

```

1\1\ GINC-UGA-PVRS-PC20PVRS\Freq\RB3LYP\6-31G(d)\C15H10\ZXWANG\28-Mar-
2002\0\#\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\OUT:c15h10
B6f.out C15H10_6565\0,1\C,0.,1.1877027,1.1928083\C,0.,1.1877027,-1.19
28083\C,0.,-1.1877027,1.1928083\C,0.,-1.1877027,-1.1928083\C,0.,0.,0.\
C,0.,1.1356342,2.5847737\C,0.,1.1356342,-2.5847737\C,0.,-1.1356342,2.5
847737\C,0.,-1.1356342,-2.5847737\C,0.,2.5035102,0.6659384\C,0.,2.5035
102,-0.6659384\C,0.,-2.5035102,0.6659384\C,0.,-2.5035102,-0.6659384\H,
0.,-2.115485,3.0535108\H,0.,-2.115485,-3.0535108\H,0.,2.115485,3.05351
08\H,0.,2.115485,-3.0535108\H,0.,3.3621051,1.324443\H,0.,3.3621051,-1
324443\H,0.,-3.3621051,1.324443\H,0.,-3.3621051,-1.324443\C,0.,0.,-3.3
52984\C,0.,0.,3.352984\H,0.,0.,-4.4356041\H,0.,0.,4.4356041\\Version=x
86-Linux-G98RevA.5\State=1-AG\HF=-577.3212164\RMSD=1.766e-09\RMSF=4.32
0e-05\ZPE=119.1197236\Dipole=0.,0.,0.\DipoleDeriv=0.0320391,0.,0.,0
0.,-0.1017099,0.1279255,0.,0.,0.0792373,0.,0.,0.,-0.1017099\Polar=4
7.680322,0.0000002,195.9042246,0.0000008,0.0000019,256.7178524\PG=D02H
 [O(C1),C2"(H1C1.C1H1),SG(C12H8)]\NImag=3\\0.04717130,0.0.,0.42376792,0
0.00006818,0.,0.,-0.35099464,0.,0.,-0.00001663,0.,0.,0.37028654\\0.,-0
.,0.,0.00000104,0.,0.,-0.00000104\\\\@

```

```

1\1\ GINC-UGA-PVRS-PC19PVRS\Freq\RB3LYP\6-31G(d)\C21H24\ZXWANG\29-Mar-
2002\0\#\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-31G(D) FREQ\OUT:c21h20
d2hB6f.out c21h20 (distorted ptC)\0,1\C,-0.7398382801,1.2750630544,0.
\C,0.7398382801,1.2750630544,0.\C,-0.7398382801,-1.2750630544,0.\C,0.7
398382801,-1.2750630544,0.\C,0.,0.,0.\C,1.2959052456,1.3375083141,-1.4
285669866\C,-1.2959052456,1.3375083141,-1.4285669866\C,1.2959052456,-1
.3375083141,-1.4285669866\C,-1.2959052456,-1.3375083141,-1.4285669866\
C,1.2959052456,1.3375083141,1.4285669866\C,-1.2959052456,1.3375083141,
1.4285669866\C,1.2959052456,-1.3375083141,1.4285669866\C,-1.2959052456
,-1.3375083141,1.4285669866\C,0.,1.665881079,-2.2551372921\C,0.,-1.665
881079,-2.2551372921\C,0.,1.665881079,2.2551372921\C,0.,-1.665881079,2
.2551372921\C,2.0194526647,0.,-1.8093582613\C,-2.0194526647,0.,-1.8093
582613\C,2.0194526647,0.,1.8093582613\C,-2.0194526647,0.,1.8093582613\
H,-2.0303675582,2.1451472799,-1.5815724731\H,2.0303675582,2.1451472799
,-1.5815724731\H,-2.0303675582,-2.1451472799,-1.5815724731\H,2.0303675
582,-2.1451472799,-1.5815724731\H,-2.0303675582,2.1451472799,1.5815724
731\H,2.0303675582,2.1451472799,1.5815724731\H,-2.0303675582,-2.145147
2799,1.5815724731\H,2.0303675582,-2.1451472799,1.5815724731\H,2.208194
7851,0.,-2.8916666315\H,-2.2081947851,0.,-2.8916666315\H,2.2081947851,
0.,2.8916666315\H,-2.2081947851,0.,2.8916666315\H,0.,-1.1587700548,-3.
228032308\H,0.,1.1587700548,-3.228032308\H,0.,-1.1587700548,3.22803230
8\H,0.,1.1587700548,3.228032308\H,0.,2.7419947084,-2.4706665803\H,0.,
2.7419947084,-2.4706665803\H,0.,2.7419947084,2.4706665803\H,0.,-2.7419
947084,2.4706665803\H,-3.0123210975,0.,-1.3350209376\H,3.0123210975,0.
,-1.3350209376\H,-3.0123210975,0.,1.3350209376\H,3.0123210975,0.,1.335
0209376\Version=x86-Linux-G98RevA.5\State=1-AG\HF=-814.4220135\RMSD=3
.974e-09\RMSF=2.712e-05\ZPE=250.4005263\Dipole=0.,0.,0.\DipoleDeriv=0.
182296\Polar=194.8734282,-0.0000015,192.8935808,-0.0000004,0.0000028,2
03.9660544\PG=D02H [O(C1),SG(C4),SG'(C4H8),SG"(C4H8),X(C8H8)]\NImag=1\
\0.51837006,-0.06329539,0.28520377,0.,0.,0.40300890,-0.23841450,0.0269
0.00042100,0.00001052,0.,0.00002248,-0.10911487,0.,0.10358701\0.00014
0000085,0.,0.00000619\ \@

