

## Supporting Information

# DFT Studies on a New Class of Cage Functionalized Organic Superbases

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### Cartesian coordinates:

**B3LYP/6-311+G\*\*//B3LYP/6-31G\* SCF energies, B3LYP/6-31G\* zero point vibrational energies (ZPVE), and Cartesian coordinates for 7-12 and their monoprotonated ions**

7

SCF ENERGY at B3LYP/6-311+G\*\* = -734.96781 au  
ZPVE = 260.994 kcal/mol

1	-3.6739925120	1.0461233418	1.3144319202
6	-3.3736384922	0.0348714783	1.0115134876
6	-2.1217574387	-0.4693229734	-1.1103367994
6	-1.4769945111	-1.7453627944	-0.5196154777
6	-1.3852496103	-1.6052565980	1.0340553719
6	-1.9324279863	-0.2200672753	1.4551499234
1	-4.0415160033	-0.6540869970	1.5445261609
1	-2.2178725488	-0.5597046404	-2.1989301396
1	-1.8962195817	-2.6824408982	-0.8984406570
1	-1.7700152337	-2.4421707327	1.6247877698
1	-1.8752171562	-0.1050412034	2.5439618785
6	-0.8558441725	0.6968431529	0.7915937372
1	-0.9678560066	1.7423477616	1.0931907432
6	-0.9914150591	0.5512423796	-0.7899462689
1	-1.1689014505	1.5292673641	-1.2486230330
6	0.1687399921	-1.4233868451	0.9283908307
1	0.7900915768	-2.1828956503	1.4102762774
6	0.0826925782	-1.5436808855	-0.6340192231
1	0.6517105509	-2.3724872603	-1.0620191218
6	0.1878856900	-0.2279697672	-1.4388572771
1	-0.1469598194	-0.5084393454	-2.4602879694
6	0.3981905918	0.0117926590	1.4308602762
1	0.1832942540	0.0135555683	2.5199815650
7	1.4559245315	0.4835667132	-1.5790581862
7	1.7509274203	0.5388825147	1.2582289056
6	1.8149905621	1.9905615805	1.2589433697
1	1.2607012171	2.3847591088	0.4045936758
1	2.8598281579	2.3032593135	1.1501296980
1	1.4223494498	2.4512332618	2.1890029578
6	2.6438724305	-0.0194988454	2.2630528997

1	2.6510174124	-1.1127710058	2.2036881301
1	2.3647814610	0.2582986090	3.3019122671
1	3.6655897362	0.3324448390	2.0826847689
6	2.6082634880	-0.3961257726	-1.6869950208
1	2.5615775656	-1.0811622600	-2.5586113069
1	2.7082346198	-0.9868112815	-0.7742286772
1	3.5146716046	0.2112233115	-1.7919575049
6	1.4029523101	1.4043984669	-2.7049375647
1	0.5767036970	2.1121790283	-2.5819838489
1	1.2655767381	0.8945421968	-3.6822993172
1	2.3336304547	1.9806336791	-2.7529226669
6	-3.4940306073	-0.1465962706	-0.5184127019
1	-4.1929767507	-0.9561860906	-0.7659214167
1	-3.8944625406	0.7580362589	-0.9932170253\

## 7H<sup>+</sup>

SCF ENERGY at B3LYP/6-311+G\*\* = -735.39540 au  
ZPVE = 269.005 kcal/mol

6	-0.2955010000	2.2885710000	-0.9195490000
6	-1.6260560000	1.7387320000	-0.3600720000
6	-1.4807460000	1.4937480000	1.1762300000
6	-0.0549930000	1.8833080000	1.6281690000
1	-0.3846820000	2.4785040000	-1.9960280000
1	-2.5164830000	2.2820310000	-0.6832100000
1	-2.2798720000	1.8804780000	1.8120190000
1	0.0610080000	1.7244790000	2.7069060000
6	0.7663670000	0.7962570000	0.8659000000
1	1.8183550000	0.8003060000	1.1637370000
6	0.6148610000	1.0439030000	-0.7033830000
1	1.5963920000	1.1701490000	-1.1671310000
6	-1.4466920000	-0.0594710000	0.9301920000
1	-2.2472780000	-0.6442810000	1.3873410000
6	-1.5906770000	0.1892390000	-0.6180310000
1	-2.4808750000	-0.2514290000	-1.0700690000
6	-0.2899520000	0.0018780000	-1.4253800000
1	-0.4730630000	0.3848760000	-2.4420540000
6	-0.0265230000	-0.4318580000	1.3897220000
1	0.0102150000	-0.4267350000	2.4855830000
7	0.2187070000	-1.3883530000	-1.5859060000
7	0.4710410000	-1.8100390000	1.0057310000
6	1.8761950000	-2.0446150000	1.4479400000
1	2.5355570000	-1.3182780000	0.9736140000
1	2.1766140000	-3.0521210000	1.1535200000
1	1.9433360000	-1.9469090000	2.5351650000
6	-0.4238790000	-2.8882270000	1.5186260000
1	-1.4215500000	-2.7662930000	1.0974930000
1	-0.4767310000	-2.8371040000	2.6098200000
1	-0.0193850000	-3.8568560000	1.2184040000
6	-0.7839670000	-2.2471190000	-2.2500250000
1	-1.0575150000	-1.8562590000	-3.2415650000
1	-1.6892950000	-2.3164140000	-1.6432240000
1	-0.3714980000	-3.2517940000	-2.3766140000
6	1.4762060000	-1.4128210000	-2.3613670000
1	2.2587080000	-0.8592950000	-1.8382850000
1	1.3435390000	-0.9706440000	-3.3601190000
1	1.8052160000	-2.4484680000	-2.4831150000
1	0.4340860000	-1.8086680000	-0.1042020000

6	0.3256240000	3.3257200000	1.2916170000
1	-0.3177120000	4.0034330000	1.8642700000
1	1.3501070000	3.5206100000	1.6292110000
6	0.1803760000	3.5690710000	-0.2283600000
1	-0.5373260000	4.3718890000	-0.4318580000
1	1.1305300000	3.8908820000	-0.6699170000

## 8

SCF ENERGY at B3LYP/6-311+G\*\* = -1189.92094 au  
ZPVE = 385.809 kcal/mol

1	4.1179890000	1.3067810000	2.0528310000
6	4.2199490000	1.0458950000	0.9914160000
6	3.4154460000	-1.0903950000	-0.0613390000
6	3.2734700000	-0.4263460000	-1.4527310000
6	2.9767160000	1.0965110000	-1.2657440000
6	2.9389510000	1.4264540000	0.2478500000
1	5.0526400000	1.6496510000	0.6071940000
1	3.6323890000	-2.1602820000	-0.1721600000
1	4.0665000000	-0.6857550000	-2.1614000000
1	3.5796620000	1.7878980000	-1.8630130000
1	2.7522010000	2.4967920000	0.3998930000
6	1.6611070000	0.6263510000	0.6486830000
1	1.3436020000	0.8262750000	1.6768130000
6	1.9538820000	-0.9243980000	0.4617390000
1	1.7940720000	-1.4534090000	1.4013540000
6	1.4807400000	0.8573330000	-1.6931070000
1	1.1251290000	1.3716900000	-2.5904480000
6	1.7839840000	-0.6709720000	-1.8824310000
1	1.5979950000	-1.0582940000	-2.8872050000
6	1.2396480000	-1.5902860000	-0.7696270000
1	1.7749350000	-2.5441400000	-0.9114900000
6	0.7005500000	1.2492240000	-0.4169770000
1	0.8357850000	2.3382240000	-0.3314500000
7	-0.1392950000	-1.9760190000	-0.9281310000
7	-0.7190460000	0.9656130000	-0.3985790000
6	4.5004960000	-0.4630590000	0.8143630000
1	5.4818700000	-0.6302810000	0.3514410000
1	4.5280580000	-0.9757180000	1.7846550000
6	-0.9883770000	-2.2061130000	-0.0087410000
6	-1.5395830000	1.9264590000	-0.1328150000
7	-1.2326150000	3.1539120000	0.4879030000
7	-2.8792520000	1.8373030000	-0.5243280000
6	-1.7447630000	4.4185170000	-0.0049700000
6	-0.4579940000	3.2255740000	1.7093890000
6	-3.9329910000	2.1528090000	0.4316570000
6	-3.2498240000	0.7990000000	-1.4720020000
1	-0.9171830000	5.1186750000	-0.1953000000
1	-2.2848080000	4.2547550000	-0.9383050000
1	-2.4281910000	4.9017630000	0.7128820000
1	-1.0214270000	3.7692040000	2.4852190000
1	-0.2557890000	2.2196950000	2.0785740000
1	0.5027530000	3.7449690000	1.5718920000
1	-4.2697610000	1.2525100000	0.9728260000
1	-3.5775810000	2.8783920000	1.1637870000
1	-4.8015700000	2.5762170000	-0.0878290000
1	-4.1740810000	1.1000080000	-1.9815550000
1	-2.4500390000	0.6771610000	-2.2026070000
1	-3.4125940000	-0.1691210000	-0.9800550000
7	-0.7482760000	-2.1174550000	1.3923320000
7	-2.3085470000	-2.5415450000	-0.3865790000

