

Supporting Information for
**Key Role of End-Capping Groups in Optoelectronic Properties of
Poly-*p*-phenylene Cation Radicals**

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Archive entries from the calculation files

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Introduction

The archive entries, formerly intended for the Browse Quantum Chemistry Database System, are organized as a simple list of data fields separated by backslash symbols, which is wrapped in 70-char text lines. The script 'Parse.Archive.pl', written in Perl, converts archive entry into human readable format. To use this script,

1. Check if the Perl interpreter is installed on the system. To do this, run the command 'perl -v' in console. If console returns a message like 'command not found', please obtain and install a Perl interpreter (www.perl.org/get.html; Perl is Open Source software licensed under GNU GPL).
2. Save the script code, listed below, as a file named 'Parse.Archive.pl'.

3. Select an archive entry of interest and save it as another file (e.g. 'B-Xb.txt').
4. Run the command 'perl Parse.Archive.pl B-Xb.txt > B-Xb-parsed.txt' in console. The parsed archive entry will be stored in the file 'B-Xb-parsed.txt' in this example. In some cases, absolute path to the Perl interpreter might need to be provided.

```
# --- Parse.Archive.pl ---

# Merge all strings in one line
my $s='';
while (<>) { chomp ; $s .= $_ }
$_ = $s;

# Some PDF viewers (like Mac OS's Preview) might substitute
# 'end of line' symbols by the white space symbols,
# To remove these extra white spaces, please uncomment the following lines:
# my $str_length = 70;
# my $index = $str_length;
# while (length($_) > $index) {
#     substr $_,$index,1,'';
#     $index += $str_length;
# }

# Replace all backslashes by new-line symbols
s:\\:\n:g;

# Print the resulting output
print;

# --- END ---
```

^{iA}PP_n (Alternant conformer)

iAPP2

```
1\1\GINC-HPC-CN56\FOpt\RBLYP\6-31G(d)\C18H22\TALIPOVM\10-Sep-2013\0\#\#
P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent=Dichl
oromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title
\0,1\C,-0.254,1.13372,0.22024\C,-0.182,3.4682,1.83028\C,-1.03502,2.25
303,-0.08845\C,0.56266,1.2082,1.35112\C,0.59469,2.35242,2.13764\C,-0.9
9809,3.39378,0.69895\H,-1.69604,2.2225,-0.94317\H,1.19731,0.372,1.6086
7\H,1.24378,2.3798,3.00305\H,-1.6231,4.23434,0.42928\C,-0.29196,-0.085
,-0.62197\C,-0.36228,-2.41996,-2.23145\C,-0.41747,-0.0033,-2.01083\C,-
0.2026,-1.361,-0.05456\C,-0.2362,-2.50139,-0.84259\C,-0.45251,-1.14864
,-2.79565\H,-0.46627,0.96564,-2.48744\H,-0.12774,-1.46295,1.01893\H,-0
.17153,-3.46885,-0.36331\H,-0.54327,-1.04983,-3.86944\C,-0.4011,-3.662
66,-3.10098\H,-0.49931,-3.32656,-4.13565\C,0.8989,-4.47031,-3.00002\H,
1.76362,-3.85949,-3.25971\H,0.87131,-5.3256,-3.67658\H,1.04992,-4.8515
7,-1.98904\C,-1.61772,-4.54165,-2.78471\H,-2.54687,-3.98155,-2.89062\H
,-1.57314,-4.9262,-1.76471\H,-1.65746,-5.39707,-3.46049\C,-0.13639,4.7
119,2.69801\H,0.57214,4.51326,3.50529\C,-1.4969,5.00788,3.34158\H,-1.8
5009,4.15769,3.92529\H,-2.25139,5.23157,2.58597\H,-1.42623,5.87043,4.0
0568\C,0.37896,5.93029,1.9218\H,1.36257,5.73739,1.49334\H,0.45854,6.79
703,2.5794\H,-0.29571,6.19351,1.10584\Version=EM64L-G09RevC.01\HF=-69
8.7571317\RMSD=2.958e-09\RMSF=3.924e-06\Dipole=0.0002684,0.0004826,0.0
```

000678\Quadrupole=-6.3354396,4.270883,2.0645566,-1.4723664,2.899904,3.3639631\PG=C01 [X(C18H22)]\@

iAPP3

1\1\GINC-HPC-CN55\FOpt\RBLYP\6-31G(d)\C24H26\TALIPOVM\10-Sep-2013\0\#\#
P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent=Dichl
oromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title
\0,1\H,0.25446,0.63616,-2.55759\C,-0.02745,0.57261,-1.51629\C,-0.6642
3,0.44231,1.17037\C,-0.37064,-0.66723,-0.96761\C,-0.00331,1.72048,-0.7
398\C,-0.32104,1.68215,0.62169\C,-0.68837,-0.70556,0.39388\H,0.29703,2
.65488,-1.19203\H,-0.98871,-1.63996,0.84611\H,-0.94614,0.37876,2.21167
\C,-0.2944,2.90857,1.4516\C,-0.24333,5.25853,3.03856\C,-0.69191,4.1449
7,0.93048\C,0.12855,2.87374,2.78256\C,0.1516,4.02634,3.55678\C,-0.6657
5,5.29301,1.70741\H,-1.04709,4.20529,-0.0886\H,0.46504,1.94121,3.21314
\H,0.49181,3.96629,4.58223\H,-0.98844,6.22739,1.26855\C,-0.39728,-1.89
365,-1.79752\C,-0.44835,-4.24361,-3.38448\C,-0.82023,-1.85882,-3.12848
\C,0.00023,-3.13006,-1.2764\C,-0.02593,-4.27809,-2.05333\C,-0.84328,-3
.01141,-3.9027\H,-1.15672,-0.92629,-3.55906\H,0.35541,-3.19037,-0.2573
2\H,0.29676,-5.21247,-1.61447\H,-1.18349,-2.95137,-4.92815\C,-0.47974,
-5.4949,-4.24178\H,-0.84365,-5.19823,-5.22801\C,0.92014,-6.09353,-4.42
812\H,1.60713,-5.36368,-4.85664\H,0.88118,-6.95608,-5.09477\H,1.33726,
-6.42765,-3.47703\C,-1.4538,-6.54164,-3.68668\H,-2.45883,-6.13133,-3.5
8749\H,-1.1376,-6.89397,-2.70377\H,-1.50364,-7.40677,-4.34927\C,-0.211
93,6.50982,3.89586\H,0.15197,6.21315,4.88209\C,-1.61182,7.10845,4.0822
\H,-2.29881,6.3786,4.51072\H,-2.02894,7.44257,3.13111\H,-1.57286,7.971
,4.74885\C,0.76213,7.55656,3.34076\H,1.76715,7.14625,3.24157\H,0.81196
,8.42169,4.00335\H,0.44592,7.90889,2.35784\Version=EM64L-G09RevC.01\H
F=-929.6807408\RMSD=2.611e-09\RMSF=2.810e-06\Dipole=0.0000064,-0.00000
21,0.0000035\Quadrupole=-12.1808726,7.845961,4.3349116,-0.7685636,2.04
81144,4.9208334\PG=C01 [X(C24H26)]\@

iAPP4

1\1\GINC-HPC-CN53\FOpt\RBLYP\6-31G(d)\C30H30\TALIPOVM\10-Sep-2013\0\#\#
P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent=Dichl
oromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title
\0,1\H,1.4402299147,-2.633700276,-0.7993391834\C,0.6919663781,-1.8748
915348,-0.9782823971\C,-1.2507119323,0.0569161448,-1.3470230004\C,-0.2
986560935,-2.0944553404,-1.9409360725\C,0.711334694,-0.7162979337,-0.2
180664071\C,-0.2597474454,0.2764009983,-0.3847218174\C,-1.2694515028,-
1.1014990461,-2.1076187682\H,1.4741901276,-0.5962665792,0.5378214969\H
, -2.0323581234,-1.2218254451,-2.8634001221\H,-1.9993027648,0.815402461
1,-1.5260522318\C,-0.2396451743,1.5135805061,0.4277815574\C,-0.2011549
519,3.8836375644,1.9851117782\C,-1.425619768,2.1246428862,0.8475571952
\C,0.9660442573,2.1144182897,0.8039842601\C,0.9846739283,3.2727611715,
1.5646248733\C,-1.4067002719,3.2826445261,1.6087776245\H,-2.3758329855
,1.6719783428,0.6027676265\H,1.9020389736,1.6887940898,0.4715426686\H,
1.9346804585,3.7257739948,1.8095283686\H,-2.342569856,3.7085013021,1.9
412437106\C,-0.1808002265,5.1205692364,2.7993086754\C,-0.1443159663,7.
4895540216,4.3578650963\C,-1.1467256766,6.1181403073,2.6259462021\C,0.
8027699273,5.3340101926,3.7681164096\C,0.8177504915,6.4955443123,4.529
0162592\C,-1.1277819434,7.2754931481,3.389070264\H,-1.9090429938,5.997
2368995,1.8692861279\H,1.5519251326,4.5756616345,3.9467993014\H,1.5889
952402,6.6265379332,5.2766040375\H,-1.8882554644,8.0253072604,3.218285

7759\C, -0.3184327772, -3.3325300828, -2.7534157886\C, -0.3588225526, -5.70
43058181, -4.3075147415\C, 0.8659634527, -3.9376753165, -3.1806163853\C, -1
.5249270383, -3.9389732481, -3.120596772\C, -1.5429581469, -5.0982162168, -
3.8808908608\C, 0.8422622507, -5.0994002064, -3.9409958003\H, 1.8167506131
, -3.4853602366, -2.936363322\H, -2.4602533958, -3.5111996202, -2.788212831
3\H, -2.4966626033, -5.5394852527, -4.136740223\H, 1.7774655914, -5.5388821
822, -4.2621154305\C, -0.3692715526, -6.9733076184, -5.1388814122\H, 0.6726
188383, -7.2353323061, -5.336082759\C, -1.0037865964, -8.1460575691, -4.380
7465553\H, -0.4955119815, -8.3238957758, -3.4329784519\H, -0.9469288896, -9
.0598431459, -4.9737782848\H, -2.0560907509, -7.9548941431, -4.1655247326\
C, -1.055853305, -6.7614057722, -6.4939928444\H, -0.5846867356, -5.95248091
47, -7.0524765924\H, -2.1103528176, -6.5114984547, -6.3681724968\H, -0.9994
059847, -7.6686922726, -7.0969737354\C, -0.116281609, 8.7529427811, 5.19732
88319\H, 0.7404923767, 8.6714076606, 5.869907244\C, -1.3731644816, 8.887840
5313, 6.0660559329\H, -1.5047142728, 8.0160618251, 6.7071154019\H, -2.26910
98614, 8.9900585606, 5.4519860832\H, -1.3046388333, 9.7708874897, 6.7028195
05\C, 0.0914383815, 10.0051745258, 4.3362075648\H, 1.00280715, 9.9290081377
, 3.74303221\H, 0.1684783157, 10.8929342549, 4.9653923599\H, -0.7430691668,
10.1562293178, 3.6499055775\\Version=EM64L-G09RevC.01\HF=-1160.604288\R
MSD=7.869e-09\RMSF=6.086e-07\Dipole=0.0009118, -0.0013407, 0.0015033\Qua
drupole=-0.7219094, 6.6367264, -5.9148171, -2.566731, 4.2909643, 14.5162506
\PG=C01 [X(C30H30)]\@

iAPP5

1\1\GINC-HPC-CN51\FOpt\RBLYP\6-31G(d)\C36H34\TALIPOVM\10-Sep-2013\0\#\#
P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent=Dichl
oromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title
\0,1\H,0.7911216716,0.266590843,-2.6178065843\C,0.3327088473,0.271237
1611,-1.6393209483\C,-0.7569348683,0.3065589167,0.9014145599\C,-0.2296
364503,-0.9051553389,-1.1331447694\C,0.3496569214,1.4384037178,-0.8924
60133\C,-0.1949126422,1.4830334598,0.3950933619\C,-0.7739273284,-0.860
5966922,0.1545304579\H,0.8210180042,2.319209615,-1.3043536588\H,-1.245
4233939,-1.7413413442,0.5663932072\H,-1.2153944083,0.3112298466,1.8798
7964\C,-0.2485190241,-2.1516615861,-1.9312154988\C,-0.2866367763,-4.53
98759174,-3.46014252\C,-0.4271926387,-2.1217308406,-3.3180742995\C,-0.
089022786,-3.4024225191,-1.3259904288\C,-0.1073748283,-4.5694153998,-2
.0733399006\C,-0.446402858,-3.2889453758,-4.0650191669\H,-0.5851737424
, -1.1760193967,-3.8164961798\H,0.0830988844,-3.4629699114,-0.260896395
\H,0.0505028312,-5.515243873,-1.5751439057\H,-0.6187422146,-3.22884449
11,-5.1300872164\C,-0.1775746728,2.7299464546,1.1925561594\C,-0.145429
6564,5.11903767975,2.7202421828\C,0.0006194532,2.7011224219,2.579474672
7\C,-0.3392644767,3.9800680758,0.5865558974\C,-0.3240040972,5.14743804
29,1.3333225099\C,0.0168330959,3.8687820569,3.3258587075\H,0.160172315
4,1.7559804178,3.0784831143\H,-0.5111157561,4.0396518107,-0.4786367813
\H,-0.4840086892,6.0926923155,0.8347278762\H,0.1885181102,3.8094217406
,4.3910759789\C,-0.1292214364,6.3668558868,3.5177614214\C,-0.101537407
7,8.7554340543,5.0461109144\C,-0.6830446402,6.4129628537,4.8020421171\
C,0.4385538919,7.5403158623,3.015623625\C,0.4496940255,8.7082331489,3.
7667348396\C,-0.6682457953,7.5813980793,5.5481925728\H,-1.1515819289,5
.5299933757,5.2133012986\H,0.8970324225,7.5371335834,2.0368465501\H,0.
9039095989,9.5982438711,3.3514732869\H,-1.1139825822,7.5767308636,6.53
36135604\C,-0.3064288817,-5.7869949921,-4.2586685435\C,-0.3459087421,-
8.1764963536,-5.7853234271\C,0.2453119874,-5.8351275711,-5.5411537118\
C,-0.8790178315,-6.9603637695,-3.755121949\C,-0.8970242697,-8.12788153
13,-4.5025786806\C,0.2236493804,-7.006939708,-6.2859992374\H,0.7174067

522, -4.955010551, -5.9544201627\H, -1.3359684599, -6.9535448013, -2.775632
5653\H, -1.356174553, -9.0110472429, -4.0796420184\H, 0.6664602181, -7.0127
212412, -7.2732915454\C, -0.3626406871, -9.4495754177, -6.6103495123\H, 0.1
298374393, -9.2230645775, -7.5586162542\C, 0.4303132157, -10.5763172854, -5
.9364246557\H, 1.4583065082, -10.2718001038, -5.7395652142\H, 0.453963501,
-11.4611369407, -6.5739593223\H, -0.0214786282, -10.8640358565, -4.9859781
755\C, -1.7929676921, -9.9019611234, -6.9303592657\H, -2.349684735, -9.1166
972152, -7.4418975418\H, -2.3382582004, -10.1613306082, -6.0217107231\H, -1
.7801668575, -10.7834219973, -7.5728556867\C, -0.0833584909, 10.0390963564
, 5.8544963757\H, 0.4151041218, 10.7950145309, 5.2436091589\C, 0.7244031293
, 9.8865788401, 7.1493583486\H, 1.7441097032, 9.561863352, 6.9419533268\H, 0
.2685010771, 9.1529320179, 7.8157641792\H, 0.7720517698, 10.8361830942, 7.6
840566908\C, -1.5007041771, 10.5461852742, 6.1492574108\H, -2.0668661406, 1
0.6908632025, 5.2290505574\H, -1.4631699593, 11.4991312235, 6.6788069736\H
, -2.0511854725, 9.8408684091, 6.7735350451\\Version=EM64L-G09RevC.01\HF=
-1391.5278478\RMSD=5.244e-09\RMSF=2.833e-07\Dipole=-0.0024314, 0.000963
3, -0.0017121\Quadrupole=-20.4969463, 14.7568221, 5.7401241, 3.2761669, -4.
2166888, 9.8813714\PG=C01 [X(C36H34)]\@

iAPP6

1\1\GINC-HPC-CN50\FOpt\RBLYP\6-31G(d)\C42H38\TALIPOVM\10-Sep-2013\0\#\#
P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent=Dichl
oromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title
\0,1\H, -2.1851124755, 0.6784126332, -0.9408468813\C, -1.2989834805, 0.939
7659675, -0.3803964958\C, 0.9750288863, 1.6877666534, 1.0029350697\C, -0.17
40371989, 0.1106560252, -0.4383441793\C, -1.2870789262, 2.1160589847, 0.352
1005465\C, -0.1497255335, 2.5172005308, 1.0605289093\C, 0.9632278214, 0.511
5655247, 0.2703308034\H, -2.1642239442, 2.7470973239, 0.347470382\H, 1.8404
336998, -0.1193917816, 0.2749338813\H, 1.8611357247, 1.9491847495, 1.563378
6824\C, -0.1865071793, -1.1451999869, -1.221639936\C, -0.2103808983, -3.550
3651612, -2.7227146125\C, -1.3384259361, -1.9337477467, -1.3086736252\C, 0.
9532060606, -1.5861677276, -1.9020061907\C, 0.9414861051, -2.7617022228, -2
.6356718544\C, -1.350036882, -3.1094042738, -2.0422087061\H, -2.2285489699
, -1.6411545391, -0.7704005312\H, 1.852145953, -0.9868424611, -1.8838371522
\H, 1.831530236, -3.0542346943, -3.1740879413\H, -2.2489634555, -3.70874615
2, -2.0604593159\C, -0.1364934125, 3.774041362, 1.8423096642\C, -0.11083278
45, 6.182625586, 3.3389724457\C, 1.0154952602, 4.5626302673, 1.9268200664\C
, -1.2752973258, 4.2164402183, 2.5231581085\C, -1.2624156651, 5.3932994263,
3.2549530795\C, 1.0277353249, 5.7399735111, 2.6578365931\H, 1.905114571, 4.
2689089698, 1.3882399477\H, -2.1744343601, 3.6172542838, 2.506928859\H, -2.
1517665841, 5.6872316797, 3.7938225802\H, 1.9267008185, 6.3393672961, 2.674
0479184\C, -0.0977535203, 7.4411471951, 4.1195370997\C, -0.0693464466, 9.85
16661529, 5.613012128\C, 1.0380390938, 7.8388363842, 4.8337187641\C, -1.217
8132677, 8.2745084189, 4.1691819583\C, -1.200373281, 9.453919472, 4.9020276
803\C, 1.0504574305, 9.0179105823, 5.5629457715\H, 1.9149388864, 7.20692425
66, 4.8370061042\H, -2.1056379425, 8.0120431431, 3.6113872116\H, -2.0821919
908, 10.0809001925, 4.913542569\H, 1.9459962773, 9.2851691624, 6.1072776726
\C, -0.2225193082, -4.8058953257, -3.5066212991\C, -0.2446963281, -7.210766
2076, -5.0093241196\C, -1.3590871611, -5.2065418354, -4.2164108544\C, 0.902
5551728, -5.6347486331, -3.5646650818\C, 0.8913917843, -6.8102584737, -4.29
85897045\C, -1.3696059691, -6.38167873, -4.9510565011\H, -2.2366642197, -4.
5760096441, -4.2206937317\H, 1.7882520325, -5.3738186121, -3.0032452535\H,
1.7686702825, -7.4411657573, -4.2943937608\H, -2.2551800143, -6.6428076637
, -5.512548884\C, -0.2556843511, -8.4660153351, -5.7951686391\C, -0.2793702
601, -10.869381741, -7.3000327697\C, 0.8801432531, -8.8998695529, -6.483028

9516\C, -1.4049776527, -9.2602785568, -5.8757300381\C, -1.4150260998, -10.4348855428, -6.612207121\C, 0.8649457601, -10.0776984668, -7.2184309228\H, 1.7795397857, -8.3007510912, -6.4634018979\H, -2.2951652429, -8.9671522554, -5.3372419074\H, -2.3215971537, -11.0239234474, -6.6425849804\H, 1.759402413, -10.3818053519, -7.745999436\C, -0.2815352805, -12.1534958999, -8.1078914451\H, 0.7143351791, -12.2591356889, -8.5439459403\C, -0.5301709507, -13.382060177, -7.2238175873\H, 0.2052948982, -13.445886253, -6.4217725858\H, -0.4688928753, -14.2968411562, -7.8148803489\H, -1.5206147049, -13.3471004494, -6.7677600308\C, -1.2876597858, -12.0977972576, -9.2642321584\H, -1.091590592, -11.2468380641, -9.9166743567\H, -2.3101840022, -12.0076594881, -8.8947103911\H, -1.2305446195, -13.0067769035, -9.8645734258\C, -0.0643122427, 11.143325131, 6.4088260533\H, -1.047759754, 11.6013601868, 6.2819438012\C, 0.978304289, 12.1353960823, 5.8784443589\H, 0.8176577599, 12.3487061857, 4.8215913491\H, 1.9901832097, 11.74332808, 5.9907249193\H, 0.9241828625, 13.0765556212, 6.4272851459\C, 0.135211408, 10.8880317478, 7.9080902869\H, -0.6256117024, 10.2114172243, 8.2974350772\H, 0.0760240924, 11.8234604524, 8.4661130758\H, 1.1116353993, 10.4439836443, 8.1071629823\\Version=EM64L-G09RevC.01\HF=-1622.451433\RMSD=7.733e-09\RMSF=3.265e-07\Dipole=0.0011648,0.0012474,-0.0024096\Quadrupole=0.3479936,11.401513,-11.7495067,-0.3130339,0.4292822,23.5716303\PG=C01 [X(C42H38)]\@\

iAPP7

1\1\GINC-HPC-CN49\F0pt\RBLYP\6-31G(d)\C48H42\TALIPOVM\10-Sep-2013\0\#\# P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRf(PCM,solvent=Dichloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title \0,1\C,10.0490615987,-0.0048650781,-0.0947408843\C,7.2131707447,-0.0013581756,-0.0986185522\C,9.3258932895,0.3627563206,-1.2340880814\C,9.3218692303,-0.3705791814,1.0426589481\C,7.9359716061,-0.3684768456,1.0410631573\C,7.9400028101,0.3639695931,-1.2363382351\H,9.8534253827,0.6817229828,-2.1215821493\H,9.8460301717,-0.690703079,1.931731692\H,7.4087919627,-0.687241228,1.9288616543\H,7.4160386829,0.684092609,-2.1255543134\C,11.5300518454,-0.0070725086,-0.0928370638\C,14.3658421843,-0.010952629,-0.0859433216\C,12.2533717775,0.3682085117,1.0447888199\C,12.2555582907,-0.3837336546,-1.2256544927\C,13.6442211746,-0.3838385896,-1.2187019807\C,13.6397942644,0.365279486,1.0466981948\H,11.7250092358,0.6880155164,1.9318222178\H,11.7316043916,-0.7023568581,-2.1157109313\H,14.1762448316,-0.6883208683,-2.1103992939\H,14.1608325249,0.6696320178,1.944252327\C,5.7329629044,0.0005726711,-0.1005258318\C,2.8976990467,0.0040902812,-0.1040035532\C,5.0091041514,-0.3658209789,-1.2398866318\C,5.0072119048,0.3688188068,1.0370363969\C,3.6214508656,0.3704249641,1.0354085619\C,3.6233353526,-0.3639920173,-1.2416550599\H,5.5354386046,-0.6868156097,-2.1273156572\H,5.5321576412,0.6885244934,1.9257512674\H,3.0951678399,0.6913682198,1.9228934785\H,3.098436934,-0.683619841,-2.1304356018\C,1.4175395909,0.0058646928,-0.1057664184\C,-1.4175905075,0.0092683291,-0.1091020536\C,0.6946323406,0.3724844449,-1.245637571\C,0.6910672318,-0.3590162819,1.0323987892\C,-0.6946827713,-0.3573515944,1.0307691196\C,-0.6911176792,0.3741503024,-1.2472670195\H,1.2216644195,0.6909940069,-2.1335415562\H,1.2152386876,-0.6787883445,1.9215419775\H,-1.221714735,-0.6758615794,1.918672997\H,-1.2152890533,0.6939222404,-2.1364102805\C,-2.8977501528,0.0110399276,-0.1108654648\C,-5.7330144332,0.0145468925,-0.1143430321\C,-3.6233884208,0.379100069,1.0267923188\C,-3.6215012332,-0.3552768424,-1.2502841504\C,-5.0072623394,-0.3536750866,-1.251912075\C,-5.0091572957,0.3809230487,1.0250241274\H,-3.0984917786,0.6987139407,1.9155789173\H,-3.095217626,-0.6762022897,-2.137775153\H,-5.5322067126,-0.673366244,-2.1406330347\H,-5.5354927251,0.70189

91945, 1.9124592967\C, -7.2132222853, 0.0164698657, -0.1162497865\C, -10.04
91127712, 0.0199573117, -0.1201275063\C, -7.940051374, -0.3488944689, 1.021
4598506\C, -7.9360250998, 0.3836154141, -1.2559213788\C, -9.3219227385, 0.3
857085139, -1.2575170133\C, -9.3259418195, -0.3476909452, 1.0192094905\H, -
7.4160841232, -0.6690379624, 1.9106667155\H, -7.4088466138, 0.702406863, -2
.1437108659\H, -9.8460855762, 0.7058547781, -2.1465805227\H, -9.8534715114
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6\C, -14.3658933932, 0.0260094493, -0.1289246888\C, -12.2556127417, 0.39877
23599, 1.0107979552\C, -12.25342012, -0.353097963, -1.2596691375\C, -13.639
8425345, -0.3501805554, -1.2615783417\C, -13.6442755596, 0.3988655941, 1.00
38458392\H, -11.7316614517, 0.7173730071, 1.9008639116\H, -11.7250551046, -
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7345852\H, 16.1887979932, -0.7252954685, 1.9469017165\H, 17.5425158405, -1.
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76472129\H, 17.5473552361, 1.3695550379, 0.0600887668\C, -15.8829858963, 0.
0315322842, -0.1221318709\H, -16.1973493183, 0.3629898137, 0.8700155632\C,
-16.4540117067, 1.0243882092, -1.1423140082\H, -16.1888631676, 0.740381067
1, -2.1617512556\H, -16.075745792, 2.0315010817, -0.9665535402\H, -17.54258
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.3545312213, -0.2749854069\H, -16.0838111544, -2.0742734781, 0.4027323802\
\Version=EM64L-G09RevC.01\HF=-1853.3749705\RMSD=2.945e-09\RMSF=1.480e-
07\Dipole=-0.0000003, -0.0000053, 0.0000006\Quadrupole=31.114752, -31.216
569, 0.1018169, -0.1506732, -0.1891631, 1.7310181\PG=C01 [X(C48H42)]\@

iAPP8

1\1\GINC-HPC-CN48\FOpt\RBLYP\6-31G(d)\C54H46\TALIPOVM\10-Sep-2013\0\#\#
P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent=Dichl
oromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title
\0, 1\C, 10.0529285604, 0.0075243882, -0.0981104367\C, 7.2170542507, 0.0041
730167, -0.1005307851\C, 9.3281209559, 0.484481053, -1.1951101762\C, 9.3273
840366, -0.4711005847, 0.9976741479\C, 7.9414781429, -0.4723685102, 0.99683
64624\C, 7.942240272, 0.4823639943, -1.1967041717\H, 9.8543028612, 0.891185
2262, -2.0468197693\H, 9.8529314893, -0.876379331, 1.8504564954\H, 7.415636
9801, -0.8788201674, 1.8489064858\H, 7.4168953117, 0.8876855187, -2.0496185
423\C, 11.5339270065, 0.0092244472, -0.0970157241\C, 14.3697411278, 0.01338
72492, -0.0919343418\C, 12.2570257387, 0.2717925897, 1.0719189847\C, 12.259
6798815, -0.2509119755, -1.2619781601\C, 13.648331795, -0.2474575082, -1.25
57524013\C, 13.6434592768, 0.2730016401, 1.0728402026\H, 11.7284210627, 0.5
003047532, 1.9865921768\H, 11.7359998591, -0.4811826289, -2.179024996\H, 14
.1805506675, -0.4602399383, -2.1735440837\H, 14.164283789, 0.4884449349, 1.
9958898599\C, 5.7368387747, 0.0027766942, -0.1016848624\C, 2.9015485146, 0.
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6960053271, -0.4767570234, 0.9916536278\C, -0.6897446775, -0.4774504069, 0.
9904923587\C, -0.6883603158, 0.4745845383, -1.2045939735\H, 1.2234996253, 0

