

Supporting Information

Tube and Cage C₆₀H₆₀: A Comparison With C₆₀F₆₀

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The Gaussian archive of calculated structure at B3LYP/6-31G(d,p)

Isomer 1:

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1\1\GINC-M0106\FOpt\RB3LYP\6-31G(d,p)\C60H60\JJF\18-Mar-2007\0\#\ B3LY
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Isomer 2:

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Isomer 3:

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839346\C, -1.2943643568, -2.4870593159, -2.4222285601\C, 0.1986353446, -2.9
719385224, -2.5395965501\C, -3.7718627166, 0.7592820229, -0.7877208097\C, -
3.5558687535, -0.608683011, -1.5810709006\C, -1.3581382093, -2.6810018233,
2.5961900369\C, 0.2225033526, -2.8473496384, 2.4718705985\C, 0.723336165, -
1.4142097674, 2.5477571813\C, -0.1021578507, -0.7587947546, 3.6335263672\C
, -1.5570444561, -1.2868205907, 3.3701129518\C, 2.2015138465, -2.8951907012
, 0.729587166\C, 0.8935085657, -3.6112115885, 1.2828654748\C, -0.0056418786
, -3.7852412579, 0.0014059394\C, -1.1762123365, -2.8313811887, 0.0452280398
\C, -2.1119847058, -2.8908874555, 1.2388926946\C, -3.1913848352, -1.8540330
638, 0.7882445869\C, -2.7109621396, -0.481004873, 1.1804251045\C, -2.538615
9671, -0.2919832764, 2.6817346155\C, -2.2137503282, 1.2268211128, 2.7501747
877\C, 0.8888630232, -3.3762067886, -1.2091966946\C, 1.7456588888, -2.28007
68787, -0.5933210958\C, -3.0288602048, 1.8992667202, 1.5887880772\C, -3.607
8534486, 0.6744502556, 0.7571043265\C, -3.3200384847, -1.9786311722, -0.781
68429\C, -2.0788014981, -2.8874862133, -1.1765288319\H, 1.1806266886, -2.22
86073213, -4.3414247844\H, -0.683919456, -0.9948935269, -4.5533992662\H, -2
.9117099294, -0.6771943622, -3.6657621228\H, -3.0893254744, 1.5795239589, -
3.5895356482\H, -3.488912657, 2.7271106328, -1.6798712145\H, -1.8270600469
, -2.8287372642, -3.3223203423\H, 0.2036986882, -3.8641089585, -3.174087405
5\H, -4.8112355287, 1.0480538287, -0.9745871573\H, -4.5065896002, -0.771429
8851, -2.0961119811\H, -1.7183159539, -3.463710039, 3.2698314454\H, 0.54985
72263, -3.3453681938, 3.3953944033\H, 0.2332861306, -1.1716150329, 4.596928
9634\H, -1.9993763678, -1.5234264583, 4.3430445125\H, 2.8858025354, -3.7072
618164, 0.4461480376\H, 1.1751014498, -4.6052288715, 1.6443289308\H, -0.370
9361558, -4.8177518016, -0.0849758172\H, -2.5713478158, -3.8894967066, 1.26
40388271\H, -4.161256208, -2.0397643905, 1.2698245387\H, -3.5310666262, -0.
4530681329, 3.1282651472\H, -2.4898046123, 1.6623164846, 3.7204716747\H, 1.
5706737484, -4.2096351445, -1.4341605498\H, -3.8691906063, 2.4489585381, 2.
0246736776\H, -4.6023900138, 0.4616098037, 1.1739666477\H, -4.2144214948, -

2.5746185497,-0.9835636085\H,-2.4452612555,-3.9191033359,-1.2795282853
\H,-1.7377667353,-0.3226828021,0.7011899799\H,0.4491116348,-0.93732119
58,1.5999102932\H,1.1130028259,-1.4073799158,-0.3903545371\H,-0.765220
1002,-0.6227693649,-1.5550501447\H,-0.7423056419,-1.8280148427,0.06360
63811\\Version=IA64L-G03RevC.02\State=1-A\HF=-2322.5331015\RMSD=4.153e
-09\RMSF=1.941e-05\Dipole=0.,0.,-0.0858953\PG=C02 [X(C60H60)]\ \@

Isomer 4:

1\1\GINC-M0104\FOpt\RB3LYP\6-31G(d,p)\C60H60\JJF\21-Nov-2007\0\ \#P B3L
YP/6-31G** OPT GEOM=ALLCHECK GUESS=READ\ \BB\ \0,1\C,-0.7614350441,1.212
1647973,3.6989732138\C,0.8535676445,1.2635107266,3.6565395267\C,3.2662
677937,0.4080955497,1.8819567477\C,2.2280934208,1.4245840306,1.4724990
891\C,1.5669399009,2.192391727,2.6148111533\C,0.7234850053,3.236810205
1,1.8286960524\C,-0.6338077556,2.6239471607,1.5546982033\C,-1.49780556
34,2.2054942468,2.7291584944\C,-2.761598415,1.6809237784,1.9586387167\
C,-2.6002818188,0.1959661466,1.6669009649\C,1.4751277747,3.4420808277,
0.4393980473\C,2.7158426366,2.5120223788,0.503133039\C,-2.802900215,2.
4703732842,0.5750304434\C,-1.5471207573,3.3761695721,0.5747354995\C,-0
.1049997129,0.9207488608,-2.8811435948\C,1.1071713102,0.3235876754,-3.
5761065995\C,-1.304430891,0.2583205072,-3.5429266015\C,2.6002818188,-0
.1959661466,-1.6669009649\C,2.4127217029,0.7078814451,-2.8594695883\C,
2.4909003141,2.1575108091,-2.226343244\C,1.1494210698,2.9604988644,-2.
1049422211\C,-0.1024338906,2.4369985593,-2.8919182118\C,-1.3755041228,
3.0117960657,-2.1591051401\C,-2.5805376793,2.0156724332,-2.0049583531\
C,-2.6574125433,0.6681623754,-2.8662950899\C,3.3110951722,1.9727937531
, -0.8423324949\C,3.6637052226,0.4329969558,-0.7708126647\C,-3.69843117
,0.343844815,-0.5989050577\C,-2.6735600573,1.4829189826,-0.5779372969\
C,-0.8064879845,3.5853086188,-0.7889596372\C,0.5875174375,2.9564916825
, -0.6979270073\H,-1.0490360861,1.5196445291,4.70881029\H,1.1660669273,
1.6259582733,4.6400332364\H,4.1077617188,0.9280080274,2.3597211468\H,2
.3684473668,2.7203566227,3.1509633965\H,0.6176847243,4.1837976117,2.37
28774648\H,-1.7797959049,3.0955640643,3.3093286139\H,-3.6833071562,1.8
411649534,2.5324241687\H,1.7494840956,4.4933577962,0.2844796012\H,3.52
7546865,3.0454395317,1.0182906473\H,-4.6391096801,-0.2984532211,1.2570
08265\H,-3.7314586428,3.0467030862,0.4761101421\H,-1.7954909298,4.3555
1505,1.0043855073\H,1.1230674364,0.7331187325,-4.5970358206\H,-1.34010
24476,0.6445268908,-4.571686431\H,3.2613798002,0.5913570624,-3.5491382
778\H,3.13586907,2.7511996137,-2.8804417066\H,1.3462580404,3.998440258
8,-2.4099204253\H,-0.0850929966,2.7693476575,-3.9388720663\H,-1.738113
9372,3.8623669554,-2.7440698386\H,-3.4970151556,2.5796090555,-2.226242
3263\H,-3.3822667034,0.8313245829,-3.6695936272\H,4.2481791672,2.51766
14392,-0.986281656\H,4.6391096801,0.2984532211,-1.257008265\H,-4.69915
98957,0.773281551,-0.740368742\H,-0.6738708182,4.6652698792,-0.9342636
323\H,-0.4148454235,1.6687855108,1.0710194865\H,0.4233423693,1.8945803
024,-0.5005865913\H,1.4340307238,0.8694826702,0.9602503282\H,1.6606275
915,-0.0826568232,-1.1183231723\H,-1.7014685164,1.0034621312,-0.436502

137\H, -0.0921209752, 0.5819880397, -1.8377136936\C, 0.7614350441, -1.21216
47973, -3.6989732138\C, -0.8535676445, -1.2635107266, -3.6565395267\C, -3.2
662677937, -0.4080955497, -1.8819567477\C, -2.2280934208, -1.4245840306, -1
.4724990891\C, -1.5669399009, -2.192391727, -2.6148111533\C, -0.7234850053
, -3.2368102051, -1.8286960524\C, 0.6338077556, -2.6239471607, -1.554698203
3\C, 1.4978055634, -2.2054942468, -2.7291584944\C, 2.761598415, -1.68092377
84, -1.9586387167\C, -1.4751277747, -3.4420808277, -0.4393980473\C, -2.7158
426366, -2.5120223788, -0.503133039\C, 2.802900215, -2.4703732842, -0.57503
04434\C, 1.5471207573, -3.3761695721, -0.5747354995\C, 0.1049997129, -0.920
7488608, 2.8811435948\C, -1.1071713102, -0.3235876754, 3.5761065995\C, 1.30
4430891, -0.2583205072, 3.5429266015\C, -2.4127217029, -0.7078814451, 2.859
4695883\C, -2.4909003141, -2.1575108091, 2.226343244\C, -1.1494210698, -2.9
604988644, 2.1049422211\C, 0.1024338906, -2.4369985593, 2.8919182118\C, 1.3
755041228, -3.0117960657, 2.1591051401\C, 2.5805376793, -2.0156724332, 2.00
49583531\C, 2.6574125433, -0.6681623754, 2.8662950899\C, -3.3110951722, -1.
9727937531, 0.8423324949\C, -3.6637052226, -0.4329969558, 0.7708126647\C, 3
.69843117, -0.343844815, 0.5989050577\C, 2.6735600573, -1.4829189826, 0.577
9372969\C, 0.8064879845, -3.5853086188, 0.7889596372\C, -0.5875174375, -2.9
564916825, 0.6979270073\H, 1.0490360861, -1.5196445291, -4.70881029\H, -1.1
660669273, -1.6259582733, -4.6400332364\H, -4.1077617188, -0.9280080274, -2
.3597211468\H, -2.3684473668, -2.7203566227, -3.1509633965\H, -0.617684724
3, -4.1837976117, -2.3728774648\H, 1.7797959049, -3.0955640643, -3.30932861
39\H, 3.6833071562, -1.8411649534, -2.5324241687\H, -1.7494840956, -4.49335
77962, -0.2844796012\H, -3.527546865, -3.0454395317, -1.0182906473\H, 3.731
4586428, -3.0467030862, -0.4761101421\H, 1.7954909298, -4.35551505, -1.0043
855073\H, -1.1230674364, -0.7331187325, 4.5970358206\H, 1.3401024476, -0.64
45268908, 4.571686431\H, -3.2613798002, -0.5913570624, 3.5491382778\H, -3.1
3586907, -2.7511996137, 2.8804417066\H, -1.3462580404, -3.9984402588, 2.409
9204253\H, 0.0850929966, -2.7693476575, 3.9388720663\H, 1.7381139372, -3.86
23669554, 2.7440698386\H, 3.4970151556, -2.5796090555, 2.2262423263\H, 3.38
22667034, -0.8313245829, 3.6695936272\H, -4.2481791672, -2.5176614392, 0.98
6281656\H, 4.6991598957, -0.773281551, 0.740368742\H, 0.6738708182, -4.6652
698792, 0.9342636323\H, 0.4148454235, -1.6687855108, -1.0710194865\H, -0.42
33423693, -1.8945803024, 0.5005865913\H, -1.4340307238, -0.8694826702, -0.9
602503282\H, -1.6606275915, 0.0826568232, 1.1183231723\H, 1.7014685164, -1.
0034621312, 0.436502137\H, 0.0921209752, -0.5819880397, 1.8377136936\Version=IA64L-G03RevC.02\State=1-AG\HF=-2322.5096205\RMSE=3.276e-09\RMSF=3
.103e-05\Dipole=0., 0., 0.\PG=CI [X(C60H60)]\@

Isomer 5:

1\1\GINC-M0106\FOpt\RB3LYP\6-31G(d,p)\C60H60\JJF\18-Mar-2007\0\#\ B3LY
P/6-31G** OPT GEOM=ALLCHECK\cluster\0,1\C, -1.3568263842, 1.8675113545
, 4.0487050641\C, -1.3555201662, 1.8657134996, 2.4877702817\H, -1.978350762
9, 2.7229662954, 4.3339471821\H, -1.9800148597, 2.7252567283, 2.2172963279\
C, 0.0000000294, 2.3071871144, 1.878811415\H, 0.000000043, 3.369103502, 2.16
07954841\C, 0.0000000169, 1.3216712932, 6.0774535718\C, 0.0000000274, 2.149

4226105,4.761385294\H,0.0000000253,1.9807788739,6.9509129346\H,0.00000
0041,3.2169572133,5.0039141381\H,-1.9828195527,2.7291170571,-0.0407163
783\C,0.0000000295,2.3094789918,0.3074924725\H,0.000000043,3.373374169
8,0.0407163783\C,0.0000000294,2.3083709615,-4.0487050641\C,0.000000029
4,2.3061486907,-2.4877702817\H,0.0000000429,3.3657714104,-4.3339471821
\H,0.000000043,3.368602541,-2.2172963279\C,-1.3561305363,1.866553602,-
1.878811415\H,-1.9803093172,2.7256620142,-2.1607954841\C,-0.7768588809
,1.0692545471,-6.0774535718\C,-1.2633988892,1.7389194361,-4.761385294\
H,-1.1642725897,1.6024837859,-6.9509129346\H,-1.890879974,2.6025730799
, -5.0039141381\C,-1.3574776681,1.8684077699,-0.3074924725\C,-2.1953912
54,-0.7133258284,4.0487050641\C,-0.0000000294,-2.3083709615,4.04870506
41\C,2.1953912358,-0.7133258844,4.0487050641\C,1.3568264318,1.86751131
99,4.0487050641\C,-2.1932777489,-0.712639109,2.4877702817\C,-0.0000000
294,-2.3061486907,2.4877702817\C,2.1932777307,-0.7126391649,2.48777028
17\C,1.3555202138,1.865713465,2.4877702817\H,-3.2010388454,-1.04008052
42,4.3339471821\H,-0.0000000429,-3.3657714104,4.3339471821\H,3.2010388
189,-1.0400806058,4.3339471821\H,1.9783508323,2.7229662449,4.333947182
1\H,-3.2037314107,-1.0409553916,2.2172963279\H,-0.000000043,-3.3686025
41,2.2172963279\H,3.2037313842,-1.0409554733,2.2172963279\H,1.98001492
92,2.7252566777,2.2172963279\C,-2.1942653303,0.7129600555,1.878811415\
C,-1.3561305839,-1.8665535674,1.878811415\C,1.3561305363,-1.866553602,
1.878811415\C,2.1942653485,0.7129599996,1.878811415\H,-3.2042078264,1.
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.9803093172,-2.7256620142,2.1607954841\H,3.2042078529,1.0411101971,2.1
607954841\C,-1.2569840906,0.4084189066,6.0774535718\C,-0.7768589082,-1
.0692545273,6.0774535718\C,0.7768588809,-1.0692545471,6.0774535718\C,1
.256984101,0.4084188746,6.0774535718\C,-2.0442223715,0.6642081408,4.76
1385294\C,-1.2633989336,-1.7389194039,4.761385294\C,1.2633988892,-1.73
89194361,4.761385294\C,2.0442223884,0.6642080887,4.761385294\H,-1.8838
326475,0.6120943581,6.9509129346\H,-1.1642726305,-1.6024837562,6.95091
29346\H,1.1642725897,-1.6024837859,6.9509129346\H,1.8838326631,0.61209
43101,6.9509129346\H,-3.0595081077,0.9940944881,5.0039141381\H,-1.8908
800404,-2.6025730316,5.0039141381\H,1.890879974,-2.6025730799,5.003914
1381\H,3.059508133,0.9940944101,5.0039141381\H,-3.2082694994,-1.042429
9059,-0.0407163783\H,-0.000000043,-3.3733741698,-0.0407163783\H,3.2082
694728,-1.0424299878,-0.0407163783\H,1.9828196223,2.7291170065,-0.0407
163783\C,-2.1964450353,0.7136682846,0.3074924725\C,-1.3574777157,-1.86
84077352,0.3074924725\C,1.3574776681,-1.8684077699,0.3074924725\C,2.19
64450535,0.7136682286,0.3074924725\H,-3.2082694728,1.0424299878,0.0407
163783\H,-1.9828196223,-2.7291170065,0.0407163783\H,1.9828195527,-2.72
91170571,0.0407163783\H,3.2082694994,1.0424299059,0.0407163783\C,-2.19
53912358,0.7133258844,-4.0487050641\C,-1.3568264318,-1.8675113199,-4.0
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133258284,-4.0487050641\C,-2.1932777307,0.7126391649,-2.4877702817\C,-
1.3555202138,-1.865713465,-2.4877702817\C,1.3555201662,-1.8657134996,-
2.4877702817\C,2.1932777489,0.712639109,-2.4877702817\H,-3.2010388189,

