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J6035-1

R. Janke, G. Haufe, E.-U. Würthwein, J. H. Borkent

-26-

penta_gs.arc

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,1.6230660546,0.0495465059\H,3.7744002049,-0.8918086721,-1.5183648274\H,2.888633
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penta_ts.arc

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,1.1981865819,-0.5693326691,-1.1296003149\C,0.7888027299,1.4182423481,1.11583272
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640935\C,-3.7126530937,-0.3764089767,-0.5894258931\C,-2.635857671,0.3884481901,-
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,4.9308433326\C,4.4373873754,-0.7347457106,-2.2688161549\C,-1.3465868741,-0.5086
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hepta_gs.arc

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hepta_ts.arc

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J6035-4

R. Janke, G. Haufe, E.-U. Würthwein, J. H. Borkent

-29-

octa_gs.arc

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629\C,1.9800694779,-2.40720156,-0.4867449399\C,1.9705973356,2.4156795349,0.48349
70538\C,1.2854060108,-3.6437653048,-0.6414572906\C,1.2701581673,3.6490716104,0.6
379422706\C,-0.0641854046,-3.6581733939,-0.8419348837\C,-0.0794208105,3.65724203
77,0.8391959679\C,-0.7708147095,-2.4448211522,-1.0979839996\C,-0.7802672576,2.44
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1,2.4830653029,1.4375915478\C,-2.8312170218,-1.376278658,-1.8297298861\C,-2.8346
933084,1.3618604747,1.8295882808\C,-2.1285498395,-0.1445367566,-2.0292585892\C,-
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65,-1.971903272\C,1.0444564773,-1.135405859,1.9775817317\C,-0.1098186424,3.00914
1941,-3.0688379738\C,-0.0871991207,-3.0041531661,3.0795726478\C,-2.5685958983,2.
9255419887,-3.4659717583\C,-2.5465387747,-2.9347742917,3.4755160308\C,-3.8329195
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889731113,-1.41356352,-2.0665057922\C,-3.8926736547,1.3936291566,2.0661630495\C,-
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701\C,-0.6113291834,-4.5934629776,-0.8856168875\C,-0.6308576248,4.5900144083,0.8
827957129\C,1.8491861543,-4.566762963,-0.5612486488\C,1.8295339599,4.5746822643,
0.5569999776\C,3.9246319214,-3.3450880291,-0.3143675103\C,3.9110525678,3.3617261
376,0.3086415455\C,5.1542352438,-1.1971574,-0.1176607317\C,5.1491906477,1.218989
8867,0.1096576258\Version=IBM-RS6000-G94RevB.1\HF=-1300.5043357\RMSE=6.285e-06\
Dipole=-0.0584371,0.000179,0.000519\PG=C01 [X(C34H20)]\@
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octa_ts.arc