.8806464568, -2.0557499811\H, 1.2210928665, -0.8814074952, 1.8449604455\H, -1.2158938559, -0.8825848113, 1.8429223441\H, -1.2134729564, 0.8791617271, -2.0579257716\C, -2.8938521935, -0.0026468397, -0.1090257125\C, -5.7289538135, -0.0041389818, -0.1117473932\C, -3.6197647747, 0.2510357811, 1.059300669\C, -3.6172537577, -0.2571232932, -1.2787346825\C, -5.0029915503, -0.2579191986, -1.280041647\C, -5.0055156558, 0.2503679135, 1.0579502213\H, -3.0951717594, 0.48317038, 1.9749950226\H, -3.0906621076, -0.4887200277, -2.1934157884\H, -5.5275560719, -0.4901713816, -2.1957142587\H, -5.5320857751, 0.4820295442, 1.9726233272\C, -7.2091255741, -0.0049535186, -0.113275408\C, -10.0443753086, -0.0070663387, -0.1166047546\C, -7.934747859, -0.480182312, 0.9839577415\C, -7.9328828805, 0.4693685558, -1.2121335975\C, -9.3186374015, 0.4684289974, -1.2136834259\C, -9.3205173547, -0.4813064443, 0.9822545092\H, -7.4098632978, -0.8837277318, 1.8379312515\H, -7.4065953128, 0.8736963594, -2.0648707882\H, -9.8435916501, 0.8720026667, -2.0675909232\H, -9.8468751105, -0.8856637426, 1.8349286316\C, -11.5245898772, -0.0085586391, -0.11857846\C, -14.3605024421, -0.0117573193, -0.122567335\C, -12.251350612, 0.2459824636, 1.048975745\C, -12.2474821804, -0.2646297677, -1.2881722019\C, -13.6333737292, -0.2666218168, -1.2898574573\C, -13.6372401115, 0.2449613462, 1.0467186698\H, -11.7273438397, 0.4793499662, 1.9647663978\H, -11.7203869444, -0.4967834033, -2.2024934015\H, -14.1575700229, -0.5000659322, -2.2054916909\H, -14.1646889464, 0.477324073, 1.9607615644\C, 15.8868357989, 0.0143744582, -0.1003096002\H, 16.2013677891, -0.2199352015, -1.119725867\C, 16.4632048791, -1.0684910984, 0.8203916715\H, 16.0888805891, -2.0559212457, 0.5500137498\H, 16.1982805466, -0.8838675711, 1.8624797239\H, 17.5518018095, -1.0874445993, 0.7531103342\C, 16.4571788035, 1.3939938008, 0.2521971483\H, 16.1921515819, 1.6832456201, 1.2701990702\H, 16.0782148897, 2.1613464551, -0.4229371494\H, 17.5457285623, 1.3867692899, 0.1818715548\C, -20.1943195387, -0.0255229597, -0.1256894988\C, -20.7709815703, 1.3932375453, -0.2114469421\H, -20.5066044033, 1.871357523, -1.1557820395\H, -20.3963581293, 2.0205874174, 0.5974661648\H, -21.8595400205, 1.3677683338, -0.1456979867\C, -20.7644058515, -0.9167578773, -1.2362144195\H, -20.4984188203, -0.5368131159, -2.2236977672\H, -21.8530150169, -0.9525975515, -1.1764716007\H, -20.3860379726, -1.9359715345, -1.1569261065\C, -15.8414995477, -0.0141190881, -0.1245485174\C, -16.5650485677, 0.4680627152, -1.2210054065\H, -16.0368748289, 0.8713881316, -2.0734406608\C, -17.951464147, 0.4647190894, -1.2231110493\H, -18.4728335855, 0.8531223365, -2.0874195228\C, -18.6772527558, -0.0185487882, -0.131677638\C, -17.9554237152, -0.4978361037, 0.9601734721\H, -18.4872645376, -0.8865382686, 1.8186175291\C, -16.5667601989, -0.4977815273, 0.9670501528\H, -16.0425880457, -0.8998599803, 1.8225234027\H, -20.5087156102, -0.450300548, 0.8302160915\\Version=EM64L-G09RevC.01\HF=-2084.2985171\RMSD=1.002e-09\RMSF=3.016e-07\Dipole=0.0007173, 0.0000417, -0.0000402\Quadrupole=36.183536, -35.67509, -0.508446, 0.1439671, -0.2159302, -3.4734916\PG=C01 [X(C54H46)]\@\

iAPP9

1\1\GINC-HPC-CN47\FOpt\RBLYP\6-31G(d)\C60H50\TALIPOVM\10-Sep-2013\0\#\P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRf(PCM,solvent=Dichloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title \0,1\C,10.0702812426, -0.0403033487, -0.0844328528\C,7.2344844913, -0.0140255212, -0.0881162523\C,9.3482465779, 0.1414166485, -1.2684607653\C,9.3419685856, -0.2079078313, 1.0978198745\C,7.9561276047, -0.194562192, 1.0962552638\C,7.9624268946, 0.1536552883, -1.2705503514\H,9.8768752321, 0.3057582992, -2.1964851587\H,9.8648692941, -0.3818967172, 2.0273319875\H,7.4278290099, -0.3586247418, 2.0245474339\H,7.4396817119, 0.3274147739, -2.2002241913\C,11.5512018853, -0.0555656112, -0.0828970954\C,14.3868380961, -0

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,0.9584963015,1.8011882746\H,11.7421788264,-1.0732939848,-1.9653501477
\H,14.1868568421,-1.0813894229,-1.9638686091\H,14.1923375795,0.9196484
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8,-2.2142214859\H,-9.8261197926,0.3997592301,-2.2154742957\H,-9.828500
0631,-0.2791433836,2.0106395951\C,-11.5066582398,0.0585670159,-0.10353
67099\C,-14.3419085623,0.0529960987,-0.1046219085\C,-12.2298784837,-0.
4920796475,-1.1665586891\C,-12.2328316661,0.606806635,0.9587162989\C,-
13.6186023728,0.6041461957,0.9581150305\C,-13.6156279783,-0.4948615669
, -1.1670244475\H,-11.7030662304,-0.9530636995,-1.9896813484\H,-11.7084
43051,1.0696687328,1.7823382136\H,-14.145533656,1.064931742,1.78127521
07\H,-14.1400872585,-0.9578654287,-1.9905111701\C,15.9037892607,-0.105
8047672,-0.0836219771\H,16.2131069981,-0.5958357669,-1.0094901062\C,16
.4671524312,-0.926847055,1.0830449014\H,16.0801031883,-1.9458178397,1.
0709157186\H,16.2050806355,-0.4806853169,2.0435134492\H,17.5553753701,
-0.9757845167,1.0255904638\C,16.4934437012,1.3101696956,-0.0925828468\
H,16.2346263416,1.8524134237,0.8180097957\H,16.123580879,1.885822926,-
0.9411551023\H,17.5816355058,1.2703679385,-0.1571717948\C,-24.49179409
62,0.0058834654,-0.1128509626\C,-25.0616014225,-0.8110917677,1.0535351
379\H,-24.7984674964,-0.3657436933,2.0140908368\H,-24.6803616213,-1.83
22643007,1.0427199299\H,-26.1499962971,-0.8538561921,0.9944515211\C,-2
5.0732391974,1.4252421389,-0.1236112172\H,-24.8125249092,1.966612716,0
.7869641285\H,-26.1615546324,1.3916994793,-0.1896767153\H,-24.69887807
54,1.9981504555,-0.9720676809\C,-15.8221134828,0.0488272576,-0.1047910
02\C,-16.5473590069,0.2206769477,-1.2882831585\H,-16.0222632904,0.3916
00197,-2.217157352\C,-17.9332269852,0.2162034326,-1.2882517404\H,-18.4
595457579,0.3835989338,-2.2170430938\C,-18.6580153732,0.0384192677,-0.
1053097009\C,-17.9323981555,-0.133389836,1.077996831\H,-18.457649141,-
0.3045434399,2.0067093722\C,-16.5465040574,-0.1278065733,1.0784911697\
H,-16.0205142718,-0.2949176558,2.0075506636\C,-20.1389993125,0.0314927
483,-0.105919207\C,-20.8664774761,0.5845118666,0.953874979\H,-20.34144
93477,1.046486756,1.7779899257\C,-22.2528950035,0.5767557145,0.9534814
238\H,-22.7773108662,1.0213348841,1.7883875062\C,-22.9747586134,0.0182

602332, -0.1041460912\C, -22.2490076113, -0.5315601446, -1.1595521743\H, -2
2.7777117194, -0.9792759302, -1.9907480763\C, -20.8603536022, -0.527459062
3, -1.1636221986\H, -20.3330377102, -0.9849446941, -1.9887614475\H, -24.802
5863811, -0.4829739737, -1.0388465167\\Version=EM64L-G09RevC.01\HF=-2315
.2220809\RMSD=9.094e-09\RMSF=8.133e-07\Dipole=-0.000028, -0.0094802, -0.
0004364\Quadrupole=41.1722581, -39.1169053, -2.0553528, -0.153292, 0.05908
09, 8.1962841\PG=C01 [X(C60H50)]\@\

iAPP10

1\1\GINC-HPC-CN57\Fopt\RBLYP\6-31G(d)\C66H54\TALIPOVM\10-Sep-2013\0\#\#
P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent=Dichl
oromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title
\0,1\C,10.0914162388, -0.0062678877, -0.1153865156\C,7.2555492807, -0.00
27639748, -0.1071777273\C,9.3634877047,0.4049966142, -1.2366516209\C,9.3
689756304, -0.4155841067,1.0101297114\C,7.9830880343, -0.4134425726,1.01
44795447\C,7.9776003978,0.4061693068, -1.2330352649\H,9.8872969442,0.75
79569652, -2.1134244703\H,9.8968284804, -0.769723254,1.8839927709\H,7.45
95931732, -0.7661319227,1.8915773632\H,7.4498990007,0.7601979489, -2.107
0691658\C,11.5724037705, -0.0085669998, -0.1198141146\C,14.4082398529, -0
.0128911415, -0.1250017832\C,12.3006073032,0.321505837,1.0286619382\C,1
2.2930832649, -0.3402583826, -1.269647997\C,13.6817570068, -0.3406902456,
-1.2685566357\C,13.6870261255,0.3183987987,1.0246423285\H,11.776081337
4,0.6061489309,1.9298319398\H,11.7653561462, -0.6235061931, -2.169372051
6\H,14.2099390693, -0.6097027206, -2.1738419103\H,14.2118340337,0.587140
3357,1.9313168502\C,5.7753522288, -0.0010053589, -0.1027841178\C,2.94008
72543,0.0016929359, -0.0940275326\C,5.0466929032, -0.3240082723, -1.25216
17957\C,5.0544103897,0.3235513293,1.051016637\C,3.668662864,0.32480894
,1.0553497821\C,3.6609303679, -0.3226314563, -1.2479288015\H,5.569291114
8, -0.6108605724, -2.1533794843\H,5.5831113233,0.6094094259,1.9489802151
\H,3.1461771326,0.6117056059,1.9566194063\H,3.1323383825, -0.6085331775
, -2.1459474315\C,1.4599277162,0.0027684605, -0.0892997201\C, -1.37511294
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1\C,0.7386257704, -0.404000072,1.0379144012\C, -0.6471055841, -0.40301002
38,1.0424655028\C, -0.6538884542,0.4112509655, -1.2073628558\H,1.2548124
438,0.7616014397, -2.0897724793\H,1.2668172017, -0.755838662,1.912443725
1\H, -1.1701148047, -0.754007056,1.9204556442\H, -1.1821435682,0.76288743
44, -2.0819489133\C, -2.8552557924,0.005371313, -0.0752722516\C, -5.690264
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78216\H, -5.4982399184, -0.6084921243, -2.116365403\H, -5.484113529,0.6213
979897,1.9833464132\C, -7.170419227,0.0069151677, -0.060864446\C, -10.005
4093118,0.0075499778, -0.0513254035\C, -7.891363874, -0.3978161872,1.0672
966288\C, -7.8987510813,0.4119991167, -1.1841430503\C, -9.2844856857,0.41
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248989\H, 16.2397325995, -0.8077342823, 1.8700901871\H, 17.588745278, -1.07
81254028, 0.7694416644\C, 16.50244972, 1.3763298602, 0.135067438\H, 16.2422
055622, 1.722781306, 1.1362756273\H, 16.1243057041, 2.1066662588, -0.580374
1035\H, 17.5907072012, 1.3605409429, 0.0617560098\C, -28.7859167179, 0.0070
148474, 0.0135848061\C, -29.3606073678, 1.4182582266, -0.1622306366\H, -29.
099480352, 1.8330853115, -1.1368894119\H, -28.9814194119, 2.0963620341, 0.6
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-0.9538235734, -1.0336738576\H, -29.1012325397, -0.6394327234, -2.04511934
01\H, -30.450999359, -0.9840073342, -0.9663112518\H, -28.9851558766, -1.966
2994357, -0.8900277586\C, -15.8007693391, 0.0086242813, -0.032172049\C, -16
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035502149\C, -17.9147521318, 0.4120785783, -1.1516940358\H, -18.4431511431
, 0.7603410634, -2.027541463\C, -18.6360121227, 0.0091419827, -0.0230709118
\C, -17.9076799509, -0.3940008077, 1.1009260381\H, -18.4305757723, -0.74204
05589, 1.9801638446\C, -16.5219175645, -0.3941714851, 1.0965396889\H, -15.9
935975953, -0.7424047852, 1.9724548893\C, -20.1162120817, 0.009333302, -0.0
184400328\C, -20.8445951071, -0.3206879199, -1.1658858585\H, -20.321830990
7, -0.6121040696, -2.0656089474\C, -22.2304846214, -0.3207706149, -1.161379
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100179134, -0.0098239817\C, -22.2233452633, 0.3405463224, 1.1373014174\H, -
22.7464504015, 0.6322104293, 2.036721835\C, -20.8374603217, 0.3396791972, 1
.1334349225\H, -20.309088648, 0.6309087615, 2.029937748\C, -24.433093365, 0
.0100377244, -0.0052297698\C, -25.1542236141, -0.4005166356, 1.1185713422\H,
-24.6268822573, -0.7473727656, 1.9959868419\C, -26.5429026739, -0.398322
4207, 1.1178050055\H, -27.0714967421, -0.7295599669, 2.0019717851\C, -27.26
88733819, 0.0106189301, 0.0003829748\C, -26.5472109242, 0.4206772095, -1.12
32762498\H, -27.0717692101, 0.753376992, -2.0086391484\C, -25.1607972039, 0
.42148899, -1.1274568846\H, -24.635827358, 0.7678227709, -2.0065154073\H, -
29.0965908358, -0.3537532764, 0.9966260223\\Version=EM64L-G09RevC.01\HF=
-2546.1456128\RMSD=4.932e-09\RMSF=3.856e-07\Dipole=0.0000658, -0.000344
7, 0.000113\Quadrupole=46.1599742, -45.4724651, -0.6875091, -0.0497042, -0.
3834976, -1.5585332\PG=C01 [X(C66H54)]\@

^{iA}PP_n⁺ (Helical conformer)

iAPP2+*

1\1\GINC-HPC-CN16\Stability\UBLYP\6-31G(d)\C18H22(1+,2)\TALIPOVM\15-Au
g-2013\0\#\#P IOP(3/76=0600004000) BLYP/6-31G(d) stable(opt) scrf(check
) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=
ultrafine)\Title\1,2\C,0,-0.3066888274,1.1006826686,0.2281937783\C,0
,-0.2180832823,3.4298436417,1.8487156708\C,0,-0.9135846753,2.321447535
2,-0.1898544198\C,0,0.3453408713,1.1007785266,1.4949781739\C,0,0.39085
54607,2.2316466665,2.2680405423\C,0,-0.8753305115,3.4390153741,0.59930
76987\H,0,-1.4445364332,2.3675357634,-1.1256340604\H,0,0.844903327,0.2
140484037,1.8465768749\H,0,0.9074724234,2.2075295127,3.2159920673\H,0,
-1.3609517828,4.340387596,0.257621037\C,0,-0.3470599757,-0.0750871627,
-0.590754773\C,0,-0.4116702825,-2.4011836849,-2.2171867163\C,0,-0.7044
289167,-0.009298315,-1.9684430614\C,0,-0.0276899519,-1.3609411006,-0.0
635423959\C,0,-0.0682357578,-2.4802335134,-0.8501234899\C,0,-0.7252668
41,-1.1357433095,-2.7490251977\H,0,-0.9281408738,0.9400324498,-2.42501
6839\H,0,0.2181479914,-1.4710793091,0.9791174262\H,0,0.1644233199,-3.4
38699607,-0.4118122724\H,0,-0.9823402875,-1.0536030657,-3.7945467862\C

,0,-0.4438506517,-3.6303288841,-3.0868265579\H,0,-0.7209294767,-3.3100363047,-4.0915925108\C,0,0.9408811071,-4.2921999053,-3.1682371902\H,0,1.6934162767,-3.5955486064,-3.5354850359\H,0,0.8987379805,-5.1395525051,-3.8517719423\H,0,1.2649432866,-4.6632904199,-2.195941442\C,0,-1.507671175,-4.627466975,-2.6001044006\H,0,-2.4949822979,-4.1688807198,-2.5633273776\H,0,-1.2720029931,-5.0104928889,-1.6072307785\H,0,-1.5508098431,-5.474778358,-3.2836509961\C,0,-0.1649313459,4.6629879954,2.7114924732\H,0,0.3924621756,4.405403098,3.6124869964\C,0,-1.5736376813,5.1045940613,3.1390086606\H,0,-2.0968870374,4.3078781611,3.6661756198\H,0,-2.1778705381,5.4001705171,2.2813693275\H,0,-1.4984125076,5.9625148008,3.806327513\C,0,0.5840420663,5.8035515157,2.0038316315\H,0,1.5922679199,5.5020826542,1.7225044864\H,0,0.6587918934,6.6596956476,2.6734629649\H,0,0.0613178473,6.1276080454,1.1039053012\\Version=EM64L-G09RevC.01\HF=-698.5465936\S2=0.785577\S2-1=0.\S2A=0.750956\RMSD=6.251e-09\Dipole=0.0306306,0.0046364,-0.0108223\Quadrupole=-19.9079462,18.1657081,1.7422381,-2.8471959,5.1716568,17.8968847\PG=C01 [X(C18H22)]\@

iAPP3+*

1\1\GINC-HPC-CN69\Stability\UBLYP\6-31G(d)\C24H26(1+,2)\TALIPOVM\12-Sep-2013\0\#\#P IOP(3/76=0600004000) BLYP/6-31G(d) stable(opt) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title\1,2\H,0,-0.3896047286,0.7511707584,-2.6320123312\C,0,-0.383903936,0.6373588944,-1.5607771409\C,0,-0.4038625398,0.3823072342,1.2092420284\C,0,-0.4235448923,-0.6622807781,-0.9864809894\C,0,-0.3773009353,1.7606729542,-0.7844049633\C,0,-0.3800718834,1.6824779334,0.6349758375\C,0,-0.4388610083,-0.7403271791,0.4327048524\H,0,-0.3410376775,2.7220562904,-1.2693822078\H,0,-0.4490197028,-1.7025224916,0.9173535295\H,0,-0.4247914327,0.268703619,2.2802823146\C,0,-0.3607059356,2.870421243,1.4565447078\C,0,-0.3227160125,5.2038549933,3.0674267324\C,0,-0.7359383604,4.1314647184,0.9349178126\C,0,0.0337371478,2.8203851164,2.8130841959\C,0,0.0579191368,3.9596164578,3.5875734859\C,0,-0.7238680103,5.2593075613,1.7224142366\H,0,-1.0748597127,4.2160055058,-0.084803328\H,0,0.3586554076,1.8904056915,3.2508330387\H,0,0.3811020493,3.8930036575,4.6163337095\H,0,-1.0339781465,6.2003045273,1.2927736243\C,0,-0.4481042324,-1.8502352344,-1.8078521339\C,0,-0.4950345898,-4.183968048,-3.4175175868\C,0,-0.0310020756,-1.8196430972,-3.1580793338\C,0,-0.8907199477,-3.0914812397,-1.2918634057\C,0,-0.919948731,-4.2191659958,-2.0791675384\C,0,-0.0481334701,-2.959545421,-3.931913145\H,0,0.344330922,-0.9061430134,-3.5903473435\H,0,-1.2489506331,-3.15902808,-0.2774264629\H,0,-1.2813027726,-5.144026208,-1.654649152\H,0,0.2941181287,-2.9091178259,-4.9554219639\C,0,-0.5151355921,-5.4236851484,-4.2810017614\H,0,-0.1443788864,-5.1369013687,-5.2661709082\C,0,0.4208879035,-6.5074058098,-3.7266949949\H,0,1.4410960705,-6.1375863363,-3.6285644284\H,0,0.4331609204,-7.3653686583,-4.3987227538\H,0,0.0911900966,-6.8556861024,-2.7474463159\C,0,-1.9422124097,-5.9621231375,-4.4572881103\H,0,-2.6031998472,-5.2036386813,-4.8756390751\H,0,-2.3637261339,-6.2923803337,-3.5074576733\H,0,-1.9344951135,-6.8169813464,-5.1333503545\C,0,-0.2982805821,6.4426327579,3.9320853865\H,0,0.0400628606,6.1375259259,4.9234059309\C,0,-1.7003049038,7.050052695,4.0834554463\H,0,-2.4045888537,6.3250360231,4.4903422261\H,0,-2.0889028956,7.3996625528,3.1265659023\H,0,-1.6626571223,7.9040900663,4.7595433538\C,0,0.6995883197,7.4794775139,3.3963066108\H,0,1.7020047603,7.0600165544,3.3161298056\H,0,0.741740116,8.3354109136,4.0697243253\H,0,0.4050298677,7.8439593759,2.4117663083\\Version=EM64L-G09RevC.01\HF=-929.4756554\S2=0.786967\S2-1=0.\S2A=0.751123\RMSD=6.675e-09\Dipole=0.0750238,0.0053864,0.0045022\Quadrupole=

-34.6490474,30.2462894,4.4027581,0.5138392,0.7122132,30.9859986\PG=C01
[X(C24H26)]\ \@

iAPP4+*

1\1\GINC-HPC-CN26\Stability\UBLYP\6-31G(d)\C30H30(1+,2)\TALIPOVM\15-Aug-2013\0\#\#P IOP(3/76=0600004000) BLYP/6-31G(d) stable(opt) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title\1,2\H,0,1.5136217022,-1.2643880841,-2.8598663791\C,0,0.7399595445,-1.1062420664,-2.1259235294\C,0,-1.2210976893,-0.6846674062,-0.2032061715\C,0,-0.2498270172,-2.0965967698,-1.9239239002\C,0,0.7629031323,0.042953823,-1.3817547203\C,0,-0.2213635994,0.3044295458,-0.3934108502\C,0,-1.2255882821,-1.8444095312,-0.9312331346\H,0,1.5342820483,0.7684201027,-1.5808237073\H,0,-2.0099826913,-2.563087456,-0.75683439\H,0,-1.9826971209,-0.5461602686,0.5462938607\C,0,-0.2056011396,1.5179190752,0.382853136\C,0,-0.1723032455,3.9116645181,1.9242337851\C,0,-1.3565901002,1.9667648077,1.0809402297\C,0,0.96203246,2.3177807046,0.4855772023\C,0,0.9797757256,3.461946488,1.2377108646\C,0,-1.3423907971,3.1249481226,1.8114328224\H,0,-2.2762431729,1.4087699506,1.0206556712\H,0,1.8694501108,2.01486591,-0.0102407668\H,0,1.8879282614,4.0413852881,1.2795879784\H,0,-2.2388421285,3.4207524315,2.3322046319\C,0,-0.1539111299,5.1349009922,2.716166452\C,0,-0.1195833495,7.5102803849,4.2598172673\C,0,-1.3345322936,5.8610999171,2.9647819918\C,0,1.0432696467,5.6317939053,3.2613115687\C,0,1.0523471296,6.7871135389,4.020113855\C,0,-1.3124646704,7.022081016,3.7106127807\H,0,-2.2703966053,5.5337954724,2.5388062069\H,0,1.9673038312,5.0918061951,3.1233158842\H,0,1.9852196725,7.1353253053,4.4406684829\H,0,-2.2361510632,7.5609305768,3.8645784687\C,0,-0.2639973946,-3.3258172904,-2.7062876221\C,0,-0.2944573558,-5.7156682601,-4.2277748289\C,0,0.3273622089,-3.3855006962,-3.9807608345\C,0,-0.8710554912,-4.4972636585,-2.2137143966\C,0,-0.8769469785,-5.6614250447,-2.9547043577\C,0,0.3023882447,-4.5521210543,-4.7216365137\H,0,0.7774314879,-2.504484102,-4.4114335549\H,0,-1.308430845,-4.5061076544,-1.2273282021\H,0,-1.3370449517,-6.5444859304,-2.5356759677\H,0,0.7502669627,-4.5625862854,-5.705307414\C,0,-0.3052944596,-6.9884523825,-5.0467552873\H,0,0.1989786348,-6.7685522162,-5.9893725424\C,0,0.4765742343,-8.1114294661,-4.3517319581\H,0,1.5022402933,-7.8085265807,-4.1423384952\H,0,0.5064050172,-8.9964039381,-4.9876765832\H,0,0.0092181117,-8.3952638629,-3.4080761554\C,0,-1.7356779573,-7.4354021677,-5.377516198\H,0,-2.2852307473,-6.6509552919,-5.8973507322\H,0,-2.2900596126,-7.6943583459,-4.4746855481\H,0,-1.7137392016,-8.3170708594,-6.0183791381\C,0,-0.091298814,8.7783661361,5.0856658073\H,0,0.9427410435,8.9354937816,5.3975480835\C,0,-0.9442931787,8.6452508795,6.3544558906\H,0,-0.6232913171,7.7977174805,6.9596540124\H,0,-1.9986196353,8.5067175571,6.1123398299\H,0,-0.8581158992,9.54758249,6.9601745892\C,0,-0.5180452486,9.9988085669,4.2586939511\H,0,0.1067536993,10.1147889925,3.3733825121\H,0,-0.431491886,10.905948539,4.8571621088\H,0,-1.5547761332,9.9139741748,3.9309739541\Version=EM64L-G09RevC.01\HF=-1160.4011569\S2=0.7855\S2-1=0.\S2A=0.751069\RMSD=1.868e-09\Dipole=0.133993,0.0138746,-0.0778652\Quadrupole=-31.6728671,41.4412884,-9.7684213,4.0581258,-5.521138,52.4589082\PG=C01 [X(C30H30)]\ \@

iAPP5+*

1\1\GINC-HPC-CN60\Stability\UBLYP\6-31G(d)\C36H34(1+,2)\TALIPOVM\12-Sep-2013\0\#\#P IOP(3/76=0600004000) BLYP/6-31G(d) stable(opt) scrf(check)

```
) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=
ultrafine)\Title\1,2\H,0,0.874569916,0.2714328986,-2.606227814\C,0,0
.3785041785,0.2812455361,-1.64971115\C,0,-0.8599923675,0.3435822519,0.
836462867\C,0,-0.2472238276,-0.8949486781,-1.1638771566\C,0,0.40357213
11,1.4340750362,-0.9130923838\C,0,-0.2192080973,1.5139515359,0.3578120
325\C,0,-0.8617800983,-0.8170529073,0.1117681929\H,0,0.8853148013,2.30
27220121,-1.3313470035\H,0,-1.3679555569,-1.6767687513,0.5189653209\H,
0,-1.332700501,0.3472411455,1.8049615293\C,0,-0.2559832386,-2.11943993
11,-1.9339068524\C,0,-0.2640104734,-4.5278084439,-3.4450040983\C,0,-0.
023019123,-2.1159346294,-3.3286143108\C,0,-0.4953257743,-3.3723200019,
-1.3236603706\C,0,-0.4887787442,-4.5359245761,-2.0541061175\C,0,-0.037
2566959,-3.2798059989,-4.0585197062\H,0,0.1445762572,-1.1859873585,-3.
8473324613\H,0,-0.6601173015,-3.4340270885,-0.2601881083\H,0,-0.684786
3202,-5.4688616305,-1.5493818417\H,0,0.1556374989,-3.2319411044,-5.118
7608045\C,0,-0.1998323649,2.7359933842,1.1332337017\C,0,-0.159833237,5
.1348092827,2.655604843\C,0,-1.1491184361,2.9772487432,2.1516801796\C,
0,0.7705970482,3.7372176098,0.9039681791\C,0,0.7942554246,4.892487856,
1.6484660881\C,0,-1.1342482113,4.143101216,2.8798332816\H,0,-1.9228834
332,2.2538360018,2.3527344612\H,0,1.530777562,3.5917787482,0.153339527
\H,0,1.5470702674,5.6351467024,1.4349783584\H,0,-1.8718744609,4.283668
9731,3.6544093063\C,0,-0.1389767658,6.3732656783,3.44203602\C,0,-0.100
1821189,8.7633089694,4.9618126888\C,0,-1.3195738451,6.9149898104,3.974
6886635\C,0,1.0600774079,7.0561659396,3.6881923334\C,0,1.0741765637,8.
2215948933,4.4364987611\C,0,-1.2979564629,8.0850394927,4.7114605954\H,
0,-2.2675622496,6.4348027671,3.7828578167\H,0,1.9944365984,6.657702971
4,3.3218837454\H,0,2.016651365,8.7181446322,4.6217172376\H,0,-2.229603
9339,8.4785468339,5.0925760151\C,0,-0.2653326119,-5.7702043599,-4.2232
824285\C,0,-0.2688150374,-8.1725157115,-5.7240974169\C,0,-0.631132637,
-5.7789078027,-5.5768422516\C,0,0.0996261597,-6.9936204464,-3.63813697
14\C,0,0.1024458712,-8.1634444966,-4.3750074971\C,0,-0.6366843592,-6.9
571759581,-6.3043778019\H,0,-0.9465451816,-4.8652662011,-6.0580384874\
H,0,0.4166393049,-7.0247242717,-2.6064400599\H,0,0.403896583,-9.082584
9562,-3.8930650763\H,0,-0.9378905162,-6.9346215808,-7.3425841037\C,0,-
0.2754190979,-9.4525128573,-6.5345373162\H,0,-0.5938573286,-9.19051320
19,-7.5453579367\C,0,1.1268057158,-10.0670835164,-6.6351489243\H,0,1.8
38945389,-9.3594190253,-7.0593243238\H,0,1.1059408697,-10.9516000921,-
7.2724402112\H,0,1.4980177856,-10.3719019755,-5.6558950854\C,0,-1.2833
535772,-10.4675276594,-5.9794892354\H,0,-2.2874455143,-10.0455813544,-
5.9393191719\H,0,-1.0117322579,-10.7860340145,-4.972262899\H,0,-1.3125
558684,-11.3550164294,-6.6123113636\C,0,-0.0691374567,10.0419699957,5.
7741238996\H,0,0.9725515407,10.3649554473,5.824112471\C,0,-0.552396687
7,9.8111081181,7.2118672948\H,0,0.035787417,9.0386987353,7.7071558111\
H,0,-1.5985992076,9.5033049988,7.2339989023\H,0,-0.4641628835,10.73009
27401,7.7921086151\C,0,-0.8696873341,11.1624039683,5.0975034389\H,0,-0
.5082987502,11.3514532244,4.0867875443\H,0,-0.7814711608,12.0871617166
,5.668525161\H,0,-1.9291025496,10.9105871448,5.0343938581\Version=EM6
4L-G09RevC.01\HF=-1391.3253373\S2=0.783642\S2-1=0.\S2A=0.750972\RMSD=1
.632e-09\Dipole=0.035308,-0.1502696,-0.2061695\Quadrupole=-50.8976406,
54.8412916,-3.943651,4.416872,-4.8819211,61.9940024\PG=C01 [X(C36H34)]
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iAPP6+*

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1\1\GINC-HPC-CN28\Stability\UBLYP\6-31G(d)\C42H38(1+,2)\TALIPOVM\15-Au
g-2013\0\#P IOP(3/76=0600004000) BLYP/6-31G(d) stable(opt) scrf(check
) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=
```