1.0400806058,-4.3339471821\H,-1.9783508323,-2.7229662449,-4.3339471821
\H,1.9783507629,-2.7229662954,-4.3339471821\H,3.2010388454,1.040080524
2,-4.3339471821\H,-3.2037313842,1.0409554733,-2.2172963279\H,-1.980014
9292,-2.7252566777,-2.2172963279\H,1.9800148597,-2.7252567283,-2.21729
63279\H,3.2037314107,1.0409553916,-2.2172963279\C,-2.1942653485,-0.712
9599996,-1.878811415\C,-0.0000000294,-2.3071871144,-1.878811415\C,2.19
42653303,-0.7129600555,-1.878811415\C,1.3561305839,1.8665535674,-1.878
811415\H,-3.2042078529,-1.0411101971,-2.1607954841\H,-0.000000043,-3.3
69103502,-2.1607954841\H,3.2042078264,-1.0411102788,-2.1607954841\H,1.
9803093867,2.7256619637,-2.1607954841\C,-1.256984101,-0.4084188746,-6.
0774535718\C,-0.0000000169,-1.3216712932,-6.0774535718\C,1.2569840906,
-0.4084189066,-6.0774535718\C,0.7768589082,1.0692545273,-6.0774535718\
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05,-4.761385294\C,2.0442223715,-0.6642081408,-4.761385294\C,1.26339893
36,1.7389194039,-4.761385294\H,-1.8838326631,-0.6120943101,-6.95091293
46\H,-0.0000000253,-1.9807788739,-6.9509129346\H,1.8838326475,-0.61209
43581,-6.9509129346\H,1.1642726305,1.6024837562,-6.9509129346\H,-3.059
508133,-0.9940944101,-5.0039141381\H,-0.000000041,-3.2169572133,-5.003
9141381\H,3.0595081077,-0.9940944881,-5.0039141381\H,1.8908800404,2.60
25730316,-5.0039141381\C,-2.1964450535,-0.7136682286,-0.3074924725\C,-
0.0000000295,-2.3094789918,-0.3074924725\C,2.1964450353,-0.7136682846,
-0.3074924725\C,1.3574777157,1.8684077352,-0.3074924725\\Version=IA64L
-G03RevC.02\State=1-A1G\HF=-2322.3065669\RMSD=5.962e-09\RMSF=4.624e-05
\Dipole=0.,0.,0.\PG=D05D [5SGD(C12H12)]\\@

Isomer 6:

1\1\GINC-C0129\FOpt\RB3LYP\6-31G(d,p)\C60H60\STUDENT\04-Nov-2007\0\\#p
b3lyp/6-31g** opt symm=loose\\BB\\0,1\C,-2.1927186815,3.3025637232,2.
3375055089\C,-1.0832614759,2.2430624295,2.1263127964\H,-2.0120483591,3
.6941808821,3.3443997144\H,-0.7660627078,1.9631756162,3.1398367863\H,1
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4022899,0.0894458096\C,-2.6599869404,3.2231923695,-1.94207423\C,-0.178
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025\H,1.2496901797,-1.1009901505,-0.3458298562\C,5.3078386002,-3.19307
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.8967308307,0.8394910347\H,3.8508073928,-5.9366683289,-1.4767630494\H,
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2.0222873325\H,-1.0143539508,-0.7287618921,-3.0608214114\C,-0.91687453
08,-1.5524427647,1.3869330292\C,-1.2983020328,-1.6992902348,-1.2543723
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969108745,-0.2292573302,2.4196764409\C,-3.0607923899,-0.5153741086,0.2
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, -5.3078386002, 3.1930781497, 0.5069430523\C, -4.8108611061, 3.8327233653, -0.8199229667\C, -4.9328366644, 1.6873376458, 0.4829238547\C, -4.1127533399, 2.7256276197, -1.6610152293\H, -6.388051408, 3.3260940708, 0.6192535587\H, -5.6468330462, 4.2705894238, -1.3736385255\H, -5.8346671178, 1.0818766354, 0.6185379015\H, -4.5997790801, 2.652620815, -2.6385578953\C, -1.8962351813, -1.5875740037, 0.174718254\C, -0.9658457916, -0.3846910622, -2.0232338876\H, -0.0772210886, -3.4014534281, 2.0124828792\H, -2.3944656198, -2.5565899606, 0.302298799\H, -3.754549539, -0.5279042671, -1.6605910774\\Version=IA32L-G03RevD.01\State=1-AG\HF=-2322.3798155\RMSD=2.976e-09\RMSF=5.533e-05\Thermal=0.\Dipole=0.,0.,0.\PG=C02H [SGH(C12H12),X(C48H48)]\\@

Isomer 7:

1\1\GINC-M0102\FOpt\RB3LYP\6-31G(d,p)\C60H60\JJF\04-Nov-2007\0\\#P B3LYP/6-31G** OPT GEOM=ALLCHECK GUESS=READ\\BB\\0,1\C, -2.2940630692, 3.3516808322, 2.1545928689\C, -1.26504166, 2.1970174083, 2.1075350012\H, -2.2072557894, 3.7538754076, 3.1695347728\H, -0.5970760027, 2.3933215267, 2.9558592596\H, 0.7861768486, 0.7841835382, 3.2914041662\C, 1.8828262707, -0.8008013508, 2.3612469697\H, 2.2632082611, -0.8180083332, 3.3917378996\C, 4.4893789483, -4.105676412, 1.2342554917\C, 3.8005014017, -2.9712515153, 2.0432697152\H, 5.2400512061, -4.6173536601, 1.8441445083\H, 4.1899507839, -2.963707053, 3.0663960669\C, 0.7385079173, 0.2976483072, 2.3123591224\C, -1.1193032791, 4.4282206117, -0.0378394012\C, -2.2565998658, 3.4433589967, -2.2791731237\C, -0.1103217817, 3.2488268416, -0.0549763945\C, -1.1218868434, 2.337719596, -2.3388861187\H, -0.4886355876, 5.3233577241, -0.0276051352\H, -2.2649350783, 3.9038318654, -3.2727428026\H, 0.8376124286, 3.6951840551, 0.2734909767\H, -0.7517838315, 2.3342756317, -3.3717778236\C, -0.3467570926, 2.053676336, 0.8845976568\C, 0.1570885128, 2.6808236387, -1.4719228657\H, 0.647909085, 3.4871370265, -2.0335772965\C, -3.3968286245, 5.1036902449, 0.7552085565\C, -3.4020202408, 5.1146952629, -0.7986733421\C, -2.0136008281, 4.5781048199, 1.2331040814\C, -2.0128967712, 4.6292585891, -1.2998568149\H, -3.5883102327, 6.1057703343, 1.1506957124\H, -3.6232401329, 6.116737683, -1.1784398691\H, -1.5304647156, 5.3326156832, 1.8621090038\H, -1.5381769998, 5.4229437649, -1.8857778177\H, 0.8348135904, 0.5952216351, -3.196103596\C, 0.9894508025, 1.4737685441, 1.3167277506\C, 1.2049965553, 1.4842168436, -1.3746147209\H, 1.5053430348, 2.2390124577, 1.9166890729\H, 2.0683001656, 1.8103977181, -1.9709539225\C, 4.2162393367, -1.6120277538, 1.4029594798\C, 3.975652518, -1.6536820681, -1.2656160327\C, 3.1529678415, -0.4351006004, 1.494192359\C, 2.6459540588, -1.0687305149, -0.8527034333\H, 5.0702917605, -1.275900636, 2.0003056944\H, 4.4951731303, -0.9250768569, -1.9040076607\H, 3.6320576096, 0.3758380779, 2.0583891133\C, 2.8879302831, 0.1306523407, 0.0752971646\C, 1.7530705555, -0.9438429736, -2.0964761992\H, 3.8420541234, 0.5674005718, -0.2536939494\H, 2.4421959474, -0.7747073742, -2.9365544056\C, 5.1446414443, -3.472966109, -0.0226634292\C, 4.4730403249, -4.0986971718, -1.2806543013\C, 4.8431780696, -1.9471947468, -0.0102731887\C, 3.749357575, -2.9684938395, -2.064768926\H, 6.2237744628, -3.6543957976, -0.0279747135\H, 5.2173712225, -4.5935662378, -1.9119312693\H, 5.776174147, -1.3822509877, -0.099

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6\H,-0.7861768486,-0.7841835382,3.2914041662\C,-1.8828262707,0.8008013
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4909767\H,0.7517838315,-2.3342756317,-3.3717778236\C,0.3467570926,-2.0
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7\C,-3.749357575,2.9684938395,-2.064768926\H,-6.2237744628,3.654395797
6,-0.0279747135\H,-5.2173712225,4.5935662378,-1.9119312693\H,-5.776174
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426\C,-1.8775211231,-1.3084338204,0.042121646\C,-0.74185626,-0.2304699
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38607,-2.1980120944,0.0923620064\H,-2.224465182,1.8564315617,-0.241489
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09\RMSF=1.344e-05\Dipole=0.,0.,0.0151838\PG=C02 [X(C60H60)]\@

Isomer 8:

1\1\GINC-C0129\FOpt\RB3LYP\6-31G(d,p)\C60H60\STUDENT\09-Nov-2007\0\#p
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44,1.7857406559,1.3202558763\H, -2.6987627965,1.6143910302,1.8767550538
\C, -1.0505260893,6.0847997537,0.7904631727\C, -1.670942056,4.7325497099
,1.2461649401\H, -1.5960828665,6.9455444045,1.1878376819\H, -2.715040765
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, -1.9285106062, -4.0787156003, -1.3912575083\C,0.5038023378, -3.903721728
, -1.4378072569\C, -1.8845798787, -2.4958086432, -1.3883259576\C,0.7261517
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4529,2.9777192398\C, -0.6839886062, -1.839584309,2.1097409411\H, -0.74887
27315, -2.147378917,3.1648263219\C, -0.4145709653, -6.0396780862,1.291124
3712\C, -0.6673852684, -4.7014195572,2.0340098334\H, -0.6343533872, -6.891
8898784,1.941346326\H, -0.9312211117, -4.9034186701,3.0766943916\C, -0.65
01937419, -0.3048538978,2.1161527275\C,1.6941603691,3.9115490229,1.3064
876286\C,1.9206025451,4.016622603, -1.3500321205\C,1.221158694,2.501449
4038,0.9877330341\C,1.9449347972,2.4362349293, -1.3623098539\H,2.576011

2778,3.7820202489,1.9493314792\H,2.7933858388,4.3194625192,-1.93749537
 14\H,0.35230445,2.5601936836,0.3512987475\H,2.8197284375,2.1444493791,
 -1.9593139628\C,0.6779313345,1.8702607005,2.2736357679\C,2.2164889459,
 1.8403855971,0.0549900242\H,3.233076789,2.1486812152,0.3442228033\C,0.
 423622157,6.0677220345,1.2841606907\C,1.3533870933,6.0401668381,0.0350
 047768\C,0.6475886096,4.7539801929,2.0955141763\C,2.1385378953,4.70218
 85497,0.0440651245\H,0.6313038385,6.9443333459,1.9051423511\H,2.039393
 6527,6.892624067,0.0433423748\H,1.0735116608,4.9919277056,3.0748089304
 \H,3.20957429,4.9046126012,0.1415824377\H,0.3907263571,-0.6858424771,-
 0.2551901168\C,0.7625120265,0.2967150502,2.3598248681\C,2.2118465542,0.
 3056705328,0.0897572281\H,1.0258220027,0.04620075,3.3968712834\H,3.22
 89046311,0.0107527622,-0.203841519\C,0.6706871488,-3.9103095582,2.0339
 657869\C,2.4531999786,-4.0862311917,0.0622331322\C,0.5267170118,-2.500
 5347346,1.4812239317\C,2.4922622335,-2.4815926116,0.0535086649\H,0.983
 9386533,-3.7801516404,3.0792501291\H,3.495897977,-4.4228084717,0.06593
 89681\H,0.2151674784,-2.5599004203,0.4502924148\C,1.9198373572,-1.8688
 986179,1.3958277777\C,1.832974803,-1.7857113605,-1.2269476738\H,2.5286
 531351,-2.2580010432,2.2227782739\H,2.6674234309,-1.6144130021,-1.9210
 079098\C,1.0725605601,-6.0669398653,0.8292702336\C,1.0967497764,-6.084
 7808937,-0.7251552292\C,1.7629324022,-4.752716684,1.3094548087\C,1.732
 2351667,-4.7325229168,-1.1595708552\H,1.5895583646,-6.9431696801,1.231
 9262611\H,1.6531257283,-6.9455198489,-1.1072472373\H,2.5451426337,-4.9
 900281931,2.0366948525\H,2.3871106154,-4.82725434,-2.0358223944\C,1.97
 24717182,-0.2952807328,1.5034602252\C,1.2523863817,-0.4248604957,-0.85
 12441221\H,1.2554614496,2.2599876598,3.1224445422\H,2.8630135083,-0.04
 41590046,2.096273875\H,3.5527863472,-2.2147904243,0.0040598031\\Versio
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 6e-05\Thermal=0.\Dipole=-0.0701402,-0.0000369,-0.0990757\PG=C02 [X(C60
 H60)]\@

Another [H10@C60H50](#) endo cage isomer:

D5 symmetry (From Dodziuk, H.; Nowinski, K. Chem. Phys. Lett. 1996, 249, 406)

1\1\GINC-M0104\FOpt\RB3LYP\6-31G(d,p)\C60H60\JJF\22-Nov-2007\0\#\P B3L
 YP/6-31G** OPT GEOM=ALLCHECK\BB\0,1\C,0.392062418,1.2939237087,3.703
 9179949\C,0.8270768899,2.429784418,2.7172303944\C,-0.2753525337,3.2139
 180172,1.9485527263\C,-1.3342601258,2.2136336551,1.5611792497\C,-2.055
 2814893,1.5374415434,2.7172303944\C,-1.1094406247,0.7727179329,3.70391
 79949\C,0.427804336,3.8496536189,0.6751715944\C,1.8583467319,3.1688254
 614,0.6717682974\C,1.6929816586,1.9530072058,1.5611792497\C,1.35174852
 47,0.0269708979,3.7039179949\C,0.4433641145,-1.277254777,3.7039179949\
 C,-1.0777344326,-0.8163577624,3.7039179949\C,-3.1417062855,0.731279464
 4,1.9485527263\C,-3.5290393496,1.5964744922,0.6751715944\C,-2.43947138
 25,2.7466136887,0.6717682974\C,2.5664431185,-0.0357521878,2.7172303944
 \C,2.9715290608,1.2550311073,1.9485527263\C,-2.0973107067,-1.479593288
 4,2.7172303944\C,-2.5175997661,-0.5849063683,1.5611792497\C,-1.8583467