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17583603,-0.7924633387\C,-1.4640086532,-1.0568760232,0.6833483335\C,-0.234147839
2,-1.0579597663,-1.5982896763\C,-0.531313555,-0.4094070014,1.5961454959\C,1.0412
537298,-0.4106374752,-1.321447106\C,-0.306283633,1.0239732644,1.6270496352\C,1.1
910190848,1.022754286,-1.1508027845\C,-1.2024209569,1.9195752162,0.9934061138\C,
0.169217753,1.9184384138,-1.5512688373\C,-2.6443451489,-1.5647999602,-1.42495796
94\C,-3.7701360601,-2.0028053132,-0.6561426004\C,-2.6211462379,-2.0038915088,-2.
7876480062\C,-3.596004002,-2.3004504024,0.6608819006\C,-1.425350598,-2.302399821
8,-3.3659934166\C,-2.3790189282,-1.9503512005,1.3172265381\C,-0.2079623293,-1.95
22251293,-2.7104951924\C,-2.0308112994,-2.5618669309,2.5637715583\C,1.0246092382
,-2.5641851068,-3.1046621553\C,-0.8336756441,-2.2860732023,3.1597932286\C,2.1807
473588,-2.2881110282,-2.4327026266\C,-0.0926366621,-1.1418522105,2.7309399058\C,
2.2301923328,-1.1433846982,-1.5786052775\C,0.9600182748,-0.6113926233,3.54913618
32\C,3.4924643547,-0.6130053863,-1.1493830918\C,1.3683252715,0.6812896921,3.4130
874174\C,3.6035146896,0.6797686818,-0.733838587\C,0.6523704674,1.5660742884,2.54
18440123\C,2.4822825963,1.5646993072,-0.8530526395\C,0.7553109887,2.9699743714,2
.6916035886\C,2.6641898635,2.9685810922,-0.8496291441\C,-0.1249248008,3.81581526
77,2.0472490412\C,1.6421768935,3.8145003005,-1.2308754443\C,-1.1294994705,3.2795
097568,1.2174854342\C,0.3967159042,3.2783128217,-1.6138265768\C,-1.9856911675,1.
5092852457,0.3692993706\C,-0.7827590258,1.5082274062,-1.8624464861\C,-1.84856004
66,3.9412592778,0.748670404\C,-0.3900897229,3.9401288169,-1.9568778629\C,-0.0645
557085,4.8870038449,2.2002955298\C,1.803363773,4.8856596048,-1.2647702128\C,1.50
263538,3.3658272365,3.3712362046\C,3.6428126438,3.3643257321,-0.5990758839\C,2.1
48178596,1.0894971673,4.0467351622\C,4.5616481395,1.0878991772,-0.4309768931\C,1
.3823373359,-1.2510725964,4.3167815126\C,4.3657859799,-1.2528053663,-1.218571544
8\C,-0.5022270347,-2.827843932,4.0383349454\C,3.0967272611,-2.8301355075,-2.6386
171605\C,-2.7050723558,-3.3055411027,2.9738268571\C,0.9962270492,-3.3084110361,-
3.8927924238\C,-4.3536047354,-2.8369727832,1.2214656585\C,-1.3737784603,-2.83972
39808,-4.3065737807\C,-4.6779576439,-2.2822168175,-1.1788048799\C,-3.5568930492,
-2.2833920517,-3.2584420116\Version=IBM-RS6000-G94RevB.1\HF=-1300.4377851\RMSE=
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0)]\@
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J6035-5

R. Janke, G. Haufe, E.-U. Würthwein, J. H. Borkent

-30-

nona_gs.arc

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,-1.5507342799\C,-0.5800192175,0.0749775818,1.5510477299\C,0.8116787512,-0.82077
50163,-1.1634157151\C,0.3828142158,1.0895780611,1.1627162904\C,1.0243633481,-1.9
128673405,-0.2196684536\C,0.1059887934,2.167393912,0.2192094189\C,-2.9521175227,
-0.3693937401,-1.3808538383\C,-2.8242998934,-0.9309717858,1.3835084983\C,-4.1278
286544,-0.7387610998,-0.6544595222\C,-4.0455909491,-1.1011347729,0.6583378758\C,
-3.0390768101,0.0196359257,-2.7523179647\C,-2.7347916634,-1.3196483935,2.7549105
284\C,-1.9219287174,0.4184858294,-3.4270156042\C,-1.5538100561,-1.2013238508,3.4
284055367\C,-0.6252259989,0.2534617518,-2.8507809338\C,-0.4534601714,-0.49664812
92,2.8510132217\C,0.5401125751,0.6452208216,-3.574992169\C,0.7680424168,-0.35117
65691,3.5740148012\C,1.7813553532,0.4516172419,-3.0436711898\C,1.8060367645,0.35
56730755,3.0416520209\C,1.9478670068,-0.322218944,-1.8551977261\C,1.6236951155,1
.1261407282,1.8533186768\C,3.2675886565,-0.6512003537,-1.4037223555\C,2.67461079
97,1.9890040057,1.4008022415\C,2.3572473075,-2.2229952569,0.1998900236\C,1.17689
16204,3.0188854822,-0.2013925999\C,3.4645345866,-1.5208261193,-0.3764514869\C,2.
4788293639,2.8590911286,0.3736957682\C,-0.013703734,-2.7823553969,0.2037807754\C
,0.2320606761,-3.8331760097,1.0649961854\C,1.5343260357,-4.0741639138,1.54903997
67\C,2.5777150872,-3.2871696782,1.110147166\C,-1.2049875031,2.5079818768,-0.2029
571296\C,-1.4342049715,3.5627341838,-1.0639293898\C,-0.361401034,4.3386625111,-1
.5490094191\C,0.9190487064,4.0748459032,-1.1113942617\H,-4.9132305561,-1.4757374
49,1.1902602923\H,-5.0728010186,-0.7722230455,-1.1854723991\H,-4.0162586118,0.04
66617566,-3.2218165759\H,-1.9907439532,0.815131469,-4.4339744834\H,0.4123820854,
1.1299133466,-4.5364721438\H,2.6680874253,0.8107373671,-3.5542196388\H,4.1081790
131,-0.1884309481,-1.9093372322\H,4.4644376216,-1.7542920737,-0.0268256187\H,3.5
943946041,-3.4903785067,1.4302386318\H,1.7153381117,-4.8931834653,2.2353988281\H
,-0.5824196277,-4.4833853197,1.362003501\H,-1.0113155786,-2.6297905526,-0.176824
2242\H,-3.6056684448,-1.762751124,3.2253117844\H,-1.4450170194,-1.5891385338,4.4
352782559\H,0.861279738,-0.843759015,4.5354490746\H,2.7615914989,0.4112862108,3.
5513017978\H,3.6328997557,1.9312221644,1.9055174479\H,3.2818275074,3.4985889944,
0.0232855237\H,1.7501809718,4.694219677,-1.4323078818\H,-0.5495896275,5.15621879
35,-2.2351829914\H,-2.4490604211,3.8010829568,-1.3599377993\H,-2.0405302726,1.94
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-09\RMSF=1.445e-05\Dipole=0.0458218,0.0102165,0.0000633\PG=C01 [X(C38H22)]\%
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nona_ts.arc