ultrafine)\Title\1,2\H,0,-0.2675122534,1.4187984616,-2.1838107731\C,
0,-0.2592487211,1.363846247,-1.1076239943\C,0,-0.2061390447,1.28156004
44,1.6671460289\C,0,-0.2409326677,0.1038450084,-0.4601451701\C,0,-0.23
24970296,2.534457942,-0.3947878927\C,0,-0.2104777549,2.536692418,1.018
0709106\C,0,-0.2083827544,0.1094942461,0.956265152\H,0,-0.2575472923,3
.469119743,-0.9317447674\H,0,-0.2107354843,-0.8204151383,1.500719608\H
,0,-0.1700402707,1.2347148465,2.7437783082\C,0,-0.2517063348,-1.130917
4141,-1.2101563088\C,0,-0.2601963159,-3.5640081532,-2.6902681461\C,0,-
0.6593323872,-1.1713902622,-2.5668504996\C,0,0.1481445555,-2.357025466
7,-0.6227866912\C,0,0.1553778092,-3.5248239895,-1.3393298099\C,0,-0.67
43431834,-2.3447258771,-3.2744758536\H,0,-0.9913437697,-0.2717386618,-
3.0582674882\H,0,0.4822570519,-2.3815913781,0.4012658527\H,0,0.4597337
189,-4.4332807814,-0.8450547803\H,0,-0.981873787,-2.3221238892,-4.3075
512937\C,0,-0.1920472578,3.7822372393,1.7741571902\C,0,-0.1562630285,6
.2079200049,3.2450066\C,0,-0.6800820509,3.8443439279,3.0928512451\C,0,
0.3150557551,4.9694452866,1.2133616587\C,0,0.33898646,6.1455460157,1.9
327080335\C,0,-0.669507165,5.026230099,3.8031039906\H,0,-1.0978670519,
2.964669834,3.5572723877\H,0,0.7199301086,4.965432657,0.2132780537\H,0
,0.7275125845,7.0373448416,1.4649649144\H,0,-1.0450950128,5.0320504064
,4.8150126747\C,0,-0.1382104402,7.4678104519,4.0084582189\C,0,-0.10560
44311,9.8896139762,5.4773836313\C,0,-1.1376737069,7.760478578,4.946441
1138\C,0,0.8766713035,8.4128774259,3.8220198626\C,0,0.8903872374,9.595
4254529,4.5460997154\C,0,-1.1214608624,8.946626479,5.6602465833\H,0,-1
.9522166099,7.0671744474,5.0977522034\H,0,1.6796544504,8.2117421435,3.
1279182413\H,0,1.6949927283,10.3008517368,4.3887222936\H,0,-1.91709748
27,9.1418344065,6.3656116007\C,0,-0.2593938016,-4.8068136136,-3.447594
4553\C,0,-0.251756657,-7.2292828393,-4.9264859962\C,0,-1.0933697523,-4
.982277311,-4.5689970759\C,0,0.5773023458,-5.8813036302,-3.0879719733\
C,0,0.5854509963,-7.0536305965,-3.8122136822\C,0,-1.0942289547,-6.1624
409927,-5.2807768973\H,0,-1.7681880994,-4.1962120031,-4.8698863392\H,0
,1.2486655185,-5.7870154772,-2.2488730255\H,0,1.2347998546,-7.85688322
06,-3.4992769458\H,0,-1.7418316613,-6.2544888778,-6.1392357817\C,0,-0.
2451900337,-8.4853552951,-5.6945930468\C,0,-0.2332278245,-10.902664978
9,-7.1715952801\C,0,0.9195430428,-9.2515329532,-5.8189202843\C,0,-1.40
50298046,-8.9550408992,-6.3267575721\C,0,-1.3973123284,-10.1385882947,
-7.0445538796\C,0,0.9213866406,-10.431989269,-6.5459161161\H,0,1.84064
17014,-8.9096601655,-5.3701082141\H,0,-2.3299434175,-8.4053614485,-6.2
309571046\H,0,-2.3150755416,-10.4739804912,-7.5069946972\H,0,1.8401924
586,-10.9956253919,-6.6339898775\C,0,-0.2170270761,-12.1981744929,-7.9
585996968\H,0,0.8001201057,-12.5918992347,-7.9068892769\C,0,-1.1510676
458,-13.2474647659,-7.3420210527\H,0,-0.8948655263,-13.4406071487,-6.3
003431083\H,0,-1.0790726575,-14.1877163502,-7.8897533999\H,0,-2.191400
2497,-12.9212917684,-7.3769265145\C,0,-0.54924049,-11.9676970766,-9.43
83822062\H,0,0.1340618083,-11.2478682642,-9.8888908727\H,0,-1.56493239
45,-11.5897106005,-9.5624014009\H,0,-0.472721334,-12.9028516145,-9.994
1623581\C,0,-0.0792545576,11.1883334576,6.2591125409\H,0,0.8060368025,
11.7394960451,5.9353474797\C,0,0.0560892371,10.9404538437,7.7669260533
\H,0,0.9449235106,10.3510228488,7.9918304067\H,0,-0.8096839659,10.4056
285725,8.1597738197\H,0,0.1320669776,11.8877716011,8.3018471336\C,0,-1
.3041362146,12.0597266807,5.9530143845\H,0,-1.3843105179,12.2671471518
,4.8859636646\H,0,-1.2336143627,13.0118689282,6.4800531954\H,0,-2.2266
857437,11.5718265803,6.270466849\Version=EM64L-G09RevC.01\HF=-1622.24
89688\S2=0.782033\S2-1=0.\S2A=0.750892\RMSD=2.126e-09\Dipole=0.0931025
, -0.2890304, -0.1945413\Quadrupole=-62.6645005,68.3915795,-5.727079,0.3
829021,2.9424018,75.4410153\PG=C01 [X(C42H38)]\@

iAPP7+*

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1\1\GINC-HPC-CN1\Stability\UBLYP\6-31G(d)\C48H42(1+,2)\TALIPOVM\15-Aug
-2013\0\#\#P IOP(3/76=0600004000) BLYP/6-31G(d) stable(opt) scrf(check)
guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)
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iAPP8+*

1\1\GINC-HPC-CN41\Stability\UBLYP\6-31G(d)\C54H46(1+,2)\TALIPOVM\02-Sep-2013\0\#\P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title\1,2\C,0,10.0143637957,0.0710866329,-0.0904777264\C,0,7.1771316203,0.0564799559,-0.0991901112\C,0,9.2850936332,0.8975371173,-0.9601551342\C,0,9.2883308406,-0.7626785967,0.774880192\C,0,7.9094322946,-0.7769617583,0.7665446712\C,0,7.9061024675,0.8975794315,-0.9603743777\H,0,9.808437842,1.5631604677,-1.6295646759\H,0,9.8142185143,-1.4228393898,1.4476802049\H,0,7.3935273316,-1.4231237099,1.459646991\H,0,7.3878665721,1.538543027,-1.6565654152\C,0,11.4877120421,0.0782111943,-0.08631017\C,0,14.3205765203,0.0893472914,-0.0762986814\C,0,12.2098553643,-0.1625657432,1.0905579413\C,0,12.2140682674,0.3247428841,-1.2566249911\C,0,13.6007281668,0.3256465438,-1.2475468372\C,0,13.5942653633,-0.1529726,1.0934483583\H,0,11.6837087135,-0.3299806808,2.0190539036\H,0,11.6941805283,0.4880836429,-2.1893558993\H,0,14.1342112703,0.5072233556,-2.1707086862\H,0,14.1151457281,-0.3307700992,2.0238761392\C,0,5.7193294869,0.0488001022,-0.1034201891\C,0,2.874339808,0.0338058973,-0.1104996793\C,0,4.9794438179,1.1734646266,-0.5317873528\C,0,4.9891944266,-1.083723766,0.3209564345\C,0,3.6180728559,-1.0966774527,0.3059645976\C,0,3.6081856335,1.1719949792,-0.5235913259\H,0,5.4953675568,2.0664363331,-0.8466068006\H,0,5.5129861942,-1.971242269,0.6382130776\H,0,3.1072201054,-1.9818368236,0.648286555\H,0,3.0898066033,2.0518217683,-0.8684107786\C,0,1.4289408676,0.026376412,-0.1134059461\C,0,-1.416704708,0.0123006264,-0.1178206617\C,0,0.6837386049,1.2309494256,-0.1112012944\C,0,0.6957160722,-1.1855551576,-0.1181826954\C,0,-0.6748002546,-1.1910412953,-0.1339526459\C,0,-0.6867743338,1.2228948881,-0.0997020527\H,0,1.1934056326,2.1803909878,-0.0885165117\H,0,1.2147293962,-2.1299753181,-0.1392753448\H,0,-1.1893203347,-2.138498223,-0.1287032741\H,0,-1.2105814674,2.1652107259,-0.1065944145\C,0,-2.8722315922,0.0052444069,-0.119532969\C,0,-5.7094451944,-0.0085170574,-0.1220394871\C,0,-3.5980617513,-1.0853399585,-0.6371054977\C,0,-3.6095350181,1.0888066403,0.3965765286\C,0,-4.9873480779,1.0761368244,0.4034210268\C,0,-4.9759526196,-1.0860437112,-0.6464045909\H,0,-3.0769678299,-1.9287653946,-1.0624180157\H,0,-3.0974379718,1.9372310955,0.8228696877\H,0,-5.5160125606,1.9290494726,0.8007367543\H,0,-5.4955769504,-1.9440754445,-1.0446599566\C,0,-7.1802299007,-0.0155826057,-0.1229496082\C,0,-10.0133785452,-0.0288678972,-0.1245556785\C,0,-7.9016350802,-0.6654590509,-1.1335156957\C,0,-7.9088591191,0.6274852937,0.8868050418\C,0,-9.2920164205,0.6164545835,0.887575819\C,0,-9.2848558403,-0.6673826642,-1.135879716\H,0,-7.3766152802,-1.1565800695,-1.9393406091\H,0,-7.389406851,1.1234961478,1.693243312\H,0,-9.8204312218,1.1315590493,1.6761308047\H,0,-9.8074962461,-1.1873831546,-1.9250696136\C,0,-11.4912144179,-0.0357837007,-0.1252247974\C,0,-14.325412607,-0.0490613881,-0.1262908726\C,0,-12.2151181582,0.

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431\C, 0, -17.9214614019, 0.6800621324, -1.0542720948\H, 0, -18.4551529892, 1
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.0661875, -4.3569751\PG=C01 [X(C54H46)]\@

iAPP9+*

1\1\GINC-HPC-CN35\Stability\UBLYP\6-31G(d)\C60H50(1+,2)\TALIPOVM\02-Sep-2013\0\#\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title\1,2\C, 0, 10.0307795079, 0.0688135895, -0.0843141247\C, 0, 7.1922561437, 0.0635635206, -0.092754499\C, 0, 9.3030612196, 0.9754018853, -0.8730623232\C, 0, 9.3017574511, -0.8403217588, 0.7002448037\C, 0, 7.9237802353, -0.849867275, 0.691227598\C, 0, 7.9250280847, 0.9798223778, -0.8723245465\H, 0, 9.8277749278, 1.6996258702, -1.4771595219\H, 0, 9.8254057014, -1.5625327148, 1.3076424969\H, 0, 7.4074765673, -1.5570583412, 1.3212230932\H, 0, 7.4098866344, 1.6852587789, -1.5052482686\C, 0, 11.502868582, 0.0711042282, -0.0802612096\C, 0, 14.3356914238, 0.072856184, -0.0706778836\C, 0, 12.2248373808, -0.2946782383, 1.0645848678\C, 0, 12.2299407053, 0.4375581943, -1.2188359492\C, 0, 13.6162765722, 0.4331072798, -1.210447215\C, 0, 13.6089520518, -0.2891983979, 1.0677040514\H, 0, 11.6989089136, -0.5570067897, 1.9708824014\H, 0, 11.710820121, 0.6993157474, -2.1292053572\H, 0, 14.1500930444, 0.7090473664, -2.1096696058\H, 0, 14.1293963428, -0.5656617469, 1.9739158955\C, 0, 5.7367591992, 0.0606348749, -0.0969167955\C, 0, 2.8901842219, 0.0548050211, -0.104062083\C, 0, 4.9987107813, 1.2146573175, -0.4473825901\C, 0, 5.0016760599, -1.0964930179, 0.2495359847\C, 0, 3.6313647182, -1.1040865499, 0.2340092397\C, 0, 3.6282895124, 1.216653653, -0.4387250591\H, 0, 5.5161168071, 2.1258252446, -0.7010526699\H, 0, 5.5215374829, -2.0055714015, 0.5056584301\H, 0, 3.1183679015, -2.009439611, 0.5146664801\H, 0, 3.1130178057, 2.1199051644, -0.7220068099\C, 0, 1.4449500564, 0.0518388254, -0.1070878851\C, 0, -1.4001734558, 0.0458307396, -0.1116584407\C, 0, 0.7032178596, 1.2556666246, -0.0312725423\C, 0, 0.7085391206, -1.1550838164, -0.1856258965\C, 0, -0.6626146263,

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1204,-0.8218005351,0.7532137875\H,0,-15.9848641491,-1.4798108615,1.428
336991\C,0,-17.8987193213,-0.8265153845,0.7535792768\H,0,-18.422128729
9,-1.4657283746,1.4500125088\C,0,-18.6269978843,-0.0081144328,-0.11591
98037\C,0,-17.9053052768,0.815781369,-0.9857157839\H,0,-18.4339926751,
1.4507079479,-1.6820815517\C,0,-16.5195262588,0.8219474493,-0.98561851
69\H,0,-15.9967651284,1.4839708687,-1.660957065\C,0,-20.1079784291,-0.
0134667709,-0.1153506422\C,0,-20.8276754727,-1.1948556871,0.0958306339
\H,0,-20.2966747263,-2.1254823017,0.2380753712\C,0,-22.2140601501,-1.1
994734371,0.0969764263\H,0,-22.7325564579,-2.1351762529,0.25590471\C,0
, -22.9434597086,-0.0266055003,-0.1126790435\C,0,-22.2252999328,1.14931
56641,-0.3233598051\H,0,-22.7600975363,2.0766488529,-0.4809878944\C,0,
-20.8366940199,1.1597699008,-0.3251635049\H,0,-20.315603297,2.09581772
71,-0.4684204668\H,0,-24.7780757031,1.0060963936,-0.2956016285\\Versio
n=EM64L-G09RevC.01\HF=-2315.0192409\S2=0.780827\S2-1=0.\S2A=0.750831\R
MSD=4.986e-09\Dipole=12.1419754,0.1033046,-0.050052\Quadrupole=152.442
5059,-71.977692,-80.4648139,0.7567419,-0.3153461,-5.6054697\PG=C01 [X(
C60H50)]\@

iAPP10+*

1\1\GINC-HPC-CN43\Stability\UBLYP\6-31G(d)\C66H54(1+,2)\TALIPOVM\02-Sep-2013\0\#\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title\1,2\C,0,10.0493875284,0.0559848107,-0.1014548271\C,0,7.210547539,0.0544837131,-0.1019371695\C,0,9.320440731,0.9701689499,-0.8808433839\C,0,9.3211503602,-0.8588916715,0.6777488419\C,0,7.9434985078,-0.8668318783,0.6723037146\C,0,7.9427903495,0.9766073413,-0.875945255\H,0,9.8443651466,1.6987198993,-1.480314873\H,0,9.8454964182,-1.5868267546,1.2775774086\H,0,7.4283435403,-1.5788733836,1.2976548529\H,0,7.4270647371,1.6881794106,-1.5013686595\C,0,11.520973195,0.0564851948,-0.1014200912\C,0,14.3537235963,0.0548898849,-0.0995732319\C,0,12.2456949496,-0.3235302709,1.0372477088\C,0,12.2454490801,0.4354659101,-1.2377734866\C,0,13.6316693182,0.4290639341,-1.2332661293\C,0,13.6296889013,-0.3193759655,1.0366783588\H,0,11.722067255,-0.5957260994,1.9419301244\H,0,11.7243049743,0.7083451962,-2.1436776077\H,0,14.1634052349,0.7145972628,-2.1306979659\H,0,14.1523449448,-0.6066158249,1.9382265619\C,0,5.7559275212,0.0537192345,-0.1018997387\C,0,2.9091442163,0.0523265034,-0.1006509716\C,0,5.0182522726,1.2100963779,-0.4471006531\C,0,5.0196674975,-1.1034725105,0.2435891944\C,0,3.6495717686,-1.1088905338,0.2317907813\C,0,3.6481431089,1.2141802389,-0.4340580888\H,0,5.5360745515,2.121210209,-0.6999018487\H,0,5.5385930002,-2.0141056489,0.4958339677\H,0,3.1357783537,-2.0141507804,0.5112813778\H,0,3.133188709,2.1189282488,-0.7130856527\C,0,1.4638858756,0.0516898351,-0.0993145581\C,0,-1.3807461134,0.050271558,-0.0949259673\C,0,0.7246326134,1.2561778033,-0.0145478403\C,0,0.7255684798,-1.1534985553,-0.1822485678\C,0,-0.645914933,-1.1517707935,-0.192831301\C,0,-0.6468221498,1.2530811507,0.0003047773\H,0,1.2382364729,2.1999912551,0.0694831761\H,0,1.2398413346,-2.0967966904,-0.2679167977\H,0,-1.1658640106,-2.0948487776,-0.2482932014\H,0,-1.1675318613,2.1956363237,0.0574530897\C,0,-2.8393970024,0.0493442368,-0.0918454243\C,0,-5.6752736055,0.0466330271,-0.0842804143\C,0,-3.5699202897,-0.9871189839,-0.7012639312\C,0,-3.5686314913,1.0846306997,0.5211052909\C,0,-4.9477732068,1.0772715826,0.5313631807\C,0,-4.9491064115,-0.9824024935,-0.7041635038\H,0,-3.0528953298,-1.7908807266,-1.202180597\H,0,-3.0504947863,1.8894274875,1.0192003988\H,0,-5.471929646,1.8933538362,1.005054315\H,0,-5.4742058042,-1.7994819019,-1.1750791547\C,0,-7.1480544849,0.0448332946,-0.0796777663\C,0,-9.980965594,0.0408575937,-0.0702796043\C,0,-7.8753835688,-0.4975806991,-1.146841903\C,0,-7.8698166046,0.5852735102,0.9922596159\C,0,-9.2535503126,0.5797189382,0.9976039483\C,0,-9.2591407481,-0.4959048809,-1.143008897\H,0,-7.3548627202,-0.9072169066,-1.999916991\H,0,-7.3447741731,0.9963408198,1.8418621582\H,0,-9.7770093143,1.0157963682,1.8356691396\H,0,-9.7868965067,-0.9334838804,-1.9775920745\C,0,-11.4594595088,0.0386579523,-0.0652448575\C,0,-14.2929948222,0.0343700694,-0.0554789014\C,0,-12.1877367674,0.2173373167,-1.2462940238\C,0,-12.1790489728,-0.1422074233,1.1207916556\C,0,-13.5643205841,-0.1452659477,1.1250613954\C,0,-13.573008408,0.2161825534,-1.2410042382\H,0,-11.666424931,0.3758730577,-2.1792645159\H,0,-11.6508184518,-0.2990820172,2.0501445891\H,0,-14.0867627873,-0.273655752,2.0619931141\H,0,-14.102296338,0.3429814596,-2.174298407\C,0,15.8694934876,0.0572886536,-0.108662907\H,0,16.1833262825,0.3822344249,-1.1026938898\C,0,16.4405815016,-1.347988091,0.1206049828\H,0,16.0636036085,-2.0530657773,-0.6201798148\H,0,16.1772599494,-1.7264904518,1.1091814693\H,0,17.5287190294,-1.330803921,0.0505746932\C,0,16.4412696312,1.0557467708,0.9061302383\H,0,16.1788684253,0.7771738874,1.9275989987\H,0,16.0641029188,2.0622443287,0.7252704475\H,0,17.5293461741,1.0832962521,0.8385096968\C,0,-28.7568822196,0.0225329809,-0.003462617\C,0,-29.3334791882,0.0552810605,-1.4245241456\H,0,-29.0697394579,-0.8463212472,-1.979299518\H,0,-28.9579949231,0.9131331534,-1.982516206\H,0,-30.421964703

1,0.1197320379,-1.3937531751\C,0,-29.3290543487,-1.1565492376,0.793277406\H,0,-29.0649988103,-2.1100811006,0.3336473649\H,0,-30.4175330526,-1.0978762082,0.8337283957\H,0,-28.9508793686,-1.1619418579,1.8156340857\C,0,-15.7729460241,0.0322243141,-0.0504029547\C,0,-16.4929817186,-0.8153718197,0.7976502299\H,0,-15.9642019225,-1.4934927566,1.4519529553\C,0,-17.8786852903,-0.8171723378,0.8023688771\H,0,-18.4012875491,-1.4748890407,1.481918493\C,0,-18.607324898,0.0282133454,-0.0406622984\C,0,-17.8868816374,0.8756297181,-0.8886817216\H,0,-18.4160076862,1.5318576055,-1.5646046787\C,0,-16.5011838372,0.8777642973,-0.8934934096\H,0,-15.9788455344,1.5574022265,-1.551391384\C,0,-20.0876855121,0.0261969681,-0.0355568293\C,0,-20.8099561091,-1.1579594878,0.1431083132\H,0,-20.2825874111,-2.0932489818,0.2650010294\C,0,-22.1958723475,-1.159478926,0.1485038834\H,0,-22.72013876,-2.0914211102,0.3044092497\C,0,-22.9230586689,0.0223760144,-0.0259390949\C,0,-22.200235455,1.2061505696,-0.2054579695\H,0,-22.728223959,2.1365468215,-0.3579775931\C,0,-20.8143491165,1.208413278,-0.2093560348\H,0,-20.2903470889,2.1451107509,-0.334919074\C,0,-24.4041516537,0.0206792639,-0.0205818254\C,0,-25.1276817075,1.073812241,0.5441281739\H,0,-24.602197123,1.896739941,1.0076752028\C,0,-26.5163377636,1.0676118508,0.5463583133\H,0,-27.0468684577,1.8949853444,0.998944377\C,0,-27.2398150787,0.0150255519,-0.0118163647\C,0,-26.5156560469,-1.0378781113,-0.5762355273\H,0,-27.0382480576,-1.8703525639,-1.0274480497\C,0,-25.1292226938,-1.0366190407,-0.5814580712\H,0,-24.6023766561,-1.8570808141,-1.0478535597\H,0,-29.0696390149,0.9407229329,0.4986621724\\Version=EM64L-G09RevC.01\HF=-2545.9427129\S2=0.780919\S2-1=0.\S2A=0.750835\RMSD=1.065e-09\Dipole=16.5795742,0.0761979,-0.0647069\Quadrupole=159.5366507,-73.835757,-85.7008937,0.4139315,-1.1062542,-3.3716096\PG=C01 [X(C66H54)]\@

^HPP_n (Alternant conformer)

HPP2

1\1\GINC-HPC-CN19\FOpt\RBLYP\6-31G(d)\C12H10\TALIPOVM\13-Sep-2013\0\#\# P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent=Dichloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title \0,1\C,-0.254403997,1.1355427535,0.2181735506\C,-0.1830829036,3.447943109,1.8100838531\C,-1.0430953876,2.2477684162,-0.0944380315\C,0.5707628309,1.2067999001,1.3454680029\C,0.605933199,2.3497769977,2.1334106845\C,-1.0077384422,3.391728428,0.6921127514\H,-1.7055547873,2.2085727236,-0.9474188568\H,1.2061815003,0.3688706281,1.5945830492\H,1.2566155602,2.3846389534,2.9959704381\H,-1.6313017502,4.2365769479,0.4351869988\C,-0.2918349329,-0.0859920955,-0.6225017645\C,-0.362398275,-2.3987343928,-2.2139744601\C,-0.3989486029,0.0025033916,-2.0144278498\C,-0.2207922095,-1.3581240199,-0.0450682102\C,-0.2549960399,-2.5020912511,-0.8316351071\C,-0.4346277867,-1.140856716,-2.8018450793\H,-0.4324641246,0.9745446725,-2.4855521328\H,-0.1604257565,-1.4528236329,1.0297865541\H,-0.205727888,-3.4748981583,-0.3627693088\H,-0.5106726716,-1.0479155478,-3.876176048\H,-0.3895493543,-3.2888029027,-2.8264364333\H,-0.1556781804,4.3379017954,2.4226973993\\Version=EM64L-G09RevC.01\HF=-463.0301523\RMSD=3.042e-09\RMSF=2.560e-06\Dipole=0.0000533,0.0004359,0.0000866\Quadrupole=-5.2363112,3.2703593,1.9659519,-1.6725416,2.8501198,1.4708599\PG=C01 [X(C12H10)]\@

HPP3

1\1\GINC-HPC-CN18\FOpt\RBLYP\6-31G(d)\C18H14\TALIPOVM\13-Sep-2013\0\#\#
P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRf(PCM,solvent=Dichl
oromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title
\0,1\H,0.1962029002,0.6453641374,-2.571204891\C,-0.0599973856,0.57767
4104,-1.5235948283\C,-0.6318226625,0.4372452802,1.177680912\C,-0.36943
00169,-0.6669679201,-0.9663315501\C,-0.0369760958,1.7260566562,-0.7477
904766\C,-0.3223935864,1.681888888,0.6204172648\C,-0.6548413136,-0.711
1372935,0.4018784668\H,0.2368416152,2.6653572738,-1.2065374061\H,-0.92
86472843,-1.650442091,0.8606237223\H,-0.8880214509,0.3695532899,2.2252
915551\C,-0.2975860768,2.9096414553,1.4498603367\C,-0.2497299507,5.236
2600979,3.0218543218\C,-0.7423768512,4.1329377535,0.9369231127\C,0.171
5345023,2.8773424039,2.7675263286\C,0.1946217966,4.0273215237,3.545437
7392\C,-0.7180626274,5.2837459509,1.7135925368\H,-1.1310763453,4.17916
51244,-0.0703657365\H,0.5419951694,1.9492900656,3.179009529\H,0.567984
1955,3.9797374419,4.558797172\H,-1.0732331012,6.2164549865,1.298272366
9\C,-0.3942318303,-1.8947236123,-1.7957700066\C,-0.4420882652,-4.22135
42269,-3.3677475058\C,-0.8633574781,-1.8624354304,-3.1134340696\C,0.05
05572204,-3.1180164059,-1.2828234732\C,0.0262462754,-4.2688295276,-2.0
594860619\C,-0.8864459584,-3.0124211843,-3.8913370141\H,-1.2338215747,
-0.9343875054,-3.5249237246\H,0.4392510193,-3.1642372883,-0.275531992\
H,0.3814185181,-5.201533606,-1.6441563212\H,-1.2598144481,-2.964841395
8,-4.9046943676\H,-0.4605523785,-5.1167592721,-3.9726771717\H,-0.23126
65301,6.1316603266,3.6267912324\Version=EM64L-G09RevC.01\HF=-693.9536
948\RMSD=7.637e-09\RMSF=9.134e-07\Dipole=-0.0000002,-0.0000015,0.00000
31\Quadrupole=-9.869742,5.6352412,4.2345008,-1.3039191,2.4316843,1.615
825\PG=C01 [X(C18H14)]\@