319,3.1688254614,-0.6717682974\C,-0.427804336,3.8496536189,-0.67517159
44\C,0.7590721876,-2.4518804852,2.7172303944\C,2.1118584918,-2.4382661
36,1.9485527263\C,2.3805803331,-1.0066088216,1.5611792497\C,3.79343696
98,0.7827422892,0.6751715944\C,3.5290393496,1.5964744922,-0.6751715944
\C,2.4394713825,2.7466136887,-0.6717682974\C,-0.2217020998,-2.57512567
09,1.5611792497\C,-1.6663287334,-2.761962453,1.9485527263\C,-3.3660229
609,-1.4713248478,0.6717682974\C,-3.5879928257,-0.7881718491,-0.671768
2974\C,-3.7934369698,0.7827422892,-0.6751715944\C,-2.9715290608,1.2550
311073,-1.9485527263\C,-1.6929816586,1.9530072058,-1.5611792497\C,0.27
53525337,3.2139180172,-1.9485527263\C,1.3342601258,2.2136336551,-1.561
1792497\C,3.5879928257,-0.7881718491,0.6717682974\C,-2.6088706017,-2.8
629781205,0.6751715944\C,-0.8270768899,2.429784418,-2.7172303944\C,1.6
663287334,-2.761962453,-1.9485527263\C,0.2217020998,-2.5751256709,-1.5
611792497\C,-0.7590721876,-2.4518804852,-2.7172303944\C,-0.4433641145,
-1.277254777,-3.7039179949\C,1.0777344326,-0.8163577624,-3.7039179949\
C,2.0973107067,-1.4795932884,-2.7172303944\C,-2.1118584918,-2.43826613
6,-1.9485527263\C,-1.9166686455,-3.3658922797,-0.6751715944\C,-0.35915
47857,-3.6559424531,-0.6717682974\C,2.6088706017,-2.8629781205,-0.6751
715944\C,3.3660229609,-1.4713248478,-0.6717682974\C,2.5175997661,-0.58
49063683,-1.5611792497\C,1.1094406247,0.7727179329,-3.7039179949\C,-0.
392062418,1.2939237087,-3.7039179949\C,-1.3517485247,0.0269708979,-3.7
039179949\C,1.9166686455,-3.3658922797,0.6751715944\C,0.3591547857,-3.
6559424531,0.6717682974\C,3.1417062855,0.7312794644,-1.9485527263\C,2.
0552814893,1.5374415434,-2.7172303944\C,-2.5664431185,-0.0357521878,-2
.7172303944\C,-2.3805803331,-1.0066088216,-1.5611792497\H,0.5205061453
,1.7381923217,4.6948974978\H,1.4311470359,3.143724416,3.2961889717\H,-
0.7308835825,3.9990903982,2.5675895963\H,-0.8271598417,1.4224376068,0.
9979770648\H,-2.5476108357,2.3325659844,3.2961889717\H,-1.4922738896,1.
.0321617282,4.6948974978\H,0.5916928312,4.9077537858,0.8981199331\H,2.
5500653763,3.8611420089,1.1735879238\H,1.0972121068,1.2262331514,0.997
9770648\H,1.8139643787,0.0421002057,4.6948974978\H,0.6005854951,-1.712
1729637,4.6948974978\H,-1.4427821296,-1.1002812918,4.6948974978\H,-4.0
292164304,0.5406753013,2.5675895963\H,-4.4847080781,2.0793126467,0.898
1199331\H,-2.8841507299,3.6184147915,1.1735879238\H,3.4321083468,-0.38
96374441,3.2961889717\H,3.5775055346,1.9308984889,2.5675895963\H,-3.00
56571225,-1.7021193566,3.2961889717\H,-1.6084250031,-0.3471183636,0.99
79770648\H,-2.5500653763,3.8611420089,-1.1735879238\H,-0.5916928312,4.
9077537858,-0.8981199331\H,0.6900125755,-3.3845335997,3.2961889717\H,2
.9419035978,-2.8057295033,2.5675895963\H,1.5052742166,-0.6645838411,0.
9979770648\H,4.8503943586,0.9538460013,0.8981199331\H,4.4847080781,2.0
793126467,-0.8981199331\H,2.8841507299,3.6184147915,-1.1735879238\H,-0
.1669014786,-1.6369685536,0.9979770648\H,-1.7593091195,-3.6649346852,2
.5675895963\H,-4.332568556,-1.6248386823,1.1735879238\H,-4.4601778059,
-1.2320977946,-1.1735879238\H,-4.8503943586,0.9538460013,-0.8981199331
\H,-3.5775055346,1.9308984889,-2.5675895963\H,-1.0972121068,1.22623315
14,-0.9979770648\H,0.7308835825,3.9990903982,-2.5675895963\H,0.8271598

417,1.4224376068,-0.9979770648\H,4.4601778059,-1.2320977946,1.1735879238\H,-3.363394853,-3.6226678969,0.8981199331\H,-1.4311470359,3.143724416,-3.2961889717\H,1.7593091195,-3.6649346852,-2.5675895963\H,0.1669014786,-1.6369685536,-0.9979770648\H,-0.6900125755,-3.3845335997,-3.2961889717\H,-0.6005854951,-1.7121729637,-4.6948974978\H,1.4427821296,-1.1002812918,-4.6948974978\H,3.0056571225,-1.7021193566,-3.2961889717\H,-2.9419035978,-2.8057295033,-2.5675895963\H,-2.4060157413,-4.318244537,-0.8981199331\H,-0.2064761037,-4.6226203234,-1.1735879238\H,3.363394853,-3.6226678969,-0.8981199331\H,4.332568556,-1.6248386823,-1.1735879238\H,1.6084250031,-0.3471183636,-0.9979770648\H,1.4922738896,1.0321617282,-4.6948974978\H,-0.5205061453,1.7381923217,-4.6948974978\H,-1.8139643787,0.0421002057,-4.6948974978\H,2.4060157413,-4.318244537,0.8981199331\H,0.2064761037,-4.6226203234,1.1735879238\H,4.0292164304,0.5406753013,-2.5675895963\H,2.5476108357,2.3325659844,-3.2961889717\H,-3.4321083468,-0.3896374441,-3.2961889717\H,-1.5052742166,-0.6645838411,-0.9979770648\\Version=IA64L-G03RevC.02\State=1-A1\HF=-2322.4979741\RMSD=9.672e-10\RMSF=4.082e-05\Dipole=0.,0.,0.\PG=D05 [X(C60H60)]\@

D5d symmetry (From Zdetsis, A. D. Phys. Rev. B 2008, 77, 115402)

1\1\GINC-M0102\FOpt\RB3LYP\6-31G(d,p)\C60H60\JJF\28-Apr-2008\0\# B3LYP/6-31G** OPT GEOM=ALLCHECK GUESS=READ\h10c60h50-d5d\0,1\C,2.0795412601,0.6756839146,2.1365051418\H,1.4369502012,0.4668934229,1.275016635\C,1.2604873273,0.4095571595,3.3926836971\C,0.7790240106,-1.0722345639,3.3926836971\C,2.7850808816,-1.7334021667,1.9049508069\C,1.2852271798,-1.7689634539,2.1365051418\C,3.2720459938,-0.2346776577,1.9049508069\C,0.,2.1865590788,2.1365051418\C,-2.0795412601,0.6756839145,2.1365051418\C,-1.2852271798,-1.7689634539,2.1365051418\C,0.,1.3253548087,3.3926836971\C,-1.2604873273,0.4095571595,3.3926836971\C,-0.7790240106,-1.0722345639,3.3926836971\C,2.5092007492,2.1131185933,1.9049508069\C,-1.2343095341,3.0393812796,1.9049508069\C,-3.2720459938,-0.2346776577,1.9049508069\C,-0.7879261029,-3.1844200485,1.9049508069\C,1.234309534,3.0393812796,1.9049508069\C,-2.5092007492,2.1131185933,1.9049508069\C,-2.7850808816,-1.7334021667,1.9049508069\C,0.7879261029,-3.1844200485,1.9049508069\C,3.9528876184,0.422408752,0.6596514551\C,3.446238895,1.9817131872,0.6596514551\C,3.9528876185,-0.4224087519,-0.6596514551\C,2.9496676253,2.665184905,-0.6596514551\C,2.9496676253,-2.665184905,0.6596514551\C,3.2720459938,0.2346776577,-1.9049508069\C,1.623244047,3.6288880448,-0.6596514551\C,3.446238895,-1.9817131872,-0.6596514551\C,2.7850808816,1.7334021667,-1.9049508069\C,0.8197748549,3.8899510106,0.6596514551\C,1.2343095341,-3.0393812796,-1.9049508069\C,0.7790240106,1.0722345639,-3.3926836971\C,-1.6232440471,3.6288880448,-0.6596514551\C,0.8197748549,-3.8899510106,-0.6596514551\C,1.2604873273,-0.4095571595,-3.3926836971\C,-0.7879261029,3.1844200485,-1.9049508069\C,2.5092007492,-2.1131185933,-1.9049508069\C,1.2852271798,1.7689634539,-2.1365051418\C,-0.8197748549,3.8899510106,0.6596514551\C,1.6232440471,-3.6288880448,0.6596514551\C,2.0795412601,-0.6756839145,-2.1365051418\C,0.7879261029,3.1844

200485,-1.9049508069\C,-1.623244047,-3.6288880448,0.6596514551\C,0.,-2.
.1865590788,-2.1365051418\C,-0.7790240106,1.0722345639,-3.3926836971\C
, -2.9496676253,2.665184905,-0.6596514551\C,-0.8197748549,-3.8899510106
, -0.6596514551\C,0.,-1.3253548087,-3.3926836971\C,-1.2852271798,1.7689
634539,-2.1365051418\C,-3.446238895,1.9817131872,0.6596514551\C,-2.949
6676253,-2.665184905,0.6596514551\C,-3.9528876185,0.4224087519,0.65965
14551\C,-3.446238895,-1.9817131872,-0.6596514551\C,-3.9528876184,-0.42
2408752,-0.6596514551\C,-2.7850808816,1.7334021667,-1.9049508069\C,-2.
5092007492,-2.1131185933,-1.9049508069\C,-3.2720459938,0.2346776577,-1
.9049508069\C,-1.234309534,-3.0393812796,-1.9049508069\C,-1.2604873273
, -0.4095571595,-3.3926836971\C,-2.0795412601,-0.6756839146,-2.13650514
18\H,1.8856569283,0.6126870764,4.2720686352\H,1.1654000728,-1.60403559
04,4.2720686352\H,3.2807898803,-2.2325550635,2.7488518129\H,0.88808406
45,-1.2223428502,1.275016635\H,3.9664777094,-0.1222249202,2.7488518129
\H,0.,1.5108988546,1.275016635\H,-1.4369502012,0.4668934229,1.27501663
5\H,-0.8880840645,-1.2223428502,1.275016635\H,0.,1.982697028,4.2720686
352\H,-1.8856569283,0.6126870764,4.2720686352\H,-1.1654000728,-1.60403
55904,4.2720686352\H,3.1371058691,2.4303191388,2.7488518129\H,-1.34195
18269,3.7345748948,2.7488518129\H,-3.9664777094,-0.1222249203,2.748851
8129\H,-1.1094662131,-3.8101140498,2.7488518129\H,1.3419518269,3.73457
48948,2.7488518129\H,-3.1371058691,2.4303191388,2.7488518129\H,-3.2807
898803,-2.2325550635,2.7488518129\H,1.1094662132,-3.8101140498,2.74885
18129\H,5.0124707094,0.5057615732,0.9128699352\H,4.3524531816,2.537086
6527,0.9128699352\H,5.0124707094,-0.5057615731,-0.9128699352\H,3.75789
47938,3.3554260683,-0.9128699352\H,3.7578947938,-3.3554260683,0.912869
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0097,-0.9128699352\H,4.3524531816,-2.5370866527,-0.9128699352\H,3.2807
898803,2.2325550635,-2.7488518129\H,1.0679307931,4.9234318521,0.912869
9352\H,1.3419518269,-3.7345748948,-2.7488518129\H,1.1654000728,1.60403
55904,-4.2720686352\H,-2.0299464729,4.6108540097,-0.9128699352\H,1.067
9307932,-4.9234318521,-0.9128699352\H,1.8856569283,-0.6126870764,-4.27
20686352\H,-1.1094662132,3.8101140498,-2.7488518129\H,3.1371058691,-2.
4303191388,-2.7488518129\H,0.8880840645,1.2223428502,-1.275016635\H,-1
.0679307932,4.9234318521,0.9128699352\H,2.0299464729,-4.6108540097,0.9
128699352\H,1.4369502012,-0.4668934229,-1.275016635\H,1.1094662131,3.8
101140498,-2.7488518129\H,-2.0299464728,-4.6108540097,0.9128699352\H,0
, -1.5108988546,-1.275016635\H,-1.1654000728,1.6040355904,-4.272068635
2\H,-3.7578947938,3.3554260683,-0.9128699352\H,-1.0679307931,-4.923431
8521,-0.9128699352\H,0., -1.982697028,-4.2720686352\H,-0.8880840645,1.2
223428502,-1.275016635\H,-4.3524531816,2.5370866527,0.9128699352\H,-3.
7578947938,-3.3554260683,0.9128699352\H,-5.0124707094,0.5057615731,0.9
128699352\H,-4.3524531816,-2.5370866527,-0.9128699352\H,-5.0124707094,
-0.5057615732,-0.9128699352\H,-3.2807898803,2.2325550635,-2.7488518129
\H,-3.1371058691,-2.4303191388,-2.7488518129\H,-3.9664777094,0.1222249
202,-2.7488518129\H,-1.3419518269,-3.7345748948,-2.7488518129\H,-1.885
6569283,-0.6126870764,-4.2720686352\H,-1.4369502012,-0.4668934229,-1.2

75016635\\Version=IA64L-G03RevC.02\\State=1-A1G\\HF=-2322.3404683\\RMSD=4
.457e-09\\RMSF=2.567e-04\\Dipole=0.,0.,0.\\PG=D05D [5SGD(C4H4),X(C40H40)]
\\@

Other isomers considered to find the stable tube-like endo isomer:

H2@C60-1/C2h:

1\\1\\GINC-C0116\\FOpt\\RB3LYP\\6-31G(d,p)\\C60H60\\STUDENT\\03-Nov-2007\\0\\#p
b3lyp/6-31g** opt geom=allcheck guess=read\\BB\\0,1\\C,-2.2375516231,3
.2760203501,2.3350959775\\C,-1.0877626588,2.2443366864,2.3158744518\\H,-
2.0256483621,4.0616351906,3.0746339688\\H,-0.5649144009,2.3505259428,3.
2741413476\\H,1.0857963906,0.7768179281,3.0923666394\\C,2.0679104462,-0.
7552071295,1.993866239\\H,2.6117541111,-0.6846592358,2.9457144329\\C,4.8
199021946,-3.8613383589,0.8386458101\\C,4.1050533815,-2.7671072785,1.67
52054466\\H,5.6669096595,-4.2816479722,1.3887903389\\H,4.6179364592,-2.6
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\C,-1.7963301912,-1.456404924,0.2287577997\C,-0.9361433575,-0.33305123
41,-2.1007046625\H,-0.116282387,-3.4394577411,2.0931112483\H,-2.335718
824,-2.4091435142,0.2925344949\H,-3.6533509558,-0.4715380476,-1.576444
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-09\RMSF=2.208e-05\Thermal=0.\Dipole=0.,0.,0.\PG=C02H [SGH(C12H12),X(C
48H48)]\\@

H2@C60-2/C2h:

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b3lyp/6-31g** opt geom=allcheck guess=read\\BB\\0,1\C,3.805516594,-0.
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839743983\H,-0.139307029,0.0000044046,3.3291953675\C,-1.9482054759,0.0
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01354371,-2.3062229816,0.8331738125\C,4.1039471165,-1.3707117975,-1.73
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94281696,-1.755705247\H,4.3598139839,-3.2979988578,1.1916277181\H,4.40
14218186,-1.9721574833,-2.5961403836\H,2.1797173949,-3.2798424812,1.13
5235748\H,2.2936711931,-1.972149814,-2.6360349441\C,1.8048432094,-1.37
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\H,2.1951027706,3.2492099832,-0.9946563327\H,2.2649408895,-0.000071613
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H48)]\\@

H2@C60-3/C2h:

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8019701\H,2.5783323174,-0.6747560007,2.8734860139\C,4.8079600318,-3.82
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7803966,-3.1066699921\H,-0.77440124,-4.1012139015,0.1308846247\H,1.847
998357,-1.8921848956,-0.4323242654\C,0.1709106947,-2.7029776933,1.4108
546359\C,0.0089210958,-2.6131543133,-1.1874822426\H,-0.2122259217,-3.2
783708151,-2.034414277\C,3.7619193777,-4.9257024738,0.4611336633\C,3.5
88143242,-4.9424237858,-1.0817261559\C,2.3959142327,-4.5321667535,1.09
79682487\C,2.127555589,-4.5216569608,-1.3970249469\H,4.0914557984,-5.9
04019462,0.8237059521\H,3.8050196546,-5.9359346899,-1.4856268245\H,2.0
834252172,-5.3115117278,1.8004938954\H,1.6649875459,-5.2518124563,-2.0
687521176\H,-1.0358584602,-0.7859292867,-3.0243972998\C,-0.9511401606,
-1.6055868523,1.5122091244\C,-1.1694085089,-1.5978795731,-1.141320784\
H,-1.656505122,-2.0043100852,2.2511352422\H,-1.961615011,-2.0885173412
, -1.7200244843\C,-4.1250774749,1.3979603896,1.8191949979\C,-4.33860161
04,1.3743050793,-0.8922780773\C,-3.0192064793,0.2712397407,1.755462829
\C,-3.2070631872,0.3059558198,-0.9644698173\H,-4.8733714844,1.03489390
19,2.531804354\H,-5.1809442578,0.9354375193,-1.4371296686\H,-3.3290872
871,-0.5008011245,2.4704573665\C,-2.9945112062,-0.4636576941,0.3791224
844\C,-2.0416938565,0.7364618544,-1.9178019701\H,-3.9228777116,-1.0478

