Supporting Information

Local versus Global Aromaticity in Azuliporphyrin and Benziporphyrin Derivatives:

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B3LYP/def2-TZVP optimized Cartesian coordinates (Å); total energies in E_h

H_3[CP]
Energy: -973.833191999

N	1.372845000	-1.416136000	-0.056541000
N	1.545696000	1.520119000	0.041117000
N	-1.566286000	-1.528818000	0.041862000
C	1.170921000	-2.765761000	-0.086888000
C	2.441780000	-3.471717000	-0.148283000
C	3.406207000	-2.526772000	-0.148227000
C	2.726290000	-1.241741000	-0.086997000
C	3.420499000	-0.029746000	-0.046180000
C	2.885222000	1.253247000	0.024835000
C	3.548112000	2.516206000	0.084837000
C	2.588419000	3.494994000	0.119456000
C	1.303254000	2.871986000	0.090448000
C	-0.055063000	-3.434960000	-0.045773000
C	-1.188226000	2.835306000	0.079544000
C	-2.473087000	3.474964000	-0.235577000
C	-3.438685000	2.528933000	-0.235237000
C	-2.825326000	1.231363000	0.080141000
C	-3.495750000	0.007603000	0.076515000
C	-2.912851000	-1.258831000	0.091617000
C	-1.326778000	-2.873492000	0.025551000
C	-2.603013000	-3.510484000	0.085838000
C	-3.561982000	-2.531022000	0.120836000
C	0.048979000	3.480573000	0.075404000
C	-1.456843000	1.472128000	0.295041000
H	-0.014480000	-4.516426000	-0.065131000
H	-4.576990000	0.020318000	0.001253000
H	0.058279000	4.561825000	-0.000231000
H	-4.630620000	-2.664802000	0.172214000
H	-2.755836000	-4.577489000	0.096419000
H	2.556733000	-4.544336000	-0.181801000
H	4.476258000	-2.663573000	-0.181720000
H	4.618011000	2.647236000	0.095498000
H	2.744024000	4.560685000	0.170584000
H	-2.591265000	4.522327000	-0.471789000
H	-4.483500000	2.668409000	-0.471117000
H	4.500897000	-0.092495000	-0.065664000
H	-0.772722000	0.774009000	0.739954000
H	0.873814000	0.778939000	-0.080786000
H	-0.811438000	-0.872230000	-0.079516000

Au[CP]
Energy: -1107.84994178

Au	-0.030520000	0.016933000	-0.002287000
N	1.437159000	-1.481557000	-0.002357000
N	1.426467000	1.447063000	-0.002390000
N	-1.490471000	-1.410194000	-0.002401000
C	1.210625000	-2.830200000	-0.002356000
C	2.477300000	-3.513608000	-0.002579000

C	3.447520000	-2.563063000	-0.002332000
C	2.790367000	-1.282627000	-0.002519000
C	3.406817000	-0.044490000	-0.002586000
C	2.782904000	1.197167000	-0.002504000
C	3.473393000	2.450067000	-0.002786000
C	2.534522000	3.436305000	-0.002090000
C	1.250259000	2.811669000	-0.002366000
C	-0.040015000	-3.420986000	-0.002320000
C	-1.200373000	2.838093000	-0.002352000
C	-2.507822000	3.508889000	-0.002400000
C	-3.470619000	2.565479000	-0.002486000
C	-2.826504000	1.244595000	-0.002481000
C	-3.486422000	0.029994000	-0.002534000
C	-2.851415000	-1.205998000	-0.002481000
C	-1.268372000	-2.771224000	-0.002353000
C	-2.535269000	-3.436108000	-0.002040000
C	-3.502054000	-2.477445000	-0.002742000
C	0.027440000	3.472360000	-0.002323000
C	-1.433706000	1.449437000	-0.002365000
H	-0.072227000	-4.502367000	-0.002291000
H	-4.569673000	0.017898000	-0.002708000
H	0.062483000	4.555126000	-0.002243000
H	-4.572149000	-2.611823000	-0.003011000
H	-2.658212000	-4.507425000	-0.001739000
H	2.596381000	-4.585607000	-0.002695000
H	4.516864000	-2.704104000	-0.002265000
H	4.546971000	2.551345000	-0.003080000
H	2.690796000	4.503415000	-0.001819000
H	-2.640711000	4.581035000	-0.002386000
H	-4.539843000	2.720080000	-0.002566000
H	4.488643000	-0.034801000	-0.002750000