```

$2^+ (C_{21}H_{24}, D_{2h})$

1\1\ GINC-UGA-PVRS-PC21PVRS\FOpt\UB3LYP\6-311+G(d,p)\C21H24(1+,2)\ZXWANG\02-Apr-2002\0\#\ UB3LYP/6-311+G** OPT=RCFC NAME=ZXWANG GEOM=CHECK GUESS=READ POP=NONE\OUT:c21h24+1B6dd.out c21h24+2\1,2\C,-0.7403893018,1.2959347279,0.\C,0.7403893018,1.2959347279,0.\C,-0.7403893018,-1.2959347279,0.\C,0.7403893018,-1.2959347279,0.\C,0.,0.,0.\C,1.2914928466,1.3354862481,-1.4353534935\C,-1.2914928466,1.3354862481,-1.4353534935\C,1.2914928466,-1.3354862481,-1.4353534935\C,-1.2914928466,-1.3354862481,-1.4353534935\C,1.2914928466,1.3354862481,1.4353534935\C,-1.2914928466,1.3354862481,1.4353534935\C,1.2914928466,-1.3354862481,1.4353534935\C,-1.2914928466,-1.3354862481,1.4353534935\C,0.,1.6736893343,-2.2643291562\C,0.,-1.6736893343,-2.2643291562\C,0.,1.6736893343,2.2643291562\C,0.,-1.6736893343,2.2643291562\C,2.0174098293,0.,-1.8040281934\C,-2.0174098293,0.,-1.8040281934\C,2.0174098293,0.,1.8040281934\C,-2.0174098293,0.,1.8040281934\H,-2.0209057116,2.1413502485,-1.5506355985\H,2.0209057116,2.1413502485,-1.5506355985\H,-2.0209057116,-2.1413502485,-1.5506355985\H,2.0209057116,-2.1413502485,-1.5506355985\H,-2.0209057116,2.1413502485,1.5506355985\H,2.0209057116,2.1413502485,1.5506355985\H,-2.0209057116,-2.1413502485,1.5506355985\H,2.2275235548,0.,-2.8770559944\H,-2.2275235548,0.,-2.8770559944\H,2.2275235548,0.,2.8770559944\H,-2.2275235548,0.,2.8770559944\H,0.,-1.17799645,-3.2361504993\H,0.,1.17799645,-3.2361504993\H,0.,-1.17799645,3.2361504993\H,0.,1.17799645,3.2361504993\H,0.,2.7472347232,-2.4622037827\H,0.,-2.7472347232,-2.4622037827\H,0.,2.7472347232,2.4622037827\H,0.,-2.7472347232,2.4622037827\H,-2.9941310377,0.,-1.3090676575\H,2.9941310377,0.,-1.3090676575\H,-2.9941310377,0.,1.3090676575\H,2.9941310377,0.,1.3090676575\Version=x86-Linux-G98RevA.5\HF=-814.450589\S2=0.754608\S2-1=0.\S2A=0.750014\RMSD=6.973e-09\RMSF=1.743e-05\PG=D02H [O(C1),SG(C4),SG'(C4H8),SG"(C4H8),X(C8H8)]\@\

