	-0.928360	-1.150581	1.318668
7	1.975226	1.043018	0.162372
1	2.294471	1.291718	1.091926

6 2.052447 -0.422466 -0.010327
1 3.102749 -0.717612 -0.020588
6 -2.628213 0.089891 0.011277
7 -3.489227 -0.703455 0.006435

#####

SP3-IV-2-COOH b3lyp/6-311g(2d,d,p) if=108.3893

6 1.803206 0.662499 1.347103
6 1.713257 1.041365 -1.121884
1 1.681423 2.112502 -0.901184
6 0.286959 0.461192 -1.246052
1 0.186457 -0.244944 -2.069993
6 0.864546 -1.550007 0.053591
1 0.703262 -1.976675 1.045016
6 0.270933 0.492875 1.237292
1 -0.277131 1.423538 1.123595
7 -0.052538 -0.337107 0.001767
7 -1.385483 -0.900622 -0.008698
1 2.214673 0.025550 2.133056
1 0.487424 -2.250249 -0.688197
1 2.048754 1.696846 1.595611
1 -0.156420 -0.062156 2.070709
1 2.245130 0.924314 -2.070089
1 -0.484393 1.221139 -1.329916
7 2.249094 -1.174490 -0.179442
1 2.527646 -1.434053 -1.119225
6 2.439137 0.279532 0.003919
1 3.508910 0.495467 0.009048
6 -2.331029 0.050492 -0.004716
8 -2.234086 1.287601 -0.001967
8 -3.574351 -0.525261 -0.010267
1 -4.177800 0.227842 -0.011463

#####

SP3-IV-2-H b3lyp/6-311g(2d,d,p) if=138.9417

6 1.075415 1.382393 -0.393027
6 1.145874 -1.070244 -0.896234
1 1.457391 -0.812871 -1.913669
6 -0.394346 -1.191228 -0.790090
1 -0.728234 -2.069764 -0.240594
6 -0.466398 -0.039021 1.380531
1 -0.773483 0.917348 1.805188
6 -0.443151 1.259089 -0.663449
1 -0.684404 1.197578 -1.726087

7 -0.993134 -0.013182 -0.036733
7 -2.414510 -0.059468 0.084825
1 1.273576 2.137349 0.370876
1 -1.015204 -0.832054 1.884190
1 1.610317 1.678566 -1.298179
1 -1.037188 2.057294 -0.223725
1 1.620455 -2.024350 -0.649350
1 -0.894451 -1.197781 -1.757907
7 0.980140 -0.235950 1.421175
1 1.192362 -1.185998 1.705428
6 1.587425 0.020927 0.100243
1 2.673394 0.039199 0.212399
1 -2.730909 0.084181 -0.881288

#####

SP3-IV-2-NH2 b3lyp/6-311g(2d,d,p) if=126.5351

6 1.294157 -0.767286 -1.289076
6 1.251372 -0.929437 1.203061
1 1.313810 -2.016598 1.089449
6 -0.217884 -0.448652 1.264601
1 -0.393437 0.286010 2.050121
6 0.209229 1.497825 -0.158900
1 0.005321 1.861270 -1.166864
6 -0.245194 -0.642345 -1.183298
1 -0.754508 -1.588665 -1.011952
7 -0.607107 0.246518 -0.015204
7 -2.018601 0.721902 -0.018087
1 1.672406 -0.193056 -2.137764
1 -0.201219 2.212143 0.553315
1 1.591825 -1.808457 -1.434323
1 -0.696089 -0.163057 -2.050902
1 1.770924 -0.675207 2.131575
1 -0.939733 -1.255016 1.381087
7 1.631463 1.229880 0.060394
1 1.912373 1.586034 0.967367
6 1.913847 -0.220421 0.004709
1 2.996420 -0.364061 0.003255
7 -2.815324 -0.465964 0.043864
1 -3.425798 -0.423053 0.856914
1 -3.418468 -0.522741 -0.774632

#####

SP3-IV-2-NO2 b3lyp/6-311g(2d,d,p) if=106.1092

6 -1.783404 -0.644743 1.348832

6 -1.696070 -1.033484 -1.119870
1 -1.664886 -2.102120 -0.888307
6 -0.269909 -0.457702 -1.261315
1 -0.187210 0.270168 -2.068086
6 -0.813341 1.543705 0.073394
1 -0.657573 1.939952 1.077695
6 -0.246407 -0.523080 1.234053
1 0.264981 -1.471350 1.113470
7 0.088152 0.307807 0.001009
7 1.423863 0.909106 -0.012962
1 -2.175028 0.010160 2.129939
1 -0.420391 2.257175 -0.647124
1 -2.054789 -1.669592 1.608336
1 0.202919 0.009335 2.070918
1 -2.231095 -0.925202 -2.066982
1 0.493943 -1.217927 -1.385851
7 -2.195020 1.192090 -0.184126
1 -2.456655 1.457019 -1.127228
6 -2.412511 -0.257661 0.003355
1 -3.485368 -0.455621 0.008004
7 2.405284 -0.022775 -0.005391
8 2.163054 -1.256999 -0.003777
8 3.542578 0.436024 -0.006872

#####

SP3-IV-2-OH b3lyp/6-311g(2d,d,p) if=136.2754

6 1.259910 -0.867982 -1.232951
6 1.229690 -0.840603 1.265816
1 1.267661 -1.934018 1.226980
6 -0.226287 -0.323308 1.309227
1 -0.371389 0.489479 2.019283
6 0.211235 1.484192 -0.296181
1 0.019078 1.744154 -1.338059
6 -0.277429 -0.739462 -1.116274
1 -0.771771 -1.669748 -0.843966
7 -0.622064 0.259767 -0.029978
7 -2.011123 0.747368 -0.038755
1 1.625896 -0.353059 -2.123901
1 -0.192762 2.271519 0.338952
1 1.557064 -1.916244 -1.310363
1 -0.744442 -0.349603 -2.019830
1 1.764520 -0.535185 2.169569
1 -0.967708 -1.090423 1.519377
7 1.625079 1.221573 -0.041052

1 1.903266 1.644653 0.837536
6 1.893268 -0.231804 0.013318
1 2.973939 -0.386490 0.016205
8 -2.795958 -0.469440 0.164944
1 -3.181250 -0.646661 -0.700568

#####

SP3-IV-3-CH3 b3lyp/6-311g(2d,d,p) if=118.3806

7 -0.613277 0.220239 0.119990
7 -1.963974 0.672652 0.316704
7 1.220477 -0.213338 -1.470882
1 1.505307 0.616352 -1.980560
7 1.658998 1.098289 0.477028
1 1.972889 1.069626 1.442033
6 -0.155485 -0.890995 1.057186
1 -0.883588 -1.694477 0.969519
1 -0.231281 -0.469135 2.058064
6 1.275633 -1.335916 0.679958
1 1.276405 -2.272072 0.115497
1 1.875710 -1.494115 1.579320
6 0.240798 1.436826 0.404084
1 -0.146914 1.857366 1.329120
1 0.013548 2.128152 -0.407908
6 -0.232042 -0.228349 -1.294605
1 -0.734511 0.457670 -1.974469
1 -0.639960 -1.231291 -1.424960
6 -2.915722 -0.319539 -0.131384
1 -2.873727 -1.313421 0.369876
1 -3.899317 0.091887 0.111036
1 -2.938046 -0.533548 -1.222249
6 1.890951 -0.212691 -0.172945
1 2.963118 -0.353911 -0.317968

#####

SP3-IV-3-CN b3lyp/6-311g(2d,d,p) if=77.4517

6 0.101152 -0.434325 -1.225076
1 0.070288 0.268028 -2.059994
6 0.070832 -0.444703 1.233761
1 0.724807 -1.310698 1.123232
7 0.354042 0.430338 0.012247
7 1.666585 1.054225 0.039183
1 0.391647 0.129690 2.101110
1 0.961328 -1.092150 -1.340008
6 -0.655460 1.541550 -0.019913