H_2[AP]

Energy: -1165.60362445

N	1.430336000	-1.473471000	-0.028554000
N	1.473211000	1.463214000	0.021979000
N	-1.506627000	-1.455357000	0.013650000
C	1.165570000	-2.820662000	-0.034813000
C	2.446069000	-3.481270000	-0.041999000
C	3.416661000	-2.530622000	-0.039221000
C	2.782755000	-1.236706000	-0.030384000
C	3.411628000	-0.008168000	-0.018923000
C	2.796672000	1.261444000	0.006038000
C	3.523049000	2.529777000	0.016370000
C	2.583004000	3.499869000	0.037102000
C	1.289402000	2.823467000	0.041152000
C	-0.075803000	-3.423880000	-0.028561000
C	-1.212276000	2.881019000	0.056136000
C	-2.475703000	3.564224000	0.001074000
C	-3.525031000	2.536437000	-0.001719000
C	-2.868337000	1.258962000	0.051498000
C	-3.492210000	-0.013093000	0.044105000
C	-2.862775000	-1.243324000	0.029484000

C	-1.332391000	-2.782684000	-0.005474000
C	-2.615596000	-3.482520000	-0.000885000
C	-3.565961000	-2.522538000	0.019740000
C	0.072499000	3.478340000	0.054063000
C	-1.489455000	1.507489000	0.095328000
C	-2.645216000	4.939697000	-0.044189000
C	-4.896585000	2.734591000	-0.049640000
C	-3.822935000	5.683148000	-0.092935000
C	-5.615312000	3.927590000	-0.097001000
C	-5.138894000	5.233993000	-0.115571000
H	-0.075246000	-4.506357000	-0.037264000
H	-4.575288000	-0.045834000	0.041106000
H	0.127760000	4.560507000	0.054291000
H	-4.638325000	-2.647859000	0.028622000
H	-2.749687000	-4.553640000	-0.014109000
H	2.572894000	-4.552040000	-0.045233000
H	4.484574000	-2.679643000	-0.039779000
H	4.596761000	2.641579000	0.006548000
H	2.730612000	4.569358000	0.049496000
H	4.493879000	-0.031235000	-0.024633000
H	-1.733143000	5.525577000	-0.040080000
H	-3.694165000	6.759278000	-0.117708000
H	-5.897223000	6.008311000	-0.154681000
H	-6.693825000	3.821254000	-0.124402000
H	-5.501273000	1.834868000	-0.049295000
H	-0.742947000	0.745193000	0.163108000
H	0.722763000	-0.751035000	-0.044285000

Pd[AP]

Energy: -1292.45686946

Pd	-0.054769000	0.042848000	-0.005606000
N	1.406084000	-1.448796000	0.003668000
N	1.415991000	1.460682000	-0.001421000
N	-1.502944000	-1.398052000	-0.009605000
C	1.186585000	-2.793925000	0.005056000
C	2.458800000	-3.489982000	0.012028000
C	3.424850000	-2.543883000	0.014721000
C	2.755497000	-1.257406000	0.009426000
C	3.381985000	-0.025961000	0.010118000
C	2.756427000	1.221745000	0.005099000
C	3.471491000	2.477828000	0.006186000
C	2.544982000	3.464597000	0.000245000
C	1.250909000	2.829046000	-0.004567000
C	-0.057637000	-3.394624000	0.000513000
C	-1.209870000	2.858429000	-0.016004000
C	-2.469045000	3.548486000	-0.023193000
C	-3.509282000	2.529711000	-0.026187000
C	-2.845638000	1.256415000	-0.020648000
C	-3.501137000	0.016559000	-0.021311000
C	-2.867530000	-1.204463000	-0.016130000
C	-1.292023000	-2.743208000	-0.006218000
C	-2.562742000	-3.431911000	-0.010702000
C	-3.529949000	-2.485002000	-0.016760000