6	-2.9575240000	-3.6375040000	0.3279570000
6	-2.5552650000	-2.6131280000	-1.8228160000
6	-1.6610020000	-1.3665010000	2.2327790000
6	-0.0435510000	-3.2062090000	2.0407040000
1	-2.6026830000	-4.6260740000	-0.0134450000
1	-2.7851620000	-3.5658040000	1.4009380000
1	-4.0385870000	-3.5923000000	0.1550280000
1	-3.6374280000	-2.6561370000	-1.9926270000
1	-2.1354520000	-1.7365550000	-2.3116530000
1	-2.0894120000	-3.5025740000	-2.2768840000
1	-2.4800930000	-1.9665830000	2.6703720000
1	-1.0980170000	-0.9290390000	3.0694320000
1	-2.0949360000	-0.5533670000	1.6497320000
1	-0.7156620000	-3.9959830000	2.4255600000
1	0.6521450000	-3.6704200000	1.3364830000
1	0.5375620000	-2.8267650000	2.8927540000

### 8H<sup>+</sup>

SCF ENERGY at B3LYP/6-311+G\*\* = -1190.39077 au  
ZPVE = 396.103 kcal/mol

1	4.0699330000	2.1914250000	2.1067400000
6	4.1983740000	1.6029000000	1.1903780000
6	3.2793620000	-0.7133680000	0.8196240000
6	3.2398140000	-0.5193080000	-0.7152860000
6	3.0609360000	0.9988960000	-1.0393480000
6	2.9836160000	1.8009680000	0.2829650000
1	5.0866130000	2.0073270000	0.6904420000
1	3.4181020000	-1.7729560000	1.0645010000
1	4.0315400000	-1.0411520000	-1.2588150000
1	3.7371820000	1.4235400000	-1.7855530000
1	2.8675560000	2.8718470000	0.0716290000
6	1.6382460000	1.2465510000	0.8438890000
1	1.2914020000	1.7902410000	1.7286570000
6	1.8180940000	-0.3039770000	1.1680380000
1	1.5499400000	-0.5130420000	2.2080350000
6	1.5732400000	0.7337290000	-1.4701520000
1	1.2915180000	0.9649930000	-2.5012180000
6	1.7526930000	-0.7926500000	-1.1446290000
1	1.5933260000	-1.4567630000	-1.9978030000
6	1.0865680000	-1.2630810000	0.1685840000
1	1.4790790000	-2.2627150000	0.3878290000
6	0.7737290000	1.5280200000	-0.4166720000
1	0.8706940000	2.5872520000	-0.6640850000
7	-0.3657570000	-1.2996340000	0.2474180000
7	-0.6624190000	1.2430130000	-0.3612550000
6	4.3745900000	0.1008070000	1.5111320000
1	5.3547180000	-0.2600690000	1.1770820000
1	4.3354300000	-0.0789420000	2.5920190000
6	-1.0005210000	-2.4071940000	0.5250450000
6	-1.6391910000	2.0663330000	-0.7298180000
7	-1.5481810000	3.4169470000	-0.5731130000
7	-2.7719640000	1.5489990000	-1.2772800000
6	-2.1082930000	4.3591480000	-1.5427440000
6	-0.8492970000	4.0254620000	0.5581480000
6	-4.0969280000	2.1209310000	-1.0316600000
6	-2.7673150000	0.2624230000	-1.9731610000
1	-1.3279740000	5.0689960000	-1.8401810000

1	-2.4467110000	3.8266740000	-2.4316730000
1	-2.9459690000	4.9271770000	-1.1207190000
1	-1.5067420000	4.7701030000	1.0218890000
1	-0.6057160000	3.2641430000	1.2990490000
1	0.0712290000	4.5313220000	0.2429910000
1	-4.7548010000	1.3410130000	-0.6311370000
1	-4.0310600000	2.9248080000	-0.2991180000
1	-4.5435430000	2.5082690000	-1.9545570000
1	-3.4254860000	0.3325010000	-2.8456130000
1	-1.7579070000	0.0212370000	-2.3062130000
1	-3.1274460000	-0.5477410000	-1.3277060000
7	-0.5323870000	-3.6897510000	0.2898750000
7	-2.2444370000	-2.3360390000	1.1250390000
6	-3.3413930000	-3.2251120000	0.7569930000
6	-2.6406580000	-1.1386840000	1.8458630000
6	-0.7305630000	-4.7843050000	1.2338530000
6	0.2063120000	-4.0339300000	-0.9162870000
1	-4.1474310000	-2.6557700000	0.2712700000
1	-2.9925480000	-3.9850300000	0.0583940000
1	-3.7637570000	-3.7217510000	1.6390820000
1	-3.3109590000	-1.4189050000	2.6665200000
1	-1.7573550000	-0.6468760000	2.2541380000
1	-3.1759650000	-0.4190550000	1.2056710000
1	-1.3718220000	-5.5745010000	0.8193450000
1	0.2389630000	-5.2341060000	1.4846950000
1	-1.1840460000	-4.4071900000	2.1511470000
1	-0.2481010000	-4.9183680000	-1.3828020000
1	0.1596100000	-3.2085590000	-1.6276220000
1	1.2601200000	-4.2666910000	-0.7113510000
1	-0.8583550000	0.2227330000	-0.1408780000

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SCF ENERGY at B3LYP/6-311+G\*\* = -736.18893 au  
ZPVE = 274.910 kcal/mol

1	4.1179890000	1.3067810000	2.0528310000
6	4.2199490000	1.0458950000	0.9914160000
6	3.4154460000	-1.0903950000	-0.0613390000
6	3.2734700000	-0.4263460000	-1.4527310000
6	2.9767160000	1.0965110000	-1.2657440000
6	2.9389510000	1.4264540000	0.2478500000
1	5.0526400000	1.6496510000	0.6071940000
1	3.6323890000	-2.1602820000	-0.1721600000
1	4.0665000000	-0.6857550000	-2.1614000000
1	3.5796620000	1.7878980000	-1.8630130000
1	2.7522010000	2.4967920000	0.3998930000
6	1.6611070000	0.6263510000	0.6486830000
1	1.3436020000	0.8262750000	1.6768130000
6	1.9538820000	-0.9243980000	0.4617390000
1	1.7940720000	-1.4534090000	1.4013540000
6	1.4807400000	0.8573330000	-1.6931070000
1	1.1251290000	1.3716900000	-2.5904480000
6	1.7839840000	-0.6709720000	-1.8824310000
1	1.5979950000	-1.0582940000	-2.8872050000
6	1.2396480000	-1.5902860000	-0.7696270000
1	1.7749350000	-2.5441400000	-0.9114900000
6	0.7005500000	1.2492240000	-0.4169770000
1	0.8357850000	2.3382240000	-0.3314500000
7	-0.1392950000	-1.9760190000	-0.9281310000
7	-0.7190460000	0.9656130000	-0.3985790000