$2^{2+} (C_{21}H_{24}, D_{2h})$

1\1\ GINC-UGA-PVRS-PC10PVRS\FOpt\RB3LYP\6-311+G(d,p)\C21H24(2+)\ZXWANG\02-Apr-2002\0\#\ RB3LYP/6-311+G** OPT NAME=ZXWANG GEOM=CHECK GUESS=READ POP=NONE\OUT:c21h24+2B6dd.out C21H24 (+2)\2,1\C,0.,0.7363697818,1.2861900259\C,0.,-0.7363697818,1.2861900259\C,0.,0.7363697818,-1.2861900259\C,0.,-0.7363697818,-1.2861900259\C,0.,0.,0.\C,1.4584372745,-1.2898220574,1.3270984668\C,1.4584372745,1.2898220574,1.3270984668\C,1.4584372745,-1.2898220574,-1.3270984668\C,1.4584372745,1.2898220574,-1.3270984668\C,-1.4584372745,-1.2898220574,1.3270984668\C,-1.4584372745,1.2898220574,1.3270984668\C,-1.4584372745,-1.2898220574,-1.3270984668\C,2.2693132366,0.,1.700352286\C,2.2693132366,0.,-1.700352286\C,-2.2693132366,0.,1.700352286\C,-2.2693132366,0.,-1.700352286\C,1.8278773023,-2.015094931,0.\C,1.8278773023,2.015094931,0.\C,-1.8278773023,-2.015094931,0.\C,-1.8278773023,2.015094931,0.\H,1.5206277955,2.0226687573,2.1345009282\H,1.5206277955,-2.0226687573,2.1345009282\H,1.5206277955,2.0226687573,-2.1345009282\H,-2.0226687573,2.1345009282\H,1.5206277955,-2.1345009282\H,-2.0226687573,2.1345009282\H,-1.5206277955,2.0226687573,-2.1345009282\H,-1.5206277955,-2.0226687573,-2.1345009282\H,2.897796881,-2.2358004635,0.\H,2.897796881,2.2358004635,0.\H,-2.897796881,-2.2358004635,0.\H,-2.897796881,2.2358004635,0.\H,3.255480094,0.,-1.2357255094\H,3.255480094,0.,1.2357255094\H,-3.255480094,0.,-1.2357255094\H,-3.255480094,0.,1.2357255094\H,2.4302620303,0.,2.7787692811\H,2

.4302620303,0.,-2.7787692811\H,-2.4302620303,0.,2.7787692811\H,-2.4302620303,0.,-2.7787692811\H,1.3272459657,2.9878392595,0.\H,1.3272459657,-2.9878392595,0.\H,-1.3272459657,2.9878392595,0.\H,-1.3272459657,-2.9878392595,0.\Version=x86-Linux-G98RevA.5\HF=-814.0584799\RMSD=7.053e-09\RMSF=2.051e-05\PG=D02H [O(C1),SG(C4),SG'(C4H8),SG"(C4H8),X(C8H8)]\@

3(C₂₃H₂₄, D_{2h})

1\1\GINC-ORIGIN\FOpt\RB3LYP\6-311+G(d,p)\C23H24\ZXWANG\13-Aug-2000\0\#\RB3LYP/6-311+G** OPT NAME=ZXWANG GEOM=(NODISTANCE, NODIHEDRAL, NOANGLE,CHECK)\Dimethanospiro[2,2] octaplane\0,1\C,0.,1.323255714,-0.7173769459\C,0.,-1.323255714,-0.7173769459\C,0.,1.323255714,0.7173769459\C,0.,-1.323255714,0.7173769459\C,0.,0.,0.\C,1.3819478674,1.3193584185,1.3103481437\C,-1.3819478674,1.3193584185,1.3103481437\C,1.3819478674,-1.3193584185,1.3103481437\C,-1.3819478674,-1.3193584185,1.3103481437\C,1.3819478674,1.3193584185,-1.3103481437\C,-1.3819478674,1.3193584185,-1.3103481437\C,1.3819478674,-1.3193584185,-1.3103481437\C,-1.3819478674,-1.3193584185,-1.3103481437\C,2.2657746282,1.5186036002,0.\C,-2.2657746282,1.5186036002,0.\C,2.2657746282,-1.5186036002,0.\C,-2.2657746282,-1.5186036002,0.\C,1.3728665147,0.,2.1699078188\C,-1.3728665147,0.,2.1699078188\C,1.3728665147,0.,-2.1699078188\C,-1.3728665147,0.,-2.1699078188\C,0.,0.,2.9972603242\C,0.,0.,-2.9972603242\H,1.5786994903,2.1565658415,-1.9981636323\H,-1.5786994903,2.1565658415,-1.9981636323\H,1.5786994903,-2.1565658415,-1.9981636323\H,-1.5786994903,-2.1565658415,-1.9981636323\H,1.5786994903,2.1565658415,1.9981636323\H,-1.5786994903,2.1565658415,1.9981636323\H,-1.5786994903,-2.1565658415,1.9981636323\H,2.1969396736,0.,2.8907121493\H,-2.1969396736,0.,2.8907121493\H,2.1969396736,0.,-2.8907121493\H,-2.1969396736,0.,-2.8907121493\H,3.185032037,-0.9357731523,0.\H,-3.185032037,-0.9357731523,0.\H,3.185032037,0.9357731523,0.\H,-3.185032037,0.9357731523,0.\H,2.5833070269,2.567564256,0.\H,-2.5833070269,2.567564256,0.\H,2.5833070269,-2.567564256,0.\H,-2.5833070269,-2.567564256,0.\H,0.,-0.8760993837,3.6551066921\H,0.,0.8760993837,3.6551066921\H,0.,-0.8760993837,-3.6551066921\H,0.,0.8760993837,-3.6551066921\Version=SGI-G94RevE.2\State=1-AG\HF=-890.7648489\RMSD=6.706e-09\RMSF=6.987e-05\Dipole=0.,0.,0.\PG=D02H [O(C1),C2(C1.C1),SG(C4H8),SG'(C4H4),SG"(C4H4),X(C8H8)]\@