C	0.043367000	3.487958000	-0.011314000
C	-1.438209000	1.455442000	-0.014478000
C	-2.637726000	4.928015000	-0.026566000
C	-4.884982000	2.727124000	-0.033204000
C	-3.814729000	5.671939000	-0.033538000
C	-5.604181000	3.919375000	-0.038892000
C	-5.132725000	5.227843000	-0.039026000
H	-0.083487000	-4.476525000	0.002340000
H	-4.583144000	-0.013614000	-0.026175000
H	0.096068000	4.569112000	-0.012979000
H	-4.599989000	-2.622856000	-0.021338000
H	-2.676772000	-4.504633000	-0.009280000
H	2.574568000	-4.562671000	0.014449000
H	4.494878000	-2.682024000	0.019798000
H	4.546351000	2.569435000	0.010930000
H	2.705140000	4.531535000	-0.000880000
H	4.464182000	-0.022645000	0.015028000
H	-1.727075000	5.515277000	-0.023369000
H	-3.683644000	6.748379000	-0.034902000
H	-5.891344000	6.002433000	-0.044072000
H	-6.683111000	3.810779000	-0.043898000
H	-5.491076000	1.828890000	-0.034461000

Au[AC1]

Energy: -1261.49845195

Au	-0.083143000	-0.225247000	0.002657000
N	1.416526000	-1.571904000	0.028926000
N	1.160822000	1.291184000	0.002433000
N	-1.515291000	-1.583580000	0.000170000
C	1.243930000	-2.915280000	0.038872000
C	2.562404000	-3.506045000	0.056765000
C	3.474531000	-2.487708000	0.057448000
C	2.755569000	-1.237542000	0.039986000
C	3.259334000	0.064285000	0.034474000
C	2.524368000	1.276654000	0.016837000
C	2.914077000	2.646433000	0.010237000
C	1.759161000	3.429016000	-0.008166000
C	0.644306000	2.557069000	-0.012699000
C	-0.020545000	-3.543043000	0.031897000
C	-0.809004000	2.537991000	-0.026869000
C	-1.916898000	3.416165000	-0.043827000
C	-3.156838000	2.571485000	-0.048723000
C	-2.742154000	1.186926000	-0.034261000
C	-3.460646000	-0.046765000	-0.030735000
C	-2.874006000	-1.307681000	-0.014786000
C	-1.279247000	-2.931244000	0.014317000
C	-2.579350000	-3.568795000	0.007458000
C	-3.530817000	-2.596036000	-0.009858000
C	-1.357338000	1.239031000	-0.022054000
C	-1.856478000	4.810066000	-0.053845000
C	-4.462811000	3.009562000	-0.063946000
C	-2.887186000	5.735865000	-0.070244000
C	-4.964144000	4.319665000	-0.078484000

C	-4.269666000	5.515571000	-0.081214000
H	-0.019958000	-4.624935000	0.041234000
H	-4.543415000	-0.032119000	-0.040815000
H	-4.600958000	-2.733723000	-0.018804000
H	-2.736593000	-4.635949000	0.015118000
H	2.768093000	-4.564860000	0.067419000
H	4.549607000	-2.580159000	0.068761000
H	3.930386000	3.007462000	0.018011000
H	1.726460000	4.506618000	-0.017054000
H	4.338216000	0.156555000	0.044835000
H	-0.854063000	5.224936000	-0.047831000
H	-2.581384000	6.775887000	-0.075336000
H	-4.881193000	6.411317000	-0.093613000
H	-6.045008000	4.402528000	-0.088988000
H	-5.215632000	2.227898000	-0.064832000

Au[AC2]