HPP4

1\1\GINC-HPC-CN17\FOpt\RBLYP\6-31G(d)\C24H18\TALIPOVM\13-Sep-2013\0\#\#
P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRf(PCM,solvent=Dichl
oromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title
\0,1\H,1.2749516504,-1.1602382686,-3.0420913335\C,0.5791455777,-1.056
9924574,-2.2217940455\C,-1.1294259258,-0.7836521686,-0.0652793668\C,-0
.2929489342,-2.1071775257,-1.9182290556\C,0.5967212424,0.1035127026,-1
.4643606045\C,-0.2572415931,0.2666632484,-0.3688449277\C,-1.1467431342
, -1.9441092125,-0.8227698281\H,1.3061863978,0.8807788166,-1.7096478499
\H,-1.8558067805,-2.7217586441,-0.577519474\H,-1.825650163,-0.68057302
04,0.7546723959\C,-0.238676994,1.5062607044,0.4401546827\C,-0.20379293
52,3.8801144471,1.9895874436\C,-0.4449707132,1.4720542617,1.8230053177
\C,-0.0143888296,2.7539219054,-0.1506771186\C,0.0026979904,3.914332553
3,0.6069273715\C,-0.4279755908,2.6325913597,2.5803827679\H,-0.58988786
67,0.5228268749,2.3185909581\H,0.1176148018,2.8227398401,-1.2209532935
\H,0.1479878161,4.8637159715,0.1117286845\H,-0.5604037659,2.5642050671
,3.6506389991\C,-0.1859129186,5.1208782676,2.799457211\C,-0.152361668,
7.4720696384,4.3346345744\C,-1.0575304649,5.2853404475,3.8814175775\C,
0.7028636769,6.1599913368,2.5032705306\C,0.7192144455,7.3230604014,3.2
616495931\C,-1.0407285712,6.4474244836,4.6412513556\H,-1.7693730239,4.
5067712852,4.1158547641\H,1.4019501162,6.0474482694,1.686876053\H,1.41
95430497,8.1098323178,3.0185789225\H,-1.7283406225,6.5551853559,5.4683
762869\C,-0.3118751424,-3.3479431737,-2.7280789798\C,-0.3480751225,-5.
6993126704,-4.2630146889\C,-0.1253893392,-3.3045510947,-4.1139804081\C
, -0.5168907875,-4.5949956613,-2.1278600363\C,-0.5356738993,-5.75779379
07,-2.8865914517\C,-0.1424054134,-4.4670363659,-4.8732322342\H,0.01155
2506,-2.3511407376,-4.6039768368\H,-0.6402505876,-4.6571608855,-1.0560

520066\H,-0.6888092732,-6.7109594362,-2.4001905601\H,-0.003047483,-4.4084401807,-5.9436045214\H,-0.3620232584,-6.6042406459,-4.8537227834\H,-0.139458469,8.3769563836,4.9254359154\\Version=EM64L-G09RevC.01\HF=-924.8772405\RMSD=6.614e-09\RMSF=5.643e-07\Dipole=-0.0004,0.0002075,0.0003118\Quadrupole=-9.6302694,6.5248916,3.1053778,4.3281813,-6.2001979,4.1236338\PG=C01 [X(C24H18)]\@

HPP5

1\1\GINC-HPC-CN19\FOpt\RBLYP\6-31G(d)\C30H22\TALIPOVM\13-Sep-2013\0\#\# P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent=Dichloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title \0,1\H,1.6655646029,-1.2883469928,-0.1995892968\C,0.8266797042,-0.6106798842,-0.2678083282\C,-1.2610961384,1.1903733478,-0.4728866469\C,-0.2326296541,-0.9054532638,-1.1322145605\C,0.8417967989,0.5578630708,0.4769143016\C,-0.2017876833,1.4851459678,0.3915208081\C,-1.2762130671,0.0218305179,-1.2176095745\H,1.6920779021,0.7666450045,1.1102050037\H,-2.126492676,-0.1869497925,-1.8509029787\H,-2.0999803861,1.8680412303,-0.541106261\C,-0.2487309257,-2.153603112,-1.9278358567\C,-0.2800338834,-4.5440436353,-3.4515114654\C,-0.7776391203,-2.1809071534,-3.2222765605\C,0.2643335952,-3.3482086048,-1.4123168947\C,0.2490434888,-4.516727149,-2.1573387721\C,-0.7930448257,-3.3496099323,-3.9670032819\H,-1.1539273275,-1.2700708002,-3.6654625108\H,0.6522755744,-3.3725265962,-0.4040771646\H,0.6257897382,-5.4276963191,-1.7147857141\H,-1.1814821914,-3.325915044,-4.97508535\C,-0.1856860449,2.7332978931,1.1871387918\C,-0.1543889787,5.1237423595,2.7108076054\C,-0.6987503036,3.9279013662,0.671615058\C,0.3432150622,2.7606046725,2.481582387\C,0.3586178943,3.9293095572,3.2263059657\C,-0.683463019,5.0964219932,1.4166336048\H,-1.086690695,3.9522150087,-0.336625403\H,0.7194987063,1.8497687929,2.9247728877\H,0.7470497725,3.9056174989,4.2343901161\H,-1.0602109652,6.0073894965,0.9740785083\C,-0.1377686531,6.3733069685,3.507021426\C,-0.1058183417,8.7416265515,5.0155574403\C,-1.1961053966,7.2855120096,3.4351458403\C,0.9368456083,6.6732872447,4.351163347\C,0.952743651,7.8439597484,5.0977289418\C,-1.1803187086,8.4570868572,4.180314316\H,-2.048220551,7.0653456787,2.8079983273\H,1.7769233178,5.995720699,4.4063215881\H,1.7970565995,8.0582485615,5.7378577049\H,-2.0124802698,9.1438793312,4.1141303359\C,-0.2966604534,-5.7936058439,-4.2477286183\C,-0.328621804,-8.1619173638,-5.7562771624\C,-1.371278824,-6.0935793122,-5.091867489\C,0.7616758583,-6.7058122558,-4.1758639528\C,0.7458836866,-7.8773832522,-4.9210385829\C,-1.3871826758,-7.2642482531,-5.8384389139\H,-2.2113549559,-5.4160101317,-5.1470187967\H,1.6137952713,-6.4856495298,-3.5487210421\H,1.5780448311,-8.5641771408,-4.8548634588\H,-2.2314988295,-7.4785323864,-6.4785650558\H,-0.3409635742,-9.0734246968,-6.3368256486\H,-0.0934807407,9.6531370182,5.5961010359\\Version=EM64L-G09RevC.01\HF=-1155.8007759\RMSD=6.168e-09\RMSF=4.753e-07\Dipole=-0.000002,0.0000012,-0.0000014\Quadrupole=-4.5228321,6.4594608,-1.9366287,-5.9595025,9.6970997,8.6920492\PG=C01 [X(C30H22)]\@

HPP6

1\1\GINC-HPC-CN55\FOpt\RBLYP\6-31G(d)\C36H26\TALIPOVM\13-Sep-2013\0\#\# P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent=Dichloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title \0,1\H,-2.05598926,0.8289700247,-1.1883507369\C,-1.2240096458,1.0298788281,-0.5287578784\C,0.9228132536,1.6225194324,1.1098915924\C,-0.1632

710827,0.1211632723,-0.4557945119\C,-1.2114575993,2.2080289482,0.20071
71113\C,-0.137817885,2.5313453045,1.0367990157\C,0.9103367444,0.444425
0105,0.3803626569\H,-2.0339387483,2.9007779421,0.0946436853\H,1.732832
3547,-0.2483026625,0.4864533973\H,1.7547613295,1.8234342427,1.76951627
45\C,-0.1759957117,-1.1371755267,-1.2351023738\C,-0.1994159711,-3.5476
680032,-2.7272128118\C,-1.3641613986,-1.841368748,-1.4555922672\C,1.00
0145562,-1.6651347887,-1.7775269616\C,0.9887061858,-2.8433752738,-2.50
6838522\C,-1.3755548603,-3.0196692801,-2.1848447008\H,-2.2873091544,-1
.4807823185,-1.025057705\H,1.9319009612,-1.1319351006,-1.6546619312\H,
1.9118297771,-3.2039672761,-2.9374120754\H,-2.3072969179,-3.5528879015
, -2.3077437361\C,-0.1246436931,3.7899510308,1.8158272179\C,-0.09979832
75,6.2005707532,3.3074513674\C,1.0637620084,4.4938932897,2.0353965287\
C,-1.3003310612,4.3182320171,2.3587398994\C,-1.2880960985,5.4968125841
,3.0878124132\C,1.0757571811,5.6723495077,2.7646334131\H,1.9865891982,
4.1329798517,1.6044085613\H,-2.2323096109,3.7852607699,2.2363874851\H,
-2.210810058,5.8584293274,3.518493435\H,2.0076132338,6.205404904,2.887
6403901\C,-0.0863348888,7.4604868816,4.0872553884\C,-0.059741577,9.848
3377606,5.564845167\C,0.980260611,7.7665876572,4.9393633094\C,-1.13944
65362,8.3765574285,3.9916574208\C,-1.126966686,9.5570974688,4.72261848
15\C,0.9942053956,8.9475865201,5.6695061478\H,1.7943851006,7.064261614
9,5.0481177434\H,-1.963676108,8.1738183989,3.3227650849\H,-1.948301015
1,10.2534363081,4.6273355795\H,1.8256292371,9.1597275774,6.3269849371\
C,-0.2118464209,-4.8062462177,-3.5062957501\C,-0.2360161844,-7.2164464
784,-4.9986105309\C,-1.2848570098,-5.1296596816,-4.343040326\C,0.84883
98058,-5.7148403431,-3.4323823913\C,0.8368624656,-6.8930897845,-4.1619
571093\C,-1.2966548362,-6.3080522174,-5.0724187426\H,-2.1074019722,-4.
4370393082,-4.4496674161\H,1.6803654308,-5.5137382457,-2.7722487509\H,
1.6594343633,-7.5857861074,-4.0559555474\H,-2.1282525843,-6.5098408888
, -5.732270963\C,-0.2481903072,-8.4762995087,-5.7785451762\C,-0.2704073
422,-10.864313578,-7.2559214552\C,0.9284701219,-8.9865948845,-6.337533
5812\C,-1.4362718541,-9.188218973,-5.9759891761\C,-1.4478121298,-10.36
87215853,-6.7070307683\C,0.9180782267,-10.1678287834,-7.06736734\H,1.8
547316866,-8.4427758296,-6.2186705693\H,-2.3541761527,-8.8268699816,-5
.5347164543\H,-2.3764853123,-10.9056258375,-6.8406096912\H,1.838308218
2,-10.5394760317,-7.4958768697\H,-0.2789358531,-11.7834292249,-7.82442
04336\H,-0.0494665986,10.7673657134,6.1334515508\\Version=EM64L-G09Rev
C.01\HF=-1386.7243324\RMSD=9.082e-09\RMSF=1.109e-06\Dipole=0.000495,0.
000351,0.0002484\Quadrupole=5.6253198,4.9718514,-10.5971712,-2.145648,
3.6180199,15.5181852\PG=C01 [X(C36H26)]\@

HPP7

1\1\GINC-HPC-CN18\FOpt\RBLYP\6-31G(d)\C42H30\TALIPOVM\13-Sep-2013\0\#\#
P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRf(PCM,solvent=Dichl
oromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title
\0,1\C,9.3873665424,4.5084862482,0.917381675\C,6.6043680215,3.9858314
793,0.7816353992\C,8.6603002675,4.7540710391,-0.2516675844\C,8.6920300
799,3.9959538685,2.017104502\C,7.3314894797,3.7403860592,1.9508814893\
C,7.2997613131,4.4987024497,-0.3181099363\H,9.1583026008,5.179200402,-
1.1112662518\H,9.2270332467,3.764703983,2.9270203541\H,6.8340010239,3.
3148062107,2.8105470226\H,6.7650652322,4.730554906,-1.2280320277\C,10.
8420801948,4.781343065,0.9881471219\C,13.5990356627,5.2982550398,1.121
8841334\C,11.4242835885,5.2774873201,2.1596003645\C,11.6710752879,4.54
98316702,-0.1148288906\C,13.0342309021,4.8059597405,-0.0493471925\C,12
.7876206783,5.5324484056,2.226385895\H,10.801356724,5.4864274569,3.017
6247672\H,11.2489928444,4.1449260211,-1.0235375475\H,13.6564182116,4.6

127652813, -0.9119666422\H, 13.2143374551, 5.9223040897, 3.1398855469\C, 5.1513352378, 3.7124507592, 0.710358792\C, 2.3684498967, 3.188709347, 0.573581963\C, 4.3198318741, 3.919367688, 1.8158152791\C, 4.5602078948, 3.2377065714, -0.4650034894\C, 3.1999420801, 2.9818011101, -0.5318936273\C, 2.9595620027, 3.6633809409, 1.7489884605\H, 4.7357975223, 4.3153870468, 2.731094156\H, 5.1761787331, 3.0358870318, -1.3295737392\H, 2.7840319308, 2.5857493835, -1.4471819923\H, 2.3436317297, 3.8651778142, 2.6135974468\C, 0.9155284239, 2.915274237, 0.502105234\C, -1.8673594545, 2.3916638862, 0.365391071\C, 0.2196361389, 2.4031741828, 1.6019913853\C, 0.1888005162, 3.1596618648, -0.6677030042\C, -1.1714672147, 2.9037644732, -0.7344948645\C, -1.1406315156, 2.1472763546, 1.5351992735\H, 0.7539316526, 2.1721009529, 2.5123193664\H, 0.6865207797, 3.5847963349, -1.5274215479\H, -1.7057625341, 3.134838555, -1.6448226717\H, -1.6383512659, 1.7221413446, 2.3949177789\C, -3.3202810061, 2.118228294, 0.2939143959\C, -6.1031657153, 1.5944842375, 0.1571383493\C, -3.9113944748, 1.6435646731, -0.8814946438\C, -4.1517716315, 2.3251273075, 1.3993928758\C, -5.5120371487, 2.0692201368, 1.3325033337\C, -5.2716641743, 1.3875770345, -0.9483213005\H, -3.2954654538, 1.4417743635, -1.7461059589\H, -3.7358606671, 2.7211729469, 2.3146834226\H, -6.1280070578, 2.2710312192, 2.1970762793\H, -5.6876314047, 0.9915645908, -1.8636025106\C, -7.5561981294, 1.3211013994, 0.0858624232\C, -10.3391957065, 0.7984419424, -0.0498825825\C, -8.283324015, 1.5665634323, -1.0833774207\C, -8.2515863346, 0.8082117786, 1.1856022484\C, -9.612124862, 0.5528405202, 1.1191603349\C, -9.6438643118, 1.3109936013, -1.1495996645\H, -7.7858390788, 1.9921574744, -1.9430380463\H, -7.7168864072, 0.5763470164, 2.0955190255\H, -10.1101229719, 0.1276958767, 1.9787538451\H, -10.1788711415, 1.5422569262, -2.0595098948\C, -11.7939089205, 0.5255822978, -0.1206474802\C, -14.5508634715, 0.0086639739, -0.2543829384\C, -12.3761159818, 0.0294604749, -1.2921083702\C, -12.6229000204, 0.7570681358, 0.9823368935\C, -13.9860550688, 0.5009368447, 0.9168560181\C, -13.7394525896, -0.2255036125, -1.3588931635\H, -11.7531925243, -0.1794602054, -2.1501399285\H, -12.2008151491, 1.1619565675, 1.8910520348\H, -14.6082389871, 0.6941111892, 1.7794824117\H, -14.166172026, -0.615341546, -2.2723991494\H, 14.660080893, 5.4971626414, 1.17333635\H, -15.6119082469, -0.1902461474, -0.305834657\Version=EM64L-G09RevC.01\HF=-1617.6479223\RMSD=5.009e-09\RMSF=4.093e-07\Dipole=0.0000021, -0.0000009, -0.0000008\Quadrupole=15.7993443, -23.0858851, 7.2865408, 7.4767855, 0.1498701, 1.7504801\PG=C01 [X(C42H30)]\@\

HPP8

1\1\GINC-HPC-CN32\F0pt\RBLYP\6-31G(d)\C48H34\ TALIPOVM\13-Sep-2013\0\#\P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM, solvent=Dichloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title \0,1\C,10.0482922037, -0.0298612705, -0.0949366112\C, 7.2135384353, -0.0056015388, -0.1124566249\C, 9.3349710667, 0.4935259388, -1.1779152458\C, 9.3128005584, -0.5407962189, 0.9791157234\C, 7.9269640843, -0.5290556744, 0.9706399501\C, 7.9491377585, 0.5055060881, -1.1865755301\H, 9.86995935, 0.9252879996, -2.0116017978\H, 9.829951427, -0.9815807906, 1.8193009626\H, 7.3924061526, -0.9614057352, 1.804278598\H, 7.4324168884, 0.9468318656, -2.0267211398\C, 11.5300016281, -0.0426698811, -0.0858995929\C, 14.3380496999, -0.0669843432, -0.0689697679\C, 12.243601927, 0.184592315, 1.0958525166\C, 12.2537722224, -0.2823911271, -1.2589719972\C, 13.6422752181, -0.2937534964, -1.2511799769\C, 13.6320921274, 0.1718849157, 1.1047928806\H, 11.7077008591, 0.3951714475, 2.0103648245\H, 11.7253482855, -0.4837779066, -2.179878932\H, 14.1803670085, -0.488216974, -2.1683429178\H, 14.1623684035, 0.3570893219, 2.0284019629\C, 5.7333511014, 0.0069083963, -0.1215988449\C, 2.8984179973, 0.0304667871, -0.1389073941\C, 5.01417258, -0.1969354253, -1.3037585688\C,

5.00325938,0.2228617298,1.0516873327\C,3.6175743697,0.2343264217,1.0432694121\C,3.6284887107,-0.185371722,-1.3122336144\H,5.5437260188,-0.3984193914,-2.223854763\H,5.5248407803,0.4156229271,1.9781791163\H,3.0880610417,0.4357951591,1.9633937576\H,3.1069522956,-0.3781408788,-2.2387504584\C,1.4183171785,0.0426640171,-0.1480177188\C,-1.4165414378,0.065849926,-0.1656254396\C,0.7046419405,0.5650477204,-1.2315676872\C,0.6827944857,-0.4678396016,0.9265439559\C,-0.702877865,-0.4564912571,0.9179479714\C,-0.6810294171,0.5763643956,-1.2401858537\H,1.2390178189,0.9970300271,-2.0654806413\H,1.1996171096,-0.9084234667,1.766982172\H,-1.237254784,-0.8884589598,1.7518694609\H,-1.1978537687,1.0169268447,-2.08063591\C,-2.8966340646,0.0779290562,-0.1747985512\C,-5.7315370249,0.1011269064,-0.1922643598\C,-3.6267900956,0.2938785596,0.9984611128\C,-3.6156961113,-0.1262133993,-1.3569907723\C,-5.0013645135,-0.1149028998,-1.3655053706\C,-5.0124622862,0.3052424002,0.9899299276\H,-3.1053221138,0.4868720466,1.9249651929\H,-3.0861031631,-0.3277851476,-2.2770415071\H,-5.5228248489,-0.3079312698,-2.2920036737\H,-5.5420459336,0.5068501969,1.9099764614\C,-7.2116375504,0.1134197256,-0.2015186834\C,-10.0465231369,0.1371714769,-0.2193595548\C,-7.9473424201,-0.3965169857,0.8731776008\C,-7.9251226603,0.6354701382,-1.2853448325\C,-9.3108030842,0.6470973371,-1.2940376839\C,-9.3330299177,-0.3849261066,0.8644267268\H,-7.4306844608,-0.8368407595,1.7138603942\H,-7.3906065893,1.0670112859,-2.1194016851\H,-9.8275198983,1.0873986362,-2.1346957804\H,-9.8676106263,-0.8163981125,1.6984807853\C,-11.5267071746,0.1497125356,-0.2286224846\C,-14.3614947197,0.1740915589,-0.2463069217\C,-12.2567627888,0.3676916054,0.9442303103\C,-12.2457011901,-0.0559000947,-1.4105095694\C,-13.6315317164,-0.0439246123,-1.4190128518\C,-13.6425965624,0.379554219,0.9354661792\H,-11.7352181001,0.5617194546,1.870505274\H,-11.7160784947,-0.2589369542,-2.3302510934\H,-14.1534831829,-0.2374450962,-2.3451744667\H,-14.172639066,0.5821063675,1.8550827607\C,-15.8432018842,0.1870452372,-0.2556739891\C,-16.5503334476,0.7310469397,-1.3333716028\H,-16.0089515776,1.1685695414,-2.1600123714\C,-17.9388255493,0.7427278334,-1.3429540745\H,-18.4639372535,1.1747045092,-2.1833114401\C,-18.6512233104,0.2117114981,-0.2735330591\C,-17.9619127337,-0.3316109922,0.8048003168\H,-18.5051725512,-0.7542058977,1.6383640463\C,-16.5734168464,-0.3443280756,0.8128830775\H,-16.0503805748,-0.7911863359,1.646303565\H,15.4187394425,-0.0763293027,-0.0624513163\H,-19.7319110587,0.2211943922,-0.2803996051\\Version=EM64L-G09RevC.01\HF=-1848.5714549\RMSD=6.154e-09\RMSF=6.631e-07\Dipole=0.0001369,0.0000284,-0.0000916\Quadrupole=19.9216417,-27.3899113,7.4682696,-0.3753378,0.0361566,-4.8123192\PG=C01 [X(C48H34)]\@

HPP9

1\1\GINC-HPC-CN69\F0pt\RBLYP\6-31G(d)\C54H38\TALIPOVM\13-Sep-2013\0\#\# P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent=Dichloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title \0,1\C,10.0582004435,-0.0375738286,-0.0921665814\C,7.2234899626,-0.0099313942,-0.1116929248\C,9.3460113847,0.4492907682,-1.1927901453\C,9.321575808,-0.51023838,0.9985160901\C,7.9357621921,-0.4967928895,0.989084316\C,7.9602003481,0.4628821211,-1.202460561\H,9.8818958738,0.8513830354,-2.0406227416\H,9.8377566613,-0.922620334,1.853595298\H,7.4002674464,-0.8993924658,1.8369129483\H,7.444417096,0.8757225718,-2.0575463278\C,11.5398869211,-0.0522075571,-0.0821055169\C,14.3479069807,-0.0801456953,-0.0632109436\C,12.2534181391,0.213635557,1.0916130995\C,12.2637326498,-0.3323308111,-1.2461467373\C,13.6522131523,-0.3454653844,-1.2374192361\C,13.6418818936,0.1991165721,1.1015620055\H,11.7175236719,0.45

57801889, 1.998271766\H, 11.7353531392, -0.5638666042, -2.1599561809\H, 14.1903395076, -0.5714635432, -2.1473052\H, 14.1721033102, 0.4144822027, 2.0186401367\C, 5.7433306286, 0.004281793, -0.1218708051\C, 2.908452647, 0.0310003594, -0.1410906764\C, 5.0242945562, -0.2398533071, -1.2964510401\C, 5.0131442645, 0.2621642478, 1.0428505587\C, 3.6274787937, 0.2752084811, 1.0334929189\C, 3.6386290252, -0.2267667136, -1.3058549625\H, 5.5539178863, -0.4742255886, -2.2086754301\H, 5.5347110866, 0.4865842103, 1.9621884514\H, 3.0979186674, 0.5096105162, 1.9457451663\H, 3.1171309915, -0.4512553857, -2.2252136057\C, 1.4283734479, 0.0447550805, -0.1511958282\C, -1.4064423448, 0.0708182012, -0.1707549358\C, 0.7157401301, 0.5295445356, -1.2527603003\C, 0.6918260111, -0.4266742269, 0.9403895139\C, -0.6938248236, -0.4139051167, 0.9308414597\C, -0.6699130901, 0.5422626243, -1.262339896\H, 1.2509488025, 0.9311998812, -2.1011815715\H, 1.2077702258, -0.8380239457, 1.7960594253\H, -1.2290379503, -0.8155425732, 1.7792704974\H, -1.1858658413, 0.9535642587, -2.1180313263\C, -2.8865130042, 0.0843338874, -0.1809117558\C, -5.721350205, 0.1100956101, -0.2001491814\C, -3.6167684823, 0.3423401103, 0.9837574631\C, -3.6054418825, -0.1605068218, -1.3554292632\C, -4.9910943334, -0.1479111545, -1.3648181863\C, -5.0024209115, 0.3549378907, 0.9743679727\H, -3.0953345769, 0.5673389668, 1.9030220704\H, -3.0757888288, -0.3950860883, -2.2675761029\H, -5.512527405, -0.3729122533, -2.2840825888\H, -5.5320731275, 0.5895190819, 1.8865146714\C, -7.2014209536, 0.123608915, -0.2103055261\C, -10.0362370377, 0.1496635984, -0.229864654\C, -7.9379490599, -0.347804865, 0.8812936827\C, -7.9140405802, 0.6082976799, -1.3119159197\C, -9.2996915224, 0.6210607293, -1.3214649286\C, -9.3236023802, -0.3350889473, 0.871715028\H, -7.4219959672, -0.7590812775, 1.7369969063\H, -7.378829769, 1.0099122943, -2.1603571058\H, -9.8156377723, 1.0323805511, -2.1771481295\H, -9.8588103319, -0.7367182564, 1.720149233\C, -11.5163161896, 0.1634120966, -0.2399703007\C, -14.3511938877, 0.1901153001, -0.2591904871\C, -12.246492861, 0.4212441561, 0.9247792693\C, -12.2353410773, -0.0808682742, -1.4145393832\C, -13.6210065023, -0.0678335086, -1.4238966905\C, -13.6321583364, 0.4343252111, 0.9153746534\H, -11.7249945008, 0.6457881052, 1.844124329\H, -11.7057791036, -0.3153203385, -2.3267777648\H, -14.1425720615, -0.2923130117, -2.3432206336\H, -14.1617819156, 0.6687510956, 1.8275849675\C, -15.8313535791, 0.2043190182, -0.269368314\C, -16.5436301505, 0.69108365, -1.3701858311\H, -16.0081394393, 1.093616237, -2.2180487274\C, -17.9294439516, 0.7045179926, -1.3796184682\H, -18.445628319, 1.116822711, -2.2347328996\C, -18.6660646992, 0.2319414285, -0.2888951909\C, -17.953871889, -0.2548246908, 0.8117694207\H, -18.4897534918, -0.6568475376, 1.6596368879\C, -16.568060659, -0.2684076403, 0.8214394691\H, -16.0522750977, -0.681174003, 1.6765595287\C, -20.1477511639, 0.2465640735, -0.2989569395\C, -20.8612809614, -0.0194001422, -1.4726488531\H, -20.3253847179, -0.2616308804, -2.3792834717\C, -22.2497446523, -0.0048922064, -1.4825983309\H, -22.7799650782, -0.2203530734, -2.3996546036\C, -22.9557709577, 0.2744811182, -0.3178529495\C, -22.2600787556, 0.5399222989, 0.8563287994\H, -22.7982062115, 0.7660075587, 1.7661924657\C, -20.8715980471, 0.5267975854, 0.8650572071\H, -20.3432192309, 0.7584272583, 1.7788433785\H, 15.4285785564, -0.0908934774, -0.0559315186\H, -24.0364426326, 0.285220777, -0.325132881\Version=EM64L-G09RevC.01\HF=-2079.4949971\RMSD=9.316e-09\RMSF=4.678e-07\Dipole=-0.0000012, -0.0000037, -0.0000016\Quadrupole=22.5983153, -31.6159792, 9.0176639, -0.5115658, 0.0697929, -2.1499409\PG=C01 [X(C54H38)]\@\

HPP10

1\1\GINC-HPC-CN20\FOpt\RBLYP\6-31G(d)\C60H42\TALIPOVM\13-Sep-2013\0\#\P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent=Dichloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title