6	4.5004960000	-0.4630590000	0.8143630000
1	5.4818700000	-0.6302810000	0.3514410000
1	4.5280580000	-0.9757180000	1.7846550000
6	-0.9883770000	-2.2061130000	-0.0087410000
6	-1.5395830000	1.9264590000	-0.1328150000
7	-1.2326150000	3.1539120000	0.4879030000
7	-2.8792520000	1.8373030000	-0.5243280000
6	-1.7447630000	4.4185170000	-0.0049700000
6	-0.4579940000	3.2255740000	1.7093890000
6	-3.9329910000	2.1528090000	0.4316570000
6	-3.2498240000	0.7990000000	-1.4720020000
1	-0.9171830000	5.1186750000	-0.1953000000
1	-2.2848080000	4.2547550000	-0.9383050000
1	-2.4281910000	4.9017630000	0.7128820000
1	-1.0214270000	3.7692040000	2.4852190000
1	-0.2557890000	2.2196950000	2.0785740000
1	0.5027530000	3.7449690000	1.5718920000
1	-4.2697610000	1.2525100000	0.9728260000
1	-3.5775810000	2.8783920000	1.1637870000
1	-4.8015700000	2.5762170000	-0.0878290000
1	-4.1740810000	1.1000080000	-1.9815550000
1	-2.4500390000	0.6771610000	-2.2026070000
1	-3.4125940000	-0.1691210000	-0.9800550000
7	-0.7482760000	-2.1174550000	1.3923320000
7	-2.3085470000	-2.5415450000	-0.3865790000
6	-2.9575240000	-3.6375040000	0.3279570000
6	-2.5552650000	-2.6131280000	-1.8228160000
6	-1.6610020000	-1.3665010000	2.2327790000
6	-0.0435510000	-3.2062090000	2.0407040000
1	-2.6026830000	-4.6260740000	-0.0134450000
1	-2.7851620000	-3.5658040000	1.4009380000
1	-4.0385870000	-3.5923000000	0.1550280000
1	-3.6374280000	-2.6561370000	-1.9926270000
1	-2.1354520000	-1.7365550000	-2.3116530000
1	-2.0894120000	-3.5025740000	-2.2768840000
1	-2.4800930000	-1.9665830000	2.6703720000
1	-1.0980170000	-0.9290390000	3.0694320000
1	-2.0949360000	-0.5533670000	1.6497320000
1	-0.7156620000	-3.9959830000	2.4255600000
1	0.6521450000	-3.6704200000	1.3364830000
1	0.5375620000	-2.8267650000	2.8927540000

## 9H<sup>+</sup>

SCF ENERGY at B3LYP/6-311+G\*\* = -736.61517 au

ZPVE = 283.616 kcal/mol

1	-3.9913737320	0.6803864787	-0.1294382789
6	-3.5215992596	-0.3094354959	-0.1697489710
6	-1.5789867585	-0.9102144054	-1.6307651674
6	-1.0404271052	-2.0083632516	-0.6786626195
6	-1.4959198099	-1.6499914608	0.7980107538
6	-2.3082003071	-0.3299570651	0.7535218553
1	-4.2676539372	-1.0163648762	0.2106268384
1	-1.2889041502	-1.1570424108	-2.6593203393
1	-1.4153626757	-3.0036659232	-0.9339250838
1	-2.0749408674	-2.4817783704	1.2090048240
1	-2.6431815399	-0.0806991828	1.7688598154
6	-1.1406008643	0.6256062023	0.3586957648
1	-1.4557613277	1.6735875601	0.3784911128
6	-0.6836343352	0.2618893092	-1.1311154419
1	-0.8078595278	1.1566335089	-1.7485247996

6	-0.3630879091	-1.2438804262	1.7765318280
1	-0.6571783880	-1.4678296556	2.8063029616
6	0.4800927162	-1.9032562100	-0.9667967182
1	0.7500941652	-2.5812754664	-1.7819593577
6	0.6939517820	-0.4189851414	-1.4174698888
1	0.7795414319	-0.4180982842	-2.5155862624
6	-0.2411953458	0.3032510402	1.5896296100
1	-0.7121815959	0.7954174994	2.4474611996
7	1.9266896362	0.2483208262	-0.9127060248
7	1.1694714725	0.8587886272	1.5906938025
6	1.1556119084	2.3527781868	1.6419197147
1	0.5502173512	2.7419523781	0.8246838851
1	2.1787584871	2.7218740783	1.5476816656
1	0.7354012477	2.6803337365	2.5964606499
6	2.0068625123	0.3317905891	2.7101193010
1	2.1271774316	-0.7457305803	2.6118756373
1	1.5281614078	0.5629685442	3.6655993971
1	2.9875161249	0.8099730943	2.6695564722
6	3.1328750727	-0.5762612035	-1.1424791069
1	3.2706603053	-0.7983533338	-2.2111811128
1	3.0682465185	-1.5184215556	-0.5968128239
1	4.0125051953	-0.0305836106	-0.7892134077
6	2.1142100272	1.5475080411	-1.5952864778
1	1.2482113586	2.1933795230	-1.4361782617
1	2.2476879060	1.4137132896	-2.6792671246
1	3.0036671272	2.0456512717	-1.1985362120
6	-3.0846775425	-0.6687911524	-1.6024563220
1	-3.5953379352	-1.5704215513	-1.9596049765
1	-3.3407552140	0.1278877322	-2.3105667457
1	1.1079312228	-2.1915973340	-0.1226366989
1	0.5709484708	-1.7787226320	1.6048221305
1	1.6095458579	0.5695874904	0.6188283103

## 10

SCF ENERGY at B3LYP/6-311+G\*\* = -1191.14939 au  
ZPVE = 400.338 kcal/mol

6	-2.4293660000	-1.8927320000	-1.1723660000
6	-0.9910850000	-2.4711090000	-1.1540380000
6	-0.7240340000	-3.0052320000	0.3142250000
6	-1.8543540000	-2.4825980000	1.2435500000
1	-2.7080990000	-1.6451880000	-2.2042110000
1	-0.8664610000	-3.3035440000	-1.8563160000
1	-0.6654930000	-4.1005840000	0.2998180000
1	-1.6174370000	-2.7608480000	2.2793680000
6	-1.5905890000	-0.9608700000	1.0540670000
1	-2.1581470000	-0.3592220000	1.7715630000
6	-2.1108290000	-0.5784080000	-0.4056490000
1	-2.9835290000	0.0778790000	-0.3019950000
6	0.4834100000	-2.3616080000	1.0042320000
1	0.8047700000	-2.9764330000	1.8544310000
6	-0.1562680000	-1.2252200000	-1.6341080000
1	0.1095660000	-1.3495280000	-2.6894040000
6	-1.1068850000	0.0058050000	-1.4303540000
1	-1.6883750000	0.1266070000	-2.3588960000
6	-0.0629460000	-0.9778390000	1.5176910000
7	-0.5552270000	1.2923460000	-1.0660360000
7	0.8750260000	0.0663580000	1.1829930000
6	1.3966000000	0.8124240000	2.0876990000
6	-0.5470840000	2.2652630000	-1.9050720000
1	-0.1551870000	-1.0580500000	2.6124920000

1	0.7688500000	-1.0657010000	-1.0820890000
1	1.3569500000	-2.2300910000	0.3624960000
7	0.9036650000	1.0436820000	3.3855760000
7	2.6197170000	1.4520690000	1.8265560000
7	-0.4697980000	3.5869360000	-1.4286570000
7	-0.6562240000	2.1902220000	-3.3056340000
6	1.7603250000	1.0359980000	4.5540880000
6	-0.4957010000	1.3233860000	3.6248930000
6	2.7716230000	2.8670890000	2.1395820000
6	3.3233040000	1.0518220000	0.6176490000
6	0.5598110000	4.4647220000	-1.9710130000
6	-0.7044350000	3.7837770000	-0.0073530000
6	0.0586220000	1.1954130000	-4.0772660000
6	-1.4615170000	3.1203860000	-4.0734980000
1	1.4116760000	0.2902020000	5.2852160000
1	2.7790890000	0.7826160000	4.2572810000
1	1.7793530000	2.0134810000	5.0640270000
1	-0.6061040000	2.2697550000	4.1795470000
1	-1.0166140000	1.4225950000	2.6716060000
1	-0.9905870000	0.5354000000	4.2138200000
1	3.8177940000	3.0888270000	2.3857480000
1	2.4804740000	3.5081160000	1.2900080000
1	2.1498090000	3.1347250000	2.9945180000
1	4.3555240000	1.4166510000	0.6771920000
1	3.3266830000	-0.0358340000	0.5375540000
1	2.8526180000	1.4538380000	-0.2915750000
1	0.2429180000	5.5115500000	-1.8911930000
1	1.5165260000	4.3564970000	-1.4309850000
1	0.7363990000	4.2350340000	-3.0227300000
1	-0.9022880000	4.8474040000	0.1709450000
1	-1.5685930000	3.1959170000	0.3047660000
1	0.1516730000	3.4736890000	0.6093250000
1	-0.6090450000	0.4504680000	-4.5369570000
1	0.6203930000	1.6833750000	-4.8897420000
1	0.7705550000	0.6728110000	-3.4372340000
1	-2.2053280000	2.5784370000	-4.6778310000
1	-1.9857690000	3.7948480000	-3.3953770000
1	-0.8518390000	3.7248060000	-4.7653810000
6	-3.2654810000	-2.9666720000	0.9212630000
6	-3.5188910000	-2.7868430000	-0.5850490000
1	-3.3782140000	-4.0156620000	1.2237870000
1	-3.9904620000	-2.3953180000	1.5168940000
1	-3.5094570000	-3.7540990000	-1.1061950000
1	-4.5059830000	-2.3465180000	-0.7749250000