Energy: -1261.49413862

Au	0.039195000	-0.736595000	-0.032161000
N	-0.194531000	-2.709501000	-0.035874000
N	2.002234000	-0.873741000	-0.035616000
N	-1.911709000	-0.866289000	-0.029450000
C	-1.481080000	-3.175739000	-0.034994000
C	-1.372108000	-4.598157000	-0.038492000
C	-0.022161000	-4.918712000	-0.041370000
C	0.727604000	-3.691103000	-0.039644000
C	2.108578000	-3.366221000	-0.041053000
C	2.669894000	-2.082999000	-0.039098000
C	4.078008000	-1.745202000	-0.040409000
C	4.203371000	-0.389890000	-0.037742000
C	2.877278000	0.188133000	-0.034675000
C	1.167589000	2.017939000	-0.028142000
C	0.705976000	3.382688000	-0.024349000
C	-0.771822000	3.354480000	-0.022093000
C	-1.185375000	1.979604000	-0.024465000
C	-2.518912000	1.469237000	-0.023469000
C	-2.858295000	0.117896000	-0.025838000
C	-2.448230000	-2.124381000	-0.031300000
C	-3.870446000	-1.937166000	-0.028688000
C	-4.121254000	-0.583296000	-0.025412000
C	2.505735000	1.526947000	-0.031234000
C	0.013080000	1.222054000	-0.028036000
C	1.524364000	4.499592000	-0.023102000
C	-1.627453000	4.448459000	-0.018333000
C	1.180811000	5.852542000	-0.019497000
C	-1.327710000	5.807720000	-0.015749000
C	-0.081805000	6.430496000	-0.016249000
H	-3.342054000	2.171888000	-0.020608000
H	3.320999000	2.238981000	-0.031139000
H	-5.091787000	-0.112364000	-0.022902000
H	-4.606528000	-2.725003000	-0.029241000
H	-2.191778000	-5.299062000	-0.038839000
H	0.396585000	-5.912735000	-0.044324000

H	4.875718000	-2.471794000	-0.043017000
H	5.119858000	0.179291000	-0.037877000
H	2.813114000	-4.187455000	-0.043855000
H	2.589525000	4.295840000	-0.025221000
H	2.014932000	6.545043000	-0.019221000
H	-0.101251000	7.514858000	-0.013765000
H	-2.183484000	6.473312000	-0.012927000
H	-2.685734000	4.212395000	-0.017214000

H_2[BP]

Energy: -1011.94531108

N	1.454903000	-1.363970000	-0.002564000
N	1.481695000	1.555601000	-0.002419000
N	-1.464046000	-1.321091000	-0.003093000
C	1.190539000	-2.710467000	-0.002333000
C	2.475095000	-3.377026000	-0.002009000
C	3.443211000	-2.431528000	-0.001377000
C	2.807295000	-1.131509000	-0.001933000
C	3.431422000	0.089945000	-0.001756000
C	2.798788000	1.359530000	-0.001930000
C	3.534612000	2.626398000	-0.001590000
C	2.602784000	3.598060000	-0.001898000
C	1.301652000	2.926960000	-0.002133000
C	-0.045435000	-3.305329000	-0.002504000
C	-1.249116000	3.149662000	-0.003178000
C	-2.250534000	4.142430000	-0.004261000
C	-3.961268000	2.471809000	-0.004689000
C	-2.992664000	1.446968000	-0.003640000
C	-3.488065000	0.089048000	-0.003522000
C	-2.830839000	-1.108387000	-0.003255000
C	-1.299491000	-2.642539000	-0.002802000
C	-2.583537000	-3.347860000	-0.003195000
C	-3.532686000	-2.393076000	-0.003298000
C	0.120349000	3.612674000	-0.002508000
C	-1.637195000	1.803120000	-0.002836000
C	-3.593897000	3.806768000	-0.005009000
H	-0.059069000	-4.387283000	-0.002413000
H	-4.570048000	0.008252000	-0.003799000
H	0.226831000	4.692413000	-0.002414000
H	-4.605115000	-2.515641000	-0.003514000
H	-2.711523000	-4.419686000	-0.003200000
H	2.597894000	-4.448251000	-0.001993000
H	4.511236000	-2.579595000	-0.000762000
H	4.609188000	2.728750000	-0.001297000
H	2.750828000	4.667270000	-0.001798000
H	4.513390000	0.077797000	-0.001310000
H	-1.956804000	5.185370000	-0.004567000
H	-4.350103000	4.581140000	-0.005771000
H	-5.010903000	2.202904000	-0.005334000
H	-0.885611000	1.033462000	-0.001773000
H	0.746564000	-0.639015000	-0.003215000