304036,0.4290389141\H,-2.5783323174,0.6747560007,-2.8734860139\C,-5.30
 69040101,3.1930200387,0.518285037\C,-4.8079600318,3.8290537521,-0.8103
 686227\C,-4.9398206111,1.6792051087,0.5147011763\C,-4.0953124194,2.725
 6534049,-1.638219664\H,-6.3865369917,3.3301123905,0.6312246617\H,-5.64
 39176569,4.2571311721,-1.3717418714\H,-5.8544822625,1.0823147721,0.590
 1083881\H,-4.5947117143,2.6234116546,-2.6068725196\C,-1.8390657997,-1.
 5235969312,0.2565980455\C,-0.9069304026,-0.3385727309,-2.029604456\H,-
 0.1153022219,-3.4809417885,2.1309017217\H,-2.3526462101,-2.4919068653,
 0.2904031684\H,-3.6368441175,-0.5021738957,-1.5677016166\\Version=IA32
 L-G03RevD.01\State=1-AG\HF=-2322.3762943\RMSD=4.037e-09\RMSF=4.220e-05
 \Thermal=0.\Dipole=0.,0.,0.\PG=C02H [SGH(C12H12),X(C48H48)]\ \@

H2@C60-4/C2h (Corresponding to isomer 6)

H2@C60H58-5/C2h:

1\1\GINC-C0110\FOpt\RB3LYP\6-31G(d,p)\C60H60\STUDENT\05-Nov-2007\0\#p
 b3lyp/6-31g** opt symm=loose\\BB\0,1\C,-1.8552816289,4.054989569,1.3
 601272839\C,-1.8612162512,2.4946644487,1.3728150646\H,-2.710606396,4.3
 470898786,1.9782764668\H,-2.7610754918,2.2333824437,1.9381534251\H,-2.
 7167427556,0.0473843055,1.6470183254\C,-1.7832979136,-1.8329543987,1.3
 601280036\H,-2.6690762206,-2.0500066686,1.9720634194\C,-1.098101084,-6
 .0509785881,0.7759919066\C,-1.7475002408,-4.7247438804,1.2642719434\H,
 -1.6438332387,-6.9161898951,1.1644565869\H,-2.6219486259,-4.9544626735
 ,1.8815210229\C,-1.7136744933,-0.2760257881,1.3373060282\C,0.714980567
 2,4.0455309264,2.2136704569\C,2.2934761851,3.9903666389,0.000000023\C,
 0.6870998645,2.4874911412,2.2428111715\C,2.2390711163,2.4293042887,0.0
 00000014\H,1.0474841358,4.3477955915,3.2125635101\H,3.3600082354,4.238
 3740583,0.0000000244\H,1.0515105098,2.2263124723,3.2429536638\H,3.2900
 413284,2.1095142249,0.0000000122\C,-0.7405064986,1.8982983518,2.295089
 8646\C,1.7832979136,1.832954383,1.3601280247\H,2.6690762206,2.05000664
 59,1.972063443\C,-0.3810265998,6.0749251443,1.2557776963\C,1.098101084
 ,6.0509785792,0.7759919764\C,-0.6528222115,4.7682498981,2.0496751483\C
 ,1.7475002408,4.7247438658,1.2642719979\H,-0.5716557822,6.9556026944,1
 .8765826729\H,1.6438332387,6.9161898817,1.1644566666\H,-0.9888505013,5
 .0192987193,3.0608340291\H,2.6219486259,4.9544626518,1.88152108\H,0.40
 27738189,-0.7324197778,-0.0000000042\C,-0.7277069425,0.3121125256,2.37
 80930215\C,1.7136744933,0.2760257727,1.3373060314\H,-1.1308030418,0.05
 21736433,3.3648884015\H,2.7167427556,-0.0473843245,1.6470183248\C,-0.7
 149805672,-4.0455309519,2.2136704103\C,1.8552816289,-4.0549895847,1.36
 01272372\C,-0.6870998645,-2.487491167,2.2428111428\C,1.8612162512,-2.4
 946644645,1.3728150358\H,-1.0474841358,-4.3477956286,3.21256346\H,2.71
 0606396,-4.3470899015,1.9782764167\H,-1.0515105098,-2.2263125097,3.242
 9536382\C,0.7405064986,-1.8982983783,2.2950898427\C,2.1320812896,-1.79
 9980448,-0.0000000104\H,1.0834870294,-2.23170132,3.2838772041\H,3.2185
 977897,-1.622020838,-0.0000000093\C,0.3810265998,-6.0749251588,1.25577
 76262\C,1.2955961481,-6.0783113796,-0.000000035\C,0.6528222115,-4.7682

499218,2.0496750934\C,2.1308630782,-4.764160229,-0.0000000275\H,0.5716
 557822,-6.955602716,1.8765825927\H,1.9513990801,-6.9542716568,-0.00000
 00401\H,0.9888505013,-5.0192987546,3.0608339713\H,3.197415795,-5.01186
 77319,-0.0000000289\C,0.7277069425,-0.312112553,2.3780930179\C,1.44519
 94933,-0.442269155,-0.0000000025\H,-1.0834870294,2.2317012821,3.283877
 2298\H,1.1308030418,-0.0521736821,3.3648884009\H,2.7610754918,-2.23338
 2466,1.9381533994\C,-2.2934761851,-3.9903666389,-0.000000023\C,-2.2390
 711163,-2.4293042887,-0.000000014\H,-3.3600082354,-4.2383740583,-0.000
 0000244\H,-3.2900413284,-2.1095142249,-0.0000000122\H,-0.4027738189,0.
 7324197778,0.0000000042\C,-2.1320812896,1.799980448,0.0000000104\H,-3.
 2185977897,1.622020838,0.0000000093\C,-1.2955961481,6.0783113796,0.000
 000035\C,-2.1308630782,4.764160229,0.0000000275\H,-1.9513990801,6.9542
 716568,0.0000000401\H,-3.197415795,5.0118677319,0.0000000289\C,-1.4451
 994933,0.442269155,0.0000000025\C,-0.7149805672,-4.0455309264,-2.21367
 04569\C,1.8552816289,-4.054989569,-1.3601272839\C,-0.6870998645,-2.487
 4911412,-2.2428111715\C,1.8612162512,-2.4946644487,-1.3728150646\H,-1.
 0474841358,-4.3477955915,-3.2125635101\H,2.710606396,-4.3470898786,-1.
 9782764668\H,-1.0515105098,-2.2263124723,-3.2429536638\H,2.7610754918,
 -2.2333824437,-1.9381534251\C,-1.7832979136,-1.832954383,-1.3601280247
 \C,0.7405064986,-1.8982983518,-2.2950898646\H,1.0834870294,-2.23170128
 21,-3.2838772298\C,-1.098101084,-6.0509785792,-0.7759919764\C,0.381026
 5998,-6.0749251443,-1.2557776963\C,-1.7475002408,-4.7247438658,-1.2642
 719979\C,0.6528222115,-4.7682498981,-2.0496751483\H,-1.6438332387,-6.9
 161898817,-1.1644566666\H,0.5716557822,-6.9556026944,-1.8765826729\H,-
 2.6219486259,-4.9544626518,-1.88152108\H,0.9888505013,-5.0192987193,-3
 .0608340291\H,2.7167427556,-0.0473843055,-1.6470183254\C,-1.7136744933
 ,-0.2760257727,-1.3373060314\C,0.7277069425,-0.3121125256,-2.378093021
 5\H,-2.7167427556,0.0473843245,-1.6470183248\H,1.1308030418,-0.0521736
 433,-3.3648884015\C,-1.8552816289,4.0549895847,-1.3601272372\C,0.71498
 05672,4.0455309519,-2.2136704103\C,-1.8612162512,2.4946644645,-1.37281
 50358\C,0.6870998645,2.487491167,-2.2428111428\H,-2.710606396,4.347089
 9015,-1.9782764167\H,1.0474841358,4.3477956286,-3.21256346\H,-2.761075
 4918,2.233382466,-1.9381533994\C,-0.7405064986,1.8982983783,-2.2950898
 427\C,1.7832979136,1.8329543987,-1.3601280036\H,-1.0834870294,2.231701
 32,-3.2838772041\H,2.6690762206,2.0500066686,-1.9720634194\C,-0.381026
 5998,6.0749251588,-1.2557776262\C,1.098101084,6.0509785881,-0.77599190
 66\C,-0.6528222115,4.7682499218,-2.0496750934\C,1.7475002408,4.7247438
 804,-1.2642719434\H,-0.5716557822,6.955602716,-1.8765825927\H,1.643833
 2387,6.9161898951,-1.1644565869\H,-0.9888505013,5.0192987546,-3.060833
 9713\H,2.6219486259,4.9544626735,-1.8815210229\C,-0.7277069425,0.31211
 2553,-2.3780930179\C,1.7136744933,0.2760257881,-1.3373060282\H,-2.6690
 762206,-2.0500066459,-1.972063443\H,-1.1308030418,0.0521736821,-3.3648
 884009\H,1.0515105098,2.2263125097,-3.2429536382\\Version=IA32L-G03Rev
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 =0.\Dipole=0.,0.,0.\PG=C02H [SGH(C12H12),X(C48H48)]\\@