## 10H<sup>+</sup>

SCF ENERGY at B3LYP/6-311+G\*\* = -1191.61100 au

ZPVE = 409.116 kcal/mol

6	-2.5286610000	-1.9472890000	-1.1499600000
6	-1.1157380000	-2.5914500000	-1.1453990000
6	-0.7049500000	-2.8783600000	0.3590520000
6	-1.8570530000	-2.3856950000	1.2761290000
1	-2.8366040000	-1.7700460000	-2.1894440000
1	-1.0877390000	-3.5291940000	-1.7090910000
1	-0.5123040000	-3.9497580000	0.4753380000
1	-1.5893460000	-2.5900020000	2.3204620000
6	-1.7011160000	-0.8594310000	1.0109750000
1	-2.3488760000	-0.2579510000	1.6588390000
6	-2.1406220000	-0.5866100000	-0.5001590000
1	-2.9706930000	0.1287130000	-0.4964660000



6	0.4664230000	-2.0337530000	0.9161560000
1	0.9655910000	-2.5758980000	1.7270300000
6	-0.3109110000	-1.4880510000	-1.8836170000
1	-0.3135510000	-1.6932840000	-2.9592770000
6	-1.0986870000	-0.1677720000	-1.5844060000
1	-1.6959920000	0.0902470000	-2.4624830000
6	-0.2126760000	-0.7348490000	1.4872230000
7	-0.2946330000	1.0238380000	-1.2934780000
7	0.5436340000	0.4783920000	1.2062760000
6	1.2225970000	1.0742100000	2.1516620000
6	-0.2823480000	2.1378860000	-2.0222800000
1	-0.2771390000	-0.8766120000	2.5698220000
1	0.7356020000	-1.4120290000	-1.5850770000
1	1.2445460000	-1.7943380000	0.1891790000
7	0.9353650000	1.0364300000	3.5081040000
7	2.3395230000	1.8130600000	1.8103770000
7	-0.1104580000	3.3402280000	-1.4107660000
7	-0.4378150000	2.1154180000	-3.3751250000
6	1.9688980000	0.8797720000	4.5251690000
6	-0.4286800000	1.0966550000	4.0103370000
6	2.7103500000	3.0480260000	2.4914410000
6	3.0302650000	1.5714420000	0.5543100000
6	0.6394070000	4.4352070000	-2.0277470000
6	-0.5146760000	3.5652530000	-0.0238800000
6	0.0880450000	1.0321530000	-4.2055760000
6	-1.1671620000	3.1578610000	-4.0987460000
1	1.7518630000	-0.0024530000	5.1420000000
1	2.9401160000	0.7358770000	4.0502930000
1	2.0254490000	1.7517360000	5.1913660000
1	-0.5078410000	1.8923420000	4.7639890000
1	-1.1154400000	1.3251260000	3.1936920000
1	-0.7429290000	0.1560230000	4.4833710000
1	3.7241060000	2.9882460000	2.9068790000
1	2.6860750000	3.8915100000	1.7863450000
1	2.0102850000	3.2574950000	3.2998860000
1	4.1043640000	1.7389120000	0.6953790000
1	2.8638170000	0.5420590000	0.2371010000
1	2.6867350000	2.2435450000	-0.2478160000
1	-0.0067390000	5.2936460000	-2.2446160000
1	1.4262640000	4.7620090000	-1.3381370000
1	1.1099450000	4.0971450000	-2.9506400000
1	-0.9920250000	4.5486650000	0.0483890000
1	-1.2246550000	2.7989540000	0.2860220000
1	0.3461940000	3.5415860000	0.6532810000
1	-0.7143180000	0.4063410000	-4.6135190000
1	0.6425110000	1.4684640000	-5.0444040000
1	0.7675890000	0.4111200000	-3.6229940000
1	-1.9159620000	2.6833800000	-4.7429450000
1	-1.6821900000	3.8134630000	-3.3964980000
1	-0.5010330000	3.7567870000	-4.7312040000
6	-3.2345560000	-2.9854800000	1.0128080000
6	-3.6324080000	-2.7369420000	-0.4540920000
1	-3.2090770000	-4.0575490000	1.2415820000
1	-3.9626110000	-2.5436110000	1.7040690000
1	-3.7884720000	-3.6800500000	-0.9915300000
1	-4.5774810000	-2.1850040000	-0.5258670000
1	0.1669730000	1.0013150000	-0.3368480000

## 11

SCF ENERGY at B3LYP/6-311+G\*\* = -774.27011 au

ZPVE = 278.925 kcal/mol

1	-1.2364498048	-3.7123239355	0.3045161161
6	-0.2063461981	-3.3515025102	0.4177859778
6	0.2856071505	-2.5373442687	-0.7750117401
6	1.6448079263	-1.9423052517	-0.2912747984
6	1.3905686315	-1.7035087691	1.2291121444
6	-0.0715612837	-2.2154684959	1.4247191482
1	0.4391961260	-4.2099866685	0.6446050435
1	0.3095278065	-3.0721742618	-1.7250044740
1	2.5373525276	-2.4997223618	-0.5864423788
1	2.1258413199	-2.0863017024	1.9412935946
1	-0.3581684746	-2.4509707980	2.4506765304
6	-0.8431503637	-1.0183977704	0.7960667054
1	-1.9169061084	-1.0502798477	1.0066214297
6	-0.5791192273	-1.2348250523	-0.7799529736
1	-1.5267152127	-1.3678952077	-1.3099690564
6	1.3202676063	-0.1517052199	0.9867473454
6	1.5932799840	-0.4001842039	-0.5510594294
6	0.3879719900	-0.2297827348	-1.5033380135
6	0.7553830423	-0.7836742833	-2.9152497793
6	-0.1217047082	0.1967313370	1.4536574135
6	-0.1288622798	0.0875343382	3.0130643527
7	-0.0836833476	1.1540403847	-1.6368445781
7	-0.6848455802	1.4993160874	1.0671756631
6	-1.9817005498	1.8084944686	1.6455634662
1	-2.6633370100	0.9595331140	1.5352663035
1	-2.4193028519	2.6562438303	1.1033902987
1	-1.9584574684	2.0834458882	2.7187700977
6	0.2205843209	2.6247121816	1.1708886868
1	1.1281139403	2.4345310256	0.5937118390
1	0.5155945135	2.8828947746	2.2089501811
1	-0.2629950856	3.5120953117	0.7442951360
6	0.8091611027	2.0781926408	-2.3098956029
1	0.8065220839	2.0106523209	-3.4162897698
1	1.8398330223	1.9305567932	-1.9728013112
1	0.5216305272	3.1054125026	-2.0507972876
6	-1.4569976299	1.3285451792	-2.0595750213
1	-2.1349269467	0.8046143393	-1.3813093212
1	-1.6655921825	0.9908599273	-3.0951387838
1	-1.7093583400	2.3948061553	-2.0105302805
1	2.0960925769	0.4404920036	1.4802329224
1	2.5206080228	0.0565231377	-0.9092630523
1	1.3765795849	-0.0618623477	-3.4532028623
1	1.3159879295	-1.7194207171	-2.8921383945
1	-0.1494809595	-0.9511470885	-3.5121950261
1	0.1955972495	1.0406529540	3.4457751832
1	-1.1331765352	-0.1255232854	3.3966521961
1	0.5417371214	-0.6827397686	3.4001972063

## 11H<sup>+</sup>

SCF ENERGY at B3LYP/6-311+G\*\* = -774.70610 au

ZPVE = 2286.923 kcal/mol

1	-1.2336630869	-3.7199220585	0.4089627172
6	-0.1993816842	-3.3623430633	0.4657704785
6	0.2366029757	-2.5600184727	-0.7563459277
6	1.6171073494	-1.9630443329	-0.3446761387