\\0,1\C,10.0749415229,-0.0459586356,-0.0955805206\C,7.2402514005,-0.0148333369,-0.1126854572\C,9.3628932679,0.4982266552,-1.1690977091\C,9.3382299429,-0.5741528605,0.969237809\C,7.9524260465,-0.5591014853,0.9609374256\C,7.9770913418,0.513605919,-1.1775295317\H,9.8989450685,0.9434505899,-1.994981243\H,9.8543487035,-1.0309505791,1.8014616403\H,7.4168417521,-1.0050119579,1.7867271328\H,7.4614389615,0.9710047197,-2.0096867146\C,11.5566109247,-0.0624471623,-0.0867873369\C,14.3645692712,-0.0938526888,-0.0703063042\C,12.2707052028,0.1427479557,1.098694237\C,12.2798193332,-0.2837266605,-1.2638194125\C,13.6682909448,-0.2986284017,-1.2562265879\C,13.6591619632,0.1265606703,1.1073907019\H,11.7352607397,0.3387978748,2.0167035158\H,11.7509186754,-0.4679364146,-2.1880485023\H,14.2059451852,-0.4786408284,-2.1765904427\H,14.1898628242,0.2946061175,2.0340316923\C,5.760095765,0.0011572492,-0.1216369921\C,2.9252195735,0.0310325355,-0.138548596\C,5.0405421256,-0.1790633589,-1.3074069644\C,5.0303877081,0.1968019705,1.0554520405\C,3.644732815,0.2113104769,1.0472340837\C,3.6548864592,-0.1643657285,-1.3156986131\H,5.5696994295,-0.3644668203,-2.2311063421\H,5.552297719,0.371149971,1.9854020418\H,3.1155753226,0.396605825,1.9709606256\H,3.1329873267,-0.3386537594,-2.2456717625\C,1.4451529868,0.0463116638,-0.1473980322\C,-1.3896512207,0.0750841495,-0.1645434971\C,0.7324886498,0.5905292218,-1.2208133246\C,0.7086621548,-0.4831251768,0.9172861242\C,-0.6769827683,-0.4690777748,0.9088995887\C,-0.6531603126,0.6046050357,-1.2291905247\H,1.2677161424,1.0372575215,-2.0463636321\H,1.2246723803,-0.9405368451,1.7491828143\H,-1.2121754528,-0.9158793139,1.7344292778\H,-1.1691429177,1.0620321691,-2.0610950662\C,-2.8697183359,0.0899349656,-0.1735053017\C,-5.7045604037,0.1180451278,-0.1905209228\C,-3.5995704965,0.2839334238,1.0037797998\C,-3.5890707223,-0.0896586526,-1.3595052867\C,-4.9747159767,-0.0759038239,-1.3678147303\C,-4.9852170331,0.2976553344,0.995478115\H,-3.0778471354,0.4577585781,1.9339283448\H,-3.0597827425,-0.2738735893,-2.2833631889\H,-5.4964481794,-0.2497118836,-2.297962789\H,-5.514517898,0.4818340947,1.9193375283\C,-7.1846262521,0.1327215608,-0.1994813684\C,-10.019420755,0.1608361734,-0.2167604263\C,-7.9210395767,-0.3973413507,0.8649475401\C,-7.8973581063,0.6771528719,-1.272743907\C,-9.2830028702,0.6908931681,-1.2811897431\C,-9.3066900884,-0.3836015595,0.8565001125\H,-7.4049803152,-0.8549547647,1.6967017077\H,-7.362215142,1.1243687647,-2.0980812934\H,-9.7990634697,1.1485181099,-2.1129355119\H,-9.8418386011,-0.8307993013,1.6818448689\C,-11.4994852767,0.1756299393,-0.2257584561\C,-14.334334818,0.2044352495,-0.2430068152\C,-12.2293772821,0.3697821286,0.9514695664\C,-12.218780905,-0.0039417995,-1.4117913045\C,-13.6044211868,0.0101036767,-1.4202008571\C,-13.615024979,0.3838937934,0.9430404574\H,-11.7076772484,0.5435248623,1.8816502213\H,-11.6894497824,-0.1883088723,-2.335597101\H,-14.126114701,-0.1636698168,-2.3503755969\H,-14.1443445021,0.5683147311,1.8668401258\C,-15.8144027747,0.2198611182,-0.2521685512\C,-16.5266703297,0.764244866,-1.3257579981\H,-15.9911504048,1.2107472106,-2.1512429044\C,-17.9123196055,0.7789130025,-1.3343452386\H,-18.4280329578,1.2364573161,-2.1663588553\C,-18.6492300579,0.2498537386,-0.2697836828\C,-17.9369596347,-0.2946042315,0.8037532285\H,-18.4725541573,-0.7410021623,1.6292513115\C,-16.5512989742,-0.3092515863,0.8123912569\H,-16.0356494015,-0.7668130623,1.6444353112\C,-20.1293777673,0.2657793702,-0.278911257\C,-20.8486634957,0.0847323021,-1.464633759\H,-20.3193604721,-0.1015553485,-2.3881011301\C,-22.2344603508,0.0999924673,-1.4730413868\H,-22.7567043786,-0.0743288191,-2.4028465096\C,-22.9640987876,0.2969100461,-0.2964041127\C,-22.2449052695,0.4777755919,0.8892055312\H,-22.7746214773,0.663621254,1.8125331531\C,-20.8591038766,0.4625936759,0.8978832457\H,-20.3372595218,0.6374038143,1.8278132824\C,-24.4457673633,0.3134903833,-0.3056672328\C,-25.1773744873,-0.2363451227,0.7525454679\H,-24.6554945335,-0.7001639032,1.5773721761

\C, -26.5658351582, -0.2202028525, 0.7445890665\H, -27.1101974441, -0.6572476532, 1.5699420557\C, -27.2537262595, 0.3451059347, -0.3232998298\C, -26.5399388158, 0.8946356946, -1.3823912996\H, -27.0639199304, 1.3437141234, -2.2144483532\C, -25.1514797133, 0.8795146499, -1.3729019816\H, -24.6089603385, 1.3313897444, -2.191024253\H, 15.4452333095, -0.1059306555, -0.0639609279\H, -28.3343877472, 0.3572594506, -0.3300772529\\Version=EM64L-G09RevC.01\HF=-2310.4185623\RMSD=2.364e-09\RMSF=8.314e-07\Dipole=0.0001542, 0.0000007, -0.0000853\Quadrupole=25.247889, -34.1576791, 8.9097901, -0.6036517, 0.0261282, -6.8363164\PG=C01 [X(C60H42)]\@

^HPP_n⁺ (Helical conformer)

HPP2+*

1\1\GINC-HPC-CN64\Stability\UBLYP\6-31G(d)\C12H10(1+,2)\TALIPOVM\25-Aug-2013\0\#\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title\1,2\C,0,-0.253950513,1.1153712354,0.2038440358\C,0,-0.1847217161,3.4260081013,1.7953899022\C,0,-0.8721983015,2.3276700315,-0.2278772523\C,0,0.4014294976,1.1188025979,1.4720971747\C,0,0.4401487016,2.2533395153,2.2423899336\C,0,-0.8437689091,3.4516061739,0.5582427927\H,0,-1.4029825738,2.3595550042,-1.1639835143\H,0,0.906888147,0.2347891254,1.8209996926\H,0,0.9547336145,2.2450689669,3.1905334195\H,0,-1.3317566417,4.3549199443,0.2269514056\C,0,-0.2904129464,-0.0655805425,-0.6084859679\C,0,-0.3628436093,-2.3770373228,-2.1987826535\C,0,-0.6276437363,0.001998078,-1.9940920675\C,0,0.0090956135,-1.3489715639,-0.0593757033\C,0,-0.0365648152,-2.4769110766,-0.8389832856\C,0,-0.6527441597,-1.1296199024,-2.7692237784\H,0,-0.8285774713,0.9539363712,-2.4549469182\H,0,0.2385236614,-1.4486323129,0.9877416469\H,0,0.1746900215,-3.4419439805,-0.4054414733\H,0,-0.8919538086,-1.060122694,-3.8188529041\H,0,-0.3907289588,-3.266113357,-2.8106411695\H,0,-0.1584610962,4.3147976073,2.4077266843\\Version=EM64L-G09RevC.01\HF=-462.8092801\S2=0.796584\S2-1=0.\S2A=0.751742\RMSD=4.005e-09\Dipole=0.0001289, -0.0001126, 0.0008834\Quadrupole=-15.3931593, 12.4568307, 2.9363286, -3.0883723, 5.4812914, 10.5774314\PG=C01 [X(C12H10)]\@

HPP3+*

1\1\GINC-HPC-CN61\Stability\UBLYP\6-31G(d)\C18H14(1+,2)\TALIPOVM\25-Aug-2013\0\#\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title\1,2\H,0,0.3014748751,0.6529293205,-2.5518069472\C,0,0.0093649775,0.5844680548,-1.5172665113\C,0,-0.7073607462,0.4322422594,1.1684698779\C,0,-0.367490621,-0.6730933027,-0.9696949081\C,0,0.047789626,1.7125241998,-0.7500222291\C,0,-0.3171659249,1.687251243,0.6245786249\C,0,-0.7172640039,-0.7013235064,0.4086927178\H,0,0.3326960938,2.6425190036,-1.2129171816\H,0,-1.0277603003,-1.6263997946,0.8650027396\H,0,-0.9738740032,0.3587674478,2.2094480393\C,0,-0.2941192884,2.8848934902,1.4343521546\C,0,-0.2520337696,5.2080407958,3.0044186925\C,0,0.4702296191,4.0110331606,1.0481904641\C,0,-1.0359976921,2.9651312261,2.6363779819\C,0,-1.0200478925,4.1126945197,3.4015036553\C,0,0.4955296102,5.1488576648,1.8275467559\H,0,1.0743364528,3.9763860044,0.1562341369\H,0,-1.6544354598,2.1392235841,2.9482890305\H,0,-1.6062184552,4.1623435461,4.3065196919\H,0,1.0981877247,5.9922746378,1.5265512164\C,0,-0.394

0985071, -1.8707927259, -1.7794198182\C, 0, -0.445383342, -4.1934530712, -3.349526884\C, 0, -0.4742845932, -1.7945481427, -3.1897871905\C, 0, -0.3407017539, -3.1531507031, -1.1844641555\C, 0, -0.3572100351, -4.2934555504, -1.9604627085\C, 0, -0.5080906846, -2.9394203586, -3.9584824552\H, 0, -0.5495546532, -0.8361125989, -3.6772705566\H, 0, -0.2463172148, -3.2511450327, -0.1152457987\H, 0, -0.2978109715, -5.2633877951, -1.4905170394\H, 0, -0.5871380833, -2.8628631429, -5.0322738881\H, 0, -0.4650354648, -5.0879114902, -3.954335188\H, 0, -0.2360255188, 6.1027170569, 3.6089876803\\Version=EM64L-G09RevC.01\HF=-693.7427237\S2=0.792971\S2-1=0.\S2A=0.751582\RMSD=6.819e-09\Dipole=0.0005025,0.0043951,0.0032349\Quadrupole=-26.5682475,22.6729567,3.8952909,3.3666855,-3.7276006,22.2498028\PG=C01 [X(C18H14)]\@

HPP4+*

1\1\GINC-HPC-CN58\Stability\UBLYP\6-31G(d)\C24H18(1+,2)\TALIPOVM\25-Aug-2013\0\#\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title\1,2\H,0,1.4775323389,-1.2709196849,-2.8408515371\C,0,0.7031677312,-1.1124357189,-2.1077421352\C,0,-1.2626030274,-0.6957138437,-0.1866989645\C,0,-0.2934245709,-2.0973982269,-1.9153646273\C,0,0.7311310726,0.0303921137,-1.354498745\C,0,-0.2555024356,0.2895299194,-0.3663006248\C,0,-1.2713841497,-1.8490977931,-0.9242155602\H,0,1.5075700334,0.7523597839,-1.54543744\H,0,-2.0601016299,-2.5653730765,-0.7594297492\H,0,-2.0257673676,-0.5588955794,0.5612407015\C,0,-0.2350166126,1.4955802076,0.4184465047\C,0,-0.1931223083,3.8783484385,1.9740745843\C,0,-1.3825391025,1.9388653167,1.1280582165\C,0,0.934011951,2.2957057593,0.5191149596\C,0,0.9556052511,3.4346376698,1.2784456412\C,0,-1.3638186497,3.0921422787,1.8654877551\H,0,-2.3020761842,1.380721888,1.0710954727\H,0,1.8383693509,1.9969153958,0.0156911801\H,0,1.8632129493,4.0149325548,1.3190671036\H,0,-2.2562358182,3.3849514215,2.3947503632\C,0,-0.1712631722,5.10033847,2.7730907175\C,0,-0.1297933635,7.4458045366,4.3070879533\C,0,-1.3501834325,5.8325198737,3.004282697\C,0,1.0291224485,5.5761121589,3.3318529306\C,0,1.0458737157,6.730078014,4.0949971477\C,0,-1.3261248255,6.9940844249,3.755587223\H,0,-2.2813393722,5.5115063821,2.5637161399\H,0,1.9449275156,5.0211745422,3.1991744111\H,0,1.9738790936,7.0711555104,4.5294241608\H,0,-2.2382844041,7.5515007835,3.9088137014\C,0,-0.3119724527,-3.3226918069,-2.7092766735\C,0,-0.3483480435,-5.6740807141,-4.2340273062\C,0,0.2568397755,-3.3575811972,-3.9955516704\C,0,-0.8988389856,-4.4989004056,-2.2077894889\C,0,-0.9090565182,-5.660554177,-2.9593139983\C,0,0.2308969445,-4.5173253332,-4.7496301863\H,0,0.6880357282,-2.4643847961,-4.4203111404\H,0,-1.3151004651,-4.5137494343,-1.2124429409\H,0,-1.3498299468,-6.5581203779,-2.5514830994\H,0,0.6580178768,-4.520698443,-5.7414669881\H,0,-0.1137202346,8.3497239505,4.8982485614\H,0,-0.3625067036,-6.5802407857,-4.8217652506\\Version=EM64L-G09RevC.01\HF=-924.6706592\S2=0.789319\S2-1=0.\S2A=0.751347\RMSD=4.061e-09\Dipole=-0.0000186,-0.0003329,-0.0014167\Quadrupole=-23.2668108,31.2588611,-7.9920503,4.0941814,-5.5111872,41.5110123\PG=C01 [X(C24H18)]\@

HPP5+*

1\1\GINC-HPC-CN56\Stability\UBLYP\6-31G(d)\C30H22(1+,2)\TALIPOVM\25-Aug-2013\0\#\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title\1,2\H,0,0.6528415542,0.3207908234,-2.6714089651\C,0

,0.2533403699,0.3009612676,-1.6709483684\C,0,-0.7387652269,0.282999149
8,0.9255751945\C,0,-0.2536548335,-0.9111106278,-1.135415822\C,0,0.2845
494665,1.450611414,-0.9311208193\C,0,-0.2168568446,1.4908730156,0.3952
250538\C,0,-0.7430039959,-0.8736730456,0.1958409417\H,0,0.6728028485,2
.3467749964,-1.3865628055\H,0,-1.1557882025,-1.7631787324,0.6423966204
\H,0,-1.1144399623,0.25733836,1.9353221382\C,0,-0.2683197881,-2.130404
9042,-1.9125278114\C,0,-0.2861623447,-4.525192768,-3.4393861519\C,0,-0
.1906373666,-2.1044408415,-3.3241133825\C,0,-0.3582640833,-3.398076983
8,-1.2928384001\C,0,-0.3555692171,-4.5559442305,-2.0334432074\C,0,-0.2
107194493,-3.2642306327,-4.0612735239\H,0,-0.1424936166,-1.1628682598,
-3.8468892945\H,0,-0.4007841787,-3.4744957608,-0.2183693747\H,0,-0.432
5229776,-5.5028968018,-1.5223419014\H,0,-0.1418107147,-3.2010136275,-5
.1360409039\C,0,-0.1957936692,2.7103265976,1.1727452959\C,0,-0.1530823
669,5.104216937,2.6990156633\C,0,-1.0559962782,2.8926971811,2.27927418
23\C,0,0.6863804001,3.7685121995,0.8568349759\C,0,0.7128349672,4.92205
72963,1.6041741845\C,0,-1.0411231728,4.0571329453,3.0098941824\H,0,-1.
7628471909,2.1242755185,2.5478688302\H,0,1.3776141072,3.670206607,0.03
53226051\H,0,1.3961377205,5.7092341898,1.3259870862\H,0,-1.7090660952,
4.1542348416,3.8515089741\C,0,-0.1305078408,6.3434467656,3.489095118\C
,0,-0.087121609,8.7076594622,4.9942691731\C,0,-1.2953247109,6.82467268
56,4.1049965332\C,0,1.0565894086,7.0742584522,3.6453044874\C,0,1.07789
02343,8.2402757726,4.394087669\C,0,-1.2736533895,7.9965791682,4.844529
2008\H,0,-2.2291085138,6.2976949228,3.977971881\H,0,1.9739445369,6.712
0406094,3.2059576979\H,0,2.004764823,8.7820942058,4.5138889145\H,0,-2.
1839900312,8.3583939312,5.299971698\C,0,-0.2910738753,-5.764213653,-4.
2291520423\C,0,-0.2983355678,-8.127525664,-5.7361886116\C,0,-0.8403319
488,-5.7919405393,-5.5197609634\C,0,0.2546853342,-6.9484050323,-3.7114
242642\C,0,0.25519598,-8.1148658321,-4.4596617559\C,0,-0.8481521535,-6
.9623579055,-6.2617392922\H,0,-1.29267822,-4.9024347724,-5.9319036822\
H,0,0.7100842966,-6.9488361166,-2.73247921\H,0,0.692420059,-9.01338562
68,-4.0491863823\H,0,-1.2880368614,-6.9672753596,-7.248364758\H,0,-0.3
011912189,-9.038435638,-6.3170373393\H,0,-0.0705585905,9.6190240399,5.
5742107319\\Version=EM64L-G09RevC.01\HF=-1155.596201\S2=0.786259\S2-1=
0.\S2A=0.751144\RMSD=4.694e-09\Dipole=-0.0094066,-0.0803068,-0.0489422
\Quadrupole=-42.3297829,43.685439,-1.3556561,3.7958945,-3.6492461,48.5
71951\PG=C01 [X(C30H22)]\@

HPP6+*

1\1\GINC-HPC-CN55\Stability\UBLYP\6-31G(d)\C36H26(1+,2)\TALIPOVM\25-Au
g-2013\0\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) scrf(check
) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=
ultrafine)\Title\1,2\H,0,-0.2224007426,1.4381717093,-2.1806714105\C,
0,-0.2138263677,1.3738194672,-1.1051489416\C,0,-0.1605203701,1.2670997
658,1.669618598\C,0,-0.1934780193,0.1074815868,-0.4680218067\C,0,-0.18
93243536,2.5378662389,-0.3827565154\C,0,-0.1679756195,2.5279966329,1.0
306312807\C,0,-0.1600875013,0.1014847816,0.949367258\H,0,-0.2163737565
,3.4770192515,-0.9116170466\H,0,-0.1596936879,-0.8326051966,1.48637065
83\H,0,-0.1241434216,1.2115275493,2.7457705095\C,0,-0.2044035868,-1.11
97747622,-1.227615436\C,0,-0.2179456259,-3.5408682057,-2.72670634\C,0,
-0.6027199313,-1.1470796896,-2.5881666883\C,0,0.18458944,-2.3535132884
, -0.6472213553\C,0,0.1894513169,-3.5153527483,-1.3729315752\C,0,-0.620
106433,-2.3146261503,-3.3047069448\H,0,-0.9255438761,-0.2418643732,-3.
0752617942\H,0,0.511247036,-2.3887143388,0.3787933883\H,0,0.4846713639
, -4.429858898,-0.8842663585\H,0,-0.9204371668,-2.2827119412,-4.3396376
416\C,0,-0.1540549248,3.7670939844,1.7969174405\C,0,-0.1298650305,6.17

96457295, 3.2858931608\C, 0, -0.6438571939, 3.8160736405, 3.1154672437\C, 0, 0.3494577021, 4.960221708, 1.2457024737\C, 0, 0.3680856131, 6.1307801854, 1.9747309022\C, 0, -0.6390931455, 4.992720042, 3.8348954102\H, 0, -1.0589108479, 2.9311964739, 3.5722629331\H, 0, 0.7558338078, 4.9655161063, 0.2462882964\H, 0, 0.7542641131, 7.0280545782, 1.5155109461\H, 0, -1.0164272794, 4.9902722961, 4.8462056811\C, 0, -0.1194297146, 7.435542814, 4.0599725837\C, 0, -0.1014697027, 9.8231926909, 5.5297295257\C, 0, -1.1406829093, 7.7227314348, 4.9746182264\C, 0, 0.9111764892, 8.3701633125, 3.8977132225\C, 0, 0.9211311293, 9.5497781444, 4.6275374753\C, 0, -1.1329605526, 8.9057044741, 5.6989741533\H, 0, -1.9605819556, 7.0305171612, 5.0987051364\H, 0, 1.7242210576, 8.160272739, 3.2182377458\H, 0, 1.7310570478, 10.2528913258, 4.4962212748\H, 0, -1.9360790153, 9.1140468375, 6.3911857388\C, 0, -0.2226163589, -4.7789744601, -3.493451289\C, 0, -0.2315110141, -7.1908944942, -4.9847105141\C, 0, -1.059000652, -4.9419105183, -4.614155694\C, 0, 0.6093547545, -5.8587817789, -3.1414372968\C, 0, 0.6096022757, -7.0275824642, -3.8729236351\C, 0, -1.0677795107, -6.1186542199, -5.3328487803\H, 0, -1.7297622307, -4.1500896233, -4.9090452829\H, 0, 1.2829596258, -5.7724127482, -2.3032442622\H, 0, 1.2553503875, -7.836671947, -3.5672052522\H, 0, -1.7172657293, -6.203736559, -6.1907402505\C, 0, -0.2369142321, -8.4458407383, -5.759826363\C, 0, -0.2480955469, -10.8324629728, -7.2313310892\C, 0, 0.9360069304, -9.194329463, -5.9220539705\C, 0, -1.4154804936, -8.9186815178, -6.3511978991\C, 0, -1.4209808762, -10.1012044201, -7.0761875065\C, 0, 0.9304532933, -10.3732518054, -6.6528606036\H, 0, 1.8635032257, -8.8378759977, -5.4985715993\H, 0, -2.3386925279, -8.3737981797, -6.2188488155\H, 0, -2.3428305591, -10.4550156067, -7.5150100693\H, 0, 1.8480637446, -10.9304104533, -6.7757728375\H, 0, -0.2524937596, -11.7523102026, -7.7981925704\H, 0, -0.0947141311, 10.7434271008, 6.0959441725\Version=EM64L-G09RevC.01\HF=-1386.5206998\S2=0.784214\S2-1=0.\S2A=0.751024\RMSD=4.640e-09\Dipole=-0.0087819, -0.1007776, -0.0613741\Quadrupole=-51.5064919, 54.6626082, -3.1561163, 0.2393817, 2.5430522, 61.2589403\PG=C01 [X(C36H26)]\ \@

HPP7+*

1\1\GINC-HPC-CN54\Stability\UBLYP\6-31G(d)\C42H30(1+,2)\TALIPOVM\25-Au g-2013\0\#\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title\1,2\C, 0, 10.0120494789, -0.0081276844, -0.1049061105\C, 0, 7.1785125308, -0.0063464983, -0.1084467207\C, 0, 9.2887227011, 0.7454590031, -1.0387585123\C, 0, 9.2854485003, -0.760893717, 0.8270592647\C, 0, 7.9035499543, -0.765730415, 0.8228928256\C, 0, 7.9068219639, 0.7520405729, -1.0380444078\H, 0, 9.8157262027, 1.3484744554, -1.7630305668\H, 0, 9.8098844295, -1.3645859234, 1.5526285716\H, 0, 7.3824749567, -1.3472739869, 1.5682164569\H, 0, 7.3883400228, 1.3342545269, -1.7846541082\C, 0, 11.4903963637, -0.0089144173, -0.1029273413\C, 0, 14.2956536635, -0.0103276076, -0.0991292091\C, 0, 12.2063811148, -0.0916145611, 1.097146015\C, 0, 12.2097089847, 0.0730709961, -1.3010550321\C, 0, 13.5974740751, 0.0706326284, -1.2990100278\C, 0, 13.5941481303, -0.0905808298, 1.0988578102\H, 0, 11.6745826841, -0.1305480301, 2.0367265941\H, 0, 11.6804861955, 0.1125728297, -2.2420628841\H, 0, 14.1335164842, 0.1250563016, -2.2357995697\H, 0, 14.1275975068, -0.1455317201, 2.0370964709\C, 0, 5.7127927214, -0.0052345839, -0.1100403035\C, 0, 2.8717138179, -0.0027866404, -0.112423947\C, 0, 4.9832993896, 1.1095410802, -0.5674869684\C, 0, 4.9806119756, -1.1188219941, 0.3459996869\C, 0, 3.6062611182, -1.1237065169, 0.3351485047\C, 0, 3.6089430743, 1.1167912815, -0.5589336963\H, 0, 5.5067745482, 1.9887903015, -0.9089845905\H, 0, 5.5020065375, -1.9989524705, 0.6884075437\H, 0, 3.0904857085, -1.9950809851, 0.7053722112\H, 0, 3.0952822123, 1.9890650771, -0.9299692301\C, 0, 1.4236575948, -0.0013910619, -0.113159567\

C, 0, -1.4236575961, 0.0013910547, -0.1131595628\C, 0, 0.6856597972, 1.208172242, -0.1205636191\C, 0, 0.6832953921, -1.2095086523, -0.1062174394\C, 0, -0.6856597979, -1.2081722314, -0.1205636518\C, 0, -0.6832953927, 1.2095086451, -0.1062174026\H, 0, 1.2026860517, 2.1537924361, -0.1068620272\H, 0, 1.1984939391, -2.1561276684, -0.1200677157\H, 0, -1.202686052, -2.1537924439, -0.1068620867\H, 0, -1.1984939395, 2.1561276617, -0.1200676489\C, 0, -2.871713817, 0.0027866337, -0.1124239393\C, 0, -5.7127927237, 0.0052345792, -0.1100402931\C, 0, -3.6089430771, -1.1167912832, -0.5589336982\C, 0, -3.6062611185, 1.1237065059, 0.3351485245\C, 0, -4.9806119751, 1.1188219844, 0.345999708\C, 0, -4.9832993915, -1.1095410814, -0.567486969\H, 0, -3.0952822179, -1.989065076, -0.9299692411\H, 0, -3.0904857096, 1.9950809706, 0.7053722391\H, 0, -5.5020065347, 1.9989524584, 0.6884075737\H, 0, -5.5067745498, -1.9887902994, -0.908984599\C, 0, -7.1785125312, 0.0063464954, -0.1084467114\C, 0, -10.0120494792, 0.0081276868, -0.1049061069\C, 0, -7.9068219639, -0.752040585, -1.0380443928\C, 0, -7.9035499551, 0.7657304237, 0.8228928264\C, 0, -9.2854485009, 0.7608937277, 0.8270592622\C, 0, -9.2887227007, -0.7454590122, -1.0387584994\H, 0, -7.3883400226, -1.3342545477, -1.7846540862\H, 0, -7.3824749581, 1.3472740025, 1.5682164525\H, 0, -9.8098844311, 1.3645859433, 1.5526285606\H, 0, -9.8157262029, -1.3484744716, -1.7630305475\C, 0, -11.490396363, 0.0089144231, -0.1029273419\C, 0, -14.2956536608, 0.0103276188, -0.099129219\C, 0, -12.2097089796, -0.0730710048, -1.3010550347\C, 0, -12.2063811171, 0.0916145842, 1.0971460116\C, 0, -13.5941481323, 0.0905808553, 1.0988578021\C, 0, -13.5974740695, -0.0706326341, -1.2990100349\H, 0, -11.6804861864, -0.1125728507, -2.2420628839\H, 0, -11.6745826888, 0.1305480634, 2.0367265916\H, 0, -14.1275975125, 0.1455317587, 2.03709646\H, 0, -14.1335164765, -0.1250563185, -2.2357995774\H, 0, 15.376224668, -0.0108670286, -0.0976684158\H, 0, -15.3762246653, 0.0108670419, -0.0976684291\\Version=EM64L-G09RevC.01\HF=-1617.4445951\S2=0.78211\S2-1=0.\S2A=0.750904\RMSD=1.361e-09\Dipole=-0.0000004,0.,-0.0046593\Quadrupole=106.6205118,-51.9912612,-54.6292506,-0.1076559,0.,0.0000003\PG=C01 [X(C42H30)]\@\

HPP8+*

1\1\GINC-HPC-CN19\Stability\UBLYP\6-31G(d)\C48H34(1+,2)\TALIPOVM\02-Sep-2013\0\#\P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title\1,2\C, 0, 10.0110695501, -0.0058952211, -0.115997913\C, 0, 7.1783867585, -0.0042778395, -0.1100442107\C, 0, 9.2854490978, 0.7931976924, -1.0067115717\C, 0, 9.2882859552, -0.8040850173, 0.7778282556\C, 0, 7.904135594, -0.8062759284, 0.7795378419\C, 0, 7.9013095072, 0.7969589601, -1.0026077257\H, 0, 9.8105956176, 1.4325739113, -1.701061627\H, 0, 9.8156094296, -1.4440345375, 1.4699966083\H, 0, 7.382480335, -1.4242469038, 1.4954536343\H, 0, 7.3773601435, 1.4155126222, -1.7163400668\C, 0, 11.491503916, -0.0068600601, -0.1192546701\C, 0, 14.2978819328, -0.0087121345, -0.1255156404\C, 0, 12.2119298035, -0.1213427696, 1.0748818973\C, 0, 12.2067496254, 0.1066553195, -1.3165955857\C, 0, 13.5949799625, 0.1051547052, -1.319784086\C, 0, 13.6001621847, -0.1216665599, 1.0718742712\H, 0, 11.682534825, -0.1860744419, 2.0146427198\H, 0, 11.6732464125, 0.1720521151, -2.2539855692\H, 0, 14.1274733318, 0.1854689338, -2.2569019717\H, 0, 14.136723823, -0.2027009348, 2.0066055379\C, 0, 5.7047669648, -0.0035770483, -0.1071198635\C, 0, 2.8691708721, -0.0023906754, -0.101948116\C, 0, 4.9780069263, 1.1534918781, -0.4273653297\C, 0, 4.9782096802, -1.1600045472, 0.2158997244\C, 0, 3.5986694997, -1.1633130962, 0.2111544062\C, 0, 3.5984951363, 1.1579520329, -0.4175885548\H, 0, 5.5025892681, 2.0661587025, -0.6662043475\H, 0, 5.5029025904, -2.0731124231, 0.4528004503\H, 0, 3.0808693796, -2.0709287256, 0.4804717419\H, 0, 3.0804837729, 2.066096335, -0.6849934784\C, 0, 1.4098075967, -0.00185725, -0.099579894\C, 0, -1.