4 (C₁₇B₄H₂₄, D_{4h})

1\1\GINC-ORIGIN\FOpt\RB3LYP\6-311+G(d,p)\C17H24B4\ZXWANG\05-Jul-2000\0\#\B3LYP/6-311+G** OPT=RCFC GEOM=(NODISTANCE, NODIHEDRAL, NOANGLE) FREQ=NORAMAN POP=NONE GEOM=CHECK GUESS=READ\Octaplane + B4\0,1\B,1.0466637718,1.0466637718,0.\B,-1.0466637718,1.0466637718,0.\B,-1.0466637718,-1.0466637718,0.\B,1.0466637718,-1.0466637718,0.\C,0.,0.,0.\C,-1.3293839815,1.3293839815,1.5819858639\C,-1.3293839815,-1.3293839815,1.5819858639\C,1.3293839815,-1.3293839815,1.5819858639\C,-1.3293839815,1.3293839815,1.5819858639\C,1.3293839815,-1.3293839815,1.5819858639\C,-1.3293839815,-1.3293839815,1.5819858639\C,1.3293839815,1.5819858639\C,1.3293839815,-1.3293839815,1.5819858639\C,1.3293839815,-1.3293839815,1.5819858639\C,1.3293839815,-1.3293839815,1.5819858639\C,0.,1.8809478789,2.1993900064\C,-1.8809478789,0.,2.1993900064\C,0.,-1.8809478789,2.1993900064\C,1.8809478789,0.,2.1993900064\C,0.,1.8809478789,-2.1993900064\C,-1.8809478789,0.,-2.1993900064\C,0.,-1.8809478789,-2.1993900064\C,1.8809478789,0.,-2.1993900064\H,2.0967405949,2.0967405949,1.7268175725\H,-2.0967405949,2.0967405949,1.7268175725\H,-2.0967405949,-2.0967405949

5 ($\text{C}_{19}\text{B}_2\text{H}_{24}$, C_{2h})

6 ($\text{C}_{21}\text{B}_2\text{H}_{24}$, D_{2h})

```
1\1\ PG[D02, 1-AG], NImag[N/A])\F0pt\RB3LYP\6-311+G(d,p)\C21H24B2\ZXWANG\18-Jan-2002\0\#\ RB3LYP/6-311+G** OPT=RCFC NAME=ZXWANG SYM=L0OSE GEOM=CHECK GUESS=READ\EN[-864.2139178], ZPE[ N/A]_ radomb2h4B6dd.log_Dimethanospiro[2,2] octaplane\0,1\C,0.,1.3116338757,-0.7213880283\C,0.,-1.3116338757,-0.7213880283\C,0.,1.3116338757,0.7213880283\C,0.,-1.3116338757,0.7213880283\C,0.,0.,0.\C,1.411282045,1.298825153,1.3136464834\C,-1.411282045,1.298825153,1.3136464834\C,1.411282045,-1.298825153,1.3136464834\C,-1.411282045,-1.298825153,1.3136464834\C,1.411282045,1.298825153,-1.3136464834\C,-1.411282045,1.298825153,-1.3136464834\C,1.41128
```

2045, -1.298825153, -1.3136464834\C, -1.411282045, -1.298825153, -1.3136464834\C, 2.2
 813218683, 1.5587761006, 0.\C, -2.2813218683, 1.5587761006, 0.\C, 2.2813218683, -1.558
 7761006, 0.\C, -2.2813218683, -1.5587761006, 0.\C, 1.4477468811, 0., 2.1634885161\C, -1
 .4477468811, 0., 2.1634885161\C, 1.4477468811, 0., -2.1634885161\C, -1.4477468811, 0.,
 -2.1634885161\B, 0., 0., 3.1360869963\B, 0., 0., -3.1360869963\H, 1.5190176324, 2.14185
 50999, -1.999239432\H, -1.5190176324, 2.1418550999, -1.999239432\H, 1.5190176324, -2.
 1418550999, -1.999239432\H, -1.5190176324, -2.1418550999, -1.999239432\H, 1.51901763
 24, 2.1418550999, 1.999239432\H, -1.5190176324, 2.1418550999, 1.999239432\H, 1.519017
 6324, -2.1418550999, 1.999239432\H, -1.5190176324, -2.1418550999, 1.999239432\H, 2.30
 63597616, 0., 2.8411589496\H, -2.3063597616, 0., 2.8411589496\H, 2.3063597616, 0., -2.8
 411589496\H, -2.3063597616, 0., -2.8411589496\H, 3.2112424113, -0.9954293719, 0.\H, -3
 .2112424113, -0.9954293719, 0.\H, 3.2112424113, 0.9954293719, 0.\H, -3.2112424113, 0.9
 954293719, 0.\H, 2.5561474612, 2.6160893875, 0.\H, -2.5561474612, 2.6160893875, 0.\H, 2
 .5561474612, -2.6160893875, 0.\H, -2.5561474612, -2.6160893875, 0.\H, 0., -1.003609847
 7, 3.8232259264\H, 0., 1.0036098477, 3.8232259264\H, 0., -1.0036098477, -3.8232259264\
 H, 0., 1.0036098477, -3.8232259264\\Version=SGI-G94RevE.2\State=1-AG\HF=-864.21391
 78\RMSD=4.688e-09\RMSF=2.003e-05\Dipole=0., 0., 0.\PG=D02H[O(C\@