6	1.4508861435	-1.7290991540	1.1891129299
6	-0.0040302886	-2.2226410554	1.4606578159
1	0.4526728795	-4.2192452001	0.6691698809
1	0.2127686790	-3.0930697971	-1.7066161348
1	2.4949907580	-2.5108855248	-0.6897615129
1	2.2179283258	-2.1187579567	1.8597960384
1	-0.2448167122	-2.4516674021	2.4990432498
6	-0.8048468936	-1.0231782375	0.8612033774
1	-1.8606120732	-1.0467186483	1.1445407850
6	-0.6301061644	-1.2624885243	-0.7236052748
1	-1.6059763081	-1.4013117573	-1.1960780271
6	1.3912713248	-0.1786087590	0.9578618879
6	1.5582497253	-0.4183888917	-0.6016338017
6	0.2962752902	-0.2604628148	-1.4875255803
6	0.5946118920	-0.7694647514	-2.9202540751
6	-0.0208213211	0.1762744730	1.4772884563
6	-0.0586063781	0.1590656998	3.0198689530
7	-0.2476621854	1.1437764578	-1.5582255111
7	-0.5321199830	1.5434301745	1.0071254895
6	-1.9481653103	1.8295869503	1.3790906585
1	-2.5913924186	1.0208528679	1.0340326325
1	-2.2511302453	2.7605480989	0.8944862579
1	-2.0468083234	1.9427027064	2.4604259201
6	0.3342635555	2.6992318046	1.3852045942
1	1.3719717892	2.4802546040	1.1362158604
1	0.2509716729	2.9194886326	2.4506874151
1	0.0043700960	3.5729185081	0.8188388147
6	0.7168871863	2.1485044190	-2.0560689187
1	0.9372586974	2.0341788228	-3.1242529367
1	1.6538488573	2.0863698893	-1.4992368253
1	0.2904490401	3.1460773723	-1.9110720696
6	-1.5130973942	1.2588957726	-2.3140866898
1	-2.2547077374	0.5583410326	-1.9254232962
1	-1.3771171704	1.0688477193	-3.3859225663
1	-1.9021430548	2.2752550328	-2.1983242236
1	2.1986919833	0.4020094777	1.4106685289
1	2.4629787215	0.0301493620	-1.0180303928
1	1.0866111109	0.0023171912	-3.5184107298
1	1.2633932593	-1.6305854241	-2.9168908584
1	-0.3218278162	-1.0675403615	-3.4403141787
1	0.3556628603	1.0775593068	3.4447420538
1	-1.0768221750	0.0314584072	3.4018073949
1	0.5419430302	-0.6587810943	3.4167132267
1	-0.4797960723	1.4566469676	-0.1131286935

**12:** SCF ENERGY at B3LYP/6-311+G\*\* = -1229.23679 au  
ZPVE = 402.794 kcal/mol

6	-4.3684390000	0.0415170000	0.2341270000
6	-3.4325850000	-1.0751100000	-0.2195650000
6	-2.8756760000	-1.6634900000	1.1151940000
6	-2.8176580000	-0.4145040000	2.0500540000
6	-3.3381030000	0.7294840000	1.1257090000
6	-2.0830680000	0.9324760000	0.2202140000
6	-2.1513360000	-0.3577630000	-0.7336190000
6	-1.2566500000	-0.4091670000	1.9602340000
6	-1.3089330000	-1.6716200000	1.0189810000
6	-1.0432990000	-1.4301940000	-0.4924780000
6	-1.3830070000	-2.7401110000	-1.2619540000
6	-0.9255340000	0.9385040000	1.2779000000
6	-1.1380630000	2.0741430000	2.3208920000

7	0.2429530000	-0.9986440000	-1.0441200000
7	0.4895600000	1.0434520000	0.9156820000
6	0.9917020000	2.0313840000	0.2691460000
6	1.3349600000	-1.6627540000	-0.9188170000
7	2.3431640000	2.3479110000	0.4566170000
7	0.2864250000	2.9141840000	-0.5907090000
7	2.3271220000	-1.5277610000	-1.8976130000
7	1.6330880000	-2.6091590000	0.0917830000
6	1.8214930000	-2.1551940000	1.4603290000
6	2.2753370000	-3.8693530000	-0.2335290000
6	1.9908270000	-0.8690240000	-3.1467180000
6	3.7277710000	-1.4087050000	-1.5245600000
6	-0.1296640000	2.4272260000	-1.8969450000
6	0.4988330000	4.3475240000	-0.5047200000
6	3.0606380000	1.7191990000	1.5513790000
6	3.1879780000	2.6984290000	-0.6744610000
1	-4.7227360000	0.6736940000	-0.5896750000
1	-5.2412140000	-0.3261070000	0.7901630000
1	-3.8613930000	-1.7988050000	-0.9151310000
1	-3.3805190000	-2.5610510000	1.4823500000
1	-3.2912990000	-0.4804100000	3.0329840000
1	-3.6826250000	1.6321270000	1.6336720000
1	-2.1339300000	1.8548120000	-0.3587640000
1	-2.2062220000	-0.0619240000	-1.7862570000
1	-0.7023800000	-0.5636360000	2.8910840000
1	-0.8139740000	-2.5570940000	1.4199420000
1	0.9732420000	-1.1342650000	-3.4340540000
1	2.6924510000	-1.2003710000	-3.9229750000
1	3.8901360000	-1.8000180000	-0.5206670000
1	4.3636320000	-1.9674540000	-2.2241850000
1	4.0599270000	-0.3581440000	-1.5351530000
1	2.8944190000	-2.1299800000	1.7267540000
1	0.5606310000	2.7613490000	-2.6940780000
1	-0.1457430000	1.3350950000	-1.8901370000
1	1.2456600000	4.7336160000	-1.2210560000
1	0.8241200000	4.6154210000	0.5028710000
1	-0.4477830000	4.8657720000	-0.7120460000
1	3.9009860000	3.4841380000	-0.3921010000
1	2.5849690000	3.0612550000	-1.5058330000
1	3.4149860000	0.7072030000	1.3002850000
1	2.4044800000	1.6376790000	2.4180130000
1	3.9316030000	2.3367920000	1.8049720000
1	-1.1294880000	2.8037330000	-2.1555310000
1	2.1024260000	-4.1155080000	-1.2831770000
1	1.8447640000	-4.6681940000	0.3866390000
1	3.3651280000	-3.8695680000	-0.0550070000
1	1.3256790000	-2.8291930000	2.1731040000
1	1.4155770000	-1.1477320000	1.5702120000
1	3.7675930000	1.8315250000	-1.0308460000
1	2.0468390000	0.2285300000	-3.0755720000
1	-0.5703320000	-3.4586200000	-1.1235650000
1	-2.3037520000	-3.2190740000	-0.9203950000
1	-1.4806290000	-2.5335170000	-2.3344710000
1	-0.2918120000	2.0756200000	3.0155510000
1	-1.1726680000	3.0482620000	1.8209170000
1	-2.0495260000	1.9586460000	2.9120060000

## 12 H+

SCF ENERGY at B3LYP/6-311+G\*\* =-1229.684911au  
ZPVE =413.866 kcal/mol

6	-4.3874530000	-0.3319940000	-0.0128790000
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6	-3.3444810000	-1.4458780000	-0.0082290000
6	-2.8677540000	-1.5019710000	1.4792430000
6	-2.9509380000	-0.0088760000	1.9253770000
6	-3.4857200000	0.7062370000	0.6448170000
6	-2.1878860000	0.7150270000	-0.2115910000
6	-2.0678970000	-0.8296060000	-0.6657960000
6	-1.3851440000	0.0990050000	1.9034990000
6	-1.3062400000	-1.4228460000	1.4779690000
6	-0.9334190000	-1.6950730000	0.0057360000
6	-1.1172710000	-3.1757690000	-0.3823580000
6	-1.1220030000	1.2016350000	0.8221260000
6	-1.5083560000	2.5466340000	1.4950230000
7	0.4218720000	-1.2526870000	-0.3994390000
7	0.2683260000	1.2347150000	0.3544910000
6	0.9650340000	2.3003250000	0.0552570000
6	1.5162710000	-1.9417320000	-0.7232710000
7	2.3269480000	2.2736200000	0.2914270000
7	0.4999810000	3.4792490000	-0.5041420000
7	2.3097620000	-1.4424610000	-1.7110170000
7	1.9180660000	-3.0858830000	-0.0999070000
6	1.7704780000	-3.2688450000	1.3426530000
6	2.5194150000	-4.2094740000	-0.8172080000
6	1.7732480000	-0.5710690000	-2.7554550000
6	3.7647900000	-1.5932720000	-1.7115230000
6	-0.5007910000	3.4865630000	-1.5578190000
6	0.9260390000	4.7939730000	-0.0375850000
6	2.8926550000	1.3581040000	1.2683930000
6	3.2980260000	2.9342960000	-0.5716230000
1	-4.7197870000	-0.0482720000	-1.0184050000
1	-5.2710880000	-0.5789350000	0.5876920000
1	-3.6739720000	-2.3907680000	-0.4408140000
1	-3.3513610000	-2.2579100000	2.1007900000
1	-3.4790620000	0.2227530000	2.8526370000
1	-3.9270850000	1.6915550000	0.8009670000
1	-2.2677340000	1.3561460000	-1.0920710000
1	-2.0512540000	-0.9136820000	-1.7572950000
1	-0.8877060000	0.3148990000	2.8531590000
1	-0.7893560000	-2.0592630000	2.2003530000
1	0.6933640000	-0.7016800000	-2.8237420000
1	2.2322730000	-0.8396620000	-3.7129590000
1	4.0999430000	-2.0106880000	-0.7622530000
1	4.1031940000	-2.2397380000	-2.5295860000
1	4.2258920000	-0.6074850000	-1.8399270000
1	2.7463710000	-3.5305980000	1.7695570000
1	-0.1617080000	4.1375380000	-2.3747130000
1	-0.6296460000	2.4777230000	-1.9507530000
1	1.4240730000	5.3676590000	-0.8307490000
1	1.6112830000	4.6867590000	0.8040090000
1	0.0532380000	5.3690120000	0.2997290000
1	3.8772490000	3.6896320000	-0.0253110000
1	2.7915160000	3.4171100000	-1.4073600000
1	3.2876090000	0.4440920000	0.7986440000
1	2.1241430000	1.0725530000	1.9862480000
1	3.7204610000	1.8513080000	1.7917880000
1	-1.4761730000	3.8608390000	-1.2180540000
1	2.4669150000	-4.0386400000	-1.8926090000
1	1.9590580000	-5.1227560000	-0.5842680000
1	3.5650750000	-4.3657760000	-0.5261950000
1	1.0668130000	-4.0745110000	1.5834830000
1	1.4229710000	-2.3425230000	1.7985420000
1	4.0062310000	2.1960030000	-0.9738850000
1	1.9915880000	0.4837470000	-2.5485230000
1	0.5390820000	-0.1960940000	-0.2742700000