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3851961073,1.1610514894,-1.5788837699\C,-0.384636419,1.1600288796,1.5798209584\C
,0.7031646906,0.209502059,-1.6039451164\C,0.703795633,0.208437944,1.6037739814\C
,0.4738497135,-1.2304690486,-1.5549975456\C,0.4743634004,-1.2314711165,1.5539804
242\C,-2.7892598555,1.5747891142,-1.3822915904\C,-2.7887808366,1.5737260157,1.38
45747584\C,-4.0304202958,1.5750869424,-0.6801805986\C,-4.0301884588,1.574534208,
0.6829125677\C,-2.7305762963,2.289237423,-2.6260265626\C,-2.7295753796,2.2871723
715,2.628809474\C,-1.5302878182,2.7374174123,-3.0876272997\C,-1.5290980574,2.735
1185362,3.0902477879\C,-0.3163803841,2.2002172921,-2.5520062973\C,-0.3154171319,
2.1984408679,-2.5537005349\C,0.9565857887,2.6133155914,-3.0462532155\C,0.95782602
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617,1.9285991813,2.698785691\C,1.9714816597,0.6545477517,-2.0718874904\C,1.97229
10843,0.6531396878,2.0714046437\C,3.0840044227,-0.2496431949,-2.08865346\C,3.084
8046298,-0.2510678341,2.0870874265\C,1.5826471699,-2.1181177506,-1.7300092914\C,
1.5832365994,-2.1192700436,1.7278620858\C,2.9024011458,-1.5836548246,-1.89195614
16\C,2.9030647527,-1.5849503192,1.8895598924\C,-0.8286128072,-1.790053529,-1.567
2335594\C,-1.0261732562,-3.1464097713,-1.7299514618\C,0.071499337,-4.0206198662,
-1.8567532853\C,1.3525995052,-3.5102154118,-1.8476734102\C,-0.8281039758,-1.7910
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.0218485026,1.8539423315\C,1.353221882,-3.5114540388,1.8446288574\H,-4.945294127
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8966\H,2.2081387805,-4.1666314918,-1.967940166\H,-0.0936045573,-5.0852093863,-1.
9744746483\H,-2.03512239,-3.5413322876,-1.7605463455\H,-1.6793279659,-1.12932455
01,-1.479477551\H,-3.661418202,2.6009771712,3.0853600282\H,-1.4666284731,3.44153
65616,3.9103747513\H,1.0027513481,3.4771929447,3.6988788584\H,3.0690322034,2.263
3748298,3.0240729926\H,4.0646113374,0.1481124221,2.3265012889\H,3.7387727668,-2.
274459536,1.9407378182\H,2.2088215462,-4.1679518021,1.9640209135\H,-0.0929457905
,-5.0865215667,1.9709409852\H,-2.0345433878,-3.5424257758,1.7591900717\H,-1.6788
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8H22)]\%
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