1 -0.307793 2.232182 -0.785021
1 -0.585138 2.044398 0.943858
6 -2.049858 0.939859 -0.305953
1 -2.355174 1.111533 -1.340640
1 -2.799548 1.400790 0.340018
6 -1.973148 -0.572251 -0.028577
1 -2.960236 -1.035273 -0.036065
7 -1.138940 -1.177323 -1.062227
1 -0.953811 -2.144604 -0.819713
7 -1.340811 -0.812647 1.289906
1 -1.821714 -0.286160 2.012555
6 2.604280 0.121742 0.012939
7 3.466060 -0.670161 -0.013740

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SP3-IV-3-COOH b3lyp/6-311g(2d,d,p) if=105.7276

6 0.302608 0.471087 -1.232862
1 0.309438 -0.236185 -2.064289
6 0.314328 0.459430 1.237607
1 -0.253849 1.378429 1.123310
7 -0.040151 -0.379712 0.002550
7 -1.375812 -0.930900 0.016365
1 -0.061853 -0.094262 2.096559
1 -0.499364 1.192720 -1.351324
6 0.887086 -1.565949 -0.037225
1 0.487031 -2.224938 -0.804119
1 0.777676 -2.068853 0.922987
6 2.325513 -1.078782 -0.319840
1 2.614150 -1.257437 -1.358297
1 3.035256 -1.612246 0.315796
6 2.371392 0.427153 -0.013516
1 3.392831 0.809772 -0.009322
7 1.590768 1.115971 -1.035695
1 1.468444 2.085918 -0.764813
7 1.756662 0.683838 1.310117
1 2.179924 0.082610 2.010436
6 -2.313870 0.029256 0.005184
8 -2.205966 1.265654 -0.017738
8 -3.560725 -0.535081 0.016359
1 -4.158767 0.222336 0.004653

#####

SP3-IV-3-H b3lyp/6-311g(2d,d,p) if=176.6052

6 0.412837 -0.658965 -1.236093

1 0.665214 0.006991 -2.062638
6 0.391181 -0.716802 1.204057
1 0.697967 -1.758347 1.071035
7 0.984253 0.021363 0.007659
7 2.405046 0.133841 0.022231
1 0.900754 -0.312630 2.076548
1 0.960739 -1.592074 -1.358185
6 0.431904 1.417214 0.018618
1 1.001631 1.950919 -0.739063
1 0.698524 1.833102 0.989190
6 -1.089975 1.379303 -0.246112
1 -1.328104 1.692041 -1.265766
1 -1.612954 2.054428 0.435025
6 -1.570229 -0.065880 -0.024293
1 -2.659212 -0.132699 -0.028637
7 -1.027675 -0.889490 -1.101920
1 -1.214979 -1.863490 -0.889324
7 -1.067765 -0.581779 1.271408
1 -1.330347 0.051644 2.020620
1 2.709435 -0.846646 0.058488

#####

SP3-IV-3-NH2 b3lyp/6-311g(2d,d,p) if=135.7371

6 0.222172 -0.486944 -1.228656
1 0.306254 0.227744 -2.049496
6 0.193747 -0.553048 1.211167
1 0.746503 -1.485259 1.099312
7 0.588692 0.292941 0.017585
7 1.999297 0.760192 0.043830
1 0.565323 -0.023267 2.087633
1 0.981998 -1.258489 -1.336291
6 -0.246411 1.529161 0.026564
1 0.192507 2.182020 -0.725853
1 -0.095198 1.996206 0.999286
6 -1.717677 1.143518 -0.252605
1 -2.012085 1.398511 -1.273699
1 -2.388152 1.676626 0.425442
6 -1.855701 -0.376455 -0.039494
1 -2.900782 -0.690377 -0.056050
7 -1.124166 -1.050036 -1.109480
1 -1.077118 -2.040138 -0.892166
7 -1.261549 -0.772044 1.258956
1 -1.673347 -0.221159 2.006409
7 2.794181 -0.434029 -0.012095

1 3.431933 -0.372036 -0.802249
1 3.370195 -0.506947 0.824289

#####

SP3-IV-3-NO2 b3lyp/6-311g(2d,d,p) if=103.4929

6 0.287971 -0.458443 1.252996
1 0.300823 0.277046 2.059268
6 0.293870 -0.508199 -1.230342
1 -0.238985 -1.442863 -1.095291
7 -0.077038 0.349166 -0.006891
7 -1.417341 0.939808 -0.019958
1 -0.103423 0.012331 -2.100606
1 -0.500462 -1.185016 1.414172
6 0.828039 1.559184 0.001102
1 0.416083 2.234745 0.746952
1 0.716947 2.030553 -0.974440
6 2.272446 1.106072 0.304816
1 2.547785 1.307265 1.342553
1 2.975053 1.645480 -0.333363
6 2.349569 -0.402466 0.020442
1 3.377329 -0.766652 0.022780
7 1.578576 -1.090220 1.051162
1 1.470835 -2.066983 0.799903
7 1.740544 -0.684197 -1.301072
1 2.147514 -0.079368 -2.007737
7 -2.390636 -0.002781 -0.006589
8 -3.531660 0.444058 -0.012376
8 -2.135790 -1.234789 0.014270

#####

SP3-IV-3-OH b3lyp/6-311g(2d,d,p) if=137.1698

6 0.233422 -0.490351 -1.233691
1 0.302665 0.219385 -2.060292
6 0.222115 -0.540977 1.213440
1 0.776610 -1.470480 1.098632
7 0.604572 0.307992 0.007679
7 1.987655 0.786912 0.037289
1 0.605966 -0.009346 2.082474
1 0.998840 -1.255364 -1.343514
6 -0.246005 1.536851 0.012374
1 0.179707 2.193906 -0.744499
1 -0.099952 2.006790 0.984002
6 -1.711596 1.130552 -0.265188
1 -2.006601 1.368378 -1.290128

1 -2.387529 1.667048 0.404385
6 -1.834165 -0.387239 -0.029792
1 -2.876205 -0.710566 -0.038348
7 -1.101187 -1.068671 -1.095272
1 -1.042890 -2.055518 -0.866564
7 -1.230165 -0.757771 1.269958
1 -1.641248 -0.201059 2.013207
8 2.769410 -0.456824 0.098647
1 3.226605 -0.470836 -0.748971

#####

SP3-IV-4-CH3 b3lyp/6-311g(2d,d,p) if=101.9524

7 -0.625420 0.305637 -0.014043
7 -1.893285 0.729023 -0.011537
7 0.223063 1.489839 -0.062085
1 -0.279591 2.088414 -0.711986
1 1.608192 -1.353815 1.878652
6 1.588107 1.137945 -0.503546
1 2.272424 1.852576 -0.038024
1 1.714660 1.188232 -1.591484
6 1.856152 -0.290675 -0.003722
1 2.924197 -0.513409 -0.012507
1 -0.967559 -1.282864 -1.213795
1 -0.650264 0.100260 1.965969
6 -2.857708 -0.357056 0.013934
1 -2.697388 -1.095041 0.815126
1 -3.832076 0.105376 0.183102
1 -2.951523 -0.918209 -0.936696
7 -0.218347 -0.598480 -1.188408
7 -0.196788 -0.479904 1.263012
1 0.979063 -2.231868 -0.432283
6 1.079635 -1.251746 -0.913391
1 1.591141 -1.385529 -1.872300
1 1.607115 0.417164 2.034822
6 1.276657 -0.420817 1.410531

#####

SP3-IV-4-CN b3lyp/6-311g(2d,d,p) if=74.5051

7 -0.343117 0.403099 -0.006192
7 -1.610224 1.014741 -0.004280
7 0.610424 1.475666 -0.254496
1 0.160747 2.019045 -0.987043
1 1.634240 -1.279273 2.005692
6 1.911120 0.891127 -0.659808