Pd[BP]

Energy: -1138.78293704

Pd	-0.088972000	0.217579000	-0.002998000
N	1.392120000	-1.299461000	-0.002404000
N	1.430696000	1.590269000	-0.002700000
N	-1.497589000	-1.268858000	-0.003240000
C	1.179705000	-2.647054000	-0.002077000
C	2.453530000	-3.349912000	-0.001743000
C	3.416716000	-2.409305000	-0.001793000
C	2.744268000	-1.119134000	-0.002243000
C	3.386759000	0.095267000	-0.002355000
C	2.762155000	1.344963000	-0.002491000
C	3.499456000	2.593769000	-0.002270000
C	2.590871000	3.589998000	-0.002190000
C	1.287526000	2.965283000	-0.002500000
C	-0.049741000	-3.260192000	-0.002155000
C	-1.213322000	3.080288000	-0.003273000
C	-2.215999000	4.078346000	-0.003718000
C	-3.897785000	2.436290000	-0.005167000
C	-2.923934000	1.409954000	-0.004479000
C	-3.505686000	0.103057000	-0.004596000
C	-2.868883000	-1.092971000	-0.003911000
C	-1.284124000	-2.605743000	-0.002737000
C	-2.550126000	-3.313081000	-0.003053000
C	-3.524454000	-2.381015000	-0.003871000
C	0.107164000	3.630601000	-0.002636000
C	-1.528157000	1.691671000	-0.003608000
C	-3.559087000	3.771577000	-0.004763000
H	-0.070600000	-4.341637000	-0.001860000
H	-4.588073000	0.057838000	-0.005230000
H	0.178311000	4.711583000	-0.002368000
H	-4.593464000	-2.524953000	-0.004361000
H	-2.647240000	-4.387406000	-0.002724000
H	2.562005000	-4.423277000	-0.001487000
H	4.487206000	-2.543214000	-0.001569000
H	4.575791000	2.665237000	-0.002143000
H	2.760190000	4.655283000	-0.001981000
H	4.468388000	0.090008000	-0.002197000
H	-1.903642000	5.116092000	-0.003245000
H	-4.314774000	4.545603000	-0.005217000
H	-4.942674000	2.148706000	-0.006024000

Pd[BP-$(CHO)_2$]

Energy: -1365.49867646

Pd	-0.000001000	0.000000000	-0.768102000
O	-0.000020000	-2.344371000	5.614511000
O	0.000023000	2.344371000	5.614511000
N	0.000000000	0.000000000	-2.896302000
N	0.000001000	-2.035321000	-0.867540000
N	-0.000002000	2.035321000	-0.867540000
C	-0.000001000	1.091722000	-3.714713000
C	0.000000000	0.672279000	-5.108982000
C	0.000001000	-0.672279000	-5.108982000

C	0.000001000	-1.091722000	-3.714713000
C	0.000002000	-2.400014000	-3.299528000
C	0.000002000	-2.820070000	-1.968685000
C	0.000003000	-4.221625000	-1.585628000
C	0.000003000	-4.262075000	-0.240752000
C	0.000002000	-2.886816000	0.217004000
C	-0.000002000	2.400014000	-3.299528000
C	0.000000000	-1.207973000	2.094991000
C	0.000001000	-1.196262000	3.527926000
C	-0.000001000	1.196262000	3.527926000
C	-0.000001000	1.207973000	2.094991000
C	-0.000002000	2.522112000	1.518514000
C	-0.000002000	2.886816000	0.217004000
C	-0.000002000	2.820070000	-1.968685000
C	-0.000003000	4.221625000	-1.585628000
C	-0.000003000	4.262075000	-0.240752000
C	0.000001000	-2.522112000	1.518514000
C	-0.000001000	0.000000000	1.330213000
C	0.000000000	0.000000000	4.213299000
C	0.000002000	-2.409642000	4.407463000
C	-0.000002000	2.409642000	4.407463000
H	-0.000002000	3.170275000	-4.058455000
H	-0.000003000	3.362684000	2.189939000
H	0.000002000	-3.362684000	2.189939000
H	-0.000004000	5.124187000	0.407337000
H	-0.000003000	5.043133000	-2.284482000
H	0.000000000	1.345926000	-5.951459000
H	0.000001000	-1.345926000	-5.951459000
H	0.000004000	-5.043133000	-2.284482000
H	0.000003000	-5.124187000	0.407337000
H	0.000002000	-3.170275000	-4.058455000
H	0.000000000	0.000000000	5.293544000
H	-0.000016000	-3.403109000	3.935621000
H	0.000018000	3.403109000	3.935621000