H2@C60H58 - 6/Cs :

```
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.3054574011,2.3862978728\C,-1.0545828808,2.2792621346,2.3641058993\H,-
2.0012081158,4.09025576,3.1277083289\H,-0.5325345744,2.3862035641,3.32
25825777\H,1.1126345243,0.8289352855,3.1338233205\C,2.1006851827,-0.69
80394668,2.044582172\H,2.6752041529,-0.5907561418,2.9716713066\C,4.847
0612232,-3.8150042572,0.8366721128\C,4.0549066702,-2.7243635186,1.5983
560788\H,5.6736882007,-4.2226330395,1.4259595311\H,4.6435944939,-2.245
4609718,2.3920481973\C,0.9684840761,0.3786053489,2.1445043935\C,-1.363
3972959,4.4314358221,0.0796785014\C,-2.6437749591,3.3405890694,-1.9745
617357\C,-0.1789724106,3.4443619332,-0.0226554406\C,-1.5020131452,2.26
29084676,-2.0539696986\H,-1.0043626904,5.4166725216,0.4104816577\H,-2.
7533664731,3.7191274797,-2.9962002529\H,0.7250696604,4.0595897221,-0.1
054271032\H,-1.1951427145,2.2850477713,-3.1059845517\C,0.0864419283,2.
7094365649,1.3543270777\C,-0.1760413315,2.6920423081,-1.3709863025\H,0
.1394820259,3.5013685235,-2.0433428468\C,-3.5319226416,4.8278427899,1.
0609909889\C,-3.7609557877,5.001633322,-0.4486213877\C,-2.3714518081,3
.8800474634,1.0240556949\C,-2.35919947,4.6290868821,-1.1260329112\H,-3
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4285208379,-1.7894552103\H,0.4332983235,0.747693755,-3.2649711614\C,1.
2246320129,1.6251172882,1.2425735432\C,0.9545215469,1.6113714857,-1.47
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44318,-2.1736714196\C,3.7026237302,-1.7492765292,0.5044393885\C,4.1560
254976,-1.3701537936,-1.8452355325\C,3.1856238452,-0.4245772674,0.9614
253102\C,3.0065869853,-0.2825994695,-1.7005961626\H,2.861180151,-2.214
6696006,-0.0314357995\H,4.9047756564,-0.9605885375,-2.5333730517\H,4.0
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6575105\C,1.6783128419,-0.7272626728,-2.3698319876\H,3.8929920368,1.02
96498109,-0.34780595\H,1.9712576406,-0.7123097027,-3.4287211438\C,5.33
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765168599\C,4.8248584436,-1.6998546913,-0.5003980919\C,3.7476308555,-2
.7720850163,-2.4267516969\H,6.4249969413,-3.2229308978,-0.6219769858\H
,5.303337525,-4.3293228211,-2.3603824438\H,5.5973665121,-0.976358301,-
0.2077678826\H,4.0290592579,-2.760310527,-3.484170093\C,1.8259346858,1
.5195413777,-0.1927563358\C,0.5281519374,0.3415813728,-2.2504454919\H,
0.5315335611,3.5376549225,1.921909564\H,2.3530691862,2.4794753646,-0.2
473851011\H,3.3258005311,0.5330760446,-2.359175405\C,2.7124576448,-3.2
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84938041,2.4465798235\H,-1.893377103,0.7964171299,3.4978763866\C,-4.56
81889134,3.9275173947,1.7517552435\C,-3.7061126904,2.8368649122,2.5454
174792\H,-5.2651796196,4.4556537508,2.4085568914\H,-3.9922445424,2.797
1122438,3.6011081644\C,-0.4400647613,-0.2442849757,2.3287397542\C,1.40
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4998791, -4.4079070957, -0.029994989\C, 2.2634652695, -3.2656193374, -2.3700247993\C, 0.2906942912, -3.3228312098, 0.0885939565\C, 1.1479333584, -2.1821766625, -2.2480901447\H, 0.8753410095, -5.3654318743, 0.013109311\H, 2.1104985885, -3.7219135571, -3.3537147034\H, -0.6354963686, -3.9029074835, 0.1717502515\H, 0.5991140013, -2.2601172906, -3.1935821663\C, 0.2724512114, -2.5979222392, 1.4623014816\C, 0.0196237552, -2.5889157718, -1.2565816159\H, -0.4238596086, -3.4181176426, -1.8240541934\C, 3.8021442812, -4.9074692178, 0.478701379\C, 3.6273607034, -4.9123646308, -1.0672361458\C, 2.4390959979, -4.5132401885, 1.140085974\C, 2.1723714125, -4.4845322438, -1.3921686878\H, 4.1315168149, -5.8885641958, 0.8337963187\H, 3.8390807394, -5.9057223494, -1.474472756\H, 2.0971462967, -5.3309415079, 1.7818875031\H, 1.6825719903, -5.2812412111, -1.9607713951\H, -1.0394658774, -0.7234308411, -3.0497204802\C, -0.8672459566, -1.5151549963, 1.5531656577\C, -1.1276645005, -1.5216496762, -1.1564903751\H, -1.5916560061, -1.9467393996, 2.2547009684\H, -1.9671022426, -1.9831758304, -1.6897420598\C, -4.0522278147, 1.4664815818, 1.8646349613\C, -4.2905007747, 1.4465241194, -0.8678959009\C, -2.8956114432, 0.4085666666, 1.7447360665\C, -3.1533478951, 0.3881103261, -0.9673841596\H, -4.7850938487, 1.0156820132, 2.5419340186\H, -5.141098871, 1.0032644845, -1.3963250694\H, -3.2169236062, -0.4051627617, 2.4050373404\C, -2.8799330156, -0.3338205745, 0.3796507362\C, -2.025286516, 0.8033842652, -1.9499664781\H, -3.8071136725, -0.9158734882, 0.4706690044\H, -2.5701843229, 0.7300023722, -2.9009845472\C, -5.2895507498, 3.2320905564, 0.5593967519\C, -4.7967001466, 3.8878846088, -0.7840279857\C, -4.8754668161, 1.736549386, 0.5550702303\C, -4.0759475614, 2.8004011263, -1.6242797348\H, -6.3745274293, 3.3360512597, 0.6529610897\H, -5.6460675106, 4.3053504326, -1.3326935259\H, -5.7714714522, 1.1130093098, 0.6387127704\H, -4.5889002909, 2.6865553886, -2.5847698463\C, -1.7411292289, -1.4145283517, 0.2712480203\C, -0.8857544369, -0.2763544356, -2.0603543924\H, -0.0618553262, -3.4175988567, 2.1131900075\H, -2.27682415, -2.3698774326, 0.323102241\H, -3.6017166703, -0.436076725, -1.5342010167\\Version=IA32L-G03RevD.01\State=1-A'\HF=-2322.2994649\RMSE=7.851e-09\RMSF=2.071e-05\Thermal=0.\Dipole=-0.1226535, -0.1618688, -0.1240132\PG=CS [SG(C12H12), X(C48H48)]\@

H2@C60H58-7/Cs:

1\1\GINC-C0130\FOpt\RB3LYP\6-31G(d,p)\C60H60\STUDENT\04-Nov-2007\0\#p
b3lyp/6-31g** opt geom=allcheck guess=read\\BB\\0,1\C, -2.1983493345, 3.314906067, 2.3803897426\C, -1.0512771926, 2.2792516928, 2.3561675781\H, -1.9839418191, 4.0979034157, 3.121923186\H, -0.5235794496, 2.3806520039, 3.312509812\H, 1.1498412152, 0.7548551167, 3.1079532299\C, 2.029895624, -0.7578603015, 1.935030697\H, 2.8187722302, -0.5116652323, 2.6603349871\C, 4.8368155423, -3.7872099812, 0.8565671744\C, 4.1146458068, -2.6934083032, 1.6880225635\H, 5.6733030116, -4.2159588484, 1.4167436786\H, 4.6734562907, -2.4936301017, 2.6079055739\C, 0.9470411983, 0.342159224, 2.1117898054\C, -1.3476815747, 4.4346585951, 0.0718405946\C, -2.6411425597, 3.3522542309, -1.9815991127\C, -0.1708102514, 3.4382295335, -0.0332508332\C, -1.5067703391, 2.2689380809, -2.0638422039\H, -0.9812960998, 5.417707847, 0.4009350041\H, -2.7510

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H2@C60H58-8/Cs:

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X(C48H48)]\\@

H2@C60H58-9/Cs

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2982395,-5.8736667821,0.8531142965\H,3.830633723,-5.9099244799,-1.4605
484762\H,2.0817033659,-5.2558203594,1.7958524379\H,1.6626552174,-5.303
8940302,-1.9594323509\H,-1.0618001989,-0.7070494222,-3.0366431458\C,-0
.8818107225,-1.5257673679,1.5853495147\C,-1.1421023742,-1.4882119911,-
1.1375927297\H,-1.6050723505,-1.9835270545,2.2730761523\H,-1.998242879
,-1.9274147313,-1.6629959164\C,-4.0659934288,1.4933766679,1.9007722422
\C,-4.2733424732,1.478444509,-0.8459624634\C,-2.9200346395,0.406720831
2,1.8251696001\C,-3.124608817,0.4384380674,-0.9295512822\H,-4.81941098
07,1.0680316004,2.5730159451\H,-5.1159903384,1.0200949202,-1.375702055
4\H,-3.283908476,-0.4132906913,2.4556991871\C,-2.8733884289,-0.2981709
851,0.4270212661\C,-2.0071183313,0.8492052162,-1.9436908301\H,-3.80979
82645,-0.8701229123,0.4859467745\H,-2.5813135924,0.7570071023,-2.87603
40677\C,-5.2791431754,3.2651853955,0.5716009904\C,-4.7873927002,3.9165
097271,-0.7741672673\C,-4.8692718474,1.766596053,0.5734959948\C,-4.069
0024659,2.8265541949,-1.6165926486\H,-6.3645999061,3.3711360464,0.6653
163582\H,-5.6382493938,4.3331885217,-1.3224793078\H,-5.7694557364,1.14
65290454,0.6456465774\H,-4.5945358396,2.7027124251,-2.5697441181\C,-1.
7484331596,-1.388225343,0.3016628896\C,-0.8868963503,-0.2471183898,-2.
0560956675\H,-0.035624264,-3.4201662042,2.1061816576\H,-2.294171175,-2
.3393268529,0.3359733027\H,-3.5610089981,-0.3946372267,-1.4922055143\\
Version=IA32L-G03RevD.01\State=1-A'\HF=-2322.2234353\RMSE=9.226e-10\RM
SF=2.291e-05\Thermal=0.\Dipole=-0.0708478,-0.229593,-0.1370065\PG=CS [
SG(C12H12),X(C48H48)]\\@

H2@C60H58-10/Cs:

1\1\GINC-C0130\FOpt\RB3LYP\6-31G(d)\C60H60\STUDENT\05-Nov-2007\0\#p b
3lyp/6-31g* opt geom=allcheck guess=read\\BB\\0,1\C,-2.2138511525,3.28
82720952,2.3669216451\C,-1.1448870529,2.1833150871,2.1834324223\H,-2.0
248272167,3.6926698323,3.3680367529\H,-0.35764323,2.4320458187,2.90845
98593\H,1.0869309895,0.8310092872,3.0451421017\C,2.0422387831,-0.74408

51893,2.0089375846\H,2.6129034287,-0.6212592973,2.9368341269\C,4.80292
13231,-3.8557604456,0.8164307913\C,4.0090922451,-2.7633096811,1.573974
8555\H,5.6286899659,-4.2621572682,1.4090473488\H,4.5973159177,-2.27983
47329,2.3662210244\C,0.8949673668,0.3133832262,2.0996439622\C,-1.36250
07071,4.4108815131,0.0557498788\C,-2.6772419927,3.3017410249,-2.002758
0103\C,-0.3153132852,3.2772092988,-0.0686219228\C,-1.5150597186,2.2590
50273,-2.1477945407\H,-0.7786640417,5.3358879969,-0.014938098\H,-2.803
4736258,3.7346727026,-3.0016782728\H,0.6407036527,3.748487971,0.198235
0152\H,-1.2575008186,2.2727622844,-3.2137001327\C,-0.4647914169,2.0507
580917,0.8250785196\C,-0.1738312829,2.7205411177,-1.4980955457\H,0.158
3308218,3.5571349779,-2.1300306499\C,-3.5748682873,4.9586420099,1.0918
923292\C,-3.7537123779,4.9451023926,-0.4518542892\C,-2.1151129045,4.52
37507903,1.4183719217\C,-2.4017732464,4.530911884,-1.0927582767\H,-3.7
828577704,5.9537105681,1.498613028\H,-4.0743747766,5.9270856998,-0.814
6446559\H,-1.6149385248,5.3151425286,1.987021781\H,-2.0464114451,5.332
2108971,-1.7496533266\H,0.4052986588,0.6960019713,-3.3533870664\C,0.94
48699158,1.4902779424,1.0721027857\C,0.9536309514,1.6077044392,-1.5794
173136\H,1.4449268656,2.2869327945,1.6432658494\H,1.7025447287,2.02506
48178,-2.2643294046\C,3.6547575994,-1.7920010484,0.4760184788\C,4.1225
809107,-1.4185517367,-1.8744263705\C,3.1291581499,-0.4661528414,0.9264
13544\C,2.976631449,-0.3283848802,-1.7419274855\H,2.8158395927,-2.2619
415254,-0.0612729688\H,4.8778876693,-1.0146890929,-2.5599274425\H,3.93
81723642,0.0431731797,1.471820345\C,2.9112460217,0.4018068643,-0.35016
73004\C,1.6546546469,-0.7649165195,-2.4213709534\H,3.8353477771,0.9906
827009,-0.3817509269\H,1.9562418322,-0.7698096863,-3.4787682165\C,5.29
70191785,-3.2042321487,-0.5249028736\C,4.5526318742,-3.9024396231,-1.6
967062172\C,4.7821283946,-1.743967216,-0.5245961061\C,3.7116361582,-2.
8201720356,-2.4522450166\H,6.3837381337,-3.2665341512,-0.6406914128\H,
5.2648619072,-4.3802974295,-2.377105295\H,5.5533629646,-1.0191700741,-
0.2291719232\H,3.9941078465,-2.8131654953,-3.5101025329\C,1.7637989214
,1.4590436189,-0.2589839911\C,0.5139387302,0.3220187495,-2.3268568275\
H,-1.0321092565,1.3073699679,0.2550123638\H,2.2905799672,2.4181672965,
-0.2224189231\H,3.3067038232,0.4880768483,-2.3949521421\C,2.6701208973
, -3.3337974487,2.0685851033\C,1.5376508531,-2.2258563358,2.164491244\H
,2.8024253066,-3.7514394021,3.0743563479\H,1.2386539194,-2.2388992294,
3.2192089526\H,-0.3789481847,-0.7196375081,3.3863255976\C,-1.653962587
9,0.7688074321,2.5200355314\H,-1.9452080461,0.7833623716,3.5804727825\
C,-4.5439698741,3.903051481,1.6934676792\C,-3.6956992554,2.8247125962,
2.4198789407\H,-5.2522442512,4.3739211102,2.3829324271\H,-3.9725333692
,2.7923841742,3.4792140959\C,-0.5029193478,-0.3129348136,2.3746981105\
C,1.3610667653,-4.4453753362,-0.0495806166\C,2.2248287438,-3.306399797
9,-2.3944461279\C,0.2489064394,-3.3563563493,0.0719258153\C,1.11385771
9,-2.2158125724,-2.2761683068\H,0.8284099407,-5.4020263649,-0.00737603
8\H,2.0698154342,-3.7650817837,-3.3774351511\H,-0.6805790244,-3.933977
3577,0.1428261329\H,0.5570559495,-2.3020046666,-3.2169971031\C,0.22618
07861,-2.6485335633,1.4565250102\C,-0.0109051156,-2.6103777135,-1.2717

879784\H, -0.4668116633, -3.4333431193, -1.8394675325\C, 3.7585763608, -4.9494986837, 0.4589262762\C, 3.5832509112, -4.9552513376, -1.0868129252\C, 2.3958028341, -4.5552587908, 1.1198642646\C, 2.128855598, -4.523298114, -1.4127451436\H, 4.089104295, -5.9306772708, 0.8147386887\H, 3.7915857865, -5.9503168929, -1.4934049357\H, 2.0523632205, -5.3735926565, 1.7611760352\H, 1.6373499495, -5.3202003135, -1.9808783678\H, -1.0674496706, -0.760823068, -3.06728773\C, -0.9216504094, -1.5709806574, 1.570355073\C, -1.142176968, -1.5298700677, -1.1636699807\H, -1.6577346042, -2.0243590537, 2.2471552907\H, -1.988190761, -1.9817691031, -1.694811954\C, -4.0847578174, 1.4457597083, 1.8182429091\C, -4.3079598144, 1.4122274, -0.9007575923\C, -2.9583872064, 0.3558469101, 1.7704247508\C, -3.1520040496, 0.3752221647, -0.9786524467\H, -4.8355025581, 1.0551946698, 2.5146962376\H, -5.1450561047, 0.9482914938, -1.4344613764\H, -3.3278826951, -0.457288784, 2.4067915979\C, -2.8996541396, -0.358066875, 0.3801829793\C, -2.0284150873, 0.7907680973, -1.9849806384\H, -3.832262376, -0.9363915969, 0.4385263808\H, -2.5942827321, 0.6960355838, -2.9222325355\C, -5.2947815245, 3.2139051152, 0.5204952367\C, -4.8062025469, 3.8581560984, -0.8058562611\C, -4.9010227069, 1.7090680621, 0.5108043449\C, -4.1029506272, 2.7614234553, -1.6557319716\H, -6.3775581163, 3.3307842188, 0.6330751099\H, -5.6447711985, 4.297053162, -1.3562307561\H, -5.805790098, 1.0971619319, 0.5922954639\H, -4.6252915583, 2.6537932644, -2.6124187752\C, -1.7661201176, -1.438247256, 0.2690868229\C, -0.8970136525, -0.2922243603, -2.0902874332\H, -0.0985736302, -3.4793345387, 2.0994651737\H, -2.3053443102, -2.3931381601, 0.2932404239\H, -3.582957769, -0.4596900312, -1.5429432338\\Version=IA32L-G03RevD.01\State=1-A'\HF=-2322.2654456\RMSD=3.410e-09\RMSF=1.921e-05\Thermal=0.\Dipole=-0.1818854, -0.1235652, -0.1270194\PG=CS [SG(C12H12), X(C48H48)]\\@