4347740828, -0.0008094938, -0.095612074\C, 0, 0.6765777413, 1.1826733827, 0.1294006348\C, 0, 0.675069792, -1.1858815135, -0.3263141765\C, 0, -0.6966792571, -1.1844901803, -0.3370039718\C, 0, -0.6951420774, 1.1822896255, 0.1439493647\H, 0, 1.1978518131, 2.1061234874, 0.3255695599\H, 0, 1.1951107109, -2.1097113238, -0.5239580591\H, 0, -1.2106756316, -2.1166718994, -0.5060391396\H, 0, -1.2079632452, 2.1148425864, 0.31452147\C, 0, -2.8803593686, -0.0002377235, -0.0939793902\C, 0, -5.7278990938, 0.0010283791, -0.091110006\C, 0, -3.6216422045, -1.0328001031, -0.7200297037\C, 0, -3.6194643642, 1.0329491922, 0.53360327\C, 0, -4.9894009834, 1.0256994096, 0.5459409221\C, 0, -4.9915917877, -1.024331577, -0.7295817283\H, 0, -3.1089297893, -1.833158512, -1.2278962853\H, 0, -3.1050004315, 1.8328713558, 1.0403799524\H, 0, -5.5060911721, 1.8384497055, 1.0301488431\H, 0, -5.5099920218, -1.8366145936, -1.2127428112\C, 0, -7.1819314011, 0.0017089672, -0.0897598452\C, 0, -10.0209163292, 0.0029899873, -0.0871170439\C, 0, -7.9161516378, -0.6907743883, -1.0736285284\C, 0, -7.9136948965, 0.6948740542, 0.8954542702\C, 0, -9.2909436588, 0.6866732786, 0.9005154074\C, 0, -9.2933984801, -0.6813405404, -1.0761114366\H, 0, -7.4020958432, -1.2191735889, -1.8609190113\H, 0, -7.3976944364, 1.2228384734, 1.6817612651\H, 0, -9.8130466395, 1.2372488296, 1.6678377181\H, 0, -9.8174224901, -1.2314547675, -1.8424530611\C, 0, -11.4914515994, 0.003634343, -0.0857469573\C, 0, -14.3246620696, 0.004806212, -0.0831006921\C, 0, -12.2179947627, -0.0811763369, -1.281401991\C, 0, -12.2156924795, 0.0890621654, 1.1112600976\C, 0, -13.5989373378, 0.0855450609, 1.1114874076\C, 0, -13.6012323008, -0.0765179628, -1.2790382152\H, 0, -11.6976936468, -0.1288395864, -2.2263455638\H, 0, -11.6935822682, 0.1362988439, 2.0552253043\H, 0, -14.1239814507, 0.1636942784, 2.0520065955\H, 0, -14.1281054244, -0.1542423002, -2.2185658054\C, 0, -15.8042889321, 0.0053901551, -0.0817445934\C, 0, -16.5213905312, -0.6248792659, 0.9415889952\H, 0, -15.9897940779, -1.139680817, 1.7288442138\C, 0, -17.9094402067, -0.6251036552, 0.942297843\H, 0, -18.443489944, -1.1253123675, 1.737704148\C, 0, -18.6102578008, 0.006452497, -0.0792020382\C, 0, -17.9108138788, 0.6374801129, -1.1019699904\H, 0, -18.4459262808, 1.138088574, -1.8964099268\C, 0, -16.5227657018, 0.6362060072, -1.1037782207\H, 0, -15.9922096756, 1.1505969593, -1.8920059189\H, 0, 15.3785284413, -0.0094227295, -0.1279228901\H, 0, -19.6908762979, 0.0068589106, -0.0782250744\\Version=EM64L-G09R evC.01\HF=-1848.3683328\S2=0.781196\S2-1=0.\S2A=0.750855\RMSD=4.161e-09\Dipole=-1.16656, 0.0006192, 0.0043247\Quadrupole=136.4170818, -69.2459433, -67.1711385, -0.0814972, 0.7138363, 0.3137435\PG=C01 [X(C48H34)]\@\

HPP9+*

1\1\GINC-HPC-CN16\Stability\UBLYP\6-31G(d)\C54H38(1+,2)\TALIPOVM\02-Sep-2013\0\#\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title\1,2\C, 0, 10.0196359438, -0.0033776758, -0.1230479741\C, 0, 7.1866359039, -0.0033175206, -0.1151390998\C, 0, 9.2931675693, 0.8581750716, -0.9520345408\C, 0, 9.2977655234, -0.8649100092, 0.7099620314\C, 0, 7.9129679435, -0.8666573004, 0.713155382\C, 0, 7.9083729524, 0.859975686, -0.9474914417\H, 0, 9.8175616379, 1.5472572421, -1.597936408\H, 0, 9.8257361155, -1.554014311, 1.352915095\H, 0, 7.3910746395, -1.5354030253, 1.3819713117\H, 0, 7.3827838383, 1.5287223514, -1.613406477\C, 0, 11.5006288295, -0.0033940197, -0.1271597149\C, 0, 14.3074711016, -0.0033344383, -0.134966166\C, 0, 12.2219398118, -0.1985818677, 1.0557838828\C, 0, 12.2153440258, 0.1918034555, -1.3140960305\C, 0, 13.6036997771, 0.191731297, -1.3181324173\C, 0, 13.610297243, -0.1984465233, 1.0520926235\H, 0, 11.6928151053, -0.3276657454, 1.9890924068\H, 0, 11.6810171091, 0.320863614, -2.2444353967\H, 0, 14.1355644683, 0.3365090794, -2.2478954378\H, 0, 14.1473349338, -0.3432003672, 1.9788798836\C, 0, 5.710502068, -0.0032785577, -0.1110251921\C, 0, 2.8761017026, -0.00324846

02, -0.1033763771\C, 0, 4.9842737887, 1.1769642052, -0.321436101\C, 0, 4.9853
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6271694\C, 0, 3.6027490149, 1.179480166, -0.3121947953\H, 0, 5.5087976872, 2.
1081232989, -0.4750743239\H, 0, 5.5107226324, -2.1146535915, 0.254227463\H,
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949\H, 0, 1.2030017078, 2.0296005105, 0.5937066996\H, 0, 1.1996271725, -2.036
1929236, -0.7919049924\H, 0, -1.2106775765, -2.0478057371, -0.7687236831\H,
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5821995\H, 0, -3.1012278699, 1.6380778742, 1.3073460884\H, 0, -5.5011014009,
1.6489362851, 1.3004576527\H, 0, -5.5081988255, -1.6544338134, -1.466464401
9\C, 0, -7.1776237178, -0.002235779, -0.0792359377\C, 0, -10.0198973902, -0.0
013780306, -0.0726831492\C, 0, -7.9166347869, -0.5778709211, -1.1369283804\
C, 0, -7.9114160766, 0.5738787325, 0.9818280323\C, 0, -9.2857301558, 0.564046
2053, 0.9884207463\C, 0, -9.2909601618, -0.5672254612, -1.1371627539\H, 0, -7
.4050690902, -1.0129599075, -1.98034669\H, 0, -7.395708015, 1.0087875891, 1.
822807124\H, 0, -9.8052875343, 1.023634316, 1.8145056632\H, 0, -9.8146028931
, -1.026463096, -1.9608547693\C, 0, -11.4849727143, -0.0009270384, -0.069335
2723\C, 0, -14.3198766121, -0.0001281341, -0.0628814588\C, 0, -12.2152769111
, 0.0004780079, -1.2684251446\C, 0, -12.2098149412, -0.0018902314, 1.1330647
212\C, 0, -13.5911869108, -0.0073702867, 1.1346563596\C, 0, -13.5966340865, 0
.0067341605, -1.2637139379\H, 0, -11.6983352751, 0.0220948771, -2.215765373
\H, 0, -11.6885847108, -0.0237998696, 2.0780416491\H, 0, -14.1136610755, 0.00
22459827, 2.0794030045\H, 0, -14.1234145515, -0.0025994612, -2.2060589002\C
, 0, -15.795873583, 0.000230703, -0.0595545501\C, 0, -16.518005469, -0.663099
4407, 0.9393788536\H, 0, -15.993071092, -1.2010093407, 1.7152290229\C, 0, -17
.9027379864, -0.6639050735, 0.9407433867\H, 0, -18.4272372942, -1.175573988
9, 1.7345075736\C, 0, -18.6290502373, 0.0008537459, -0.0531634456\C, 0, -17.9
069352021, 0.6652860499, -1.0503412934\H, 0, -18.4347719885, 1.1771617933, -
1.841754861\C, 0, -16.5222100143, 0.6638703116, -1.0552327166\H, 0, -16.0005
657645, 1.2015172997, -1.8334864295\C, 0, -20.1099880536, 0.001162824, -0.04
98053333\C, 0, -20.8273155982, -1.1296475131, 0.3557688291\H, 0, -20.2951762
609, -2.0234440709, 0.6484249684\C, 0, -22.2156635195, -1.1295966471, 0.3587
60514\H, 0, -22.7495484962, -2.0169638606, 0.6683641678\C, 0, -22.9168347874
, 0.0017313917, -0.0433505408\C, 0, -22.2170605458, 1.1327708611, -0.4486923
686\H, 0, -22.7520041649, 2.0203550378, -0.7558365793\C, 0, -20.8287131417, 1
.1322609988, -0.4520887951\H, 0, -20.2975770468, 2.0258478797, -0.747196231
8\H, 0, 15.3881437845, -0.00330609, -0.1379688591\H, 0, -23.9975080693, 0.001
951831, -0.0408644005\\Version=EM64L-G09RevC.01\HF=-2079.2919029\S2=0.7
80471\S2-1=0.\S2A=0.750815\RMSD=3.034e-09\Dipole=-0.1325455, -0.0009744
, 0.001708\Quadrupole=173.4023668, -86.9822774, -86.4200894, 0.0046228, 0.8
828024, -0.9331754\PG=C01 [X(C54H38)]\@

HPP10+*

1\1\GINC-HPC-CN20\Stability\UBLYP\6-31G(d)\C60H42(1+,2)\TALIPOVM\02-Sep-2013\0\#\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title\1,2\C,0,10.0335469704,-0.0143927429,-0.1200857099\C

,0,7.200234723,-0.0078778931,-0.117247076\C,0,9.3106576975,0.885216400
7,-0.9104183177\C,0,9.3081135483,-0.9107026529,0.6716604194\C,0,7.9228
815073,-0.9086514258,0.6726870025\C,0,7.925423517,0.8895366099,-0.9086
67013\H,0,9.8378894843,1.6015954533,-1.5236626164\H,0,9.8332763799,-1.
6295145078,1.2838322832\H,0,7.3975024586,-1.6056279797,1.3093772319\H,
0,7.4019618899,1.5888883313,-1.5443327911\C,0,11.5148980084,-0.0177937
607,-0.1214983148\C,0,14.3221107109,-0.0243126153,-0.1241303834\C,0,12
.2336062154,-0.2636198582,1.0534762975\C,0,12.2325296375,0.2247079922,
-1.297818088\C,0,13.6209702855,0.2216279799,-1.2993371695\C,0,13.62204
47753,-0.2669973622,1.0523923004\H,0,11.7021532107,-0.4302557842,1.979
5091894\H,0,11.7001179235,0.3938234823,-2.2228489325\H,0,14.1549114233
,0.4038380269,-2.2213363501\H,0,14.1568605489,-0.4516914614,1.97338999
64\C,0,5.7224187965,-0.0044522583,-0.1156522568\C,0,2.8886230922,0.002
0727617,-0.1121448314\C,0,4.9999125661,1.1873048827,-0.2536088278\C,0,
4.9947750504,-1.1928742301,0.0240004813\C,0,3.6117586145,-1.1912868931
,0.0217175208\C,0,3.6169016301,1.1920851545,-0.247893306\H,0,5.5271459
388,2.1249901562,-0.3486763136\H,0,5.5179085668,-2.1329771247,0.117803
2037\H,0,3.0886068915,-2.1274590009,0.1475839107\H,0,3.0977174885,2.13
06521599,-0.3723822535\C,0,1.4181490024,0.0053936469,-0.1099057152\C,0
, -1.4202733402,0.0111949904,-0.1042736725\C,0,0.6927133772,1.105473446
3,0.3788096999\C,0,0.6862923364,-1.0915395653,-0.5960905744\C,0,-0.691
2075648,-1.086702686,-0.6025022589\C,0,-0.6847657779,1.1062600147,0.39
07130936\H,0,1.2184508503,1.9604989394,0.7750748478\H,0,1.2069355415,-
1.9486964575,-0.9944691415\H,0,-1.2095492351,-1.9573473222,-0.97238414
03\H,0,-1.1981064151,1.9789759005,0.7626943576\C,0,-2.875128429,0.0135
85913,-0.1005040597\C,0,-5.7213139573,0.0161034547,-0.0910448466\C,0,-
3.6151920551,-0.7874046334,-1.0004949823\C,0,-3.6078029914,0.816521738
,0.8037995954\C,0,-4.978271456,0.8084845125,0.8179544636\C,0,-4.985703
2464,-0.7769372653,-1.0054850841\H,0,-3.0995443578,-1.4009734001,-1.72
15852556\H,0,-3.0862533877,1.4292590437,1.5213275577\H,0,-5.4893280542
,1.4449395286,1.5219118653\H,0,-5.5025580264,-1.4124384314,-1.70603648
99\C,0,-7.1674896837,0.0160768283,-0.0853326137\C,0,-10.0121276147,0.0
135572158,-0.0728857945\C,0,-7.9106069383,-0.4073482289,-1.2130428066\
C,0,-7.9014763703,0.4387524912,1.0486171386\C,0,-9.2731557637,0.425463
9863,1.0576313531\C,0,-9.2823340655,-0.3964733484,-1.210017933\H,0,-7.
4001191954,-0.7204055706,-2.1091928907\H,0,-7.3836646195,0.7526696729,
1.9402347735\H,0,-9.7896248139,0.7649050362,1.9413094503\H,0,-9.805949
2865,-0.7369091827,-2.0890818771\C,0,-11.4709537191,0.0111083623,-0.06
61880191\C,0,-14.307413492,0.0045818129,-0.0529360517\C,0,-12.20686728
32,0.1279591567,-1.2594584671\C,0,-12.1951655174,-0.1087875572,1.13390
344\C,0,-13.5743031399,-0.1197874042,1.1377564613\C,0,-13.5860324375,0
.1326293833,-1.2504013858\H,0,-11.6941179727,0.2437349308,-2.201778760
8\H,0,-11.6730945478,-0.2221516474,2.0713562294\H,0,-14.0937209522,-0.
204569395,2.0800721969\H,0,-14.1146326131,0.2150172484,-2.1878128249\C
,0,-15.7803306671,0.0006886925,-0.0460310873\C,0,-16.4988338103,-0.738
1852934,0.9027476221\H,0,-15.9716774962,-1.3323468519,1.6345174867\C,0
, -17.8825748326,-0.7440044631,0.9063941598\H,0,-18.4028901427,-1.31595
59043,1.6605244376\C,0,-18.6137137227,-0.0069315475,-0.0327278272\C,0,
-17.8953937091,0.734011426,-0.9786776171\H,0,-18.4258236819,1.30311225
36,-1.7279070533\C,0,-16.5116648361,0.7356211046,-0.9880263508\H,0,-15
.9945470079,1.3325026229,-1.7247221791\C,0,-20.092247337,-0.0108686158
, -0.0257549877\C,0,-20.8114542119,-1.1594079085,0.3214577043\H,0,-20.2
830361845,-2.0672051178,0.5744407103\C,0,-22.1968662139,-1.1627148298,
0.3273048324\H,0,-22.7193723223,-2.0637199372,0.614472128\C,0,-22.9256
967129,-0.0183172678,-0.0123112912\C,0,-22.2061497514,1.1298766659,-0.
3588230489\H,0,-22.7361056027,2.0281051695,-0.6409819029\C,0,-20.82074
93379,1.1338541593,-0.3661147822\H,0,-20.299514208,2.0443962063,-0.624

0767378\C,0,-24.4071994119,-0.0221699108,-0.0052219058\C,0,-25.1264367
847,1.1023920691,0.4137895658\H,0,-24.5951430615,1.9777794907,0.759054
1971\C,0,-26.5148967736,1.099099517,0.4203923289\H,0,-27.0498900591,1.
9765702865,0.7554261414\C,0,-27.2146400434,-0.0294949526,0.0083376241\
C,0,-26.513029106,-1.1544234945,-0.4105085899\H,0,-27.0466429883,-2.03
46844646,-0.7403838722\C,0,-25.1245731121,-1.150467573,-0.4173183195\H
,0,-24.5920816139,-2.0230800169,-0.7677140928\H,0,15.4028028442,-0.026
8231483,-0.125145588\H,0,-28.2953304387,-0.0323153645,0.0135581317\Ver
sion=EM64L-G09RevC.01\HF=-2310.2154102\S2=0.779853\S2-1=0.\S2A=0.7507
84\RMSD=1.675e-09\Dipole=0.9285902,0.0215395,-0.0180419\Quadrupole=219
.5458996,-109.4195291,-110.1263705,-0.1560488,1.1349415,0.4501403\PG=C
01 [X(C60H42)]\@

^{RO}PP_n (Alternant conformer)

ROPP2

1\1\GINC-HPC-CN55\F0pt\RBLYP\6-31G(d)\C14H1402\TALIPOVM\13-Sep-2013\0\
\#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRFF(PCM,solvent=Dic
hloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Tit
le\0,1\C,-0.2573472471,1.0870751744,0.2286615293\C,-0.1919885077,3.39
58953877,1.8455184444\C,-1.0199403619,2.2198943479,-0.088688241\C,0.53
34176952,1.149639508,1.3760625577\C,0.5724693231,2.2820761001,2.183042
5201\C,-0.9893223803,3.3547498286,0.6998216346\H,-1.6640595114,2.20401
89361,-0.9563849983\H,1.1537010589,0.3057744328,1.6430919439\H,1.20504
4805,2.2846844625,3.0562147268\H,-1.5863420304,4.2202295164,0.45193478
02\C,-0.2903358641,-0.1257633887,-0.6206742008\C,-0.3514266551,-2.4340
860254,-2.2384897604\C,-0.3878379647,-0.0385037488,-2.0094336356\C,-0.
2240308879,-1.4092891539,-0.0606184682\C,-0.2513974539,-2.5436640638,-
0.849940647\C,-0.4211724046,-1.1699299616,-2.818116023\H,-0.4180528768
,0.9330424428,-2.4820482894\H,-0.1713695543,-1.521227196,1.0130219994\
H,-0.2077672893,-3.5288505562,-0.4090143191\H,-0.4900273004,-1.0507698
904,-3.8875182171\0,-0.3736389419,-3.6024293285,-2.9283599187\C,-0.484
0782991,-3.5507079351,-4.3368351967\H,-0.4897528651,-4.5817426813,-4.6
757686088\H,0.3633645105,-3.028956152,-4.7837442123\H,-1.4103385843,-3
.064110018,-4.6457396791\0,-0.2294515405,4.5512643087,2.5562637533\C,0
.5527448442,4.6452535714,3.7301422877\H,0.36902708,5.6353062331,4.1350
924801\H,1.6157350113,4.5373605485,3.5098644486\H,0.2591641923,3.89451
53008,4.4652013093\Version=EM64L-G09RevC.01\HF=-691.9629175\RMSD=4.73
8e-09\RMSF=6.883e-07\Dipole=0.3475839,0.0754922,-0.12125\Quadrupole=-7
.9797727,-5.3620671,13.3418398,2.2654736,6.055262,7.9264081\PG=C01 [X(
C14H1402)]\@

ROPP3

1\1\GINC-HPC-CN53\F0pt\RBLYP\6-31G(d)\C20H1802\TALIPOVM\13-Sep-2013\0\
\#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRFF(PCM,solvent=Dic
hloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Tit
le\0,1\H,0.108728168,0.5934011502,-2.5456563922\C,-0.1422962898,0.542
5524516,-1.495679666\C,-0.697348509,0.4508986173,1.2097006135\C,-0.433
1481913,-0.6957020345,-0.9135276115\C,-0.1288511613,1.7065565631,-0.74
33177707\C,-0.40649678,1.6891530457,0.6275485517\C,-0.7107932461,-0.71
31056271,0.4573389432\H,0.1326975598,2.6389338674,-1.2231964049\H,-0.9

723419029, -1.6454829767, 0.9372175726\H, -0.9483730315, 0.4000498347, 2.2596772999\C, -0.3937637484, 2.9323174432, 1.4311082216\C, -0.3702826908, 5.299091447, 2.9605866289\C, -0.8345683525, 4.1448612462, 0.9006329007\C, 0.0619614534, 2.9368462411, 2.7569809599\C, 0.0748486407, 4.094958486, 3.5107923929\C, -0.8270070903, 5.3195410681, 1.6450207391\H, -1.2153374594, 4.1782493135, -0.1102041951\H, 0.4329528283, 2.022616345, 3.1978048589\H, 0.4360969084, 4.0919211322, 4.5287600178\H, -1.1855959321, 6.2308752479, 1.1940838596\C, -0.445880916, -1.938866601, -1.7170874397\C, -0.4693596748, -4.3056400842, -3.246565923\C, -0.9016101595, -1.9433962155, -3.0429587332\C, -0.0050720596, -3.1514095158, -1.186613178\C, -0.0126323168, -4.3260891898, -1.9310011358\C, -0.9144964198, -3.1015084936, -3.796770074\H, -1.2726053916, -1.0291670982, -3.4837810421\H, 0.3756998051, -3.1847963499, -0.1757770999\H, 0.3459588151, -5.2374228332, -1.4800650525\H, -1.275747801, -3.0984723011, -4.8147365537\O, -0.3196615022, 6.380846546, 3.7767182724\C, -0.7502030391, 7.6289166961, 3.2701403873\H, -0.6196217683, 8.3417879895, 4.0779586936\H, -1.8016960558, 7.5996576365, 2.9812677677\H, -0.1494164612, 7.939177949, 2.4141306747\O, -0.5199797371, -5.3873950305, -4.0626982504\C, -0.0894382202, -6.6354654378, -3.5561214865\H, -0.2200167462, -7.3483359439, -4.3639410209\H, -0.6902258588, -6.9457281674, -2.7001129773\H, 0.9620543342, -6.6062064173, -3.2672473483\\Version=EM64L-G09RevC.01\HF=-922.8867185\RMSD=4.242e-09\RMSF=4.771e-07\Dipole=-0.0000001, 0.0000015, 0.0000009\Quadrupole=-14.3041189, 25.6872054, -11.3830866, -7.167216, -0.8956841, -0.3877946\PG=C01 [X(C20H1802)]\@

ROPP4

1\1\GINC-HPC-CN51\FOpt\RBLYP\6-31G(d)\C26H22O2\TALIPOVM\13-Sep-2013\O\ \#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRf(PCM,solvent=Dichloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Tit le\ \O,1\H,1.2747825363, -1.1692493292, -2.9607080012\C, 0.5691141993, -1.0572626095, -2.1499164823\C, -1.161012557, -0.7593643471, -0.0151731882\C, -0.3090130295, -2.1034940193, -1.8478018516\C, 0.5806758159, 0.1106796641, -1.4038947354\C, -0.2837080692, 0.2869075279, -0.3185278558\C, -1.1744585049, -1.925990504, -0.7631297425\H, 1.2947042092, 0.8837882431, -1.6494424965\H, -1.8901829879, -2.6980829586, -0.5192551679\H, -1.8660115553, -0.6474009224, 0.7961868511\C, -0.2712894365, 1.5340244675, 0.4785642311\C, -0.2489910148, 3.9251688304, 2.0067183259\C, -0.4983535221, 1.5154241689, 1.8585839433\C, -0.0321322425, 2.7753923135, -0.1198317631\C, -0.0224832889, 3.9432380607, 0.6263930648\C, -0.4857841284, 2.6830092418, 2.6050558755\H, -0.6547322355, 0.5718818799, 2.3616818786\H, 0.1163767795, 2.8337011709, -1.18864537\H, 0.1330269976, 4.8867212307, 0.1228797524\H, -0.6319339213, 2.6246134222, 3.6742076384\C, -0.2391404991, 5.1728087749, 2.8031533551\C, -0.2221078963, 7.5475794112, 4.3195409758\C, -1.1064493907, 5.3530084649, 3.8807609388\C, 0.6424964059, 6.2207224996, 2.5028396721\C, 0.6541270088, 7.3871010622, 3.2437030052\C, -1.1071804684, 6.5200690276, 4.6368983663\H, -1.8174187504, 4.5779664047, 4.1291669081\H, 1.3457992657, 6.1114438727, 1.6897017524\H, 1.3430002034, 8.1862049277, 3.0121502001\H, -1.802547843, 6.6169274375, 5.4551033411\C, -0.3219449835, -3.3501754867, -2.645699774\C, -0.347698514, -5.7233845731, -4.1644474751\C, -0.0994148712, -3.3299836091, -4.0297752656\C, -0.5556237593, -4.590492098, -2.0515534755\C, -0.5713764267, -5.7684653501, -2.7904630641\C, -0.1108700507, -4.4913609793, -4.7784185859\H, 0.0630335806, -2.3867794949, -4.5314697968\H, -0.7080306096, -4.6505035025, -0.983358606\H, -0.7476741637, -6.704615331, -2.285506894\H, 0.0519991441, -4.4665842075, -5.8459140986\O, -0.3402418301, -6.8059610637, -4.980630696\C, -0.5856154899, -8.0787709638, -4.4152116135\H, -0.5410369469, -8.7858665722, -5.2372798459\H, -1.5723314192, -8.1245115811, -3.952425135\H, 0.172444148

8, -8.3378925537, -3.674899585\0, -0.1364346115, 8.7251864749, 4.9859705606
\C, -0.9926397844, 8.938969669, 6.0910227313\H, -0.7513416758, 9.9265248881
, 6.4708701461\H, -0.8226802169, 8.199209298, 6.8744423312\H, -2.0414535998
, 8.9137396221, 5.7922847205\\Version=EM64L-G09RevC.01\HF=-1153.8103151\
RMSD=6.562e-09\RMSF=8.577e-07\Dipole=-0.5719608, -0.549721, 0.8663092\Qu
adrupole=-14.5355843, 14.6517952, -0.1162108, -1.1713398, -10.6499798, 11.7
119769\PG=C01 [X(C26H22O2)]\@

ROPP5

1\1\GINC-HPC-CN50\FOpt\RBLYP\6-31G(d)\C32H26O2\TALIPOVM\13-Sep-2013\0\
\#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCR(PCM,solvent=Dic
hloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Tit
le\0,1\H,1.6824997201, -1.2812424565, -0.2686115314\C, 0.8385322771, -0.6
078466308, -0.3124780347\C, -1.2629394471, 1.1826633691, -0.4573328151\C, -
0.2465341768, -0.9115696785, -1.1412512147\C, 0.8721177299, 0.5639162647, 0
.4265918214\C, -0.1778721631, 1.4863872449, 0.3714392617\C, -1.2965255137,
0.0108997213, -1.1964014669\H, 1.7415154079, 0.7792026974, 1.0311498934\H,
-2.1659236936, -0.2043871865, -1.8009585882\H, -2.1069077525, 1.8560580838
, -0.50119803\C, -0.2823848679, -2.1630542563, -1.9307139373\C, -0.35133693
94, -4.5621597811, -3.4442073189\C, -0.8548769098, -2.1998241664, -3.206299
3992\C, 0.2552616337, -3.3527926374, -1.4291510315\C, 0.220179761, -4.52484
72029, -2.1679005347\C, -0.886810673, -3.3712103388, -3.9461691876\H, -1.25
14358446, -1.2931778969, -3.6405184475\H, 0.6778180956, -3.3710064049, -0.4
346997082\H, 0.6158023355, -5.4315903312, -1.7330118184\H, -1.3069548424, -
3.3525426759, -4.9416385324\C, -0.142020645, 2.7378715493, 1.160902958\C, -
0.0730592756, 5.1369769723, 2.6743962261\C, -0.679647177, 3.9276161936, 0.6
593329871\C, 0.43045769, 2.7746357501, 2.4364947394\C, 0.4623946078, 3.9460
215683, 3.1763650213\C, -0.6445597145, 5.0996708735, 1.3980820391\H, -1.102
1890617, 3.9458353223, -0.3351243423\H, 0.8270024072, 1.8679852949, 2.87071
81517\H, 0.8825274376, 3.9273497736, 4.1718390795\H, -1.0401648733, 6.00641
88575, 0.9631876145\C, -0.0361435975, 6.3890961353, 3.4628967044\C, 0.03568
46108, 8.7730375838, 4.962977106\C, -1.0897773273, 7.3125227145, 3.41107408
41\C, 1.047486852, 6.6974492804, 4.285459945\C, 1.0943113014, 7.8704754018,
5.0308020391\C, -1.0586236541, 8.4829872868, 4.1448608223\H, -1.9576450271
, 7.1000494957, 2.8032694989\H, 1.8898353747, 6.0222144795, 4.3342783298\H,
1.9573458389, 8.0699613817, 5.6454482103\H, -1.878560171, 9.1850870776, 4.1
06973655\C, -0.3882458992, -5.8142785925, -4.2327090378\C, -0.4600593626, -
8.1982173203, -5.7327938839\C, -1.4718872227, -6.1226498757, -5.0552513258
\C, 0.665406034, -6.7376857364, -4.1809093178\C, 0.6342599404, -7.908148806
1, -4.9146987734\C, -1.518704725, -7.2956753083, -5.8005949017\H, -2.314249
7525, -5.4474311959, -5.1040504261\H, 1.5332819673, -6.525197572, -3.573121
6737\H, 1.4542107492, -8.6102329005, -4.8768306203\H, -2.38174877, -7.49517
76765, -6.4152224689\0, -0.0242025749, 9.9438787059, 5.643842372\C, 1.05235
99364, 10.2847189193, 6.4952486594\H, 0.7946585741, 11.2423085329, 6.936122
7383\H, 1.9845558667, 10.3833501428, 5.9374360362\H, 1.1821368264, 9.545681
1442, 7.2870053483\0, -0.4001653246, -9.3690556701, -6.4136627813\C, -1.476
720514, -9.7098895869, -7.2650816088\H, -1.2189974705, -10.6674580435, -7.7
05988697\H, -1.606514018, -8.9708267651, -8.0568119962\H, -2.4089139938, -9
.8085611247, -6.7072718903\\Version=EM64L-G09RevC.01\HF=-1384.733871\RM
SD=8.856e-09\RMSF=2.524e-07\Dipole=0.000006, 0.0000042, -0.0000083\Quadr
upole=-9.7419337, 2.4920421, 7.2498917, 15.7063132, 24.3376415, 24.2015571\
PG=C01 [X(C32H26O2)]\@