Pd[BP-Me$_2$]

Energy: -1217.43671357

Pd	-0.000001000	0.000000000	-0.467446000
N	0.000000000	0.000000000	-2.596964000
N	0.000000000	-2.040670000	-0.564158000
N	0.000000000	2.040670000	-0.564158000
C	0.000000000	1.092626000	-3.415101000
C	0.000000000	0.673152000	-4.807132000
C	0.000000000	-0.673152000	-4.807132000
C	0.000000000	-1.092626000	-3.415101000
C	0.000000000	-2.401300000	-2.998719000
C	0.000000000	-2.825080000	-1.668996000
C	0.000000000	-4.223069000	-1.287499000
C	0.000000000	-4.263911000	0.060570000
C	0.000000000	-2.892949000	0.518147000
C	0.000000000	2.401300000	-2.998719000
C	0.000000000	-1.207994000	2.385270000
C	0.000000000	-1.202989000	3.815442000

C	0.000000000	1.202989000	3.815442000
C	0.000000000	1.207994000	2.385270000
C	0.000000000	2.519687000	1.821388000
C	0.000000000	2.892949000	0.518147000
C	0.000000000	2.825080000	-1.668996000
C	0.000000000	4.223069000	-1.287499000
C	0.000000000	4.263911000	0.060570000
C	0.000000000	-2.519687000	1.821388000
C	0.000000000	0.000000000	1.623007000
C	0.000000000	0.000000000	4.492546000
C	0.000000000	-2.460453000	4.651262000
C	0.000000000	2.460453000	4.651262000
H	0.000000000	3.170862000	-3.758744000
H	0.000000000	3.351014000	2.508746000
H	0.000000000	-3.351014000	2.508746000
H	0.000000000	5.126957000	0.707741000
H	0.000000000	5.044843000	-1.986251000
H	0.000000000	1.346224000	-5.650280000
H	0.000000000	-1.346224000	-5.650280000
H	0.000000000	-5.044843000	-1.986251000
H	0.000000000	-5.126957000	0.707741000
H	0.000000000	-3.170862000	-3.758744000
H	0.000000000	0.000000000	5.575610000
H	-0.880118000	-3.079409000	4.463229000
H	0.880118000	-3.079408000	4.463229000
H	0.000000000	-2.202763000	5.709498000
H	0.880118000	3.079408000	4.463229000
H	-0.880118000	3.079409000	4.463229000
H	0.000000000	2.202763000	5.709498000

Pd[BP-(OMe)$_2$]

Energy: -1367.92554863

Pd	-0.094025000	0.222754000	-0.003584000
O	-1.822975000	5.394953000	-0.003256000
O	-5.223498000	2.074722000	-0.004887000
N	1.389699000	-1.296847000	-0.002662000
N	1.431284000	1.585717000	-0.002882000
N	-1.493041000	-1.269561000	-0.003361000
C	1.179174000	-2.646193000	-0.002371000
C	2.449855000	-3.347345000	-0.001903000
C	3.414299000	-2.405670000	-0.001871000
C	2.743692000	-1.118602000	-0.002300000
C	3.389590000	0.094591000	-0.002266000
C	2.767277000	1.341986000	-0.002458000
C	3.498705000	2.589670000	-0.002144000
C	2.583978000	3.583375000	-0.002305000
C	1.285820000	2.953662000	-0.002736000
C	-0.049100000	-3.262927000	-0.002501000
C	-1.211049000	3.099220000	-0.003425000
C	-2.232204000	4.107946000	-0.003602000
C	-3.927090000	2.453086000	-0.004355000
C	-2.943021000	1.408130000	-0.004041000
C	-3.503917000	0.104032000	-0.004036000