H2@C60H58-11/Cs:

1\1\GINC-C0124\FOpt\RB3LYP\6-31G(d)\C60H60\STUDENT\05-Nov-2007\0\#p b 3lyp/6-31g* opt geom=allcheck guess=read\\BB\\0,1\C, -2.1692900538, 3.3471264463, 2.4179852748\C, -1.0613118522, 2.2564569451, 2.3083243941\H, -2.0320004841, 3.7913634626, 3.4100208386\H, -0.4721871662, 2.3870227422, 3.2217774278\H, 1.176014154, 1.0492770583, 2.8055557389\C, 2.0604755243, -0.7118004184, 2.0262497734\H, 2.5903638106, -0.5405133916, 2.9708560609\C, 4.8627201296, -3.8062751473, 0.861928584\C, 4.0613739137, -2.7165619964, 1.6159204366\H, 5.6887968721, -4.2078067728, 1.4574287564\H, 4.6449357742, -2.2278822189, 2.4084752251\C, 0.8933605782, 0.3137161182, 2.0397540434\C, -1.3148863173, 4.4740160436, 0.0998982325\C, -2.6298131962, 3.3155955974, -1.9591879695\C, -0.200372709, 3.3919662166, -0.0274938929\C, -1.4798068113, 2.2640812863, -2.0904419902\H, -0.7878542906, 5.4322919171, 0.0345215908\H, -2.7440243337, 3.7453116584, -2.96088443\H, 0.7287283699, 3.9709334474, -0.0364325076\H, -1.2045936096, 2.2866754907, -3.1525379196\C, 0.0105841782, 2.4533501473, 1.1965465646\C, -0.1559207742, 2.7248977787, -1.4310684407\H, 0.1314056261, 3.5683928553, -2.0748452944\C, -3.5398563443, 4.9873882439, 1.1197899652\C, -3.7106427714, 4.9676091481, -0.4244024158\C, -2.0783771075, 4.5674545748, 1.4543220269\C, -2.3540676232, 4.553321356, -1.0575906362\H, -3.75

9731102,5.9816617732,1.5220935307\H,-4.0299937538,5.9481699297,-0.7921
540282\H,-1.5912359502,5.3673488381,2.0227250786\H,-2.0056741971,5.348
1883944,-1.7258902613\H,0.4642602336,0.7288060708,-3.3486239656\C,0.60
87204246,1.1047963325,0.7614371821\C,1.0212067026,1.6721445835,-1.5764
864035\H,-0.1575689002,0.5504012323,0.209489602\H,1.7631670256,2.13093
07755,-2.2436290751\C,3.7042669252,-1.7492807503,0.5149480437\C,4.1805
232459,-1.3777195136,-1.8363235592\C,3.1654007224,-0.4262762288,0.9594
830057\C,3.0300517826,-0.2936719534,-1.7141681124\H,2.8710093811,-2.22
68838723,-0.0243519593\H,4.9379231945,-0.9732517841,-2.5191633691\H,3.
9641029081,0.0955473082,1.507543378\C,2.9269206503,0.4309708001,-0.324
5068228\C,1.7157636297,-0.7287110085,-2.4029063672\H,3.8146162384,1.07
4176791,-0.3506693119\H,2.0202389868,-0.7431388984,-3.4594559515\C,5.3
569440455,-3.154433675,-0.4789527892\C,4.6188124996,-3.8583923522,-1.6
516532443\C,4.834745075,-1.6965478283,-0.4823167215\C,3.7764362412,-2.
7811425875,-2.4120054019\H,6.4442291007,-3.2114526096,-0.592138194\H,5
.335114881,-4.3352504207,-2.328464502\H,5.6009106659,-0.9670284623,-0.
1851850255\H,4.0609508364,-2.7759831093,-3.4693358487\C,1.7303377925,1
.4176215387,-0.2310530147\C,0.5812096758,0.369728719,-2.3185514738\H,0
.8365090033,2.9396573924,1.7373751915\H,2.1763302847,2.3686133315,0.09
15930517\H,3.3625913412,0.5274939736,-2.3598476756\C,2.726026561,-3.29
60832959,2.109878657\C,1.5858755392,-2.1984239059,2.2040336623\H,2.860
9859504,-3.712564447,3.1157854351\H,1.2912398632,-2.2044515144,3.25994
63588\H,-0.3477996119,-0.6532639119,3.4836450464\C,-1.6054825514,0.813
0427416,2.5017448527\H,-1.9411880087,0.8348090626,3.548318842\C,-4.501
234878,3.9248819425,1.7205569749\C,-3.6452433406,2.8503647535,2.445504
6478\H,-5.2109983899,4.3905200953,2.4120355449\H,-3.9324481803,2.80692
89578,3.5016498503\C,-0.4646236523,-0.2875457815,2.4547273491\C,1.4253
048151,-4.4105817173,-0.0083245038\C,2.2904730138,-3.2694946628,-2.355
6166624\C,0.308150142,-3.3255667036,0.1129131286\C,1.1762959856,-2.180
5523756,-2.2424576934\H,0.8958479669,-5.3690715367,0.0321667009\H,2.13
79256166,-3.7308713246,-3.3377203703\H,-0.619604767,-3.9069496151,0.17
33224975\H,0.6165330454,-2.2765835691,-3.1804491717\C,0.2754387594,-2.
6283833106,1.504846228\C,0.0552456075,-2.5752037734,-1.23151852\H,-0.4
007200131,-3.3978062791,-1.799469987\C,3.8245905282,-4.9059070565,0.50
31543507\C,3.6510626773,-4.9130556862,-1.0426651544\C,2.459200966,-4.5
184696443,1.1617921985\C,2.1955713705,-4.4852521842,-1.3711644217\H,4.
1599954171,-5.885138188,0.8597579815\H,3.862305473,-5.9078579141,-1.44
84073163\H,2.1180094773,-5.3385660103,1.8020680511\H,1.7076322796,-5.2
842420503,-1.9394219231\H,-1.0002662245,-0.7380487986,-3.0311722906\C,
-0.8760125473,-1.5522298282,1.6350454136\C,-1.072377488,-1.4964464513,
-1.1227240643\H,-1.6169595202,-2.0161548768,2.2979437371\H,-1.91991301
98,-1.9457109361,-1.6535104313\C,-4.0275030333,1.4721554645,1.83289130
41\C,-4.2647533622,1.4297527182,-0.8768637847\C,-2.901109328,0.3894979
338,1.7657009627\C,-3.1097784096,0.3848259219,-0.9591308515\H,-4.76945
76419,1.0739285317,2.5343287887\H,-5.1040772668,0.9693523702,-1.410036
966\H,-3.2568738092,-0.4201165197,2.4155137343\C,-2.8504787986,-0.3400

606999,0.3968183003\C,-1.9840651638,0.8026689843,-1.953852857\H,-3.777
 5657901,-0.9263355207,0.4645653625\H,-2.5380728975,0.7084556055,-2.898
 3089916\C,-5.2504476154,3.2345752206,0.5466792638\C,-4.7618571618,3.87
 89866106,-0.7789179346\C,-4.8540001622,1.7308123311,0.5351861538\C,-4.
 0573626841,2.781512894,-1.6261749646\H,-6.3334991702,3.3497428655,0.65
 83616443\H,-5.6005322303,4.3164671254,-1.3302546191\H,-5.7567976335,1.
 1168357436,0.6234797754\H,-4.5736178143,2.6773544692,-2.5866112982\C,-
 1.7063089048,-1.4111083594,0.3116081381\C,-0.8325151419,-0.2586448817,
 -2.0590860815\H,-0.0442094777,-3.4659798685,2.1416094823\H,-2.23786933
 58,-2.3703474556,0.3265748883\H,-3.5466885393,-0.4466443285,-1.5243696
 881\\Version=IA32L-G03RevD.01\State=1-A'\HF=-2322.2659634\RMSD=3.419e-
 09\RMSF=2.106e-05\Thermal=0.\Dipole=-0.2106504,-0.0972153,-0.124901\PG
 =CS [SG(C12H12),X(C48H48)]\ \@

H2@C60H58-12/Cs:

1\1\GINC-C0127\FOpt\RB3LYP\6-31G(d,p)\C60H60\STUDENT\06-Nov-2007\0\#p
 b3lyp/6-31g** opt geom=allcheck guess=read\\BB\\0,1\C,-2.159017151,3.
 3529915525,2.4231110715\C,-1.0562268688,2.257878553,2.3101848378\H,-2.
 0179146861,3.7953689215,3.4147063556\H,-0.4638691301,2.3826916141,3.22
 1900243\H,1.201749259,0.9816769112,2.7870412377\C,2.0021242444,-0.7817
 26829,1.9090072387\H,2.7579495916,-0.489431887,2.6511304679\C,4.857472
 1556,-3.7812523032,0.863575424\C,4.130650811,-2.6892138179,1.694365534
 5\H,5.6945571318,-4.2069745979,1.4251876999\H,4.6883365422,-2.48553317
 52,2.6140878816\C,0.8735737794,0.2804691017,2.0085689594\C,-1.30520296
 56,4.4789523748,0.1040167831\C,-2.6324980589,3.3288188044,-1.952651748
 7\C,-0.1955613717,3.3928744893,-0.0275186961\C,-1.4886783708,2.2733524
 398,-2.0884989668\H,-0.7748696955,5.4346248435,0.0383996755\H,-2.74715
 20661,3.7604157943,-2.952802847\H,0.7367148947,3.9659524673,-0.0390757
 422\H,-1.2172091214,2.2971079233,-3.1507566531\C,0.014214515,2.4534073
 273,1.1964024548\C,-0.1617872021,2.7275115129,-1.4335209458\H,0.126442
 0104,3.5710820742,-2.0756346208\C,-3.5251376086,5.0009742405,1.1302177
 745\C,-3.7002361915,4.9838913356,-0.413485092\C,-2.0647196106,4.573820
 8355,1.4605051665\C,-2.3474571408,4.5639380935,-1.0504698939\H,-3.7390
 934134,5.995166205,1.5341438699\H,-4.0157138313,5.9657867118,-0.779066
 4661\H,-1.5726406804,5.3702149126,2.0283356801\H,-1.9971769054,5.35710
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 05,-2.2483713268\C,4.1201026075,-1.4003382428,0.8369944574\C,4.1611470
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66551571,2.930407427,1.7344715878\H,2.2047990618,2.3044410441,0.062599
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132,2.0911563203\C,1.5568105953,-2.2126867003,2.2590043232\H,2.8730889
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H,0.6064316941,-2.2758138938,-3.1745190272\C,0.2461839023,-2.641733633
8,1.5401791377\C,0.0548040263,-2.5550024955,-1.2203243554\H,-0.3943019
936,-3.3810200814,-1.7867163892\C,3.8171670347,-4.8790533315,0.5112944
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04988,-5.8569179428,0.8723128805\H,3.8582772129,-5.8872103985,-1.43785
59117\H,2.1145753509,-5.2949438667,1.8104332079\H,1.6992992759,-5.2657
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, -4.2698901743,1.4484540785,-0.8687862553\C,-2.9085181725,0.4009497344
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18559\C,-5.2456296525,3.2568127722,0.5589618865\C,-4.7575266964,3.9004
947526,-0.7668028957\C,-4.8559952396,1.751285681,0.5441504348\C,-4.060
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638916,-1.4069826211,0.3140673531\C,-0.8454392563,-0.2521275633,-2.064
5391805\H,-0.0900220757,-3.4843827161,2.1589108935\H,-2.258347735,-2.3
623735134,0.3174215299\H,-3.5616493275,-0.430079665,-1.5200962622\\Ver
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2.408e-05\Thermal=0.\Dipole=-0.1850718,-0.1556355,-0.1437011\PG=CS [SG
(C12H12),X(C48H48)]\\@

H2@C60H58-13/Cs:

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b3lyp/6-31g** opt geom=allcheck guess=read\BB\0,1\C,-2.1611369893,3
.325733467,2.4028749299\C,-1.0978489558,2.2164366525,2.2158521957\H,-1
.9683499356,3.7278980556,3.403416003\H,-0.3056374655,2.4585036319,2.93
72611771\H,1.1771102203,0.7918278218,3.052095199\C,2.0263901217,-0.769
4851845,1.9259499539\H,2.8127698775,-0.5089761466,2.6482820035\C,4.848
4759411,-3.7883684379,0.8564828389\C,4.1252988175,-2.6949252188,1.6878
047822\H,5.6850258715,-4.2166076065,1.4169571043\H,4.6862011063,-2.491
0875068,2.6055471708\C,0.9255815238,0.3137748656,2.0998441433\C,-1.310
775295,4.4472814394,0.0913396992\C,-2.6355897018,3.3456903684,-1.96551
62842\C,-0.2689337434,3.3096987104,-0.0373851381\C,-1.4782635098,2.300
7010373,-2.1149830077\H,-0.7237476922,5.3694126392,0.0202180614\H,-2.7
629629395,3.7805228989,-2.9627830684\H,0.691025289,3.7730090935,0.2280
362843\H,-1.2245916973,2.3149770082,-3.1810634085\C,-0.4250687125,2.08
2709786,0.8541575777\C,-0.1355451785,2.7583947057,-1.4694858472\H,0.19
53040938,3.5962309587,-2.0992596022\C,-3.5188557481,5.002215677,1.1325
560718\C,-3.7013425238,4.9907460698,-0.4107206619\C,-2.0599422719,4.56
16444702,1.4554939971\C,-2.352453466,4.5724147636,-1.0546877901\H,-3.7
221047357,5.9970490928,1.5404746855\H,-4.0192424899,5.9735382692,-0.77
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457452,1.3998196847\H,4.9176610169,-0.9950833547,-2.4937809509\H,2.147
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1752507\C,1.7051432633,-0.7030570028,-2.4273150199\H,3.8113857771,0.80
81053318,-0.066252117\H,1.9852975582,-0.7213824609,-3.488921393\C,5.33
74220003,-3.1434940686,-0.4726175303\C,4.5958369648,-3.83825769,-1.646
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.3087755823,-4.3117122802,-2.3282423401\H,5.8081549102,-1.0113348058,-
0.4442559451\H,4.0349981511,-2.7421815819,-3.4478437172\C,1.788195031,
1.4514818397,-0.2449951479\C,0.548764743,0.369041482,-2.3195173528\H,-
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.490681484,3.9496814071,1.7349366835\C,-3.6448490402,2.8678652224,2.45
84265962\H,-5.1955462158,4.4221030769,2.4257852107\H,-3.9191396719,2.8

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 127678186,-3.7093003739,-3.3292831253\H,-0.6325496209,-3.8878659096,0.
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 ,-0.4039132717,-3.3790765545,-1.788097465\C,3.8041899957,-4.8823664016
 ,0.5054573102\C,3.6298658306,-4.8952408225,-1.039798132\C,2.4471147201
 ,-4.4820538404,1.156507511\C,2.1739705134,-4.46591917,-1.367083985\H,4
 .1337123506,-5.861511376,0.8659279483\H,3.8416318591,-5.8896424132,-1.
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 262923946,-1.9344306274\H,-1.0393900058,-0.7263779892,-3.0312805738\C,
 -0.9007182075,-1.542691696,1.6206071012\C,-1.0943296689,-1.4831661122,
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 7\C,-4.2657349399,1.4594700833,-0.8611304321\C,-2.9207694242,0.3981699
 209,1.8061757934\C,-3.1122599244,0.4187055616,-0.9417679097\H,-4.79224
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H2@C60H58-14/Cs:

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 H,-2.2676629922,-1.9817450418,4.3997694264\H,-0.4488156758,-1.44198573
 33,3.3335614932\H,1.1853143416,-1.4418265903,2.4236767026\C,2.47196411
 8,-1.356828523,0.7367165553\H,3.0480560089,-1.9789685356,1.4360367009\
 C,5.8505273301,-0.77579526,-1.8953159348\C,5.0004452063,-1.2630620387,
 -0.6875583693\H,6.8714942653,-1.1645482302,-1.833525745\H,5.6214814018
 ,-1.8824568002,-0.0324772868\C,1.0464749341,-1.2996539242,1.3463538514
 \C,-2.5528773492,1.3513155548,3.5497985681\C,-3.8739743649,2.246671186
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\H,-4.330974026,3.2348100129,1.2719027846\H,-0.4488156758,1.4419857333
,3.3335614932\H,-2.4983647837,3.3171903727,0.1606966901\C,-1.094851719
7,0.,1.8859290803\C,-1.2755520656,2.3928191082,1.5777448427\H,-1.36778
94159,3.362629649,2.0858238069\C,-4.5754080968,0.,4.1512995703\C,-5.04
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,2.93596262\H,-5.713939617,-1.8698483112,3.9830832082\H,-3.8287754393,
-3.0606252255,3.3752914272\C,0.1058142342,-2.3967404224,0.8059647109\C
,2.6780429539,-1.3590072697,-3.5264182316\C,2.6780429539,1.3590072697,
-3.5264182316\C,1.3041555095,-1.3679103554,-2.7793597099\C,1.304155509
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\H,2.5207323727,1.977798161,-4.4162118586\H,0.6521927305,-1.9665862862
, -3.4262789801\H,0.6521927305,1.9665862862,-3.4262789801\C,1.326723139
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\C,3.1701445389,0.,-4.1098414421\H,5.8390479564,-1.8772793151,-3.79423
1905\H,5.1771705281,0.,-5.0030338892\H,3.9405224862,-3.0600959044,-3.2