1	2.695165	1.551750	-0.282487
1	2.013922	0.804028	-1.746732
6	1.984216	-0.496397	-0.001861
1	3.004603	-0.879750	-0.007026
1	-1.032537	-1.188758	-0.978944
1	-0.393480	0.477573	1.959614
7	-0.182907	-0.628819	-1.051684
7	-0.023983	-0.210359	1.307365
1	0.823839	-2.329356	-0.188169
6	1.035377	-1.426932	-0.771557
1	1.459639	-1.720040	-1.735065
1	1.918515	0.476476	1.944205
6	1.447637	-0.368682	1.431032
6	-2.573558	0.104539	0.013817
7	-3.466393	-0.647703	0.001604

#####

SP3-IV-4-COOH b3lyp/6-311g(2d,d,p) if=97.9920

7	0.020397	-0.349204	-0.045961
7	1.320918	-0.886476	-0.083361
7	-0.853606	-1.455295	-0.444786
1	-0.358115	-1.864812	-1.232240
1	-2.086173	0.882303	2.142973
6	-2.189728	-0.921337	-0.793635
1	-2.923981	-1.685442	-0.526424
1	-2.290884	-0.690154	-1.859638
6	-2.372782	0.351668	0.047496
1	-3.419885	0.653431	0.083938
1	0.596858	1.392351	-0.743988
1	0.057144	-0.719002	1.881246
7	-0.215476	0.793105	-0.949833
7	-0.349127	0.038014	1.336596
1	-1.353271	2.272917	0.123585
6	-1.493602	1.442431	-0.577939
1	-1.939218	1.832048	-1.497134
1	-2.239658	-0.865879	1.847419
6	-1.829772	0.071659	1.456055
6	2.291937	0.046804	-0.010456
8	2.233994	1.282541	-0.010049
8	3.505649	-0.569165	0.048612
1	4.141985	0.156883	0.054055

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SP3-IV-4-H b3lyp/6-311g(2d,d,p) if=216.2134

7	-0.998257	-0.002398	0.011524
7	-2.332535	-0.051554	0.046670
7	-0.480741	-1.343273	0.258185
1	-1.103790	-1.687903	0.983592
1	1.528486	0.782093	-2.026444
6	0.937419	-1.281790	0.674743
1	1.416713	-2.200774	0.326482
1	1.062285	-1.209721	1.761266
6	1.547958	-0.047438	-0.011996
1	2.637247	-0.106381	-0.019214
1	-0.930396	1.759082	0.994123
1	-1.019606	-0.051131	-1.956903
7	-0.352852	0.927155	1.078272
7	-0.421152	0.466638	-1.316889
1	1.204258	2.094703	0.129664
6	1.061474	1.197502	0.743859
1	1.611396	1.327260	1.682065
1	1.091535	-0.939888	-1.941264
6	0.992416	0.029554	-1.440132
1	-2.634973	0.869724	-0.276552

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SP3-IV-4-NH2 b3lyp/6-311g(2d,d,p) if=141.0034

7	-0.589705	0.289973	0.012921
7	-1.920866	0.739264	0.064464
7	0.217994	1.464580	-0.269775
1	-0.326894	1.934329	-0.988529
1	1.711601	-1.092650	1.978133
6	1.558047	1.033495	-0.730729
1	2.276383	1.792139	-0.408362
1	1.618832	0.932368	-1.820494
6	1.842635	-0.319929	-0.055991
1	2.902710	-0.570905	-0.114611
1	-1.138226	-1.353837	-0.862661
1	-0.528096	0.426936	1.974444
7	-0.331855	-0.738279	-1.006628
7	-0.111966	-0.258905	1.348630
1	0.896993	-2.279159	-0.125871
6	0.973014	-1.381193	-0.751217
1	1.395177	-1.665408	-1.719708
1	1.760294	0.682629	1.873272
6	1.370545	-0.226931	1.401565
7	-2.742946	-0.438001	-0.020948
1	-3.229274	-0.586276	0.860974

1 -3.449536 -0.263240 -0.729009

SP3-IV-4-NO2 b3lyp/6-311g(2d,d,p) if=97.3811

7 0.044490 0.333249 0.038689
7 1.367930 0.914999 0.077284
7 -0.807926 1.493055 0.297114
1 -0.335924 1.966039 1.063994
1 -1.995571 -1.117714 -2.051759
6 -2.169023 1.019965 0.648196
1 -2.875646 1.758874 0.263147
1 -2.314031 0.919564 1.728916
6 -2.344525 -0.340424 -0.043762
1 -3.394243 -0.632330 -0.077880
1 0.577995 -1.322182 0.930681
1 0.144326 0.506879 -1.913697
7 -0.219526 -0.689378 1.059258
7 -0.278286 -0.185681 -1.300021
1 -1.355852 -2.271166 0.140730
6 -1.502418 -1.360951 0.732680
1 -1.976450 -1.629307 1.679913
1 -2.147198 0.653677 -1.969461
6 -1.756632 -0.232306 -1.457852
7 2.362179 -0.018031 0.006076
8 2.145748 -1.251616 0.012164
8 3.482522 0.465675 -0.052035

SP3-IV-4-OH b3lyp/6-311g(2d,d,p) if=124.2627

7 -0.602521 0.294037 0.011969
7 -1.919479 0.759649 0.055113
7 0.203765 1.466751 -0.279304
1 -0.329254 1.926338 -1.013324
1 1.689663 -1.080003 1.990695
6 1.550919 1.038017 -0.722592
1 2.262294 1.798472 -0.390010
1 1.624050 0.940004 -1.811790
6 1.830290 -0.314236 -0.047349
1 2.891083 -0.562792 -0.097904
1 -1.115807 -1.392158 -0.825001
1 -0.579437 0.377052 1.983423
7 -0.345967 -0.749792 -1.010275
7 -0.132467 -0.271079 1.339175
1 0.903461 -2.280373 -0.140836

6 0.973408 -1.375954 -0.755507
1 1.402000 -1.643727 -1.725604
1 1.724049 0.694842 1.876659
6 1.345766 -0.220731 1.406648
8 -2.731137 -0.457662 0.095393
1 -3.248611 -0.375891 -0.713406

#####

SP3-IV-5-CH3 b3lyp/6-311g(2d,d,p) if=92.7395

7 -0.630050 0.210873 -0.118291
7 -1.897782 0.612912 -0.365597
6 1.323388 -0.999921 -1.020055
1 1.619851 -0.546947 -1.970346
1 1.739325 -2.011280 -0.965283
6 1.864422 -0.158732 0.145098
1 2.941526 -0.276887 0.270487
6 -0.195570 -0.043647 1.333531
1 -0.896007 -0.756616 1.756989
1 -0.323100 0.924001 1.823817
6 -2.894374 -0.310854 0.153172
1 -2.969228 -0.363136 1.256737
1 -3.859733 0.056029 -0.201160
1 -2.785731 -1.345549 -0.210331
7 -0.151921 -1.089732 -0.843880
1 -0.615297 -0.949999 -1.740624
7 0.253722 1.268480 -0.729736
1 -0.243936 2.130981 -0.512246
7 1.551517 1.250989 -0.119975
1 1.549825 1.729880 0.783288
7 1.171987 -0.534508 1.397463
1 1.173015 -1.544657 1.498304

#####

SP3-IV-5-CN b3lyp/6-311g(2d,d,p) if=62.0739

7 0.363159 0.347495 0.007705
7 1.621123 0.974854 -0.023473
6 -1.477872 -0.293288 1.412287
1 -1.894052 0.592086 1.900054
1 -1.750437 -1.183090 1.984238
6 -2.011961 -0.403109 -0.024204
1 -3.056427 -0.712685 -0.050753
6 0.118424 -0.757759 -1.024247
1 0.934290 -1.469588 -0.922104
1 0.194308 -0.251078 -1.988231

7 0.010482 -0.255248 1.307571
1 0.410079 0.406607 1.970325
7 -0.631052 1.462899 -0.189889
1 -0.201225 2.056012 -0.899011
7 -1.870293 0.914067 -0.660530
1 -1.850985 0.758939 -1.670549
7 -1.183178 -1.355571 -0.794349
1 -1.084853 -2.228419 -0.285578
6 2.608736 0.088974 0.011231
7 3.529093 -0.628166 0.025995