1	-0.3540850000	-3.8159340000	0.0575220000
1	-2.0774130000	-3.5599280000	-0.0437650000
1	-1.0732860000	-3.2940310000	-1.4719580000
1	-0.6644000000	2.9050430000	2.0935720000
1	-1.7748600000	3.3250340000	0.7770640000
1	-2.3537520000	2.4308830000	2.1749700000

## 13

SCF ENERGY at B3LYP/6-311+G\*\* = -774.29152 au  
ZPVE = 278.663kcal/mol

1	-1.2571854140	-3.6590894357	0.1237540457
6	-0.2316718034	-3.3118428484	0.3018231741
6	0.3236227967	-2.4475749255	-0.8347257565
6	1.6568213613	-1.8917204059	-0.2581659814
6	1.3288379587	-1.7110925102	1.2540314166
6	-0.1405415179	-2.2094244430	1.3613398516
1	0.3972530592	-4.1825211504	0.5270990799
1	0.3995340489	-2.9154750928	-1.8203038136
1	2.5566299501	-2.4512735381	-0.5294532892
1	2.0243824903	-2.1311618892	1.9859143449
H	-0.4756379416	-2.4622832283	2.3712185020
6	-0.8692063243	-0.9919073477	0.7325885403
1	-1.9499405274	-1.0009053489	0.9030429519
6	-0.5409180219	-1.1508465627	-0.8131772394
1	-1.4558769956	-1.2493785374	-1.4023944649
6	1.3305992526	-0.1431615562	1.0887245012
6	2.3803971177	0.5625192028	1.9482161597
6	1.6736602327	-0.3366823436	-0.4636641515
6	3.0006490009	0.2460920604	-0.9355084975
6	0.4606330708	-0.1327906257	-1.4166047317
1	0.7696074308	-0.5930875674	-2.3792897974
6	-0.1537943192	0.1926146035	1.4194759451
1	-0.2182073732	0.0073529969	2.5136072391
7	0.0255160262	1.2419768299	-1.7045992230
7	-0.7659334161	1.4976103675	1.1449931401
6	-1.9364465767	1.6985155314	1.9873456070
1	-2.6426604734	0.8700455260	1.8704318345
1	-2.4497574873	2.6197828072	1.6895231250
1	-1.6902444092	1.7790068337	3.0667712189
6	0.1069809322	2.6584785109	1.1962779961
1	0.8953756700	2.5585632314	0.4494215787
1	0.5568410236	2.8407262861	2.1919998874
1	-0.4800292349	3.5468312545	0.9344040722
6	0.7625322461	1.8110981730	-2.8290033155
1	0.5757631620	1.2751666388	-3.7829799583
1	1.8376709866	1.7943499497	-2.6446864611
1	0.4632532860	2.8560812081	-2.9679039408
6	-1.4048480201	1.3771080883	-1.9552544553
1	-1.9670520655	1.0710509433	-1.0734699172
1	-1.7543290231	0.8028326612	-2.8369969219
1	-1.6306879235	2.4335481890	-2.1411235117
1	2.5530827384	1.6020374634	1.6566748800
1	2.0663603757	0.5605755984	2.9996783756
1	3.3444048736	0.0435399934	1.8990944115
1	3.0192669275	1.3402674491	-0.8781835877
1	3.8380340253	-0.1257410979	-0.3346953721

1 3.1966720616 -0.0429210119 -1.9760879264

### 13H<sup>+</sup>

SCF ENERGY at B3LYP/6-311+G\*\* = -774.71466 au  
ZPVE = 278.615 kcal/mol

1	-1.2788250000	-3.6450650000	0.3998250000
6	-0.2391640000	-3.3068430000	0.4744810000
6	0.2310870000	-2.5012510000	-0.7419180000
6	1.6047630000	-1.9334210000	-0.3032210000
6	1.4189860000	-1.7019350000	1.2267680000
6	-0.0392280000	-2.1661560000	1.4786860000
1	0.3943430000	-4.1752890000	0.6852460000
1	0.2204180000	-3.0109510000	-1.7079000000
1	2.4773850000	-2.4995480000	-0.6343450000
1	2.1675500000	-2.1114540000	1.9076610000
1	-0.2945980000	-2.3702290000	2.5213460000
6	-0.8132880000	-0.9683960000	0.8590600000
1	-1.8689210000	-0.9715210000	1.1387720000
6	-0.6194650000	-1.2020650000	-0.7040030000
1	-1.5822810000	-1.3236780000	-1.2035770000
6	1.4387010000	-0.1413290000	1.0160230000
6	2.5794240000	0.5618060000	1.7537530000
6	1.6274930000	-0.3816040000	-0.5613170000
6	2.9407510000	0.1115370000	-1.1715330000
6	0.3222200000	-0.1861520000	-1.3959640000
1	0.5381300000	-0.5745710000	-2.4064560000
6	-0.0162120000	0.2236380000	1.4305450000
1	-0.0761020000	0.2006360000	2.5266790000
7	-0.2460580000	1.1876290000	-1.5676030000
7	-0.5702020000	1.5914570000	1.0434190000
6	-2.0052680000	1.7448000000	1.4340060000
1	-2.6134890000	1.0060770000	0.9155970000
1	-2.3393820000	2.7452010000	1.1529500000
1	-2.1090590000	1.6162610000	2.5149710000
6	0.2166920000	2.7383020000	1.5859840000
1	1.2034340000	2.7552660000	1.1308830000
1	0.3114640000	2.6451090000	2.6708260000
1	-0.3052800000	3.6660200000	1.3447190000
6	0.6764920000	2.1119140000	-2.2595150000
1	1.0028090000	1.7113180000	-3.2304580000
1	1.5571910000	2.3080770000	-1.6500870000
1	0.1632220000	3.0612510000	-2.4347670000
6	-1.5179740000	1.1472450000	-2.3235580000
1	-2.2818680000	0.5964570000	-1.7727000000
1	-1.3890600000	0.6759110000	-3.3093110000
1	-1.8750500000	2.1693350000	-2.4754190000
1	2.8056740000	1.5649430000	1.3804420000
1	2.3565730000	0.6416500000	2.8246720000
1	3.5030180000	-0.0178460000	1.6634700000
1	3.1114820000	1.1859910000	-1.0606790000
1	3.7934490000	-0.3929490000	-0.7058790000
1	2.9746890000	-0.1240010000	-2.2416310000
1	-0.4994990000	1.5991240000	-0.0588570000