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, -2.3231537404\C,-0.0539121177,-2.3314851072,-0.7511056719\C,-0.798135
6969,0.,-2.06073368\H,-0.4577163602,-3.3243782,-0.9831793304\H,-1.5542
477504,0.,-2.8531306619\C,-3.8739743649,-2.2466711867,1.3939247411\C,-

4.5993579786,0.,0.0195097876\C,-2.5106932075,-2.3235137133,0.6235384547\C,-3.2234170109,0.,-0.7085496367\H,-4.330974026,-3.2348100129,1.2719027846\H,-5.344169621,0.,-0.7831670871\H,-2.4983647837,-3.3171903727,0.1606966901\C,-2.5029046216,-1.3981571626,-0.6430567201\C,-2.5029046216,1.3981571626,-0.6430567201\H,-3.1857504287,-1.9687063478,-1.2863798457\H,-3.1857504287,1.9687063478,-1.2863798457\C,-5.7788392422,-0.7764625257,2.0822578466\C,-5.7788392422,0.7764625257,2.0822578466\C,-4.9659929425,-1.2693906086,0.8505871976\C,-4.9659929425,1.2693906086,0.8505871976\H,-6.8014076304,-1.164759007,2.0517343817\H,-6.8014076304,1.164759007,2.0517343817\H,-5.615061465,-1.871625158,0.2068596213\H,-5.615061465,1.871625158,0.2068596213\C,-1.1342057567,-1.400197965,-1.4094138832\C,-1.1342057567,1.400197965,-1.4094138832\H,1.4517120446,-3.251479458,-1.9641120178\H,-1.3381356313,-1.9703622016,-2.3231537404\H,-3.4864463037,0.,-1.7715434155\\Version=IA64L-G03RevC.02\State=1-A'\HF=-2322.3623928\RMSD=7.694e-09\RMSF=1.917e-05\Dipole=-0.1196646,0.,-0.2405098\PG=CS [SG(C12H12),X(C48H48)]\ \@

H4@C60H56-1/C2 (Corresponding to 7)

H4@C60H56-2/Cs:

1\1\GINC-M0101\FOpt\RB3LYP\6-31G(d,p)\C60H60\JJF\05-Nov-2007\0\#\#P B3LYP/6-31G** OPT GEOM=ALLCHECK GUESS=READ\BB\0,1\C,-1.7898118256,-3.9986262829,1.3519379471\C,-1.7102933033,-2.4480139265,1.3305867927\H,-2.663582051,-4.2141142755,1.9758943056\H,-2.7125675665,-2.1194258933,1.6364325275\H,-2.7502148259,0.0562899374,1.9360819778\C,-1.820415317,1.8803230095,1.400541855\H,-2.729579876,2.1689068645,1.9388541662\C,-1.0371655144,6.0868598532,0.7859388964\C,-1.6073431442,4.7164851916,1.2328728569\H,-1.5968914595,6.9304746396,1.2003600213\H,-2.6666164208,4.7672597471,1.5177268762\C,-1.8343681729,0.3185651668,1.3977848\C,-1.7898118256,-3.9986262829,-1.3519379471\C,0.7439768357,-4.0774801551,-2.2793046224\C,-1.7102933033,-2.4480139265,-1.3305867927\C,0.721146996,-2.4998742462,-2.3770270181\H,-2.663582051,-4.2141142755,-1.9758943056\H,1.0785921236,-4.426359996,-3.2621453728\H,-2.7125675665,-2.1194258933,-1.6364325275\H,1.1268549221,-2.2490412755,-3.3641215274\C,-1.4300448886,-1.7246797285,0.\C,-0.7310343445,-1.886714235,-2.3897246498\H,-1.1379316373,-2.1840242299,-3.3659686912\C,-1.2998763696,-6.0469115557,0.\C,-0.3856166404,-6.068700656,-1.2571788941\C,-2.0975082738,-4.7103752889,0.\C,-0.635196631,-4.7670854009,-2.0676750945\H,-1.9802762487,-6.9038425751,0.\H,-0.5885519364,-6.9530180317,-1.868802505\H,-3.1711108546,-4.9247373115,0.\H,-1.011388373,-5.0227877824,-3.0635183405\H,1.0639113802,0.0011547261,-3.3258769999\C,-2.0992190581,-0.3595665915,0.\C,-0.7447347295,-0.2985983097,-2.3503835924\H,-3.187563212,-0.5239158098,0.\H,-1.1259769003,-0.0014388761,-3.3349382041\C,-1.3998972886,3.8719777136,0.\C,-0.7063838448,4.1094991622,-2.3282315054\C,-2.0793862684,2.5429541268,0.\C,-0.7209146896,2.518438917,-2.3496670011\H,-0.3268929189,3.6503221274,0.\H,-1.0576021811,4.4487469826,-3.309873866\H,-3.16287047

49,2.7300784328,0.\C,-1.820415317,1.8803230095,-1.400541855\C,0.708052
1538,1.8889888586,-2.3792237361\H,-2.729579876,2.1689068645,-1.9388541
662\H,1.1118066106,2.1778672914,-3.3598555864\C,-1.0371655144,6.086859
8532,-0.7859388964\C,0.4430726801,6.0896502207,-1.2610535528\C,-1.6073
431442,4.7164851916,-1.2328728569\C,0.6847683875,4.79012147,-2.0942285
838\H,-1.5968914595,6.9304746396,-1.2003600213\H,0.653335888,6.9789568
67,-1.8627668774\H,-2.6666164208,4.7672597471,-1.5177268762\H,1.077500
1009,5.0550155669,-3.0805817418\C,-1.8343681729,0.3185651668,-1.397784
8\C,0.6799966463,0.3029471213,-2.3442593425\H,-0.3863120257,-1.4443604
771,0.\H,-2.7502148259,0.0562899374,-1.9360819778\H,-1.1148321408,2.26
09537142,-3.3388319108\C,-0.7063838448,4.1094991622,2.3282315054\C,-0.
7209146896,2.518438917,2.3496670011\H,-1.0576021811,4.4487469826,3.309
873866\H,-1.1148321408,2.2609537142,3.3388319108\H,-1.1259769003,-0.00
14388761,3.3349382041\C,-0.7310343445,-1.886714235,2.3897246498\H,-1.1
379316373,-2.1840242299,3.3659686912\C,-0.3856166404,-6.068700656,1.25
71788941\C,-0.635196631,-4.7670854009,2.0676750945\H,-0.5885519364,-6.
9530180317,1.868802505\H,-1.011388373,-5.0227877824,3.0635183405\C,-0.
7447347295,-0.2985983097,2.3503835924\C,1.8126695765,3.994930022,1.362
737866\C,1.8126695765,3.994930022,-1.362737866\C,1.6834150411,2.450698
3616,1.3244841198\C,1.6834150411,2.4506983616,-1.3244841198\H,2.702051
6007,4.1785566354,1.9749940287\H,2.7020516007,4.1785566354,-1.97499402
87\H,2.685055122,2.0846547909,1.586435238\H,2.685055122,2.0846547909,-
1.586435238\C,0.7080521538,1.8889888586,2.3792237361\C,1.3172007282,1.
7751592164,0.\H,0.2355017683,1.6251215515,0.\C,0.4430726801,6.08965022
07,1.2610535528\C,1.3534470189,6.0486812401,0.\C,0.6847683875,4.790121
47,2.0942285838\C,2.1270879895,4.6996854055,0.\H,0.653335888,6.9789568
67,1.8627668774\H,2.050097017,6.8925261006,0.\H,1.0775001009,5.0550155
669,3.0805817418\H,3.2036318488,4.8972622714,0.\H,2.6642644671,-0.1075
004623,-1.9070729905\C,0.6799966463,0.3029471213,2.3442593425\C,1.9618
345375,0.3837796204,0.\H,1.0639113802,0.0011547261,3.3258769999\H,3.04
26588917,0.5859124205,0.\C,0.7439768357,-4.0774801551,2.2793046224\C,2
.1480611475,-3.933670452,0.\C,0.721146996,-2.4998742462,2.3770270181\C
,1.4390872376,-2.5982503051,0.\H,1.0785921236,-4.426359996,3.262145372
8\H,3.2334175686,-3.7594729098,0.\H,1.1268549221,-2.2490412755,3.36412
15274\C,1.6949025558,-1.8868978158,1.3403356279\C,1.6949025558,-1.8868
978158,-1.3403356279\H,2.7002823244,-2.2056039073,1.6497989952\H,2.700
2823244,-2.2056039073,-1.6497989952\C,1.0926683949,-6.0629308639,0.777
6304291\C,1.0926683949,-6.0629308639,-0.7776304291\C,1.7570885886,-4.7
460509649,1.2691778342\C,1.7570885886,-4.7460509649,-1.2691778342\H,1.
6267013257,-6.9350327067,1.1670566203\H,1.6267013257,-6.9350327067,-1.
1670566203\H,2.6734761449,-4.9737776537,1.8224238826\H,2.6734761449,-4
.9737776537,-1.8224238826\C,1.7338184534,-0.3271452798,1.3746091124\C,
1.7338184534,-0.3271452798,-1.3746091124\H,1.1118066106,2.1778672914,3
.3598555864\H,2.6642644671,-0.1075004623,1.9070729905\H,0.4012284548,-
2.903690186,0.\Version=IA64L-G03RevC.02\State=1-A'\HF=-2322.4097327\RM
SD=7.805e-09\RMSF=1.291e-05\Dipole=-0.0213057,-0.065891,0.\PG=CS [SG(

C12H12),X(C48H48)]\ \@

H4@C60H56 - 3/C2h:

1\1\GINC-M0102\FOpt\RB3LYP\6-31G(d,p)\C60H60\JJF\04-Nov-2007\0\#\#P B3LYP/6-31G** OPT GEOM=ALLCHECK GUESS=READ\BB\0,1\C,1.8301229169,3.9693714806,1.3519136392\C,1.7252271053,2.4205917687,1.330590791\H,2.707019108,4.1711171072,1.975982987\H,2.7193378046,2.0726882785,1.6427710977\H,2.7082905339,-0.1625760847,1.9365261024\C,1.7050143194,-1.9195010788,1.3428690861\H,2.7007070178,-2.265485412,1.6547243535\C,1.017748114,-6.0824674914,0.7775732674\C,1.7052797136,-4.777416589,1.2687981915\H,1.536581701,-6.9636919317,1.1669672378\H,2.6171041724,-5.0216156527,1.8225276174\C,1.7881070168,-0.3614437691,1.3782769877\C,1.8301229169,3.9693714806,-1.3519136392\C,-0.704463902,4.0903205631,-2.2776331773\C,1.7252271053,2.4205917687,-1.330590791\C,-0.7113500129,2.5122870173,-2.3739220432\H,2.707019108,4.1711171072,-1.975982987\H,-1.0326004794,4.4438619871,-3.26097093\H,2.7193378046,2.0726882785,-1.6427710977\H,-1.1166409422,2.2690902454,-3.3631484547\C,1.4377137957,1.7022390724,0.\C,0.7309616005,1.8746850643,-2.3822336018\H,1.1403334099,2.1585824269,-3.3614003048\C,1.3739635413,6.0251521397,0.\C,0.4602175142,6.0622023767,-1.2571563612\C,2.149515217,4.6758178559,0.\C,0.6872592154,4.7559115546,-2.0671314088\H,2.0683611252,6.8707627275,0.\H,0.6785903664,6.942411205,-1.8693507539\H,3.2265173323,4.8721749515,0.\H,1.0665674582,5.0047750005,-3.0634939925\H,-1.0912459836,0.0166782762,-3.3164344551\C,2.0871947417,0.3267067324,0.\C,0.7156820127,0.2895942787,-2.3332133734\H,3.1784437061,0.4694773467,0.\H,1.0912459836,-0.0166782762,-3.3164344551\C,2.1115710282,-3.9729250537,0.\C,0.704463902,-4.0903205631,-2.2776331773\C,1.4327186638,-2.6213985184,0.\C,0.7113500129,-2.5122870173,-2.3739220432\H,3.2001960265,-3.8209397696,0.\H,1.0326004794,-4.4438619871,-3.26097093\H,0.3872392022,-2.9002749913,0.\C,1.7050143194,-1.9195010788,-1.3428690861\C,-0.7309616005,-1.8746850643,-2.3822336018\H,2.7007070178,-2.265485412,-1.6547243535\H,-1.1403334099,-2.1585824269,-3.3614003048\C,1.017748114,-6.0824674914,-0.7775732674\C,-0.4602175142,-6.0622023767,-1.2571563612\C,1.7052797136,-4.777416589,-1.2687981915\C,-0.6872592154,-4.7559115546,-2.0671314088\H,1.536581701,-6.9636919317,-1.1669672378\H,-0.6785903664,-6.942411205,-1.8693507539\H,2.6171041724,-5.0216156527,-1.8225276174\H,-1.0665674582,-5.0047750005,-3.0634939925\C,1.7881070168,-0.3614437691,-1.3782769877\C,-0.7156820127,-0.2895942787,-2.3332133734\H,0.3893073901,1.4372392095,0.\H,2.7082905339,-0.1625760847,-1.9365261024\H,1.1166409422,-2.2690902454,-3.3631484547\C,0.704463902,-4.0903205631,2.2776331773\C,0.7113500129,-2.5122870173,2.3739220432\H,1.0326004794,-4.4438619871,3.26097093\H,1.1166409422,-2.2690902454,3.3631484547\H,1.0912459836,-0.0166782762,3.3164344551\C,0.7309616005,1.8746850643,2.3822336018\H,1.1403334099,2.1585824269,3.3614003048\C,0.4602175142,6.0622023767,1.2571563612\C,0.6872592154,4.7559115546,2.0671314088\H,0.6785903664,6.942411205,1.8693507539\H,1.0665674582,5.0047750005,3.0634939925\C,0.7156820127,0.2895942787,2.3332133734\C

, -1.8301229169, -3.9693714806, 1.3519136392\C, -1.8301229169, -3.9693714806, -1.3519136392\C, -1.7252271053, -2.4205917687, 1.330590791\C, -1.7252271053, -2.4205917687, -1.330590791\H, -2.707019108, -4.1711171072, 1.975982987\H, -2.707019108, -4.1711171072, -1.975982987\H, -2.7193378046, -2.0726882785, 1.6427710977\H, -2.7193378046, -2.0726882785, -1.6427710977\C, -0.7309616005, -1.8746850643, 2.3822336018\C, -1.4377137957, -1.7022390724, 0.\H, -0.3893073901, -1.4372392095, 0.\C, -0.4602175142, -6.0622023767, 1.2571563612\C, -1.3739635413, -6.0251521397, 0.\C, -0.6872592154, -4.7559115546, 2.0671314088\C, -2.149515217, -4.6758178559, 0.\H, -0.6785903664, -6.942411205, 1.8693507539\H, -2.0683611252, -6.8707627275, 0.\H, -1.0665674582, -5.0047750005, 3.0634939925\H, -3.2265173323, -4.8721749515, 0.\H, -2.7082905339, 0.1625760847, -1.9365261024\C, -0.7156820127, -0.2895942787, 2.3332133734\C, -2.0871947417, -0.3267067324, 0.\H, -1.0912459836, 0.0166782762, 3.3164344551\H, -3.1784437061, -0.4694773467, 0.\C, -0.704463902, 4.0903205631, 2.2776331773\C, -2.1115710282, 3.9729250537, 0.\C, -0.7113500129, 2.5122870173, 2.3739220432\C, -1.4327186638, 2.6213985184, 0.\H, -1.0326004794, 4.4438619871, 3.26097093\H, -3.2001960265, 3.8209397696, 0.\H, -1.1166409422, 2.2690902454, 3.3631484547\C, -1.7050143194, 1.9195010788, 1.3428690861\C, -1.7050143194, 1.9195010788, -1.3428690861\H, -2.7007070178, 2.265485412, 1.6547243535\H, -2.7007070178, 2.265485412, -1.6547243535\C, -1.017748114, 6.0824674914, 0.7775732674\C, -1.017748114, 6.0824674914, -0.7775732674\C, -1.7052797136, 4.777416589, 1.2687981915\C, -1.7052797136, 4.777416589, -1.2687981915\H, -1.536581701, 6.9636919317, 1.1669672378\H, -1.536581701, 6.9636919317, -1.1669672378\H, -2.6171041724, 5.0216156527, 1.8225276174\H, -2.6171041724, 5.0216156527, -1.8225276174\C, -1.7881070168, 0.3614437691, 1.3782769877\C, -1.7881070168, 0.3614437691, -1.3782769877\H, -1.1403334099, -2.1585824269, 3.3614003048\H, -2.7082905339, 0.1625760847, 1.9365261024\H, -0.3872392022, 2.9002749913, 0.\Version=IA64L-G03RevC.02\State=1-AG\HF=-2322.4135604\RMSD=1.354e-09\RMSF=4.213e-05\Dipole=0., 0., 0.\PG=C02H [SGH(C12H12), X(C48H48)]\ \@

H4@C60H56 -4/C2h:

1\1\GINC-M0109\FOpt\RB3LYP\6-31G(d,p)\C60H60\JJF\05-Nov-2007\0\ \#P B3LYP/6-31G** OPT GEOM=ALLCHECK GUESS=READ\BB\0,1\C, -1.8198409677, -4.0008871134, 1.3659123038\C, -1.6974235547, -2.4560378176, 1.3240795254\H, -2.7106649239, -4.1862883622, 1.9755597198\H, -2.7042658922, -2.0968590228, 1.5742961342\H, -2.7088799063, 0.0346848592, 1.8966639775\C, -1.7945403304, 1.8669554817, 1.3890389138\H, -2.7114768159, 2.1379097521, 1.9230849554\C, -1.0480424583, 6.0802103382, 0.7691309551\C, -1.6098613578, 4.70668398, 1.2173110208\H, -1.6148923394, 6.9207779683, 1.1799729852\H, -2.6707796708, 4.7497307307, 1.4974631841\C, -1.7792789035, 0.3062452598, 1.3880141519\C, -1.8113283518, -4.006983621, -1.3593406956\C, 0.7085158618, -4.1099431727, -2.3181715728\C, -1.6891530725, -2.4619609155, -1.323656082\C, 0.7113405991, -2.5192426154, -2.3457087581\H, -2.6983289757, -4.195123038, -1.9737057082\H, 1.0656795555, -4.4503024208, -3.2972291833\H, -2.6944076104, -2.1039192602, -1.581762141\H, 1.1111931113, -2.2625620414, -3.3326356236\C, -1.324014

2435, -1.7821057731, -0.0001490516\C, -0.7204097562, -1.8987146615, -2.3851
268836\H, -1.1225452422, -2.198765597, -3.3630349271\C, -1.3452486045, -6.0
553966977, 0.0093441553\C, -0.4307750967, -6.0942066728, -1.2487003334\C, -
2.126259263, -4.7106067465, 0.0038962332\C, -0.6782332033, -4.7987014703, -
2.0860862245\H, -2.0374077444, -6.9029199282, 0.0090780688\H, -0.633359663
6, -6.9865748862, -1.8484769893\H, -3.2016444049, -4.9143287673, 0.00099288
89\H, -1.0674148467, -5.0686224501, -3.0724780403\H, 1.1095729922, 0.001180
1522, -3.3420897971\C, -1.9733032481, -0.3933751811, -0.0052838243\C, -0.70