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SP3-IV-5-COOH b3lyp/6-311g(2d,d,p) if=83.9531

7 0.041381 -0.293770 -0.002513
7 1.324723 -0.855187 0.026943
6 -1.837752 0.190483 -1.416213
1 -2.180033 -0.724803 -1.906830
1 -2.175851 1.056077 -1.990768
6 -2.394789 0.259264 0.014444
1 -3.461182 0.485191 0.026706
6 -0.309219 0.780870 1.040543
1 0.451974 1.548467 0.945073
1 -0.214100 0.263769 1.997482
7 -0.352291 0.272598 -1.302552
1 0.098687 -0.359438 -1.960646
7 -0.877209 -1.488647 0.185344
1 -0.400931 -2.050957 0.889514
7 -2.154809 -1.042471 0.654424
1 -2.150080 -0.881493 1.663770
7 -1.651605 1.271089 0.791615
1 -1.611701 2.147237 0.280264
6 2.320986 0.062331 -0.004428
8 2.288446 1.291348 -0.026348
8 3.521562 -0.591876 -0.000503
1 4.176462 0.117208 -0.008661

#####

SP3-IV-5-H b3lyp/6-311g(2d,d,p) if=236.2625

7 -0.990958 0.029025 -0.036549
7 -2.335727 0.063062 0.105692
6 1.074703 1.371291 -0.114064
1 1.177465 1.923010 0.824777
1 1.694786 1.851087 -0.877814
6 1.533146 -0.082005 0.087080

1 2.617907 -0.163044 0.165578
6 -0.391601 -1.072048 -0.907110
1 -0.891947 -1.001616 -1.870153
1 -0.684323 -2.001411 -0.414500
7 -0.325446 1.305928 -0.615217
1 -0.905829 2.009726 -0.161527
7 -0.416261 -0.048220 1.354613
1 -1.055426 -0.684536 1.828849
7 0.912347 -0.592426 1.315320
1 0.896352 -1.611740 1.236804
7 1.052935 -0.923844 -1.033120
1 1.276511 -0.473544 -1.915193
1 -2.701211 0.013963 -0.847436

#####

SP3-IV-5-NH2 b3lyp/6-311g(2d,d,p) if=123.5522

7 -0.609509 -0.177538 -0.148172
7 -1.924761 -0.519579 -0.489026
6 1.385692 -0.913067 1.046752
1 1.712377 -1.882034 0.657952
1 1.812256 -0.766480 2.043622
6 1.855039 0.209572 0.109881
1 2.928964 0.385063 0.184942
6 -0.259816 1.300292 -0.025786
1 -0.988030 1.716412 0.663190
1 -0.429602 1.704746 -1.026208
7 -0.095575 -0.784788 1.143910
1 -0.541528 -1.699309 1.096856
7 0.233446 -0.825472 -1.204036
1 -0.299449 -0.663500 -2.057774
7 1.516615 -0.176168 -1.267148
1 1.463730 0.690089 -1.807440
7 1.118573 1.457050 0.414127
1 1.144060 1.635267 1.413238
7 -2.795127 0.295843 0.321273
1 -3.475796 0.721543 -0.301638
1 -3.318105 -0.308006 0.951685

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SP3-IV-5-NO2 b3lyp/6-311g(2d,d,p) if=93.3650

7 -0.072676 -0.274453 0.021019
7 -1.366318 -0.888055 0.020108
6 1.782984 0.354729 1.392654
1 2.108275 -0.496907 1.996149

1 2.117888 1.281300 1.864108
6 2.362675 0.246058 -0.026313
1 3.430875 0.460483 -0.049383
6 0.300518 0.651811 -1.149048
1 -0.448667 1.433782 -1.180247
1 0.221658 0.010830 -2.029315
7 0.299337 0.434033 1.245441
1 -0.169289 -0.099576 1.974254
7 0.832751 -1.499211 -0.010025
1 0.366379 -2.139992 -0.651934
7 2.118536 -1.121265 -0.507558
1 2.134639 -1.088701 -1.528782
7 1.639815 1.160430 -0.933919
1 1.600009 2.093978 -0.537237
7 -2.388218 0.026797 0.003106
8 -2.185184 1.254405 0.002531
8 -3.499994 -0.484245 -0.006103

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SP3-IV-5-OH b3lyp/6-311g(2d,d,p) if=125.4522

7 0.620600 0.246001 0.020584
7 1.935292 0.737163 0.009839
6 -1.355084 -0.191749 1.389126
1 -1.693103 0.733457 1.864688
1 -1.763758 -1.044631 1.939078
6 -1.836063 -0.234903 -0.068303
1 -2.908607 -0.418444 -0.140436
6 0.275361 -0.831772 -0.999309
1 1.008130 -1.619951 -0.867141
1 0.434970 -0.348699 -1.965131
7 0.129945 -0.322243 1.348896
1 0.558329 0.343028 1.990441
7 -0.232812 1.457305 -0.186200
1 0.278280 1.989421 -0.890519
7 -1.519364 1.057184 -0.692773
1 -1.481885 0.893968 -1.701136
7 -1.095362 -1.279386 -0.809683
1 -1.109842 -2.149820 -0.287590
8 2.779822 -0.439136 -0.068345
1 3.065536 -0.586875 0.840782

#####

SP3-IV-6-CN b3lyp/6-311g(2d,d,p) if=70.6198

7 0.352902 0.379930 -0.029300

7 1.603657 0.984810 -0.062941
1 -1.692778 -0.934895 1.965126
1 -0.889535 -2.300636 0.106918
6 -1.977516 -0.408729 0.048766
1 -3.018999 -0.724970 0.099505
1 0.209338 0.814828 1.864426
7 -0.644998 1.457084 -0.362685
1 -0.221630 1.917682 -1.168911
7 -1.871922 0.831437 -0.754394
1 -1.802617 0.539511 -1.731051
7 -1.514105 -0.105278 1.402984
1 1.018305 -1.296377 -0.859348
6 -1.063573 -1.474800 -0.592271
7 -0.029444 -0.039732 1.359217
1 -1.488504 -1.877725 -1.515859
7 0.170173 -0.736986 -0.948968
6 2.573471 0.081568 0.007067
7 3.461184 -0.674931 0.032920

#####

SP3-IV-6-COOH b3lyp/6-311g(2d,d,p) if=92.8299

7 0.028577 -0.330377 0.051088
7 1.310986 -0.865220 0.103793
1 -2.095499 0.674366 -2.018455
1 -1.411123 2.223607 -0.275254
6 -2.355139 0.268499 -0.072816
1 -3.417090 0.501837 -0.149369
1 -0.094476 -0.957326 -1.782256
7 -0.894752 -1.456841 0.472899
1 -0.435775 -1.819965 1.308675
7 -2.162553 -0.894333 0.825624
1 -2.109795 -0.517338 1.773901
7 -1.865821 -0.102623 -1.402555
1 0.580044 1.434771 0.686870
6 -1.522480 1.438204 0.482801
7 -0.380226 -0.071024 -1.364020
1 -1.979115 1.877238 1.374839
7 -0.233751 0.833637 0.887522
6 2.287542 0.064124 0.009172
8 2.220629 1.298936 -0.021333
8 3.497916 -0.549887 -0.028812
1 4.137705 0.172929 -0.053183

#####

SP3-IV-6-H b3lyp/6-311g(2d,d,p) if=206.8973

7 -0.994110 -0.034267 -0.040327
7 -2.316732 -0.061849 -0.013247
1 1.512775 1.684125 -1.056725
1 1.299845 -0.551028 -1.938932
6 1.507931 0.079127 0.136972
1 2.588037 0.155053 0.268375
1 -0.937856 1.909233 -0.244764
7 -0.483891 0.105526 1.361262
1 -1.068575 -0.553043 1.875404
7 0.884537 -0.323658 1.419653
1 0.908790 -1.345049 1.436749
1 -2.615641 0.034997 -0.985686
7 0.993476 1.397871 -0.229115
1 -0.854276 -1.425501 -1.484384
6 1.116735 -0.958264 -0.936492
7 -0.390954 1.204638 -0.740606
1 1.688325 -1.886968 -0.829232
7 -0.302243 -1.252119 -0.649574