### 14:

SCF ENERGY at B3LYP/6-311+G\*\* = -1229.25606 au  
ZPVE = 405.180 kcal/mol

6C1 -4.0219060000 -0.6962590000 -0.1865360000

6C2	-2.8889270000	-1.6631230000	0.1652620000
6C3	-2.5546960000	-1.3235340000	1.6516360000
6C4	-2.8259360000	0.2088930000	1.7234780000
6C5	-3.2679260000	0.5555610000	0.2681660000
6C6	-1.8860930000	0.4868600000	-0.4567820000
6C7	-1.6262540000	-1.0741950000	-0.5310830000
6C8	-1.2912710000	0.4958610000	1.8478660000
6C9	-1.0038320000	-1.0783520000	1.7668770000
6C10	-0.5153590000	-1.6224040000	0.3961660000
1H11	-0.7183530000	-2.7052070000	0.4497060000
6C12	-1.0162220000	1.2925590000	0.5453530000
1H13	-1.5595260000	2.2446720000	0.6917110000
7N14	0.8380100000	-1.3780550000	-0.0366400000
7N15	0.3747650000	1.5701060000	0.2886090000
6C16	0.7786370000	2.7794510000	0.1165820000
6C17	1.5049960000	-2.3002830000	-0.6363820000
7N18	2.1188750000	3.1023410000	0.3746760000
7N19	0.0062020000	3.8895420000	-0.2720840000
7N20	2.5723910000	-1.9505200000	-1.4705640000
7N21	1.2676220000	-3.6931500000	-0.6041180000
6C22	1.0645650000	-4.4072320000	0.6367510000
6C23	1.2227320000	-4.4962110000	-1.8090970000
6C24	2.7344170000	-0.5596590000	-1.8538230000
6C25	3.8183950000	-2.6998080000	-1.4407880000
6C26	-0.9879540000	3.7989980000	-1.3204350000
6C27	0.1614980000	5.1973180000	0.3352190000
6C28	2.9023810000	2.1387060000	1.1319940000
6C29	2.8868620000	3.8187470000	-0.6350510000
1H30	-4.2725650000	-0.6915340000	-1.2550910000
1H31	-4.9405550000	-0.8781650000	0.3865380000
1H32	-3.0609770000	-2.7225990000	-0.0441480000
1H33	-3.0268710000	-1.9686230000	2.3986900000
1H34	-3.4834180000	0.5826150000	2.5140260000
1H35	-3.7855720000	1.5128430000	0.1545430000
1H36	-1.9075310000	0.9242750000	-1.4593770000
1H37	-1.5022830000	-1.4090900000	-1.5659430000
6C38	-0.8242900000	1.2269530000	3.0985850000
6C39	-0.2810420000	-1.7035720000	2.9521170000
1H40	1.7740320000	-0.0505490000	-1.7880150000
1H41	3.1346000000	-0.5078310000	-2.8759330000
1H42	3.6448660000	-3.7118770000	-1.0748520000
1H43	4.2529810000	-2.7603250000	-2.4472160000
1H44	4.5609830000	-2.2174030000	-0.7828990000
1H45	1.7753840000	-5.2468610000	0.7142530000
1H46	-0.8194320000	4.5898040000	-2.0688330000
1H47	-0.9070090000	2.8335840000	-1.8214870000
1H48	0.4983830000	5.9555920000	-0.3906460000
1H49	0.8945130000	5.1396190000	1.1408080000
1H50	-0.7961940000	5.5434430000	0.7538730000
1H51	3.6627910000	4.4306770000	-0.1584310000
1H52	2.2325730000	4.4747260000	-1.2107760000
1H53	3.2176790000	1.2776010000	0.5273740000
1H54	2.3077670000	1.7544220000	1.9611310000
1H55	3.7933320000	2.6449670000	1.5235570000
1H56	-2.0169150000	3.9109740000	-0.9449520000
1H57	1.3774900000	-3.8575470000	-2.6804300000
1H58	0.2452710000	-4.9944410000	-1.9100600000
1H59	1.9955610000	-5.2830940000	-1.8142780000
1H60	0.0491920000	-4.8260520000	0.7269750000
1H61	1.2364720000	-3.7369630000	1.4801820000
1H62	3.3836860000	3.1270020000	-1.3365550000
1H63	3.4349110000	-0.0327070000	-1.1873140000
1H64	0.2693410000	1.2658800000	3.1526270000



1H65	-1.1941640000	2.2609190000	3.0878220000
1H66	-1.1916570000	0.7604130000	4.0193960000
1H67	0.7816510000	-1.4318670000	2.9492190000
1H68	-0.7050240000	-1.3979700000	3.9146270000
1H69	-0.3494900000	-2.7979160000	2.9036330000

### 14H<sup>+</sup>:

SCF ENERGY at B3LYP/6-311+G\*\* = -1229.71978 au

ZPVE = 412.998

6	-4.1407970000	-0.6990690000	-0.2504460000
6	-3.0362350000	-1.6799940000	0.1547890000
6	-2.7265090000	-1.2972360000	1.6338720000
6	-2.9627340000	0.2442080000	1.6534870000
6	-3.3720790000	0.5535220000	0.1822360000
6	-1.9854020000	0.4358580000	-0.5184850000
6	-1.7547350000	-1.1350680000	-0.5407450000
6	-1.4236460000	0.5000610000	1.8033900000
6	-1.1765930000	-1.0841630000	1.7857310000
6	-0.6652900000	-1.6371080000	0.4319950000
1	-0.7411800000	-2.7277090000	0.4721270000
6	-1.0844510000	1.2203210000	0.4686690000
1	-1.5289370000	2.2197770000	0.5692060000
7	0.7161760000	-1.3111220000	0.0371870000
7	0.3356780000	1.3371990000	0.1729830000
6	0.9177640000	2.5033050000	0.0889470000
6	1.5415400000	-2.1142180000	-0.6359660000
7	2.2772300000	2.5965390000	0.3273440000
7	0.2918360000	3.7039140000	-0.2117000000
7	2.3592950000	-1.5927700000	-1.5878840000
7	1.6090120000	-3.4523460000	-0.3910320000
6	1.4271550000	-4.0178600000	0.9442720000
6	1.8393210000	-4.4307280000	-1.4550710000
6	2.0111420000	-0.3831450000	-2.3333570000
6	3.7167110000	-2.0924930000	-1.8165970000
6	-0.7549200000	3.8023000000	-1.2174910000
6	0.6190270000	4.9504310000	0.4712130000
6	2.9649110000	1.5571300000	1.0732380000
6	3.1488660000	3.4655180000	-0.4567110000
1	-4.3721890000	-0.7221540000	-1.3218820000
1	-5.0710080000	-0.8478990000	0.3101080000
1	-3.2255880000	-2.7421110000	-0.0238460000
1	-3.2251480000	-1.9079060000	2.3901730000
1	-3.6238410000	0.6541380000	2.4204160000
1	-3.8693000000	1.5147040000	0.0289990000
1	-1.9760670000	0.8467620000	-1.5326680000
1	-1.6146740000	-1.5117920000	-1.5592560000
6	-0.9575090000	1.2652770000	3.0338270000
6	-0.5125480000	-1.6972370000	3.0114210000
1	0.9421280000	-0.1882610000	-2.2585310000
1	2.2766880000	-0.5311280000	-3.3857110000
1	3.9889150000	-2.8122600000	-1.0450080000
1	3.8123580000	-2.5636000000	-2.8015490000
1	4.4168880000	-1.2509640000	-1.7678390000
1	2.2567130000	-4.7036310000	1.1531410000
1	-0.5060810000	4.6017600000	-1.9287650000
1	-0.8308760000	2.8642840000	-1.7687000000
1	1.0485920000	5.6947130000	-0.2136430000
1	1.3310670000	4.7587950000	1.2746590000
1	-0.2908520000	5.3815340000	0.9095040000
1	3.7410460000	4.1230900000	0.1913580000
1	2.5578260000	4.0793110000	-1.1355950000
1	3.3596790000	0.7610070000	0.4216170000
1	2.2823620000	1.1053470000	1.7933950000

1	3.8116280000	2.0012270000	1.6088090000
1	-1.7353480000	4.0364940000	-0.7803240000
1	1.7692320000	-3.9499790000	-2.4308500000
1	1.0670630000	-5.2058730000	-1.3946870000
1	2.8187910000	-4.9143250000	-1.3592350000
1	0.4900110000	-4.5821670000	1.0217750000
1	1.4314310000	-3.2234040000	1.6887310000
1	3.8473720000	2.8642680000	-1.0569360000
1	2.5530630000	0.4913000000	-1.9549290000
1	0.1362360000	1.2965720000	3.1039640000
1	-1.3165010000	2.3010900000	2.9880190000
1	-1.3393910000	0.8333650000	3.9641760000
1	0.5476750000	-1.4237830000	3.0843800000
1	-0.9955560000	-1.3753310000	3.9383340000
1	-0.5825500000	-2.7918010000	2.9810300000
1	0.8728670000	-0.2670150000	0.0191450000