C	-2.857120000	-1.091494000	-0.003649000
C	-1.281276000	-2.610999000	-0.002932000
C	-2.546066000	-3.312434000	-0.003025000
C	-3.517648000	-2.374243000	-0.003480000
C	0.106077000	3.628814000	-0.002986000
C	-1.551429000	1.715382000	-0.003650000
C	-3.577215000	3.790108000	-0.004114000
C	-2.773558000	6.450393000	-0.003379000
C	-6.255968000	3.050201000	-0.005024000
H	-0.066920000	-4.344539000	-0.002201000
H	-4.580509000	0.037444000	-0.004252000
H	0.198349000	4.703508000	-0.002791000
H	-4.587442000	-2.512763000	-0.003667000
H	-2.647090000	-4.386440000	-0.002761000
H	2.557818000	-4.420833000	-0.001624000
H	4.484900000	-2.539252000	-0.001560000
H	4.574816000	2.665022000	-0.001814000
H	2.748010000	4.649555000	-0.002136000
H	4.471319000	0.086566000	-0.001934000
H	-4.328258000	4.559419000	-0.004327000
H	-3.401982000	6.419785000	0.890281000
H	-2.191971000	7.368883000	-0.002994000
H	-3.401357000	6.420141000	-0.897490000
H	-6.210813000	3.677321000	0.888937000
H	-6.210396000	3.677508000	-0.898835000
H	-7.188061000	2.490674000	-0.005304000

Pd[BP-$(NH_2)_2$]

Energy: -1249.54933404

Pd	-0.015973000	-0.000001000	-0.117242000
N	0.110060000	0.000000000	-2.234794000
N	-0.074166000	-2.040315000	-0.208293000
N	-0.074167000	2.040315000	-0.208294000
N	0.328491000	2.355144000	4.870024000
N	0.328497000	-2.355146000	4.870017000
C	0.173937000	1.093825000	-3.050257000
C	0.305992000	0.674859000	-4.431224000
C	0.305991000	-0.674859000	-4.431224000
C	0.173935000	-1.093825000	-3.050258000
C	0.079185000	-2.403682000	-2.636919000
C	-0.073787000	-2.827099000	-1.319602000
C	-0.260322000	-4.208331000	-0.942235000
C	-0.382426000	-4.237702000	0.404834000
C	-0.244278000	-2.878070000	0.862788000
C	0.079189000	2.403682000	-2.636920000
C	0.002357000	-1.211652000	2.715912000
C	0.201273000	-1.195412000	4.150951000
C	0.201267000	1.195414000	4.150953000
C	0.002352000	1.211656000	2.715913000
C	-0.206086000	2.500045000	2.174337000
C	-0.244282000	2.878071000	0.862787000
C	-0.073785000	2.827100000	-1.319604000
C	-0.260321000	4.208332000	-0.942237000

C	-0.382429000	4.237702000	0.404831000
C	-0.206079000	-2.500042000	2.174338000
C	-0.017125000	0.000002000	1.965246000
C	0.285340000	0.000000000	4.839023000
H	0.102600000	3.171251000	-3.399054000
H	-0.388144000	3.314822000	2.861533000
H	-0.388133000	-3.314818000	2.861537000
H	-0.532123000	5.092321000	1.046265000
H	-0.292741000	5.032208000	-1.637831000
H	0.378915000	1.346706000	-5.272291000
H	0.378912000	-1.346706000	-5.272292000
H	-0.292744000	-5.032207000	-1.637829000
H	-0.532117000	-5.092320000	1.046269000
H	0.102594000	-3.171253000	-3.399051000
H	0.487289000	-0.000001000	5.904398000
H	0.604165000	2.266964000	5.833380000
H	0.668853000	3.181207000	4.412307000
H	0.668850000	-3.181209000	4.412292000
H	0.604175000	-2.266973000	5.833372000