ROPP6

1\1\GINC-HPC-CN49\FOpt\RBLYP\6-31G(d)\C38H3002\TALIPOVM\13-Sep-2013\0\
\#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRf(PCM,solvent=Dic
hloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Tit
le\0,1\H,-2.0677072858,0.8523827566,-1.1965417206\C,-1.2400947668,1.0
446289165,-0.5288860379\C,0.8960748864,1.6155645468,1.1309500812\C,-0.
1847106695,0.1298799417,-0.4534612641\C,-1.2272394767,2.2181201761,0.2
080498896\C,-0.1589052254,2.530857743,1.055041319\C,0.8835574723,0.442
315037,0.3936125987\H,-2.0450881727,2.9159449812,0.0993724256\H,1.7016
349344,-0.2553198804,0.5019162976\H,1.723595127,1.8077055723,1.7987233
297\C,-0.197356131,-1.1228682017,-1.2416742869\C,-0.220839009,-3.52224
38543,-2.7527062314\C,-1.3871604083,-1.81937347,-1.4773729022\C,0.9804
342532,-1.6530852595,-1.7783309087\C,0.9689142077,-2.8255414997,-2.516
9315452\C,-1.3985245667,-2.9921125783,-2.215552275\H,-2.3120311438,-1.
4572917609,-1.0517491331\H,1.91392193,-1.1257276167,-1.643744698\H,1.8
937154536,-3.1873941724,-2.9428501888\H,-2.3319645132,-3.5195827083,-2
.3499811361\C,-0.1453014934,3.7849345335,1.8411065269\C,-0.1200974339,
6.1907894895,3.3450021858\C,1.0450501439,4.4801616797,2.077283026\C,-1
.3226368909,4.3191440343,2.3746909007\C,-1.3099027954,5.4932404584,3.1
108179234\C,1.0569725232,5.6560968339,2.8105767166\H,1.9702699712,4.11
53067915,1.6546294251\H,-2.2570372421,3.7931019542,2.2406406325\H,-2.2
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361315,5.6138518148\C,0.9622079036,7.7623610143,4.9784316834\C,-1.1542
214757,8.3645422502,4.04632543\C,-1.1525801606,9.548790709,4.775212772
9\C,0.979638254,8.9350570591,5.709089718\H,1.7826213709,7.0673663639,5
.0864773572\H,-1.985130706,8.1689666346,3.3835971838\H,-1.9808953081,1
0.2312782419,4.6727623791\H,1.8022284096,9.1664856181,6.3697735707\C,-
0.233399158,-4.7743183874,-3.5419681177\C,-0.2576681646,-7.1739166715,
-5.0558802716\C,-1.3019901312,-5.0871658093,-4.3883996434\C,0.82291810
84,-5.6881107154,-3.4697485273\C,0.8101374857,-6.8609031671,-4.2080212
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438066,-4.4949815936\H,1.651381791,-5.4961888673,-2.8029406443\H,1.628
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981531029\C,-0.2698677237,-8.4264169192,-5.8445673294\C,-0.292891925,-
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\C,-1.4538411699,-9.1259511592,-6.078657003\C,-1.4780823408,-10.303791
4172,-6.8175014721\C,0.903505765,-10.1262953585,-7.12073036\H,1.844828
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447684\H,-2.4163744043,-10.8141907726,-6.9643047275\H,1.8153900977,-10
.5236569623,-7.5418022414\0,0.0270898537,10.9623000386,6.3678605104\C,
-1.0189949453,11.9125799038,6.3154286501\H,-0.7312961739,12.7128931312
,6.9895823386\H,-1.9642364846,11.481999038,6.6485938132\H,-1.140500300
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012\C,-1.3805479207,-12.67914166,-8.3425409508\H,-1.077204604,-13.5331
375886,-8.9395521792\H,-2.0991565199,-12.0818832696,-8.9053437766\H,-1
.8464412501,-13.0303425318,-7.4208640106\Version=EM64L-G09RevC.01\HF=
-1615.6574189\RMSD=7.426e-09\RMSF=8.134e-07\Dipole=-1.1545399,0.114103
4,-0.1666261\Quadrupole=-2.8455673,23.96134,-21.1157727,0.3072393,6.92
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ROPP7

1\1\GINC-HPC-CN48\FOpt\RBLYP\6-31G(d)\C44H3402\TALIPOVM\13-Sep-2013\0\
\#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRf(PCM,solvent=Dic
hloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Tit

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ROPP8

1\1\GINC-HPC-CN47\FOpt\RBLYP\6-31G(d)\C50H38O2\TALIP0VM\13-Sep-2013\0\

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\Version=EM64L-G09RevC.01\HF=-2077.5045589\RMSD=7.510e-09\RMSF=5.629e-07\Dipole=0.0046909,0.3756998,0.0531096\Quadrupole=45.5741899,-40.8538839,-4.7203061,-8.4614642,41.1287357,-6.0070366\PG=C01 [X(C50H38O2)]\@

ROPP9

1\1\GINC-HPC-CN46\FOpt\RBLYP\6-31G(d)\C56H42O2\TALIPOVM\13-Sep-2013\0\ \#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRf(PCM,solvent=Dichloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Tit le\0,1\C,10.0655162803,-0.0215853842,-0.0361343008\C,7.2285402167,0.0111385781,-0.0658496423\C,9.3564785242,0.4744761281,-1.135324746\C,9.3223757606,-0.5014499681,1.0476219228\C,7.9366892838,-0.4837182143,1.0340777026\C,7.9707575035,0.4891394768,-1.150601754\H,9.8951690032,0.8830251174,-1.9783696387\H,9.8340127207,-0.9230436279,1.9010160141\H,7.397773608,-0.8911841561,1.8775053095\H,7.4592290766,0.9083108956,-2.0052483851\C,11.5455365328,-0.0377640519,-0.0210680845\C,14.3628009407,-0.0674187682,0.0075913432\C,12.2626239499,0.1984391269,1.151948679\C,12.2817023853,-0.2905982095,-1.1871460648\C,13.6633751313,-0.3059745941,-1.177687432\C,13.6529254107,0.1859900265,1.1788546638\H,11.7317995871,0.420603284,2.0666826238\H,11.7633901003,-0.5007579509,-2.1117610142\H,14.2234744862,-0.5109763513,-2.0782276273\H,14.1635388779,0.3833160129,2.1077333089\C,5.7485730217,0.0278367395,-0.0815548804\C,2.9133382414,0.0598860159,-0.1116599471\C,5.0333610179,-0.2037671296,-1.2611212571\C,5.0138767481,0.2757473294,1.0826144277\C,3.6282626566,0.291090883,1.0680457491\C,3.6477781919,-0.187770352,-1.2759350203\H,5.5660362168,-0.4304863538,-2.1735060617\H,5.5321086459,0.4905130157,2.0061446528\H,3.0955521157,0.5173902117,1.9805440233\H,3.1295529771,-0.4022266792,-2.1995564269\C,1.4333614575,0.0767020954,-0.1276498261\C,-1.4014017182,0.1086518674,-0.1587622795\C,0.7262232235,0.574089813,-1.2271585113\C,0.6912618067,-0.4042750545,0.9559947964\C,-0.6943198836,-0.3886236852,0.9408102891\C,-0.6593485478,0.5896703176,-1.242400268\H,1.265787494,0.9832767772,-2.0692001202\H,1.2028271932,-0.8253342866,1.8095689437\H,-1.2338613137,-0.7978057508,1.7828752345\H,-1.1708846852,1.010704315,-2.0960060423\C,-2.8813864029,0.1252109614,-0.1749929021\C,-5.7161377521,0.1567824185,-0.2058465025\C,-3.6160811951,0.3723596934,0.9892450178\C,-3.5958680112,-0.1057982002,-1.3550237542\C,-4.9814429459,-0.0903654105,-1.3700845911\C,-5.0016561238,0.3877925725,0.9741841706\H,-3.0981091783,0.5866004987,1.9130291703\H,-3.062858896,-0.3317549149,-2.2673975127\H,-5.4994149611,-0.3046064423,-2.2938687012\H,-5.5346652878,0.6137491101,1.8865579581\C,-7.1961225079,0.1733369498,-0.2220765605\C,-10.0308857615,0.2052700851,-0.2531901161\C,-7.9381732743,-0.307684167,0.8615619079\C,-7.9032067958,0.6706078889,-1.3216496285\C,-9.2887885736,0.6862510114,-1.3368347092\C,-9.3237450724,-0.2921116962,0.8463196429\H,-7.4266349729,-0.7287146754,1.7151681083\H,-7.3636673827,1.0797919159,-2.1637149312\H,-9.8003561829,1.1073058976,-2.1904096685\H,-9.8633072775,-0.7013012002,1.6883613123\C,-11.5108626447,0.2220736014,-0.2691817098\C,-14.346097923,0.2540912578,-0.2992893213\C,-12.2453063396,0.4697253018,0.895091978\C,-12.2257834672,-0.0091412378,-1.4488875918\C,-13.6113977745,0.0061866933,-1.4634575245\C,-13.6308893836,0.4857067284,0.8802769743\H,-11.7270843481,0.6841893874,1.8187133872\H,-11.6930696512,-0.2354368895,-2.3613848618\H,-14.1296263637,-0.2085873708,-2.3869876711\H,-14.1635678552,0.7124222144,1.7926608203\O,15.7150508079,-0.1032665507,-0.0822286531\C,16.4751543675,0.1231664331,1.0886738802\H,16.2590095602,-0.6240294526,1.8534221898\H,16.2922344348,1.11878003,1.4950566403\H,17.5156825021,0.0423802215,0.7911640625\O,-24.3125778921,0.

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ROPP10

1\1\GINC-HPC-CN56\FOpt\RBLYP\6-31G(d)\C62H46O2\TALIPOVM\13-Sep-2013\0\ \#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRf(PCM,solvent=Dichloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Tit le\0,1\C,10.0806971667, -0.0444515747, -0.0510358598\C, 7.2435883436, -0.0148228692, -0.0700617522\C, 9.3673714558, 0.5005208759, -1.1239535552\C, 9.3418270031, -0.5748437865, 1.0118697148\C, 7.9560741216, -0.5587825465, 1.0035697001\C, 7.9815940329, 0.5138147666, -1.1340033737\H, 9.9027614208, 0.9482289703, -1.9490106363\H, 9.8569489155, -1.0343712126, 1.8432926346\H, 7.4205571814, -1.0056184312, 1.8290074089\H, 7.4666890212, 0.9712196476, -1.9667080841\C, 11.5607731525, -0.0588613092, -0.0414303231\C, 14.3781181245, -0.0849000301, -0.0230041957\C, 12.2812340324, 0.1260880809, 1.1386856226\C, 12.2935304033, -0.2583000942, -1.2199377008\C, 13.6752518021, -0.271810517, -1.2155005815\C, 13.6716373398, 0.1149402238, 1.1606189567\H, 11.752941292, 0.3062020919, 2.0640828961\H, 11.7725375752, -0.4278945649, -2.151368056\H, 14.2327715486, -0.4357142686, -2.1260067042\H, 14.1849063861, 0.2716158606, 2.0957624228\C, 5.7635490153, 0.0004892527, -0.0802785493\C, 2.928201278, 0.030677574, -0.100239026\C, 5.0449101665, -0.175095672, -1.2674252735\C, 5.0321614947, 0.1912308993, 1.0966949338\C, 3.6464862028, 0.2055343745, 1.0870844011\C, 3.659284854, -0.1598864911, -1.2772965062\H, 5.5749547839, -0.3570256334, -2.1913039409\H, 5.5529306073, 0.3619606495, 2.0279628967\H, 3.1162913658, 0.386817672, 2.0110463762\H, 3.1384225729, -0.3300825817, -2.2086348881\C, 1.4481840971, 0.0469361053, -0.1110274971\C, -1.3866761612, 0.0779888092, -0.1323972969\C, 0.7375303621, 0.5974935293, -1.1825548836\C, 0.709596921, -0.4876094003, 0.9496540269\C, -0.6760496784, -0.472497555, 0.9391834071\C, -0.6480725646, 0.612728462, -1.1929771118\H, 1.2744127489, 1.0482499178, -2.004836683\H, 1.2240249609, -0.9498116506, 1.7798926813\H, -1.212825874, -0.9233841246, 1.7614624747\H, -1.1623664667, 1.0751508751, -2.0231589372\C, -2.8667148892, 0.0941912992, -0.1438489435\C, -5.7015238043, 0.1261840603, -0.1662967701\C, -3.5986943341, 0.2808623492, 1.033313381\C, -3.5839962957, -0.076440671, -1.3324431932\C, -4.9695812889, -0.060700655, -1.3434270022\C, -4.9843244899, 0.2963890115, 1.0223746142\H, -3.0786414972, 0.4476037367, 1.9656922947\H, -3.0531528719, -0.2550169218, -2.256510195\H, -5.4897054797, -0.2272966394, -2.2757958844\H, -5.515262614, 0.4747431804, 1.9464457982\C, -7.181528309, 0.1435075289, -0.1784105939\C, -10.016

2493053,0.1767178661,-0.2023205594\C,-7.9214249432,-0.393419192,0.8801353786\C,-7.8907139979,0.6975391187,-1.2491024751\C,-9.2762889824,0.7138286919,-1.2607530913\C,-9.3070467784,-0.3772555807,0.8684063296\H,-7.4081386481,-0.8582881836,1.709585706\H,-7.3527652128,1.1501986761,-2.0696354374\H,-9.7895158239,1.1788819535,-2.0901204486\H,-9.8449589328,-0.8299540319,1.6889406793\C,-11.4962561666,0.1941110004,-0.2150947455\C,-14.3311093651,0.2285326908,-0.2401084069\C,-12.2291581018,0.3792313704,0.9617219666\C,-12.2125706072,0.0262408788,-1.404649558\C,-13.5981373775,0.0430165226,-1.4168459949\C,-13.6147657931,0.3960949582,0.9494870945\H,-11.7098128263,0.5437932916,1.894892629\H,-11.6809943713,-0.1510544896,-2.3285531898\H,-14.1175128769,-0.1216128052,-2.3499788641\H,-14.146376812,0.5733656151,1.8733761625\O,15.7301254798,-0.1143372574,-0.1186124857\C,16.493647597,0.0607851741,1.0588404104\H,16.2812237127,-0.7202882735,1.7900420737\H,16.3104036881,1.0368751696,1.5099597322\H,17.5333379239,-0.0047285263,0.7547196071\O,-28.6133596624,0.373438271,-0.2824829347\C,-29.3645521717,0.9208626495,-1.3483674239\H,-29.1568936058,1.9840744563,-1.4761738544\H,-30.4075295456,0.788525111,-1.0792395653\H,-29.1642167099,0.3988976378,-2.2850094167\C,-15.8110860035,0.2471931269,-0.2535503731\C,-16.5189545389,0.8023147217,-1.3245495653\H,-15.9799321565,1.2548863856,-2.1444580828\C,-17.9045277669,0.8201024296,-1.3372469095\H,-18.4166016402,1.2861864594,-2.1667696816\C,-18.6462604002,0.2831287621,-0.2798967701\C,-17.9381623429,-0.2721642008,0.7909687834\H,-18.4772135835,-0.7249083985,1.6107448432\C,-16.5525457414,-0.2894770155,0.8040301791\H,-16.0404969523,-0.7552631485,1.6337590827\C,-20.1262057074,0.3020713794,-0.2938638488\C,-20.8423632504,0.1359265809,-1.4837007375\H,-20.3104875457,-0.0413058344,-2.4075670652\C,-22.2280394798,0.1520509268,-1.4964986986\H,-22.7466060926,-0.0138613413,-2.4299630387\C,-22.9632162015,0.3392696681,-0.3210892689\C,-22.2461354384,0.5063464186,0.8684260222\H,-22.7776713213,0.6848673572,1.7922364426\C,-20.8604341171,0.4866050778,0.8821049473\H,-20.3419554776,0.6496479406,1.816139034\C,-24.4431828314,0.3603929785,-0.3352808605\C,-25.1885736586,-0.1775632348,0.7232916158\H,-24.6780874087,-0.6378709265,1.5570854186\C,-26.5702348778,-0.1591227518,0.713868356\H,-27.1376956684,-0.5840162267,1.5288189585\C,-27.2603649641,0.4019361905,-0.3631449967\C,-26.5412041851,0.9423436864,-1.4264967183\H,-27.0442174463,1.3909075844,-2.2680117025\C,-25.1510944516,0.9164463653,-1.4009478494\H,-24.612483665,1.3624656717,-2.2248394779\\Version=EM64L-G09RevC.01\HF=-2539.3516649\RMSD=8.740e-09\RMSF=6.888e-07\Dipole=0.0054754,0.3779443,0.0576078\Quadrupole=58.3099758,-51.3618472,-6.9481286,-13.8331106,50.0704597,-8.0788041\PG=C01 [X(C62H46O2)]\@\

^{RO}PP_n⁺ (Helical conformer)

ROPP2+*

1\1\GINC-HPC-CN21\Stability\UBLYP\6-31G(d)\C14H14O2(1+,2)\TALIPOVM\25-Aug-2013\0\#\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title\1,2\C,0,-0.2150205013,1.0803864417,0.1960599195\C,0,-0.1394234295,3.3933337215,1.8115966624\C,0,-0.801374902,2.3066317167,-0.2341220724\C,0,0.4074185481,1.079550313,1.4753077561\C,0,0.4550689901,2.1982425575,2.264333962\C,0,-0.7724255079,3.4234890284,0.5472152269\H,0,-1.3123906072,2.3595126041,-1.1807519052\H,0,0.8916359077,0.1882240247,1.8371783513\H,0,0.9526350957,2.1566887385,3.2185849886\H,0,

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, -0.6206726605\C,0,-0.2955444321,-2.4076119568,-2.2423520407\C,0,-0.56
9101657,-0.0338693388,-2.0045540538\C,0,0.0507646762,-1.387118949,-0.0
877603072\C,0,0.0209079957,-2.505063063,-0.8673904927\C,0,-0.589620838
7,-1.1476481727,-2.8017725913\H,0,-0.7735914762,0.9179823686,-2.465257
4583\H,0,0.2723832772,-1.5018909334,0.9599654072\H,0,0.2292738279,-3.4
813793979,-0.4586909319\H,0,-0.8230211736,-1.0494309995,-3.8486651006\
0,0,-0.2891872627,-3.5431038495,-2.9136859959\C,0,-0.5940145918,-3.561
5844149,-4.3110737331\H,0,-0.5133421476,-4.5997748038,-4.608327912\H,0
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711,-4.4835472406\0,0,-0.1566805114,4.5253941637,2.4886198089\C,0,0.45
27503335,4.6080138712,3.7800802313\H,0,0.2959367091,5.6286998894,4.106
1217478\H,0,1.5179854675,4.3996414231,3.7119827608\H,0,-0.0269624679,3
.9192449733,4.4715054149\\Version=EM64L-G09RevC.01\HF=-691.7683344\S2=
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8,-0.0560515\Quadrupole=-23.8927956,6.7072711,17.1855245,2.1293825,9.4
939315,26.4920249\PG=C01 [X(C14H1402)]\@

ROPP3+*

1\1\GINC-HPC-CN50\Stability\UBLYP\6-31G(d)\C20H18O2(1+,2)\TALIPOVM\25-
Aug-2013\0\#\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) scrf(che
ck) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(gri
d=ultrafine)\Title\1,2\H,0,0.3590471178,0.5950593211,-2.5234013152\C
,0,0.0617310458,0.5435450017,-1.4889374789\C,0,-0.6603871967,0.4535095
853,1.1906088963\C,0,-0.332177338,-0.6985672134,-0.926596679\C,0,0.11
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17576019\C,0,-0.6864716738,-0.6939193561,0.4478654159\H,0,0.4077927822
,2.602416975,-1.2231686491\H,0,-1.0132669348,-1.6045915231,0.922463799
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2495195404\C,0,-0.4079680688,-1.8654477721,-3.1328021157\C,0,-0.367400
7883,-3.1833989467,-1.1085316313\C,0,-0.3908466527,-4.3435352296,-1.84
8156883\C,0,-0.4467835303,-3.011611461,-3.8799248082\H,0,-0.4445645612
, -0.9180272335,-3.6456630342\H,0,-0.307868556,-3.2700814759,-0.0357311
293\H,0,-0.3685063795,-5.2952466557,-1.3438814553\H,0,-0.4941469206,-2
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6,4.1748092849\H,0,0.2069355186,7.8991607956,2.4354192684\H,0,1.632394
6364,7.2949990954,3.3237596228\0,0,-0.4656882511,-5.3246179885,-4.0593
345378\C,0,-0.4574949074,-6.6403531206,-3.5113303368\H,0,-0.4858480251
, -7.3099974686,-4.3626815656\H,0,-1.3331449851,-6.8027179285,-2.885515
2512\H,0,0.4510290865,-6.8127742372,-2.9371719398\\Version=EM64L-G09Re
vC.01\HF=-922.6912851\S2=0.775084\S2-1=0.\S2A=0.75043\RMSD=5.125e-09\D
ipole=0.3742777,-0.0530317,0.1080038\Quadrupole=-39.1914976,54.2518487
, -15.0603511,10.7855072,-0.7185354,30.8262943\PG=C01 [X(C20H18O2)]\@

ROPP4+*

```
1\1\GINC-HPC-CN64\Stability\UBLYP\6-31G(d)\C26H22O2(1+,2)\TALIPOVM\25-
Aug-2013\0\#\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) scrf(che
ck) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(gri
d=ultrafine)\Title\1,2\H,0,1.518398823,-1.287960573,-2.7762709115\C,
0,0.7413263033,-1.1194759104,-2.0481571706\C,0,-1.218552173,-0.6623081
712,-0.1369648803\C,0,-0.2476327938,-2.1076495737,-1.8324876966\C,0,0.
7616499449,0.0438790431,-1.3244196725\C,0,-0.2215877477,0.3228374386,-
0.3434380528\C,0,-1.2232312865,-1.8354457697,-0.8447901183\H,0,1.53298
17183,0.7664076419,-1.5357319592\H,0,-2.0099445354,-2.5482659738,-0.65
67733571\H,0,-1.9808533273,-0.5106104404,0.6097502105\C,0,-0.207841753
3,1.5540884552,0.4116435528\C,0,-0.1797377467,3.9814418961,1.904884873
2\C,0,-1.3637670614,2.0262197529,1.0804962488\C,0,0.9622854982,2.34513
17556,0.5180917939\C,0,0.9778385735,3.5061275309,1.2461942204\C,0,-1.3
524330736,3.1995196126,1.788502032\H,0,-2.2870095328,1.4737504181,1.01
71641751\H,0,1.8754762999,2.0245859683,0.0436447552\H,0,1.8911734541,4
.0775970707,1.2877180776\H,0,-2.2559440309,3.5094701645,2.2887355586\C
,0,-0.1633223838,5.2187615349,2.6679080732\C,0,-0.1362677047,7.6207461
366,4.1399248929\C,0,-1.3432324522,5.9470213056,2.9077190895\C,0,1.038
0490243,5.7410465361,3.1967664803\C,0,1.0533069335,6.9074276095,3.9207
044329\C,0,-1.3402296108,7.1291182927,3.6212093604\H,0,-2.2803260823,5
.6050101507,2.4970235204\H,0,1.9643585796,5.2033940259,3.0677459183\H,
0,1.9703718901,7.2933239716,4.3388591831\H,0,-2.2648753834,7.663618004
4,3.7637664068\C,0,-0.2601193107,-3.3462306604,-2.5919992613\C,0,-0.28
11277486,-5.7533813248,-4.0564047023\C,0,0.3696475172,-3.4431511843,-3
.8533319218\C,0,-0.8975698943,-4.5008630732,-2.1000118289\C,0,-0.90763
38227,-5.6870998729,-2.8057461006\C,0,0.3548613977,-4.6122344256,-4.57
23264009\H,0,0.8444895481,-2.5779711153,-4.2885321495\H,0,-1.364820515
1,-4.4857868886,-1.1279325438\H,0,-1.3916472414,-6.5511431871,-2.38151
98009\H,0,0.821315848,-4.6767443155,-5.5433918489\O,0,-0.23524205,-6.8
453031206,-4.8258330141\C,0,-0.8587982568,-8.0425675972,-4.3784659093\
H,0,-0.6861848418,-8.7729571583,-5.1606068562\H,0,-1.9296547259,-7.896
4953656,-4.2437266474\H,0,-0.4115827827,-8.3897842387,-3.4481069246\O,
0,-0.0188688313,8.7481057969,4.8494378031\C,0,-1.1770385667,9.52838635
89,5.1164720712\H,0,-0.832886713,10.3744226401,5.7003135513\H,0,-1.905
9810083,8.9589983651,5.6914931621\H,0,-1.6293763647,9.8821024631,4.190
9602858\Version=EM64L-G09RevC.01\HF=-1153.6131002\S2=0.776045\S2-1=0.
\S2A=0.750512\RMSD=9.960e-09\Dipole=-0.8960427,-0.3207447,0.2897643\Qu
adrupole=-39.2069916,64.2860186,-25.079027,-2.5405488,-9.2074453,58.13
02208\PG=C01 [X(C26H22O2)]\@
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ROPP5+*