7(C₂₁B₂H₂₈, C_{2h})

1\1\ GINC-UGA-PVRS-PC17PVRS\F0pt\RB3LYP\6-311+G(d,p)\C21H28B2\ZXWANG\0
 4-Mar-2002\0\#\ RB3LYP/6-311+G** OPT=RCFC NAME=ZXWANG GEOM=CHECK GUESS
 =READ POP=NONE\OUT:cc4octbh3NbrB6dd.out Octaplane + CC4 + exo-(BH3)2\
 \0, 1\C, -0.6704542931, -1.2779835245, 0.3029929773\C, -0.6704542931, 1.2779
 835245, 0.3029929773\C, 0.6704542931, -1.2779835245, -0.3029929773\C, 0.670
 4542931, 1.2779835245, -0.3029929773\C, 0., 0., 0.\C, 1.7669348851, -1.330923
 8255, 0.7962175495\C, 1.7669348851, 1.3309238255, 0.7962175495\C, -1.766934
 8851, -1.3309238255, -0.7962175495\C, -1.7669348851, 1.3309238255, -0.79621
 75495\C, -0.5786894057, 1.3082959618, 1.8707814303\C, -0.5786894057, -1.308
 2959618, 1.8707814303\C, 0.5786894057, 1.3082959618, -1.8707814303\C, 0.578
 6894057, -1.3082959618, -1.8707814303\C, 0.9267004747, -1.7074974526, 2.058
 9834342\C, 0.9267004747, 1.7074974526, 2.0589834342\C, -0.9267004747, -1.70
 74974526, -2.0589834342\C, -0.9267004747, 1.7074974526, -2.0589834342\C, 2.
 5776430883, 0., 0.8392798445\C, -2.5776430883, 0., -0.8392798445\C, -1.05568
 81928, 0., 2.5438039049\C, 1.0556881928, 0., -2.5438039049\H, -1.2231772684,
 -2.1064395805, 2.244297054\H, -1.2231772684, 2.1064395805, 2.244297054\H, 1
 .2231772684, -2.1064395805, -2.244297054\H, 1.2231772684, 2.1064395805, -2.
 244297054\H, 2.469958615, -2.131283193, 0.5541016682\H, 2.469958615, 2.1312
 83193, 0.5541016682\H, -2.469958615, -2.131283193, -0.5541016682\H, -2.4699
 58615, 2.131283193, -0.5541016682\H, 3.212988734, 0., 1.7287507424\H, -3.212
 988734, 0., -1.7287507424\H, 1.3058440044, 1.2457925221, 2.9730773965\H, 1.3
 058440044, -1.2457925221, 2.9730773965\H, -1.3058440044, 1.2457925221, -2.9
 730773965\H, -1.3058440044, -1.2457925221, -2.9730773965\B, -0.8033344279,
 0., 4.1822046679\B, 0.8033344279, 0., -4.1822046679\H, 0.9844789191, -2.7896
 578366, 2.1907935196\H, 0.9844789191, 2.7896578366, 2.1907935196\H, -0.9844
 789191, -2.7896578366, -2.1907935196\H, -0.9844789191, 2.7896578366, -2.190
 7935196\H, 3.2507358752, 0., -0.0244682599\H, -3.2507358752, 0., 0.024468259
 9\H, -2.1516977394, 0., 2.4419556484\H, 2.1516977394, 0., -2.4419556484\H, -1
 .2729145536, -1.0119689368, 4.6732795276\H, -1.2729145536, 1.0119689368, 4.
 6732795276\H, 1.2729145536, -1.0119689368, -4.6732795276\H, 1.2729145536, 1
 .0119689368, -4.6732795276\H, 0.4224463484, 0., 4.3781531734\H, -0.42244634
 84, 0., -4.3781531734\\Version=x86-Linux-G98RevA.5\HF=-866.6282522\RMSD=
 9.405e-09\RMSF=2.202e-05\PG=C02H [O(C1),SGH(C4H8B2),X(C16H20)]\@