#####

SP3-IV-6-NH2 b3lyp/6-311g(2d,d,p) if=137.8848

7 0.608145 0.272964 -0.029830
7 1.907430 0.702459 -0.016784
1 -1.743078 -0.704437 1.935000
1 -0.954955 -2.223707 0.222769
6 -1.823796 -0.234863 -0.006810
1 -2.897517 -0.425394 -0.025827
1 0.362664 0.838747 1.838890
7 -0.238108 1.435604 -0.430108
1 0.262247 1.804758 -1.238702
7 -1.523972 0.944270 -0.852822
1 -1.437126 0.587929 -1.806828
7 -1.425273 0.076082 1.363448
1 1.115940 -1.475216 -0.693982
6 -1.001821 -1.433081 -0.536859
7 0.055585 -0.035769 1.411843
1 -1.438849 -1.852002 -1.449036
7 0.314886 -0.866670 -0.886400
7 2.733567 -0.480602 0.040292
1 3.458002 -0.364980 -0.661891
1 3.200545 -0.516390 0.944146

#####

SP3-IV-6-NO2 b3lyp/6-311g(2d,d,p) if=97.4700

7	0.056326	-0.313966	0.042881
7	1.352911	-0.895526	0.102687
1	-2.001830	0.918419	-1.946085
1	-1.407089	2.237316	0.010194
6	-2.323870	0.260337	-0.078122
1	-3.386393	0.487272	-0.161187
1	0.005916	-0.718341	-1.853788
7	-0.856196	-1.505922	0.292311
1	-0.419609	-1.964437	1.093397
7	-2.139219	-1.005636	0.669940
1	-2.126837	-0.756844	1.660706
7	-1.783289	0.071239	-1.426168
1	0.555555	1.357553	0.909544
6	-1.530534	1.358378	0.653917
7	-0.299850	0.106716	-1.335883
1	-2.019649	1.667962	1.581635
7	-0.241874	0.720506	1.016965
7	2.354577	0.035322	0.009393
8	3.473336	-0.445844	-0.029003
8	2.129496	1.267054	-0.015256

#####

SP3-IV-6-OH b3lyp/6-311g(2d,d,p) if=123.4128

7	0.625925	0.279400	-0.019682
7	1.904849	0.718704	0.006723
1	-1.747763	-0.785078	1.900801
1	-0.941279	-2.227952	0.099520
6	-1.810092	-0.229609	-0.019549
1	-2.883968	-0.415803	-0.050415
1	0.395250	0.689289	1.906654
7	-0.229527	1.465015	-0.346595
1	0.263190	1.888579	-1.133297
7	-1.505850	0.991362	-0.802759
1	-1.414816	0.688160	-1.774489
7	-1.410288	0.011291	1.363170
1	1.105035	-1.455416	-0.768142
6	-0.992285	-1.399149	-0.616138
7	0.065731	-0.138912	1.409339
1	-1.434008	-1.765933	-1.547914
7	0.328352	-0.819156	-0.942409
8	2.709349	-0.501558	0.135824
1	3.343480	-0.384764	-0.579695

#####

SP3-IV-7-CH3 b3lyp/6-311g(2d,d,p) if=90.1237

7	-0.648980	0.256189	-0.099332
7	-1.888017	0.656090	-0.174958
1	1.573701	-1.845087	-1.071868
1	1.170105	-1.678811	1.333145
6	1.820369	-0.204359	0.048926
1	2.895207	-0.388584	0.088432
1	-0.552358	-0.604204	-1.865683
7	0.236428	1.354985	-0.623504
1	-0.218894	2.202550	-0.286330
7	1.546750	1.231378	-0.062205
1	1.577870	1.600760	0.890634
7	1.274995	-0.873527	-1.122991
7	-0.203728	-0.953842	-0.971709
1	-0.211541	0.666973	1.840354
7	1.192368	-0.661554	1.308503
7	-0.163467	-0.220900	1.339792
6	-2.860040	-0.384841	0.152281
1	-2.682440	-0.847510	1.131149
1	-3.837446	0.099392	0.170502
1	-2.900627	-1.192001	-0.592743

#####

SP3-IV-7-CN b3lyp/6-311g(2d,d,p) if=68.8071

7	0.366320	0.332259	0.072797
7	1.603997	0.914784	0.125629
1	-1.590430	-1.747704	1.367124
1	-1.088652	-1.962834	-1.041266
6	-1.983361	-0.381385	-0.053887
1	-3.021868	-0.709346	-0.094155
1	0.365291	-0.161937	1.949567
7	-0.622680	1.444048	0.360136
1	-0.233175	2.250448	-0.128612
7	-1.886988	1.075032	-0.193628
1	-1.928651	1.274584	-1.195369
7	-1.415542	-0.753611	1.237579
7	0.067646	-0.678343	1.120515
1	0.102319	0.379858	-1.898138
7	-1.228472	-0.964584	-1.184672
7	0.075282	-0.376117	-1.214868
6	2.606022	0.044101	-0.012083
7	3.563180	-0.607662	-0.118249

#####

SP3-IV-7-COOH b3lyp/6-311g(2d,d,p) if=70.5891

7	0.047455	-0.289140	-0.082017
7	1.303121	-0.825200	-0.137790
1	-2.038033	1.724589	-1.268840
1	-1.545772	1.823057	1.145396
6	-2.351997	0.256551	0.062045
1	-3.408484	0.520206	0.112950
1	0.026947	0.326909	-1.921756
7	-0.882843	-1.443112	-0.459611
1	-0.436438	-2.250891	-0.024738
7	-2.167138	-1.196659	0.112044
1	-2.197524	-1.461434	1.099133
7	-1.798605	0.737926	-1.198816
7	-0.313730	0.765297	-1.065412
1	-0.261994	-0.521270	1.862963
7	-1.637701	0.812847	1.232659
7	-0.308157	0.291331	1.250034
6	2.313473	0.092278	0.004388
8	2.282123	1.304466	0.086122
8	3.496196	-0.594559	0.030399
1	4.169070	0.093574	0.106498

#####

SP3-IV-7-H b3lyp/6-311g(2d,d,p) if=194.6807

7	0.998268	0.048172	0.046788
7	2.312947	0.010023	0.011999
1	-1.619149	1.908237	0.127559
1	-1.304296	0.265836	1.916936
6	-1.496187	-0.077369	-0.105828
1	-2.582755	-0.139607	-0.179734
1	0.824163	1.829619	-0.755170
7	0.473674	-0.545563	-1.237649
1	1.105712	-1.327329	-1.407238
7	-0.862022	-1.018464	-1.033196
1	-0.863698	-1.925283	-0.560176
1	2.618302	0.409387	0.899986
7	-1.074415	1.272718	-0.451511
7	0.320548	1.447137	0.046134
1	0.615542	-1.573670	1.151784
7	-1.071668	-0.473648	1.257395
7	0.357425	-0.595085	1.280187

#####

SP3-IV-7-NH2 b3lyp/6-311g(2d,d,p) if=99.7512

7 -0.629262 0.194897 -0.102141
7 -1.904888 0.623133 -0.213836
1 1.591232 -1.940555 -0.857848
1 1.197045 -1.489733 1.519832
6 1.823770 -0.175764 0.059070
1 2.901211 -0.338904 0.110103
1 -0.594477 -0.877166 -1.733615
7 0.203102 1.249081 -0.777544
1 -0.279629 2.115443 -0.539536
7 1.522385 1.231792 -0.223883
1 1.553593 1.715961 0.676377
7 1.272436 -0.987335 -1.018583
7 -0.202741 -1.082690 -0.814025
1 -0.236607 0.870860 1.736678
7 1.208764 -0.483157 1.369415
7 -0.161060 -0.064672 1.336907
7 -2.784154 -0.443742 0.184292
1 -3.227008 -0.185571 1.063270
1 -3.520051 -0.476902 -0.513893