## 15:

SCF ENERGY at B3LYP/6-311+G\*\* = -1268.53321

ZPVE = 440.973 kcal/mol

1	4.2755330000	1.5391520000	1.7655590000
6	4.3881490000	1.1400190000	0.7487650000
6	3.4828680000	-1.0698090000	-0.0029510000
6	3.3416860000	-0.6157450000	-1.4785840000
6	3.1453060000	0.9343060000	-1.5151610000
6	3.1354110000	1.4714250000	-0.0623190000
1	5.2468970000	1.6657050000	0.3102840000
1	3.6756520000	-2.1408580000	0.0609670000
1	4.1004910000	-1.0242190000	-2.1541220000
1	3.7895750000	1.4909300000	-2.2035360000
1	3.0381010000	2.5565880000	-0.0446310000
6	1.8064960000	0.8230270000	0.4298760000
1	1.5323940000	1.1805650000	1.4225790000
6	2.0316250000	-0.7768040000	0.4811620000
1	1.8460160000	-1.1394000000	1.4942690000
6	1.6358450000	0.7356370000	-1.9034210000
1	1.3140070000	1.1180910000	-2.8770190000
6	1.8241490000	-0.8214030000	-1.8578140000
1	1.6088060000	-1.3279120000	-2.8028280000
6	1.2549970000	-1.5901230000	-0.6281740000
6	1.7618300000	-3.0697820000	-0.8029500000
6	0.8437970000	1.3604170000	-0.7265630000
6	0.9225240000	2.9174730000	-0.8869690000
7	-0.1815200000	-1.7708910000	-0.6179320000
7	-0.5710640000	0.9986170000	-0.8089730000
6	4.6095920000	-0.3795550000	0.7642970000
1	5.5707340000	-0.6489940000	0.3059730000
1	4.6426390000	-0.7701790000	1.7898750000
6	-0.9999050000	-1.9195300000	0.3444100000
6	-1.5491960000	1.6712480000	-0.3104570000
7	-1.5917040000	2.4494980000	0.8621110000
7	-2.7737450000	1.7054820000	-0.9911820000
6	-2.2050270000	3.7664640000	0.8875340000
6	-0.8064540000	2.1321960000	2.0325430000
6	-4.0433110000	1.5276500000	-0.3095370000
6	-2.8216960000	1.5254560000	-2.4291550000
1	-1.4434590000	4.5469910000	1.0461210000
1	-2.7052550000	3.9604290000	-0.0615390000
1	-2.9433600000	3.8518650000	1.6989800000

1	-1.4239870000	2.2598570000	2.9341970000
1	-0.4749500000	1.0967480000	1.9817500000
1	0.0752840000	2.7836520000	2.1444850000
1	-4.4724610000	0.5376530000	-0.5284730000
1	-3.8999550000	1.6077110000	0.7688220000
1	-4.7725740000	2.2888860000	-0.6231600000
1	-3.4908030000	2.2774850000	-2.8734310000
1	-1.8176980000	1.6384020000	-2.8373170000
1	-3.1964730000	0.5337220000	-2.7165270000
7	-0.7442000000	-1.8465920000	1.7483280000
7	-2.3706610000	-2.1031710000	0.0203120000
6	-3.0099870000	-3.2875230000	0.5910990000
6	-2.6914190000	-1.9646370000	-1.3946280000
6	-1.7365780000	-1.2573490000	2.6335890000
6	0.0428760000	-2.8809460000	2.3972520000
1	-2.7292890000	-4.2065590000	0.0463950000
1	-2.7387470000	-3.4204380000	1.6383200000
1	-4.0995480000	-3.1816220000	0.5322950000
1	-3.7786960000	-1.8595780000	-1.4995430000
1	-2.1822990000	-1.0881880000	-1.7875480000
1	-2.3642650000	-2.8380110000	-1.9828870000
1	-2.4112020000	-1.9995510000	3.0955860000
1	-1.2242090000	-0.7361420000	3.4539780000
1	-2.3462240000	-0.5403020000	2.0840280000
1	-0.5936080000	-3.6690760000	2.8406120000
1	0.7149360000	-3.3538740000	1.6840990000
1	0.6479240000	-2.4533120000	3.2087620000
1	0.9913390000	-3.6164120000	-1.3514930000
1	2.6884970000	-3.1461020000	-1.3772740000
1	1.9237060000	-3.5760350000	0.1550840000
1	0.0807700000	3.2455470000	-1.5035510000
1	0.8654660000	3.4434870000	0.0729600000
1	1.8278540000	3.2529670000	-1.3976570000

### 15H<sup>+</sup>:

SCF ENERGY at B3LYP/6-311+G\*\* = -1268.99540  
ZPVE = 432.783kcal/mol

1	4.1098340000	2.7174450000	1.7291160000
6	4.2809710000	1.9228730000	0.9926480000
6	3.4201860000	-0.4319280000	1.1117350000
6	3.4494070000	-0.5919590000	-0.4301400000
6	3.2359540000	0.8062520000	-1.0933920000
6	3.1036640000	1.8740980000	0.0209900000
1	5.1839300000	2.2108430000	0.4402380000
1	3.6118910000	-1.3828490000	1.6044400000
1	4.2843470000	-1.1855850000	-0.8117180000
1	3.9242240000	1.0703030000	-1.9007210000
1	3.0006970000	2.8749850000	-0.4002310000
6	1.7383420000	1.4247260000	0.6158220000
1	1.3602360000	2.1229940000	1.3680090000
6	1.9217920000	-0.0464940000	1.2789130000
1	1.5908590000	-0.0230200000	2.3222600000
6	1.7642340000	0.3958480000	-1.4978480000
1	1.5299260000	0.3741840000	-2.5667090000
6	1.9961080000	-1.0217160000	-0.8518300000
1	1.9318890000	-1.8431710000	-1.5675420000
6	1.2700480000	-1.2784060000	0.4965260000
6	1.7406580000	-2.6210100000	1.1288080000
6	0.9012240000	1.4404300000	-0.7160120000
6	0.9627970000	2.7503310000	-1.5464800000
7	-0.2010620000	-1.2316560000	0.5229800000
7	-0.5230080000	1.0729940000	-0.5619240000

6	4.4472270000	0.5542010000	1.6686440000
1	5.4527280000	0.1478500000	1.5052810000
1	4.3224340000	0.6263690000	2.7559680000
6	-1.0595050000	-2.2192710000	0.5063210000
6	-1.6234980000	1.8087050000	-0.7088210000
7	-1.7322760000	3.1132700000	-0.3276450000
7	-2.7229140000	1.2138470000	-1.2517210000
6	-2.4565450000	4.1077600000	-1.1180820000
6	-1.1092710000	3.6180050000	0.8927650000
6	-4.0876380000	1.5627970000	-0.8580890000
6	-2.6076810000	0.0812720000	-2.1683950000
1	-1.7919780000	4.9562920000	-1.3192820000
1	-2.7640250000	3.6780110000	-2.0717070000
1	-3.3410670000	4.4827770000	-0.5893160000
1	-1.8691980000	4.1359790000	1.4903820000
1	-0.7103990000	2.7880260000	1.4742110000
1	-0.3035600000	4.3293380000	0.6782660000
1	-4.6277760000	0.6482170000	-0.5882840000
1	-4.0711440000	2.2233540000	0.0086720000
1	-4.6305710000	2.0532060000	-1.6746420000
1	-3.3257360000	0.2105990000	-2.9858160000
1	-1.5983880000	0.0423650000	-2.5783160000
1	-2.8241580000	-0.8680520000	-1.6644150000
7	-0.9489400000	-3.4354330000	-0.1496110000
7	-2.2489590000	-2.0460720000	1.1912390000
6	-3.5254350000	-2.5748140000	0.7268870000
6	-2.3439260000	-1.0698470000	2.2657130000
6	-1.3721720000	-4.6985300000	0.4502300000
6	-0.2555240000	-3.5585350000	-1.4216430000
1	-4.2381970000	-1.7521880000	0.5721380000
1	-3.3955580000	-3.1013920000	-0.2187680000
1	-3.9678860000	-3.2650640000	1.4563720000
1	-3.0120170000	-1.4551490000	3.0448310000
1	-1.3546280000	-0.8932250000	2.6861870000
1	-2.7494100000	-0.1079170000	1.9166420000
1	-2.1601330000	-5.1854870000	-0.1389640000
1	-0.5179160000	-5.3864340000	0.5073960000
1	-1.7404340000	-4.5264710000	1.4618280000
1	-0.8450240000	-4.1980140000	-2.0907320000
1	-0.1525630000	-2.5758810000	-1.8827510000
1	0.7423120000	-4.0070870000	-1.3182570000
1	-0.6261750000	0.0817960000	-0.1578590000
1	1.0618500000	-3.4301320000	0.8682070000
1	2.7326490000	-2.9283940000	0.7941540000
1	1.7565130000	-2.5475410000	2.2224220000
1	0.1757510000	2.7332990000	-2.3071920000
1	0.8458460000	3.6567030000	-0.9474180000
1	1.9050670000	2.8363910000	-2.0869030000