7a (C₂₁A₁₂H₂₈, C_{2h})

```
1\1\ PG[C02H, N/A], NImag[N/A])\Fopt\RB3LYP\6-311+G(d,p)\C21H28A12\ZXWANG\15-Mar-2002\0\#\ RB3LYP/6-311+G** OPT=RCFC NAME=ZXWANG POP=NONE GEOM=CHECK GUESS=READ SYM=L00SE\EN[-1301.8208667], ZPE[ N/A]OUT:cc4oct_alh3dB6dda.out cc4octplane_alh3d (Long)\0,1\C,0.6618040689,-1.267364326,0.3222439534\C,0.6618040689,1.267364326,0.3222439534\C,-0.6618040689,-1.267364326,-0.3222439534\C,-0.6618040689,1.267364326,-0.3222439534\C,0.,0.,0.\C,0.5360279432,1.2999562328,1.9047957436\C,0.5360279432,-1.2999562328,1.9047957436\C,-0.5360279432,1.2999562328,-1.9047957436\C,-0.5360279432,-1.2999562328,-1.9047957436\C,1.7871094041,-1.3286580908,-0.7465964078\C,1.7871094041,1.3286580908,-0.7465964078\C,-1.7871094041,-1.3286580908,0.7465964078\C,-1.7871094041,1.3286580908,0.7465964078\C,0.9922019643,0.,2.5663999639\C,-0.9922019643,0.,-2.5663999639\C,2.6006052762,0.,-0.7751546531\C,-2.6006052762,0.,0.7751546531\C,-0.9823812463,1.7081898976,2.0328596082\C,-0.9823812463,-1.7081898976,2.0328596082\C,0.9823812463,1.7081898976,-2.0328596082\C,0.9823812463,-1.7081898976,-2.0328596082\A1,0.6341181342,0.,4.6575101382\A1,-0.6341181342,0.,-4.6575101382\H,1.1633865917,-2.1110860727,2.280480874\H,1.1633865917,2.1110860727,2.280480874\H,-1.1633865917,-2.1110860727,-2.280480874\H,-1.1633865917,2.1110860727,-2.280480874\H,2.4816636451,2.1314284404,-0.4888044203\H,2.4816636451,-2.1314284404,-0.4888044203\H,-2.4816636451,2.1314284404,0.4888044203\H,-2.4816636451,-2.1314284404,0.4888044203\H,-1.4113115867,-1.262763339,2.9332751204\H,-1.4113115867,1.262763339,2.9332751204\H,1.4113115867,-1.262763339,-2.9332751204\H,1.4113115867,1.262763339,-2.9332751204\H,-3.2510657693,0.,1.6535814106\H,3.2510657693,0.,-1.6535814106\H,2.0887712056,0.,2.6039997796\H,-2.0887712056,0.,-2.6039997796\H,3.2589812212,0.,0.0998920107\H,-3.2589812212,0.,-0.0998920107\H,-1.0324488119,2.7923096477,2.1508199708\H,-1.0324488119,-2.7923096477,2.1508199708\H,1.0324488119,2.7923096477,-2.1508199708\H,1.0324488119,-2.7923096477,-2.1508199708\H,1.2784412533,-1.3747581488,5.1933604746\H,1.2784412533,1.3747581488,5.1933604746\H,-1.2784412533,-1.3747581488,-5.1933604746\H,-1.2784412533,1.3747581488,-5.1933604746\H,-1.003365451,0.,4.6996316823\H,1.003365451,0.,-4.6996316823\Version=x86-Linux-G98RevA.5\HF=-1301.8208667\RMSE=4.415e-9\RMSE=1.758e-05\PG=C02H [O(\@
```

8 (C₂₃B₂H₂₈, C_{2h})

```
1\1\ GINC-UGA-PVRS-PC20PVRS\Fopt\RB3LYP\6-311+G(d,p)\C23H28B2\ZXWANG\06-Mar-2002\0\#\ RB3LYP/6-311+G** OPT POP=NONE NAME=ZXWANG GEOM=CHECK GUESS=READ\OUT:cc4oct2bh3NbrB6dd.out Dimethanospiro[2,2] octaplane + (BH3)2\0,1\C,0.4655339095,-0.6175858609,1.295743973\C,-0.2673297748,0.6175858609,1.3506328353\C,0.2673297748,-0.6175858609,-1.3506328353\C,-0.4655339095,0.6175858609,-1.295743973\C,0.,0.,0.\C,-1.769125634,0.4148471573,1.4433328579\C,1.9643835278,-0.4148471573,1.1637064077\C,-1.9643835278,0.4148471573,-1.1637064077\C,1.769125634,-0.4148471573,-1.4433328579\C,0.6287398082,1.8399914137,1.2473015856\C,-0.4359307341,-1.8399914137,1.3270415919\C,0.4359307341,1.8399914137,-1.3270415919\C,-0.6287398082,-1.8399914137,-1.2473015856\C,-1.8419766821,-1.1668353985,1.6646673394\C,2.0693912004,1.1668353985,1.3717199087\C,-2.0693912004,-1.1668353985,-1.3717199087\C,1.8419766821,1.1668353985,-1.6646673394\C,-2.2817773551,1.1704610793,0.1708969429\C,2.2817773551,-1.1704610793,-0.1708969429\C,0.1250373251,2.6215962094,-0.0093648473\C,-0.1250373251,-2.6215962094,0.0093648473\C,-1.4881821523,2.5879508284,0.1114595075\C,1.4881821523,-2.5879508284,-0.1114595075\H,-0.1403050616,-2.4984857824,2.1482809123\H,0.4587418004,2.4984857824,2.1034144501\H,-0.4587418004,-2.4984857824,-2.1034144501\H,0.1403050616,2.4984857824,-2.1482809123\H,2.4855563725,-0.9312993877,1.9734612999\H,-2.1638652164,0.9312993
```