#####

SP3-IV-7-NO2 b3lyp/6-311g(2d,d,p) if=79.1943

7 -0.074208 -0.273996 0.091990
7 -1.339514 -0.864586 0.166495
1 2.020865 1.718903 1.263935
1 1.494350 1.824789 -1.155527
6 2.315143 0.255523 -0.079334
1 3.371039 0.516869 -0.144967
1 -0.040689 0.323749 1.934926
7 0.855214 -1.445739 0.465123
1 0.405140 -2.254625 0.034207
7 2.124032 -1.197464 -0.130154
1 2.142831 -1.466017 -1.116225
7 1.778992 0.733113 1.190213
7 0.292274 0.763681 1.076140
1 0.195675 -0.519735 -1.850981
7 1.583289 0.814019 -1.238812
7 0.255345 0.290344 -1.236378
7 -2.376940 0.053438 -0.009119
8 -2.173638 1.262566 -0.074615
8 -3.472543 -0.485907 -0.065116

#####

SP3-IV-7-OH b3lyp/6-311g(2d,d,p) if=115.9010

7 -0.637127 0.202736 -0.102610
 7 -1.919525 0.629394 -0.239849
 1 1.637445 -1.839677 -1.004385
 1 1.129321 -1.640066 1.375683
 6 1.806828 -0.173314 0.093414
 1 2.882084 -0.331934 0.184632
 1 -0.489113 -0.608814 -1.875691
 7 0.204015 1.338483 -0.638535
 1 -0.280678 2.171641 -0.303140
 7 1.505298 1.254767 -0.049228
 1 1.505939 1.639430 0.898123
 7 1.322544 -0.875454 -1.087348
 7 -0.160297 -0.976727 -0.982222
 1 -0.383581 0.631029 1.818070
 7 1.130026 -0.623146 1.330060
 7 -0.243206 -0.222311 1.279529
 8 -2.766582 -0.405250 0.284989
 1 -3.121818 -0.833918 -0.502263

Table S2. The bond length (Å) of N-N ylide bond at the B3LYP/6-311G(2d,d,p) level.

Bond length	N ⁻¹ NH	N ⁻³ NCH ₃	N ⁻¹ NOH	N ⁻¹ NNH ₂	N ⁻¹ NCOOH	N ⁻¹ NCN	N ⁻¹ NNO ₂
sp ² -I-1	1.31	1.31	1.31	1.32	1.36	1.35	1.39
sp ² -I-2	1.30	1.30	1.30	1.30	1.34	1.34	1.36
sp ² -I-3	1.27	1.28	1.28	1.28	1.30	1.31	1.29
sp ² -I-4	1.26	1.26	1.27	1.27	1.26	1.29	1.28
sp ² -I-5	1.26	1.27	1.27	1.27	1.30	1.29	1.27
sp ² -I-6	1.25	1.24	1.25	1.26	1.25	1.27	1.25
sp ² -II-1	1.30	1.31	1.30	1.30	1.34	1.34	1.35
sp ² -II-2	1.31	1.32	1.31	1.31	1.37	1.36	1.38
sp ² -II-3	1.28	1.27	1.29	1.29	1.32	1.31	1.33
sp ² -II-4	1.29	1.28	1.28	1.30	1.31	1.31	1.33
sp ² -II-5	1.27	1.27	1.27	1.26	1.29	1.30	1.32
sp ³ -I-1	1.44	1.47	1.52	1.57	1.47	1.48	1.49
sp ³ -I-2	1.45	1.47	1.51	1.56	1.46	1.48	1.49
sp ³ -I-3	1.43	1.46	1.49	1.52	1.45	1.46	1.48
sp ³ -I-4	1.34	1.34	1.39	1.39	1.40	1.41	1.44
sp ³ -I-5	-	-	-	-	1.41	1.41	1.43
sp ³ -I-6	-	-	-	-	1.40	1.38	1.44
sp ³ -II-1	1.43	1.45	1.48	1.51	1.45	1.47	1.48
sp ³ -II-2	1.44	1.46	1.47	1.51	1.45	1.47	1.47
sp ³ -II-3	1.44	1.44	1.46	1.50	1.45	1.47	1.47
sp ³ -II-4	1.33	-	-	-	1.41	1.40	1.43

sp ³ -II-5	-	-	-	-	1.39	1.39	1.40
sp ³ -III-1	1.43	1.45	1.48	1.51	1.45	1.46	1.48
sp ³ -III-2	1.43	1.45	1.48	1.51	1.45	1.46	1.47
sp ³ -III-3	1.43	1.45	1.48	1.50	1.45	1.46	1.47
sp ³ -III-4	1.33	1.35	1.40	1.38	1.39	1.39	1.43
sp ³ -III-5	1.32	-	-	-	1.40	1.39	1.42
sp ³ -III-6	-	-	-	-	1.38	1.37	1.42
sp ³ -III-7	-	-	-	-	1.38	1.37	1.41
sp ³ -IV-1	1.43	1.45	1.48	1.50	1.45	1.47	1.48
sp ³ -IV-2	1.43	1.44	1.47	1.49	1.45	1.46	1.46
sp ³ -IV-3	1.43	1.44	1.46	1.49	1.44	1.45	1.46
sp ³ -IV-4	1.34	1.37	1.40	1.41	1.41	1.41	1.45
sp ³ -IV-5	1.35	1.38	1.40	1.40	1.40	1.41	1.43
sp ³ -IV-6	1.32	-	1.35	1.37	1.39	1.39	1.42
sp ³ -IV-7	1.32	1.30	1.36	1.35	1.37	1.37	1.40

* The bond lengths of N₂H₂, H₃NNH and N₂H₄ are 1.24, 1.46 and 1.49 Å, respectively.

Table S3. The bond dissociation energy (BDE) (kJ/mol) of N-N ylide bond at the CBS-QB3 level.

Bond dissociation energy	Bond						
	N- ¹ NH	N- ³ NCH ₃	N- ¹ NOH	N- ¹ NNH ₂	N- ¹ NCOOH	N- ¹ NCN	N- ¹ NNO ₂
sp ² -I-1	341.21	140.33	158.11	25.69	253.47	259.07	177.78
sp ² -I-2	392.12	155.10	187.82	84.39	264.30	279.53	181.00
sp ² -I-3	354.26	215.81	173.76	42.01	253.01	257.86	169.66
sp ² -I-4	413.04	241.33	211.50	111.88	261.21	284.09	189.87
sp ² -I-5	437.52	187.19	241.21	143.34	278.82	294.43	205.56
sp ² -I-6	409.24	235.39	211.29	119.37	250.71	260.66	169.49
sp ² -II-1	426.27	135.69	232.76	140.79	258.82	261.83	175.31
sp ² -II-2	358.95	88.78	185.10	53.05	267.65	280.96	211.63
sp ² -II-3	311.92	143.13	136.15	4.48	249.37	249.53	196.27
sp ² -II-4	353.55	179.66	158.99	36.94	257.11	246.23	166.69
sp ² -II-5	349.74	154.22	159.37	29.25	237.53	241.25	158.95
sp ³ -I-1	291.33	70.17	107.61	-17.36	268.99	262.04	203.51
sp ³ -I-2	290.79	72.05	105.94	-18.70	268.82	259.37	203.59
sp ³ -I-3	292.71	65.40	101.75	-22.43	263.34	254.60	194.56
sp ³ -I-4	323.13	102.34	113.89	-16.74	238.07	253.09	171.00
sp ³ -I-5	-	-	-	-	266.56	254.64	193.80
sp ³ -I-6	-	-	-	-	232.09	214.89	140.08
sp ³ -II-1	288.91	71.17	107.49	-17.24	270.04	260.96	205.31
sp ³ -II-2	287.32	66.07	102.72	-24.43	271.92	257.19	208.70
sp ³ -II-3	304.64	70.50	129.79	3.05	297.02	277.52	231.88
sp ³ -II-4	304.76	-	-	-	266.94	250.20	197.19
sp ³ -II-5	-	-	-	-	277.57	257.57	202.05
sp ³ -III-1	290.91	72.51	104.73	-19.83	269.95	259.49	204.22