```
1\1\GINC-HPC-CN80\Stability\UBLYP\6-31G(d)\C32H26O2(1+,2)\TALIPOVM\25-
Aug-2013\0\#\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) scrf(che
ck) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(gri
d=ultrafine)\Title\1,2\H,0,0.809316399,0.1926590343,-2.5140205808\C,
0,0.3333947663,0.2071489781,-1.5458087501\C,0,-0.851024939,0.270385032
,0.9608825769\C,0,-0.2957477753,-0.9537249101,-1.0591826631\C,0,0.3846
444046,1.3605637843,-0.7976123996\C,0,-0.2113624535,1.432773456,0.4796
626912\C,0,-0.8815279935,-0.8875685164,0.2186074714\H,0,0.8681527227,2
.2274772498,-1.2190878018\H,0,-1.3879641914,-1.751158072,0.6209493683\
H,0,-1.3035935875,0.2673912022,1.9397147844\C,0,-0.3386264319,-2.18679
1379,-1.8534831955\C,0,-0.4173932776,-4.571329588,-3.38792647\C,0,-0.3
397326299,-2.1494391727,-3.2558135249\C,0,-0.3789579894,-3.446599333,-
1.2379147956\C,0,-0.4130139078,-4.6077921441,-1.9867447435\C,0,-0.3820
176197,-3.3118999339,-4.0022913248\H,0,-0.3295904947,-1.2001580406,-3.
```

7701742207\H,0,-0.3604255189,-3.52138407,-0.1609530569\H,0,-0.45537729
73,-5.5584651352,-1.4762990076\H,0,-0.3681538403,-3.2424990813,-5.0799
024526\C,0,-0.1681558732,2.6507650307,1.2650020236\C,0,-0.0844648243,5
.0470838057,2.8084023637\C,0,-1.1106881663,2.9026209479,2.2920376731\C
,0,0.8181658898,3.6420738132,1.0391638182\C,0,0.8670358465,4.786143147
3,1.788142925\C,0,-1.0793195607,4.058239134,3.024212768\H,0,-1.8929663
693,2.1879278708,2.4897880404\H,0,1.5702042379,3.488591006,0.282401326
8\H,0,1.6343810433,5.5099936749,1.5685374071\H,0,-1.8168680892,4.19512
34965,3.7977217436\C,0,-0.0434638144,6.2591066275,3.5893099438\C,0,0.0
480495561,8.6253896934,5.1197312201\C,0,-1.1718060265,6.7061266256,4.3
261686297\C,0,1.1260470766,7.0542987089,3.6571232484\C,0,1.1838010752,
8.2050626937,4.4062791765\C,0,-1.1330002372,7.857235886,5.0630803558\H
,0,-2.0973773754,6.1559241163,4.2844160259\H,0,2.0194240208,6.74338321
58,3.1407166625\H,0,2.1007511638,8.768936658,4.4444191444\H,0,-1.99764
44624,8.2044815288,5.607005471\C,0,-0.4577163506,-5.8126613298,-4.1848
519144\C,0,-0.5393393788,-8.1825810374,-5.7041272836\C,0,-1.1207757434
, -5.8662538925,-5.4127065462\C,0,0.1679633348,-6.9858282235,-3.7356875
824\C,0,0.1321681198,-8.1486097296,-4.4784946567\C,0,-1.1695071106,-7.
0297188287,-6.1698293657\H,0,-1.6368458387,-4.9918205,-5.7816974744\H,
0,0.7131584597,-6.9804186239,-2.8030722768\H,0,0.6259180213,-9.0447834
09,-4.133106345\H,0,-1.7035995771,-7.0269230667,-7.1061989316\0,0,-0.0
101595994,9.7197067234,5.8667861862\C,0,1.1340476663,10.5633190443,5.9
88678273\H,0,0.8266013613,11.3762910055,6.6353555872\H,0,1.427608384,1
0.9551525916,5.0169067426\H,0,1.9621818562,10.0230763659,6.443185484\0
,0,-0.5217588847,-9.3665423064,-6.3566803208\C,0,-1.1819618331,-9.4639
202643,-7.6052256807\H,0,-1.0367799034,-10.4853771903,-7.9409468617\H,
0,-0.751310133,-8.7781732313,-8.3355673469\H,0,-2.2493263065,-9.264231
1386,-7.5051915585\\Version=EM64L-G09RevC.01\HF=-1384.5353222\S2=0.778
004\S2-1=0.\S2A=0.750618\RMSD=2.349e-09\Dipole=0.5505272,6.8405377,3.6
204602\Quadrupole=-70.1371973,75.4581815,-5.3209842,24.9079607,9.58649
77,93.4235003\PG=C01 [X(C32H26O2)]\@

ROPP6+*

1\1\GINC-HPC-CN112\Stability\UBLYP\6-31G(d)\C38H30O2(1+,2)\TALIPOVM\26
-Aug-2013\0\#\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) scrf(ch
eck) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(gr
id=ultrafine)\Title\1,2\H,0,0.433363793,1.4059309659,-2.0949189822\C
,0,0.1953670108,1.3636589635,-1.0432418214\C,0,-0.3790411169,1.2867533
07,1.6681038018\C,0,-0.0984113455,0.1265601491,-0.4435013254\C,0,0.214
52208,2.528196974,-0.3088102026\C,0,-0.0795029044,2.5283039136,1.07033
52589\C,0,-0.3785568977,0.12186496,0.9341426098\H,0,0.4317290313,3.454
6738222,-0.8162089109\H,0,-0.6236504554,-0.8060234094,1.4274247754\H,0
, -0.5882303054,1.2310372523,2.724624907\C,0,-0.1161705412,-1.116423699
8,-1.2278855601\C,0,-0.1659855402,-3.5144578282,-2.7368469578\C,0,-0.4
783653461,-1.1140411647,-2.5820518718\C,0,0.2236257064,-2.3461651672,-
0.6471063437\C,0,0.2033680176,-3.5152019069,-1.3857651875\C,0,-0.50661
61299,-2.2856834835,-3.3162824043\H,0,-0.7645864861,-0.1901592023,-3.0
622201935\H,0,0.5278942137,-2.3879807136,0.3881878053\H,0,0.4596077901
, -4.4458164556,-0.9014377941\H,0,-0.7813088975,-2.2440597318,-4.359878
3679\C,0,-0.0778034337,3.7572388475,1.8430899933\C,0,-0.0813503765,6.1
720002989,3.359235558\C,0,-0.799039706,3.8670010093,3.0570287857\C,0,0
.6421993964,4.8994014202,1.4156043931\C,0,0.6515790423,6.054643161,2.1
487869704\C,0,-0.8117635195,5.0292867433,3.7789124954\H,0,-1.379010596
8,3.0315258998,3.4142301484\H,0,1.2219292462,4.8600016469,0.5077249878
\H,0,1.2088928514,6.8961080588,1.7715114084\H,0,-1.3717792836,5.054963

7148, 4.6989968742\C, 0, -0.0877139415, 7.3933013444, 4.1229959492\C, 0, -0.0
979591744, 9.7930673323, 5.6027665684\C, 0, -1.0840179702, 7.6530380809, 5.1
026480872\C, 0, 0.9007262826, 8.3905359779, 3.9286448429\C, 0, 0.9094368357,
9.5593896369, 4.6490468774\C, 0, -1.0956852964, 8.818053173, 5.8163299334\H
, 0, -1.8754392228, 6.9414746285, 5.2710785705\H, 0, 1.6981933885, 8.22637483
01, 3.2228265273\H, 0, 1.6904083854, 10.2819755139, 4.4814802115\H, 0, -1.864
4258558, 9.0225333406, 6.5451078317\C, 0, -0.1983310001, -4.7656705991, -3.5
219765269\C, 0, -0.2668403305, -7.1697433893, -5.0248076316\C, 0, -1.1549395
086, -4.9676622066, -4.5229615308\C, 0, 0.7242473667, -5.7916638178, -3.2901
509836\C, 0, 0.6901386796, -6.9656996837, -4.0243244229\C, 0, -1.1875035987,
-6.141700517, -5.2570231075\H, 0, -1.8940382335, -4.2047962891, -4.72075204
37\H, 0, 1.4887815153, -5.6660455832, -2.5371440547\H, 0, 1.40908113, -7.7419
77102, -3.8056959079\H, 0, -1.9310955402, -6.2552244868, -6.0326032601\C, 0,
-0.3046811266, -8.4255652342, -5.8058605914\C, 0, -0.3795947032, -10.819122
0801, -7.2897592109\C, 0, 0.8731382806, -9.1036839906, -6.1510838104\C, 0, -1
.5130675272, -8.98246203, -6.2257688734\C, 0, -1.5628934424, -10.163046854,
-6.9581219541\C, 0, 0.8408878123, -10.2773554293, -6.879011646\H, 0, 1.83093
1491, -8.6934265132, -5.8649633862\H, 0, -2.4439101586, -8.5028863615, -5.95
90014335\H, 0, -2.52102694, -10.5604512323, -7.2518717389\H, 0, 1.7527361082
, -10.7888674349, -7.1500289597\O, 0, -0.1942446344, 10.8872176481, 6.342274
4105\C, 0, 0.7549709957, 11.9428825671, 6.1894501721\H, 0, 0.448532252, 12.71
01292587, 6.8899913657\H, 0, 0.7295342754, 12.3359641411, 5.17522573\H, 0, 1.
756423826, 11.5962327661, 6.4356247281\O, 0, -0.3098950846, -11.9719842972,
-7.9977141879\C, 0, -1.5140071947, -12.5630447559, -8.4473421634\H, 0, -1.22
46135387, -13.4582477348, -8.9881055844\H, 0, -2.0576595791, -11.895948891,
-9.1174702303\H, 0, -2.1576303192, -12.8386320712, -7.6110034155\Version=
EM64L-G09RevC.01\HF=-1615.4584138\S2=0.778983\S2-1=0.\S2A=0.750664\RMS
D=2.068e-09\Dipole=0.1183691, 10.8964101, 6.3315636\Quadrupole=-91.76685
89, 122.0602254, -30.2933665, 29.100151, 13.4321786, 112.9416259\PG=C01 [X(
C38H3002)]\@

ROPP7+*

1\1\GINC-HPC-CN49\Stability\UBLYP\6-31G(d)\C44H34O2(1+,2)\TALIPOVM\26-
Aug-2013\0\#\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) scrf(che
ck) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(gri
d=ultrafine)\Title\1,2\C, 0, 9.3716651646, 4.5800436424, 0.9254315005\C,
0, 6.5689912029, 4.0642297481, 0.8210534712\C, 0, 8.588438396, 4.9498320428,
-0.199631861\C, 0, 8.6921048784, 3.9415730125, 1.9964424042\C, 0, 7.34961135
46, 3.6837244107, 1.9397215158\C, 0, 7.2414886436, 4.7131597352, -0.24310949
47\H, 0, 9.0470072075, 5.4539757475, -1.034124417\H, 0, 9.2383422027, 3.62155
77137, 2.8683126886\H, 0, 6.8804992263, 3.2037779585, 2.7831501547\H, 0, 6.69
49903597, 5.0057169046, -1.1249518059\C, 0, 10.7874861843, 4.8387394707, 0.9
759762177\C, 0, 13.5598687476, 5.3405251938, 1.0857041896\C, 0, 11.498938706
3, 4.8179700597, 2.2022639831\C, 0, 11.5336853702, 5.1271148783, -0.19906610
16\C, 0, 12.8783182348, 5.3631448624, -0.1501202328\C, 0, 12.8470744085, 5.06
8477072, 2.2678206182\H, 0, 10.9742146993, 4.6370101412, 3.1257621261\H, 0, 1
1.0488047731, 5.1267657817, -1.1612525172\H, 0, 13.446718932, 5.5622385348,
-1.0452028381\H, 0, 13.3439866976, 5.0614535598, 3.2234174692\C, 0, 5.142223
5395, 3.7995499214, 0.7671264141\C, 0, 2.35328635, 3.2787251022, 0.658046311
\C, 0, 4.2894845457, 4.5427085606, -0.0746444517\C, 0, 4.5535927676, 2.787907
0791, 1.5534609794\C, 0, 3.2021332087, 2.5308982024, 1.4922735835\C, 0, 2.935
7474737, 4.2945634538, -0.1194579354\H, 0, 4.6875652049, 5.3411088299, -0.68
05044908\H, 0, 5.1656821496, 2.177886552, 2.1987033423\H, 0, 2.7898686172, 1.
7533144284, 2.1165799414\H, 0, 2.3199701745, 4.8797525171, -0.7848463873\C,
0, 0.9094477039, 3.0071086246, 0.599443667\C, 0, -1.8721135591, 2.4813651039

,0.4790853949\C,0,-0.0108486024,4.029100333,0.329054937\C,0,0.40546573
16,1.7163758226,0.8104286595\C,0,-0.9522240912,1.4600969843,0.74723725
32\C,0,-1.3688013127,3.7721064244,0.2746926834\H,0,0.3351624921,5.0411
834299,0.1806357216\H,0,1.0826849872,0.8978809714,1.0040490251\H,0,-1.
3052014741,0.4551635883,0.9255987638\H,0,-2.0471122726,4.5823120143,0.
0517566849\C,0,-3.3225823994,2.2060816545,0.412443003\C,0,-6.103807415
8,1.6781303567,0.2808300825\C,0,-3.8065744274,0.9957827377,-0.09602934
42\C,0,-4.2597228854,3.1464657124,0.8539921209\C,0,-5.6189611183,2.887
5591932,0.7903739945\C,0,-5.1660399347,0.7385319045,-0.1609369588\H,0,
-3.1136862599,0.2518354048,-0.4617413667\H,0,-3.9234944401,4.086015786
7,1.2680821616\H,0,-6.3139253966,3.643147258,1.1268782697\H,0,-5.50282
80402,-0.2126216417,-0.5470168584\C,0,-7.5561133725,1.4030383715,0.210
7306874\C,0,-10.3402414088,0.8773507518,0.074705501\C,0,-8.1058201997,
0.6784676828,-0.8517553689\C,0,-8.4291692412,1.8589233148,1.2037585441
\C,0,-9.7894860851,1.6036973794,1.1359662971\C,0,-9.4657559007,0.42052
35817,-0.9171087276\H,0,-7.4651292368,0.323263429,-1.6461428348\H,0,-8
.0394532845,2.4091002771,2.0482457402\H,0,-10.4351891302,1.9872744667,
1.9128835614\H,0,-9.8513538096,-0.1568823821,-1.7451047223\C,0,-11.792
8119357,0.6023124103,0.0032625974\C,0,-14.5575778001,0.0772581747,-0.1
324105899\C,0,-12.4696377256,0.5835430649,-1.2244643011\C,0,-12.541698
6252,0.3508957439,1.1530603433\C,0,-13.9065913752,0.0908236327,1.09891
7727\C,0,-13.8253983947,0.3267085686,-1.2955627251\H,0,-11.9299821597,
0.7959434728,-2.1362466261\H,0,-12.0520633153,0.3331227457,2.116251076
7\H,0,-14.4417046643,-0.1069215663,2.0137427074\H,0,-14.3418259851,0.3
234529599,-2.2442102235\O,0,14.8595959544,5.5851709276,1.0314529293\C,
0,15.6418564955,5.5784754683,2.2261970971\H,0,16.6551786917,5.79215663
84,1.9085940757\H,0,15.6016308208,4.6020544376,2.704308577\H,0,15.2985
001208,6.3499701862,2.9122824854\O,0,-15.8802619857,-0.1644792048,-0.3
027724616\C,0,-16.6730545694,-0.4187749338,0.840634209\H,0,-17.6828080
459,-0.5773815225,0.4760474496\H,0,-16.6656071052,0.429691703,1.526089
3749\H,0,-16.3351934336,-1.3119065608,1.3678853283\\Version=EM64L-G09R
evC.01\HF=-1846.3818138\S2=0.779371\S2-1=0.\S2A=0.750682\RMSD=3.226e-0
9\Dipole=16.4874516,2.9514485,1.9284256\Quadrupole=241.2963138,-93.664
0223,-147.6322915,157.9178493,35.1308344,17.7958839\PG=C01 [X(C44H3402
)]\@

ROPP8+*

1\1\GINC-HPC-CN1\Stability\UBLYP\6-31G(d)\C50H38O2(1+,2)\TALIPOVM\29-A
ug-2013\0\#\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) scrf(chec
k) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid
=ultrafine)\Title\1,2\C,0,10.0431387302,0.0323194514,-0.058035952\C,
0,7.1918120649,0.0420458339,-0.0345395937\C,0,9.2927950151,0.658190899
7,-1.088220619\C,0,9.3054804483,-0.5865486126,0.9856736566\C,0,7.93718
64526,-0.5921368846,0.9890179455\C,0,7.9247589169,0.6733426817,-1.0688
185971\H,0,9.7991767418,1.159977466,-1.8960699544\H,0,9.8215178572,-1.
092299551,1.7849028164\H,0,7.4251337489,-1.0692788642,1.8087554597\H,0
,7.4026915913,1.1544989527,-1.8797755739\C,0,11.4830606903,0.024449839
, -0.0734477119\C,0,14.3022106231,0.0071563331,-0.094242494\C,0,12.2334
316339,-0.258002092,1.0961643453\C,0,12.2152839776,0.3002507658,-1.260
3119366\C,0,13.5810366188,0.285250029,-1.2753586978\C,0,13.6062286317,
-0.2615270938,1.0988075002\H,0,11.7264011309,-0.4421494425,2.028976167
6\H,0,11.6950495695,0.4905757722,-2.184469419\H,0,14.1352194721,0.4755
039198,-2.1811996275\H,0,14.1368187235,-0.46319577,2.0142908236\C,0,5.
7395800628,0.0435949571,-0.025767763\C,0,2.9002885782,0.0425283703,-0.
014474533\C,0,5.0029320353,1.0173684869,-0.7307007762\C,0,5.0093198977

, -0.929989489, 0.6860529727\C, 0, 3.6321691583, -0.9341987652, 0.6827466547\C, 0, 3.6259293561, 1.020569832, -0.7163677451\H, 0, 5.5147741486, 1.7962893342, -1.2733115141\H, 0, 5.5261668081, -1.7087530716, 1.2241678573\H, 0, 3.1116742587, -1.6925367187, 1.2470707458\H, 0, 3.1004884136, 1.7782912013, -1.2768889046\C, 0, 1.4296985645, 0.0405347906, -0.0118174699\C, 0, -1.4041113014, 0.0357639946, -0.01522955\C, 0, 0.7022751224, 1.2337472208, -0.1191902711\C, 0, 0.7060540673, -1.1549639636, 0.0956669372\C, 0, -0.6770771051, -1.1565003572, 0.0900687935\C, 0, -0.680828667, 1.2306311343, -0.1168841807\H, 0, 1.2216655162, 2.17816159, -0.1839780383\H, 0, 1.2284681147, -2.0976432671, 0.1614333417\H, 0, -1.2004343113, -2.0963216688, 0.1855977104\H, 0, -1.2070845351, 2.1686571499, -0.2140003646\C, 0, -2.8820590915, 0.0332486264, -0.0214811373\C, 0, -5.7159705624, 0.0312085539, -0.0408427412\C, 0, -3.6015143771, -1.0114815626, -0.6118511621\C, 0, -3.6109977705, 1.0761895764, 0.5603576639\C, 0, -4.9960713526, 1.0746369125, 0.5510363827\C, 0, -4.9865327324, -1.011966476, -0.6213676163\H, 0, -3.0735598315, -1.8262954503, -1.0855307011\H, 0, -3.0907199252, 1.8919784783, 1.0408267646\H, 0, -5.525165696, 1.9046063066, 0.9963971563\H, 0, -5.5083261231, -1.8426157771, -1.0739905326\C, 0, -7.1956594036, 0.0317297575, -0.0543239193\C, 0, -10.030745604, 0.035385656, -0.0832267372\C, 0, -7.9097999592, -0.4805793624, -1.1423522783\C, 0, -7.9304547078, 0.545376596, 1.0192047979\C, 0, -9.3160213066, 0.5479015677, 1.0045358519\C, 0, -9.2952834601, -0.4795939361, -1.1558830635\H, 0, -7.3764916945, -0.8716146392, -1.9968526718\H, 0, -7.4136316265, 0.9353225583, 1.8842791123\H, 0, -9.8493634284, 0.968099123, 1.8450012893\H, 0, -9.812464577, -0.8984555914, -2.0070202469\C, 0, -11.5109566798, 0.0384958173, -0.0994597661\C, 0, -14.3481119, 0.0448344997, -0.1318051767\C, 0, -12.2223350503, 0.2523740833, -1.2845070461\C, 0, -12.250014748, -0.1724798569, 1.0689827885\C, 0, -13.6358232447, -0.1670500132, 1.0533571643\C, 0, -13.6080112934, 0.252639113, -1.3005599172\H, 0, -11.686584469, 0.4340196063, -2.2052147624\H, 0, -11.736192931, -0.3569916773, 2.0015479498\H, 0, -14.1717897741, -0.3163054244, 1.979758453\H, 0, -14.1222988769, 0.4029699503, -2.238987575\O, 0, 15.6207074805, 0.021492077, -0.2082079262\C, 0, 16.4423733034, -0.2539939958, 0.9268139022\H, 0, 16.2466028598, -1.254544445, 1.3063570624\H, 0, 16.2764940307, 0.485805634, 1.7070842806\H, 0, 17.4621134784, -0.1885565216, 0.567504606\O, 0, -19.9981108591, -0.0155086931, -0.1267937379\C, 0, -20.7546714031, 0.8303681518, -0.970849399\H, 0, -20.5400348817, 0.6368378791, -2.022691439\H, 0, -20.5665262649, 1.8822511693, -0.7517130058\H, 0, -21.796176153, 0.6022097292, -0.7685773521\C, 0, -15.8282731547, 0.0490413635, -0.1485768276\C, 0, -16.5677021707, -0.8112647413, 0.675333726\H, 0, -16.0523814503, -1.5082250963, 1.3206314518\C, 0, -17.9494524421, -0.8106514432, 0.6617205317\H, 0, -18.5121007017, -1.4833268154, 1.2922853512\C, 0, -18.6456966633, 0.0569185934, -0.183041899\C, 0, -17.9324724357, 0.9211395948, -1.0102875876\H, 0, -18.4405107347, 1.6093991091, -1.6664402561\C, 0, -16.5422422338, 0.9083067974, -0.9840137837\H, 0, -16.009048228, 1.6035102432, -1.616628462\\Version=EM64L-G09RevC.01\HF=-2077.30528221\S2=0.779422\S2-1=0.\S2A=0.750685\RMSD=9.319e-10\Dipole=20.9466733, 0.2250733, 0.2951307\Quadrupole=304.8900746, -156.6604298, -148.2296448, -22.1659311, 37.1688733, -8.6737714\PG=C01 [X(C50H38O2)]\@

ROPP9+*

1\1\GINC-HPC-CN4\Stability\UBLYP\6-31G(d)\C56H42O2(1+,2)\TALIPOVM\29-Aug-2013\0\#\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\Title\1,2\C, 0, 10.054057766, 0.0637903507, -0.0765000178\C, 0, 7.2031326663, 0.0583554087, -0.0425177727\C, 0, 9.2969033476, 0.7192938853, -1.083079028\C, 0, 9.3234499141, -0.5926218879, 0.9491272473\C, 0, 7.9551805218, -0.6055051409, 0.9569572326\C, 0, 7.9288800498, 0.7270621855, -1.0580

854678\H,0,9.7977710066,1.2498920649,-1.8758657769\H,0,9.8450309944,-1.1214819303,1.729614676\H,0,7.4482117504,-1.11188545,1.7622310554\H,0,7.4010982501,1.2318944295,-1.8507737869\C,0,11.4937804282,0.0640684968,-0.0972852972\C,0,14.3127541944,0.0660453946,-0.1282215159\C,0,12.2501747269,-0.2494111664,1.0606469162\C,0,12.2199001179,0.3801055565,-1.2779470478\C,0,13.5855399789,0.3744679319,-1.2981946608\C,0,13.6228530492,-0.2436774836,1.0585469646\H,0,11.7475389539,-0.465337526,1.9890134568\H,0,11.694820104,0.5946520009,-2.1939887202\H,0,14.1352690515,0.5957121787,-2.1997072161\H,0,14.1583193959,-0.4691876968,1.9655728837\C,0,5.7507396007,0.0524451249,-0.0286448686\C,0,2.9121345241,0.0365927949,-0.0082743737\C,0,5.0072385179,1.0485043697,-0.6938386288\C,0,5.028044286,-0.9509654592,0.6483201674\C,0,3.6507762478,-0.9623756276,0.6488186043\C,0,3.6301679816,1.0444630255,-0.6745368814\H,0,5.5136313541,1.8496452797,-1.2085423557\H,0,5.5508850491,-1.7463806594,1.1554466836\H,0,3.1354928074,-1.7443154568,1.1851394879\H,0,3.0986050236,1.8202683181,-1.2037598008\C,0,1.4413950844,0.027148112,-0.001229696\C,0,-1.3917798452,0.008463066,0.0032083966\C,0,0.7082971857,1.2206522421,-0.0477610669\C,0,0.7242564156,-1.1758330901,0.0495214275\C,0,-0.6589736446,-1.1839754864,0.0474025074\C,0,-0.674856572,1.210504788,-0.0412842184\H,0,1.2234183094,2.169478951,-0.0676688489\H,0,1.2519598423,-2.1177442264,0.0674648973\H,0,-1.1779002856,-2.1297486947,0.097523742\H,0,-1.206360737,2.1493010284,-0.0901309406\C,0,-2.8698180806,-0.0009557783,0.0010278517\C,0,-5.7033114778,-0.0159558967,-0.0099957875\C,0,-3.5859600335,-1.0151939681,-0.6438925785\C,0,-3.6016252836,1.0049265203,0.6414440211\C,0,-4.9867598676,0.996702814,0.6366577924\C,0,-4.9710568748,-1.0216830313,-0.6498322753\H,0,-3.0554190617,-1.8002813003,-1.1628260345\H,0,-3.0835055367,1.7959187069,1.163988482\H,0,-5.5185882528,1.7978606573,1.1290346525\H,0,-5.4905778642,-1.8282157273,-1.1465586423\C,0,-7.1831222344,-0.0222693611,-0.0185893408\C,0,-10.0175136811,-0.0321714313,-0.037538388\C,0,-7.8983565372,-0.4652284514,-1.1359079433\C,0,-7.9162416131,0.4152603155,1.0892203726\C,0,-9.3018747976,0.4105175889,1.0797494202\C,0,-9.2839149336,-0.4702249883,-1.1449601848\H,0,-7.365976294,-0.7961722894,-2.0160047162\H,0,-7.3980146422,0.7501873601,1.9762470208\H,0,-9.8345599011,0.7704225438,1.948174844\H,0,-9.8023758704,-0.833718685,-2.0204650049\C,0,-11.4977723934,-0.0366113765,-0.0481363756\C,0,-14.3330527366,-0.0454935268,-0.0693972406\C,0,-12.2146427422,0.260576792,-1.2116772373\C,0,-12.230091101,-0.3381334308,1.1046073942\C,0,-13.6158445254,-0.3416988994,1.0943150673\C,0,-13.6003249204,0.2554174835,-1.2221839103\H,0,-11.6832645455,0.5137009489,-2.1178389691\H,0,-11.7107499229,-0.5878278348,2.018683323\H,0,-14.1476021124,-0.5641196519,2.0082602786\H,0,-14.1196888792,0.4745085701,-2.1440261186\O,0,15.6305059214,0.0936311309,-0.2459171353\C,0,16.4583882744,-0.2057690126,0.8785930601\H,0,16.2731020183,-1.2182233445,1.2307320064\H,0,16.2879983557,0.5106231159,1.6794395962\H,0,17.4762827327,-0.1208606183,0.5181721738\O,0,-24.300227919,0.0167422636,-0.1729006071\C,0,-25.0648863405,-1.1704397248,-0.09519349\H,0,-24.8630051198,-1.8294374077,-0.9406745028\H,0,-26.1044147608,-0.8600030839,-0.1221496473\H,0,-24.872114732,-1.707042149,0.8347147835\C,0,-15.8133714913,-0.0505438912,-0.0811009069\C,0,-16.5415704021,-0.9760368312,0.6732991716\H,0,-16.0187328774,-1.7125746978,1.2665707366\C,0,-17.927412283,-0.9794868239,0.6631501392\H,0,-18.4553211649,-1.6985897739,1.2730250663\C,0,-18.6505801043,-0.0614661115,-0.1056988294\C,0,-17.9213308917,0.8630417029,-0.8608926221\H,0,-18.4437111207,1.5790184679,-1.4791652609\C,0,-16.535509232,0.8699233186,-0.8473219128\H,0,-16.0081640944,1.6108127721,-1.4310853922\C,0,-20.1308285493,-0.0681790164,-0.1206075652\C,0,-20.8523480845,-1.2600581434,-0.0506432978\H,0,-20.3246323845,-2.2020839879,-0.0069117788\C,0,-22.2427297499,-1.2798008774,-0.0644931594\H,0,-22.7564382761,-2.22655295

41, -0.0175712389\C, 0, -22.9484092487, -0.0821137139, -0.1511751306\C, 0, -2
2.2445303686, 1.1222471203, -0.2223706188\H, 0, -22.8014462334, 2.045966138
7, -0.2795197058\C, 0, -20.8628326652, 1.1244615773, -0.2070143522\H, 0, -20.
3420199047, 2.0706798808, -0.2401377107\\Version=EM64L-G09RevC.01\HF=-23
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985669, -0.6378705, 0.6819722\Quadrupole=313.8626328, -157.0484059, -156.8
142268, 25.5940968, 17.1015519, -8.4207664\PG=C01 [X(C56H42O2)]\@

ROPP10+*

1\1\GINC-HPC-CN5\Stability\UBLYP\6-31G(d)\C62H46O2(1+,2)\TALIPOVM\30-A
ug-2013\0\#\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) scrf(chec
k) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid
=ultrafine)\Title\1,2\C,0,10.0706338676, -0.0501031907, -0.0256547622\
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098, -0.9890653938\C,0,9.3120636657, -0.7608836747,0.9421474407\C,0,7.94
40382211, -0.7423411965,0.9342902525\C,0,7.9720637285,0.7303492561, -0.9
800847998\H,0,9.861043842,1.2700672233, -1.7362265784\H,0,9.8101564666,
-1.3552239884,1.6899462462\H,0,7.416390605, -1.291349655,1.6971407269\H
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4538, -0.0322201562\C,0,14.3295816649, -0.1513536347, -0.0336027555\C,0,1
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, -1.1687357213\C,0,13.6248605895,0.2886305387, -1.175003366\C,0,13.6166
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0.6411557771\C,0, -4.9585181255,1.0871966943,0.6370702426\C,0, -4.966375
5055, -0.8209356188, -0.808192295\H,0, -3.0597879347, -1.5791086144, -1.382
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1.0545429885\C,0, -9.2755535303, -0.1892235703, -1.2405684636\H,0, -7.3637
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0.5580391508, -1.2186808575\C,0, -12.2051749013, -0.2640742436,1.02844171
74\C,0, -13.5909426985, -0.2682663958,1.0268409596\C,0, -13.5909123546,0.
5535795987, -1.22025863\H,0, -11.6794144414,0.8982387509, -2.0993207186\H

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^{RO}PP₅⁺ (Helical conformer; hole in the middle of the chain)

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BLYP IOP(3/76=0600004000)/6-31G(d) td(nstates=20) scrf(check) guess(read) geom(allcheck)
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