877, 2.321686307\H, 2.1638652164, -0.9312993877, -2.321686307\H, -2.4855563
 725, 0.9312993877, -1.9734612999\H, -3.350201895, 1.3837924553, 0.250918110
 2\H, 3.350201895, -1.3837924553, -0.2509181102\B, 0.6805631685, 4.154937161
 8, -0.0509717413\B, -0.6805631685, -4.1549371618, 0.0509717413\H, -2.806989
 6024, -1.6523620301, -0.7408122611\H, 2.6653244403, 1.6523620301, -1.150668
 9627\H, -2.6653244403, -1.6523620301, 1.1506689627\H, 2.8069896024, 1.65236
 20301, 0.7408122611\H, -2.0185427744, -1.3184050457, 2.7307731583\H, 2.4027
 916561, 1.3184050457, 2.3996310616\H, -2.4027916561, -1.3184050457, -2.3996
 310616\H, 2.0185427744, 1.3184050457, -2.7307731583\H, -1.8870817778, 3.157
 7358092, -0.7326015703\H, 1.7569024848, -3.1577358092, -1.0055229266\H, -1.
 7569024848, 3.1577358092, 1.0055229266\H, 1.8870817778, -3.1577358092, 0.73
 26015703\H, -0.2506477496, -4.7331001345, 1.0396419499\H, 0.4027136457, 4.7
 331001345, 0.990707524\H, -0.4027136457, -4.7331001345, -0.990707524\H, 0.2
 506477496, 4.7331001345, -1.0396419499\H, -1.9127599828, -4.0872600037, 0.1
 432588648\H, 1.9127599828, 4.0872600037, -0.1432588648\Version=x86-Linux
 -G98RevA.5\HF=-942.7757447\RMSD=4.515e-09\RMSF=9.776e-06\PG=C02H [O(C1
),SGH(C6H4B2),X(C16H24)]\@

9 (C₂₁B₂H₂₄, C_{2h})

1\1\ GINC-UGA-PVRS-MAC9PVRS\F0pt\RB3LYP\6-311+G(d,p)\C21H24B2\ZXWANG\2
 3-Jan-2002\0\#\# RB3LYP/6-311+G** OPT NAME=ZXWANG SYM=LOOSE GEOM=CHECK
 GUESS=READ POP=NONE\Pagdone + exo-(BH3)2\0,1\C,0.,0.,0.\C,-1.2617159
 335,0.8043669791,1.8678511921\C,1.2617159335,0.8043669791,-1.867851192
 1\C,-1.2617159335,-0.8043669791,1.8678511921\C,1.2617159335,-0.8043669
 791,-1.8678511921\C,0.6168014878,1.2716503906,0.4201444902\C,-0.616801
 4878,1.2716503906,-0.4201444902\C,0.6168014878,-1.2716503906,0.4201444
 902\C,-0.6168014878,-1.2716503906,-0.4201444902\C,0.2603817664,-1.1894
 322913,1.963680809\C,-0.2603817664,-1.1894322913,-1.963680809\C,0.2603
 817664,1.1894322913,1.963680809\C,-0.2603817664,1.1894322913,-1.963680
 809\C,-1.8854524342,-1.2113552973,0.4810115737\C,1.8854524342,-1.21135
 52973,-0.4810115737\C,-1.8854524342,1.2113552973,0.4810115737\C,1.8854
 524342,1.2113552973,-0.4810115737\C,0.9077283466,0.,2.6794561873\C,-0.
 9077283466,0.,-2.6794561873\C,-2.772961996,0.,0.1130684723\C,2.7729619
 96,0.,-0.1130684723\H,-1.8266324166,1.1791157522,2.7160690187\H,1.8266
 324166,1.1791157522,-2.7160690187\H,-1.8266324166,-1.1791157522,2.7160
 690187\H,1.8266324166,-1.1791157522,-2.7160690187\H,0.4556354404,2.153
 52047,2.4355580449\H,-0.4556354404,2.15352047,-2.4355580449\H,0.455635
 4404,-2.15352047,2.4355580449\H,-0.4556354404,-2.15352047,-2.435558044
 9\H,-2.4106227337,2.1671067773,0.4793834853\H,2.4106227337,2.167106777
 3,-0.4793834853\H,-2.4106227337,-2.1671067773,0.4793834853\H,2.4106227
 337,-2.1671067773,-0.4793834853\B,0.5656292919,0.,4.3270379718\B,-0.56
 56292919,0.,-4.3270379718\H,-3.6538992979,0.,0.7611195085\H,3.65389929
 79,0.,-0.7611195085\H,1.9960078567,0.,2.5949879757\H,-1.9960078567,0.,
 -2.5949879757\H,-3.1198904645,0.,-0.918558402\H,3.1198904645,0.,0.9185
 58402\H,1.0628946098,1.0070696724,4.8021173042\H,-1.0628946098,1.00706
 96724,-4.8021173042\H,1.0628946098,-1.0070696724,4.8021173042\H,-1.062
 8946098,-1.0070696724,-4.8021173042\H,-0.647397399,0.,4.4961877669\H,0
 .647397399,0.,-4.4961877669\Version=x86-Linux-G98RevA.5\HF=-864.17340
 78\RMSD=3.698e-09\RMSF=2.106e-05\PG=C02H [O(C1),SGH(C4H8B2),X(C16H16)]
 \@