47717531, -0.3098883442, -2.3641325735\H, -3.0519395654, -0.6068923202, -0.
0081754119\H, -1.0886729233, -0.0161482218, -3.3489174864\C, -1.3905322039
, 3.8614063549, -0.0129816057\C, -0.693962705, 4.0995205915, -2.3409172848\
C, -2.0573180709, 2.5258419907, -0.0120766672\C, -0.6966375893, 2.508712713
5, -2.3613544782\H, -0.3154150984, 3.6508542111, -0.0091523496\H, -1.044998
383, 4.4354911188, -3.3237000096\H, -3.1425487147, 2.7026559287, -0.0158620
403\C, -1.78580173, 1.8606971301, -1.4085614093\C, 0.7353224053, 1.88803462
15, -2.3890508704\H, -2.6993802868, 2.1292465418, -1.9495321511\H, 1.143563
3457, 2.1837129941, -3.3657602895\C, -1.0431321831, 6.0766937306, -0.802858
475\C, 0.4386526377, 6.0885649889, -1.2732379656\C, -1.6021594802, 4.701168
1016, -1.2483898754\C, 0.6913190603, 4.7893297299, -2.1032571194\H, -1.6073
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784273, -2.9911020837, -2.0738306414\H, -4.9704396555, -5.2366683053, -0.02
13669092\H, -5.6845127419, -4.0461715864, -1.8946766873\H, -2.6566617619, -
5.3062090677, -0.0869234575\H, -3.7762642384, -3.4506211437, -3.0669235149
\C, 0.4566862621, -1.5701047666, 0.0095760032\C, 0.0657265661, -0.787167278
6, -2.3167773488\H, 1.5900182664, 0.5034073433, 0.3701523755\H, -0.20172755
45, -0.7246969488, -0.0235403429\H, -2.3258352641, -1.7467943542, -0.340923
2341\\Version=IA32L-G03RevD.01\State=1-A\HF=-2322.3968663\RMSD=9.822e-
09\RMSF=1.913e-05\Thermal=0.\Dipole=0., 0., 0.023271\PG=C02 [X(C60H60)]\
\@

H6@C60H54-2/Ci:

1\1\GINC-C0132\FOpt\RB3LYP\6-31G(d,p)\C60H60\STUDENT\07-Nov-2007\0\\#p
b3lyp/6-31g** opt geom=allcheck guess=read\\BB\\0,1\C, -1.809619463, -3
.9907768412, 1.3262397221\C, -1.7501321589, -2.4429389043, 1.2730894822\H,
-2.6816438679, -4.2121221966, 1.9494202936\H, -2.7040737123, -2.1038936292
, 1.6926010297\H, -2.4532793749, 0.049490539, 2.0304167112\C, -1.6885281026
, 1.8661117528, 1.2732915831\H, -2.6845575888, 2.1731190585, 1.6254543931\C
, -1.0866992401, 6.0511239662, 0.7696772845\C, -1.7376506404, 4.7231736718,
1.249171591\H, -1.6350411695, 6.9134281398, 1.1610214826\H, -2.6529234068,
4.9414669114, 1.8079909355\C, -1.7197334242, 0.3259975736, 1.2628307547\C,

-1.8523626182,-4.0569922847,-1.4019502665\C,0.7250604199,-4.0505658273
, -2.252225926\C, -1.86509936, -2.5068049724, -1.4465416476\C, 0.6864265851
, -2.4720203564, -2.3171144808\H, -2.7076627564, -4.3660178555, -2.01224518
33\H, 1.0751395216, -4.3718005859, -3.2387724926\H, -2.845660662, -2.216066
1249, -1.846175066\H, 1.1084022584, -2.1886598641, -3.2903178805\C, -1.6353
499344, -1.7816386173, -0.1184222999\C, -0.7926641349, -1.8967114027, -2.40
42561499\H, -1.1103968947, -2.1567785186, -3.4230740824\C, -1.307777203, -6
.0533127043, -0.0028460233\C, -0.3871859844, -6.0721581484, -1.2574168525\
C, -2.1206595226, -4.728128256, -0.0177405071\C, -0.6460137074, -4.77720437
79, -2.078364206\H, -1.9765860941, -6.9193213131, -0.0026866268\H, -0.58092
88275, -6.9620980516, -1.8638072486\H, -3.1916046882, -4.9541171508, 0.0053
956118\H, -0.9797513404, -5.0435248412, -3.0864956972\H, -0.0429080469, 0.5
291157986, -0.663388454\C, -2.2429152733, -0.3614778328, -0.0890173877\C, -
0.8055762919, -0.3211265484, -2.31588087\H, -3.33392415, -0.4407330982, 0.0
162993445\H, -0.8806836447, 0.0358076312, -3.3500509753\C, -2.1415355655, 3
.9299478171, -0.0258576305\C, -0.7367825247, 4.0702358236, -2.2822881475\C
, -1.4853713669, 2.5658943378, -0.0699706848\C, -0.756134127, 2.4924372596,
-2.3830663712\H, -3.2303497821, 3.7799187816, -0.0176329879\H, -1.05353722
7, 4.4262452149, -3.2684079689\H, -0.4284160644, 2.8058634237, -0.124649419
8\C, -1.833173594, 1.8979219682, -1.4250705735\C, 0.6411007644, 1.778363845
4, -2.1870788059\H, -2.8046880389, 2.3024929608, -1.7373683935\H, 1.0799108
216, 1.6879039788, -3.1912579525\C, -1.079672252, 6.0602384899, -0.78588301
59\C, 0.4004358262, 6.0573548701, -1.2598221317\C, -1.74861674, 4.750733702
2, -1.2854487438\C, 0.651585157, 4.7445919598, -2.0568269559\H, -1.60571134
31, 6.9384536479, -1.1723955671\H, 0.6065554174, 6.9334574867, -1.882108315
1\H, -2.6607384339, 4.9836870678, -1.8435721598\H, 1.0368069623, 4.99028569
98, -3.0518338848\C, -1.9978360438, 0.3239712882, -1.5055568638\C, 0.393446
789, 0.3573385344, -1.6315426093\H, -0.5858117003, -1.5904467414, -0.212210
2769\H, -2.9170583502, 0.1453862254, -2.075803289\H, -1.0583929157, 2.25357
90447, -3.4085891383\C, -0.7250604199, 4.0505658273, 2.252225926\C, -0.6864
265851, 2.4720203564, 2.3171144808\H, -1.0751395216, 4.3718005859, 3.238772
4926\H, -1.1084022584, 2.1886598641, 3.2903178805\H, 0.0429080469, -0.52911
57986, 0.663388454\C, -0.6411007644, -1.7783638454, 2.1870788059\H, -1.0799
108216, -1.6879039788, 3.1912579525\C, -0.4004358262, -6.0573548701, 1.2598
221317\C, -0.651585157, -4.7445919598, 2.0568269559\H, -0.6065554174, -6.93
34574867, 1.8821083151\H, -1.0368069623, -4.9902856998, 3.0518338848\C, -0.
393446789, -0.3573385344, 1.6315426093\C, 1.8523626182, 4.0569922847, 1.401
9502665\C, 1.809619463, 3.9907768412, -1.3262397221\C, 1.86509936, 2.506804
9724, 1.4465416476\C, 1.7501321589, 2.4429389043, -1.2730894822\H, 2.707662
7564, 4.3660178555, 2.0122451833\H, 2.6816438679, 4.2121221966, -1.94942029
36\H, 2.845660662, 2.2160661249, 1.846175066\H, 2.7040737123, 2.1038936292,
-1.6926010297\C, 0.7926641349, 1.8967114027, 2.4042561499\C, 1.6353499344,
1.7816386173, 0.1184222999\H, 0.5858117003, 1.5904467414, 0.2122102769\C, 0
.3871859844, 6.0721581484, 1.2574168525\C, 1.307777203, 6.0533127043, 0.002
8460233\C, 0.6460137074, 4.7772043779, 2.078364206\C, 2.1206595226, 4.72812
8256, 0.0177405071\H, 0.5809288275, 6.9620980516, 1.8638072486\H, 1.9765860

941,6.9193213131,0.0026866268\H,0.9797513404,5.0435248412,3.0864956972
 \H,3.1916046882,4.9541171508,-0.0053956118\H,2.4532793749,-0.049490539
 ,-2.0304167112\C,0.8055762919,0.3211265484,2.31588087\C,2.2429152733,0
 .3614778328,0.0890173877\H,0.8806836447,-0.0358076312,3.3500509753\H,3
 .33392415,0.4407330982,-0.0162993445\C,0.7367825247,-4.0702358236,2.28
 22881475\C,2.1415355655,-3.9299478171,0.0258576305\C,0.756134127,-2.49
 24372596,2.3830663712\C,1.4853713669,-2.5658943378,0.0699706848\H,1.05
 3537227,-4.4262452149,3.2684079689\H,3.2303497821,-3.7799187816,0.0176
 329879\H,1.0583929157,-2.2535790447,3.4085891383\C,1.833173594,-1.8979
 219682,1.4250705735\C,1.6885281026,-1.8661117528,-1.2732915831\H,2.804
 6880389,-2.3024929608,1.7373683935\H,2.6845575888,-2.1731190585,-1.625
 4543931\C,1.079672252,-6.0602384899,0.7858830159\C,1.0866992401,-6.051
 1239662,-0.7696772845\C,1.74861674,-4.7507337022,1.2854487438\C,1.7376
 506404,-4.7231736718,-1.249171591\H,1.6057113431,-6.9384536479,1.17239
 55671\H,1.6350411695,-6.9134281398,-1.1610214826\H,2.6607384339,-4.983
 6870678,1.8435721598\H,2.6529234068,-4.9414669114,-1.8079909355\C,1.99
 78360438,-0.3239712882,1.5055568638\C,1.7197334242,-0.3259975736,-1.26
 28307547\H,1.1103968947,2.1567785186,3.4230740824\H,2.9170583502,-0.14
 53862254,2.075803289\H,0.4284160644,-2.8058634237,0.1246494198\\Versio
 n=IA32L-G03RevD.01\State=1-AG\HF=-2322.3762066\RMSE=1.816e-09\RMSE=1.6
 59e-05\Thermal=0.\Dipole=0.,0.,0.\PG=CI [X(C60H60)]\@

H6@C60H54-3/C2 (Corresponding to isomer 8)

The Gaussian archive for modeling the stabilities of five-membered rings and six-membered rings in Isomer 1 and 5:

Five-membered ring from Isomer 1:

1\1\GINC-M0109\FOpt\RB3LYP\6-31G(d,p)\C5H10\JJF\04-Apr-2008\0\#P OPT(
 MODREDUNDANT) B3LYP/6-31G(D,P)\b\0,1\C,1.2642249343,-0.0000000007,0
 .4120218203\H,1.2642249361,-0.0000000022,1.5082037855\H,2.3367333202,-
 0.0000000004,0.1990574527\H,0.8747750732,2.1480685966,-0.3471546556\C,
 0.4043304924,1.2634507519,0.0907508422\C,0.4043304923,-1.2634507522,0.
 0907508385\H,0.874775073,-2.1480685956,-0.3471546618\C,-0.9870079415,0
 .7808555086,-0.4290765238\C,-0.9870079415,-0.7808555072,-0.429076526\H
 ,-1.4907230607,1.3275794044,-1.2309444182\H,-1.4907230608,-1.327579400
 7,-1.230944422\H,0.1560012066,1.6283232394,1.0941528227\H,0.1560012064
 ,-1.6283232426,1.094152818\H,-1.6371424551,1.0063591071,0.424204287\H,
 -1.6371424552,-1.0063591081,0.4242042841\\Version=IA64L-G03RevC.02\Sta
 te=1-A1\HF=-196.516665\RMSE=1.280e-09\RMSE=8.961e-03\Dipole=-0.0671835
 ,0.,0.1798192\PG=C05V [5SGV(C1H2)]\@

Five-membered ring (1) from Isomer 5:

1\1\GINC-M0109\FOpt\RB3LYP\6-31G(d,p)\C5H10\JJF\04-Apr-2008\0\#P OPT(
 MODREDUNDANT) B3LYP/6-31G(D,P)\b\0,1\C,1.1263488067,0.0000000001,0.
 7005957556\H,1.1263488079,0.0000000002,1.7936293629\H,2.1478559529,0.0

000000002,0.3126872361\C,0.3504992687,-1.2615226472,0.2126191909\C,-0.9048516541,-0.7796638737,-0.5769434767\C,-0.9048516542,0.7796638735,-0.5769434769\C,0.3504992685,1.2615226473,0.2126191907\H,0.0101183802,-1.8149781563,1.0915676063\H,-1.7959803913,-1.1217181896,-0.0443921785\H,-1.7959803915,1.1217181893,-0.0443921787\H,0.0101183799,1.8149781565,1.091567606\H,0.9870364596,-1.887479477,-0.4174191581\H,-0.8912089356,-1.1665264701,-1.5987561196\H,-0.8912089358,1.1665264697,-1.5987561197\H,0.9870364593,1.8874794771,-0.4174191584\\Version=IA64L-G03RevC.02\\State=1-A1\\HF=-196.5599875\\RMSD=6.048e-09\\RMSF=5.164e-03\\Dipole=-0.0056437,0.,0.0089731\\PG=C05V [5SGV(C1H2)]\\@

Five-membered ring (2) from Isomer 5:

1\1\GINC-M0109\FOpt\RB3LYP\6-31G(d,p)\C5H10\JJF\04-Apr-2008\0\\#P OPT(MODREDUNDANT) B3LYP/6-31G(D,P)\\BB\\0,1\H,-0.6662833277,-0.8991118983,-1.8856121514\C,-0.5831531304,-1.1053984982,0.4236854413\H,1.5874307073,-0.8991121141,1.21635933\H,-0.5858648769,-2.1986419391,0.4256555642\H,-1.4385766334,-0.8150680223,1.0451869699\H,0.6154397712,0.9171737917,-1.8222573401\C,-0.0270620452,0.9218412154,-0.9379239969\C,0.8836561359,0.9218411282,0.3155721351\H,1.9232511283,0.9171736665,-0.0222092996\C,-0.862362221,-0.3955824742,-0.9344434319\C,0.6222238291,-0.3955826163,1.1089141183\H,-0.6820890092,1.7964791507,-0.9402289727\H,0.6834338485,1.79647902,0.9392521398\H,-1.9296000744,-0.1490419859,-0.9350889423\H,0.293043057,-0.1490421987,2.1241171061\\Version=IA64L-G03RevC.02\\State=1-A'\HF=-196.5533373\\RMSD=2.999e-09\\RMSF=5.355e-03\\Dipole=-0.0243949,0.0269143,0.0177239\\PG=CS [SG(C1H2),X(C4H8)]\\@

Six-membered ring from Isomer 1:

1\1\GINC-M0109\FOpt\RB3LYP\6-31G(d,p)\C6H12\JJF\04-Apr-2008\0\\#P B3LYP/6-31G(D,P) OPT(MODREDUNDANT)\\BB\\0,1\H,1.0571002593,-0.8703545237,-2.1429659755\C,1.2910695595,-0.870354516,0.146890472\H,2.3851577004,-0.8703545068,0.1441766411\C,0.5124064335,-0.8703545259,-1.1941009371\C,-0.7628922389,0.0394501523,-1.3646953943\H,-0.7654274289,0.4298461687,-2.3867622943\C,-1.2391669168,0.9347292914,-0.1915748049\C,0.8070675137,0.0394501722,1.339044478\H,-1.5777429336,1.9567993309,-0.3859335968\C,-0.4478702903,0.9347293014,1.1711736583\H,-0.446901945,1.9567993453,1.5615684746\H,1.6934710008,0.4298461999,1.8478823937\H,1.0667880776,-1.8734839318,0.523686075\H,0.07398548,-1.8734839444,-1.1860902196\H,-1.5658414813,-0.7036228969,-1.405446984\H,-2.1730960458,0.4378661825,0.0902924823\H,0.4444400572,-0.7036228714,2.0566024994\H,-1.1556171049,0.4378661954,1.8425656711\\Version=IA64L-G03RevC.02\\State=1-A1\\HF=-235.8134663\\RMSD=4.546e-09\\RMSF=8.420e-03\\Dipole=-0.1077236,-0.1392704,0.062551\\PG=C03V [X(C6H12)]\\@

Six-membered ring (1) from Isomer 5:

1\1\GINC-M0109\FOpt\RB3LYP\6-31G(d,p)\C6H12\JJF\04-Apr-2008\0\\#P OPT(MODREDUNDANT) B3LYP/6-31G(D,P)\\bb\\0,1\C,-0.7480736863,0.158541282,-1

.3557191456\C, -0.7480737641, 0.1585412875, 1.355719102\C, 0.8062405511, 0.1514508496, -1.3544184143\C, 0.8062404733, 0.1514508551, 1.3544184599\H, -1.0384975697, -0.6961493073, -1.9778836538\H, -1.0384976832, -0.6961492993, 1.977883597\H, 1.0725699286, -0.7121230666, -1.9807257809\H, 1.0725698149, -0.7121230586, 1.9807258454\H, 1.2414101784, 0.9639486967, -1.9473924767\C, 1.4121741855, -0.293133209, 0.0000000411\H, 1.2414100667, 0.9639487046, 1.9473925441\H, 1.1239305292, -1.3541460661, 0.000000035\H, -2.3839996443, 0.4683568511, -0.0000000693\H, -1.2437509091, 1.0064643597, -1.8384758306\C, -1.4617701043, -0.1190667547, -0.0000000417\H, -1.2437510145, 1.0064643671, 1.8384757552\H, -1.7101655595, -1.1842171983, -0.0000000467\H, 2.5063459309, -0.3009808457, 0.0000000725\\Version=IA64L-G03RevC.02\State=1-A'\HF=-235.842346\RMSE=8.169e-09\RMSF=6.799e-03\Dipole=-0.0225969, -0.121012, 0.\PG=CS [SG(C2H4), X(C4H8)]\ \@

Six-membered ring (2) from Isomer 5:

1\1\GINC-M0109\FOpt\RB3LYP\6-31G(d,p)\C6H12\JJF\04-Apr-2008\0\ \#P OPT(MODREDUNDANT) B3LYP/6-31G(D,P)\ \BB\0,1\H, -2.16596536, 0.327574845, -1.2117231442\H, -2.1630312824, 0.3283426173, 1.2167358615\H, 0.1421893367, 0.1999861503, -2.4836266758\C, 0.1419063913, 0.1974911342, -1.389038272\H, 0.9738636552, -1.9594934389, -1.2161246819\H, 0.7686275289, 1.0573701792, -1.1175148915\C, -1.2069664403, 0.6380484312, -0.7813868033\C, 0.9760399497, -0.952065124, -0.7844470288\H, -1.2058341315, 1.7017031153, -1.0625486175\H, 1.9875698498, -0.6243894611, -1.0670252588\H, 0.7723362266, 1.0581407186, 1.1277005055\C, -1.2060566954, 0.6385645609, 0.7830452636\C, 0.9791178846, -0.9531283154, 0.7799819986\H, -1.2046011036, 1.7052664476, 1.0518045459\H, 1.9944563131, -0.6249441214, 1.0473199794\H, 0.1451666516, 0.1945037586, 2.4889227651\C, 0.1454721368, 0.1970301004, 1.3941360375\H, 0.9781429551, -1.9597055337, 1.212332438\\Version=IA64L-G03RevC.02\State=1-A'\HF=-235.8339765\RMSE=6.044e-09\RMSF=8.077e-03\Dipole=0.1080065, 0.1482783, -0.0001233\PG=CS [SG(C2H4), X(C4H8)]\ \@