sp ³ -III-2	283.38	66.36	95.27	-28.53	261.96	248.61	195.39
sp ³ -III-3	278.15	61.21	88.70	-35.40	250.58	236.69	183.51
sp ³ -III-4	310.29	91.04	92.97	-31.13	224.10	232.09	152.17
sp ³ -III-5	292.34	-	-	-	239.20	220.29	165.69
sp ³ -III-6	-	-	-	-	235.85	213.34	156.94
sp ³ -III-7	-	-	-	-	229.07	204.01	148.49
sp ³ -IV-1	295.10	77.70	109.91	-15.82	276.23	266.02	212.51
sp ³ -IV-2	291.88	75.27	104.18	-21.05	272.75	260.08	208.20
sp ³ -IV-3	287.52	67.40	97.82	-26.28	264.18	250.71	198.32
sp ³ -IV-4	298.40	79.66	97.65	-16.90	255.64	239.87	178.24
sp ³ -IV-5	298.32	77.11	94.64	-29.12	242.34	235.85	167.57
sp ³ -IV-6	287.86	-	80.75	-29.58	241.17	220.16	185.56
sp ³ -IV-7	301.83	82.38	78.37	-42.22	209.91	211.58	159.62

* The bond dissociation energies of N₂H₂, H₃NNH and N₂H₄ are 853.12, 198.41 and 259.24 kJ/mol, respectively.

Table S4. Calculated detoanation properties of title structures at the B3LYP/6-311G(2d,d,p) level.

$\Delta H_{f,solid}$ (kJ/mol)	R: H	R: CH ₃	R: OH	R: NH ₂	R: COOH	R: CN	R: NO ₂
sp ² -I-1	450.65	506.40	399.26	565.38	44.40	533.76	413.67
sp ² -I-2	450.96	511.05	392.64	559.11	74.87	562.65	450.50
sp ² -I-3	493.99	562.20	443.07	578.55	152.68	619.32	534.74
sp ² -I-4	545.64	600.37	495.05	618.45	218.94	689.76	600.32
sp ² -I-5	744.01	808.58	703.56	805.56	425.92	902.55	811.24
sp ² -I-6	884.99	935.20	828.56	937.37	572.77	1060.88	961.72
sp ² -II-1	438.61	477.38	367.67	537.64	34.18	514.69	381.27
sp ² -II-2	469.94	507.11	412.82	577.05	28.94	520.17	369.39
sp ² -II-3	524.36	587.88	485.41	645.07	141.97	644.11	523.41
sp ² -II-4	617.96	681.62	571.77	737.34	234.93	724.82	604.12
sp ² -II-5	726.86	801.55	704.46	853.67	368.20	856.12	737.81
sp ³ -I-1	613.47	679.43	549.77	709.03	140.73	637.48	487.68
sp ³ -I-2	644.01	708.46	586.03	742.25	173.80	671.52	520.18
sp ³ -I-3	621.04	697.33	567.37	727.44	159.42	653.59	507.44
sp ³ -I-4	779.16	845.99	746.80	913.07	375.18	844.72	727.48
sp ³ -I-5	-	-	-	-	494.08	986.75	845.42
sp ³ -I-6	-	-	-	-	578.23	1075.73	947.43
sp ³ -II-1	584.93	688.40	519.47	679.14	109.64	607.18	455.93
sp ³ -II-2	601.09	664.81	537.47	701.65	125.09	621.63	470.48
sp ³ -II-3	674.95	736.45	610.88	773.85	200.92	702.23	545.71
sp ³ -II-4	742.67	-	-	-	307.23	809.21	659.71
sp ³ -II-5	-	-	-	-	433.62	939.15	788.72
sp ³ -III-1	732.17	796.80	676.06	835.37	262.37	760.08	609.21
sp ³ -III-2	809.01	873.55	757.07	913.66	343.82	842.70	691.91
sp ³ -III-3	875.71	776.2	823.79	981.49	416.47	913.58	764.10
sp ³ -III-4	929.30	997.24	910.04	1067.68	531.06	1005.22	889.44

sp ³ -III-5	1113.75	-	-	-	686.31	1183.28	1040.45
sp ³ -III-6	-	-	-	-	775.70	1272.27	1135.12
sp ³ -III-7	-	-	-	-	915.93	1412.84	1276.21
sp ³ -IV-1	676.56	740.54	618.98	777.97	204.02	703.43	551.27
sp ³ -IV-2	693.57	756.98	640.33	798.13	224.12	724.35	571.55
sp ³ -IV-3	709.34	776.71	658.06	815.46	244.40	743.31	591.76
sp ³ -IV-4	895.95	961.67	858.06	1007.08	453.64	956.77	815.11
sp ³ -IV-5	924.77	992.92	886.89	1047.20	494.53	984.05	851.88
sp ³ -IV-6	1079.05	-	1046.70	1193.05	646.30	1149.83	1008.93
sp ³ -IV-7	1132.50	1215.12	1118.50	1273.15	740.44	1217.95	1103.15
2,4,6-trinitrotoluene (TNT)					77.57		
1,3,5-Trinitro-1,3,5-triazinane (RDX)					118.53		
1,3,5,7-Tetranitro-1,3,5,7-tetrazocane (HMX)					163.31		

ρ (g/cm ³)	R: H	R: CH ₃	R: OH	R: NH ₂	R: COOH	R: CN	R: NO ₂
sp ² -I-1	1.25	1.19	1.33	1.25	1.49	1.37	1.54
sp ² -I-2	1.36	1.26	1.46	1.38	1.52	1.43	1.59
sp ² -I-3	1.39	1.36	1.57	1.45	1.60	1.52	1.6
sp ² -I-4	1.61	1.37	1.62	1.55	1.65	1.57	1.66
sp ² -I-5	1.54	1.47	1.73	1.69	1.71	1.63	1.73
sp ² -I-6	1.59	1.49	1.77	1.73	1.74	1.67	1.76
sp ² -II-1	1.65	1.10	1.26	1.17	1.38	1.26	1.44
sp ² -II-2	1.20	1.23	1.35	1.27	1.59	1.46	1.66
sp ² -II-3	1.32	1.33	1.49	1.37	1.56	1.46	1.63
sp ² -II-4	1.38	1.41	1.57	1.46	1.69	1.58	1.77
sp ² -II-5	1.50	1.48	1.66	1.57	1.78	1.69	1.85
sp ³ -I-1	1.08	1.07	1.16	1.11	1.29	1.21	1.34
sp ³ -I-2	1.17	1.16	1.24	1.19	1.38	1.31	1.45
sp ³ -I-3	1.34	1.3	1.42	1.34	1.53	1.49	1.63
sp ³ -I-4	1.27	1.23	1.38	1.31	1.5	1.44	1.58
sp ³ -I-5	-	-	-	-	1.59	1.58	1.72
sp ³ -I-6	-	-	-	-	1.69	1.67	1.82
sp ³ -II-1	1.09	1.08	1.18	1.12	1.31	1.23	1.39
sp ³ -II-2	1.17	1.16	1.27	1.19	1.40	1.34	1.48
sp ³ -II-3	1.31	1.28	1.4	1.31	1.51	1.46	1.62
sp ³ -II-4	1.31	-	-	-	1.54	1.46	1.64
sp ³ -II-5	-	-	-	-	1.57	1.51	1.68
sp ³ -III-1	1.21	1.19	1.28	1.22	1.39	1.33	1.46
sp ³ -III-2	1.32	1.29	1.38	1.32	1.49	1.44	1.56
sp ³ -III-3	1.42	1.30	1.49	1.42	1.59	1.56	1.69
sp ³ -III-4	1.42	1.35	1.50	1.44	1.61	1.57	1.70
sp ³ -III-5	1.48	-	-	-	1.67	1.75	1.79
sp ³ -III-6	-	-	-	-	1.73	1.75	1.86
sp ³ -III-7	-	-	-	-	1.79	1.83	1.94

sp ³ -IV-1	1.13	1.12	1.21	1.16	1.32	1.20	1.37
sp ³ -IV-2	1.24	1.22	1.31	1.26	1.42	1.36	1.49
sp ³ -IV-3	1.34	1.30	1.4	1.34	1.51	1.46	1.59
sp ³ -IV-4	1.3	1.26	1.38	1.31	1.48	1.41	1.55
sp ³ -IV-5	1.44	1.38	1.52	1.44	1.61	1.58	1.71
sp ³ -IV-6	1.49	-	1.57	1.49	1.65	1.62	1.76
sp ³ -IV-7	1.61	1.52	1.69	1.61	1.80	1.78	1.89
2,4,6-trinitrotoluene (TNT)						1.63	
1,3,5-Trinitro-1,3,5-triazinane (RDX)						1.77	
1,3,5,7-Tetranitro-1,3,5,7-tetrazocane (HMX)						1.80	

D (km/s)	R: H	R: CH ₃	R: OH	R: NH ₂	R: COOH	R: CN	R: NO ₂
sp ² -I-1	5.43	5.25	6.03	5.96	5.59	5.46	6.81
sp ² -I-2	6.17	5.85	6.72	6.65	5.98	5.97	7.24
sp ² -I-3	6.74	6.62	7.48	7.24	6.61	6.67	7.78
sp ² -I-4	7.51	7.03	8.05	7.95	7.21	7.27	8.41
sp ² -I-5	8.79	8.16	8.95	9.24	8.20	8.21	9.36
sp ² -I-6	9.68	8.69	9.74	10.01	8.93	8.88	9.07
sp ² -II-1	5.89	5.62	6.60	6.42	5.96	5.85	7.25
sp ² -II-2	6.90	6.54	7.38	7.23	6.79	6.79	8.21
sp ² -II-3	8.01	7.48	8.38	8.10	7.28	7.47	8.65
sp ² -II-4	9.01	8.36	9.22	9.02	8.16	8.38	9.58
sp ² -II-5	10.10	9.36	10.19	10.06	9.02	9.39	10.20
sp ³ -I-1	5.82	5.68	6.37	6.21	5.87	5.80	6.98
sp ³ -I-2	6.57	6.38	7.02	6.87	6.44	6.48	7.61
sp ³ -I-3	7.42	7.13	7.86	7.64	7.07	7.28	8.42
sp ³ -I-4	7.88	7.53	8.38	8.23	7.70	7.84	8.89
sp ³ -I-5	-	-	-	-	8.45	8.90	9.81
sp ³ -I-6	-	-	-	-	9.16	9.66	10.59
sp ³ -II-1	6.10	5.90	6.65	6.49	6.05	6.01	7.28
sp ³ -II-2	6.82	6.60	7.34	7.12	6.57	6.70	7.85
sp ³ -II-3	7.90	7.54	8.26	8.04	7.33	7.60	8.73
sp ³ -II-4	8.40	-	-	-	7.92	8.14	9.23
sp ³ -II-5	-	-	-	-	8.50	8.85	9.85
sp ³ -III-1	6.43	6.25	6.88	6.73	6.32	6.34	7.41
sp ³ -III-2	7.29	7.02	7.64	7.49	6.99	7.11	8.10
sp ³ -III-3	8.10	6.88	8.40	8.24	7.65	7.91	8.86
sp ³ -III-4	8.48	8.03	8.86	8.73	8.17	8.38	9.30
sp ³ -III-5	9.37	-	-	-	8.83	9.29	10.09
sp ³ -III-6	-	-	-	-	9.40	9.99	10.71
sp ³ -III-7	-	-	-	-	10.04	10.80	11.43
sp ³ -IV-1	5.71	5.58	6.25	6.12	5.78	5.69	6.82
sp ³ -IV-2	6.45	6.27	6.90	6.77	6.33	6.36	7.46
sp ³ -IV-3	7.12	6.85	7.52	7.36	6.83	6.97	8.02

sp ³ -IV-4	7.70	7.38	8.07	7.90	7.38	7.51	8.46
sp ³ -IV-5	8.54	8.14	8.88	8.67	8.07	8.37	9.27
sp ³ -IV-6	9.35	-	9.60	9.40	8.68	9.05	9.90
sp ³ -IV-7	10.16	9.20	10.44	10.27	9.57	10.03	10.75
2,4,6-trinitrotoluene (TNT)						7.13	
1,3,5-Trinitro-1,3,5-triazinane (RDX)						8.81	
1,3,5,7-Tetranitro-1,3,5,7-tetrazocane (HMX)						8.91	

P (GPa)	R: H	R: CH ₃	R: OH	R: NH ₂	R: COOH	R: CN	R: NO ₂
sp ² -I-1	10.22	9.19	13.15	12.26	12.24	11.03	18.66
sp ² -I-2	14.07	11.94	17.47	16.45	14.23	13.52	21.51
sp ² -I-3	17.00	16.14	22.75	20.22	18.05	17.71	24.94
sp ² -I-4	22.10	18.32	26.94	25.53	21.83	21.53	29.81
sp ² -I-5	31.66	25.64	35.77	36.45	28.93	28.13	37.91
sp ² -I-6	39.36	29.23	41.71	43.45	34.71	33.39	36.09
sp ² -II-1	10.99	9.88	15.17	13.58	13.20	11.91	20.22
sp ² -II-2	16.58	14.65	20.00	18.37	18.92	17.88	28.51
sp ² -II-3	24.34	20.36	27.56	24.28	21.49	21.68	31.16
sp ² -II-4	31.97	26.43	34.67	31.61	28.40	28.75	40.34
sp ² -II-5	41.97	33.29	43.74	41.18	35.77	37.69	46.88
sp ³ -I-1	10.40	9.87	13.26	12.10	12.17	11.32	17.82
sp ³ -I-2	14.14	13.24	17.01	15.71	15.42	15.06	22.30
sp ³ -I-3	20.10	18.10	23.45	21.27	20.04	20.87	29.50
sp ³ -I-4	21.77	19.46	26.20	24.37	23.41	23.65	32.37
sp ³ -I-5	-	-	-	-	29.29	32.37	41.48
sp ³ -I-6	-	-	-	-	35.76	39.57	50.06
sp ³ -II-1	11.54	10.69	14.66	13.35	13.15	12.35	19.84
sp ³ -II-2	15.28	14.21	18.89	16.90	16.23	16.40	24.07
sp ³ -II-3	22.38	20.05	25.60	23.22	21.35	22.44	31.64
sp ³ -II-4	25.32	-	-	-	25.23	25.75	35.64
sp ³ -II-5	-	-	-	-	29.43	31.04	41.28
sp ³ -III-1	13.94	13.01	16.67	15.42	14.96	14.59	21.28
sp ³ -III-2	19.13	17.43	21.72	20.21	19.19	19.36	26.63
sp ³ -III-3	24.93	16.92	27.71	25.75	23.99	25.31	33.51
sp ³ -III-4	27.27	23.70	31.02	29.23	27.64	28.58	37.05
sp ³ -III-5	34.36	-	-	-	32.99	43.56	45.02
sp ³ -III-6	-	-	-	-	38.24	43.56	51.93
sp ³ -III-7	-	-	-	-	44.59	52.32	60.64
sp ³ -IV-1	10.44	9.88	13.18	12.23	12.04	11.17	17.26
sp ³ -IV-2	14.35	13.36	21.89	15.96	15.25	14.88	21.89
sp ³ -IV-3	18.48	16.71	21.30	19.78	18.49	18.84	26.46
sp ³ -IV-4	21.18	19.03	24.22	22.40	21.32	21.39	28.89
sp ³ -IV-5	27.99	24.75	31.41	28.82	26.97	28.68	36.90
sp ³ -IV-6	34.40	-	37.56	34.80	31.65	34.06	42.84

sp ³ -IV-7	42.67	33.11	46.49	43.69	40.55	44.38	52.80
2,4,6-trinitrotoluene (TNT)						20.90	
1,3,5-Trinitro-1,3,5-triazinane (RDX)						34.13	
1,3,5,7-Tetranitro-1,3,5,7-tetrazocane (HMX)						35.23	