10 ($C_{19}B_2H_{20}$, C_{2h})

```
1\1\ GINC-UGA-PVRS-PC9PVRS\F0pt\RB3LYP\6-311+G(d,p)\C19H20B2\ZXWANG\30
-Mar-2002\0\#\ RB3LYP/6-311+G** OPT=RCFC NAME=ZXWANG POP=NONE GEOM=CHE
CK GUESS=READ\ \Pagdone-B2H4\ \0,1\C,0.,0.,0.\C,0.0016815868,0.810416942
4,2.2315252838\C,-0.0016815868,0.8104169424,-2.2315252838\C,0.00168158
68,-0.8104169424,2.2315252838\C,-0.0016815868,-0.8104169424,-2.2315252
838\C,0.7486119986,1.2884248577,0.0165537563\C,-0.7486119986,1.2884248
577,-0.0165537563\C,0.7486119986,-1.2884248577,0.0165537563\C,-0.74861
19986,-1.2884248577,-0.0165537563\C,1.3036084973,-1.2489414027,1.46816
18873\C,-1.3036084973,-1.2489414027,-1.4681618873\C,1.3036084973,1.248
9414027,1.4681618873\C,-1.3036084973,1.2489414027,-1.4681618873\C,-1.3
007831092,-1.2109903881,1.436902989\C,1.3007831092,-1.2109903881,-1.43
6902989\C,-1.3007831092,1.2109903881,1.436902989\C,1.3007831092,1.2109
903881,-1.436902989\B,2.3578117157,0.,1.7491565711\B,-2.3578117157,0.,
-1.7491565711\C,-2.2440870482,0.,1.6114830667\C,2.2440870482,0.,-1.611
4830667\H,-0.0108392009,1.175837832,3.2569350796\H,0.0108392009,1.1758
37832,-3.2569350796\H,-0.0108392009,-1.175837832,3.2569350796\H,0.0108
392009,-1.175837832,-3.2569350796\H,1.6373652835,2.2551600052,1.738805
2692\H,-1.6373652835,2.2551600052,-1.7388052692\H,1.6373652835,-2.2551
600052,1.7388052692\H,-1.6373652835,-2.2551600052,-1.7388052692\H,-1.7
4006966,2.1654262153,1.7320130367\H,1.74006966,2.1654262153,-1.7320130
367\H,-1.74006966,-2.1654262153,1.7320130367\H,1.74006966,-2.165426215
3,-1.7320130367\H,-2.6387913726,0.,2.6322449849\H,2.6387913726,0.,-2.6
322449849\H,3.3696274837,0.,1.0819584502\H,-3.3696274837,0.,-1.0819584
502\H,-3.077791999,0.,0.9120901086\H,3.077791999,0.,-0.9120901086\H,2.
6417504564,0.,2.9351112097\H,-2.6417504564,0.,-2.9351112097\ \Version=x
86-Linux-G98RevA.5\HF=-785.6073179\RMSD=6.999e-09\RMSF=2.157e-05\PG=C0
2H [O(C1),SGH(C2H8B2),X(C16H12)]\ \@
```

11 ($C_{21}B_2H_{24}$, C_{2h})

```
1\1\ GINC-UGA-PVRS-PC19PVRS\F0pt\RB3LYP\6-311+G(d,p)\C21H24B2\ZXWANG\3
0-Mar-2002\0\#\ RB3LYP/6-311+G** OPT NAME=ZXWANG GEOM=CHECK GUESS=READ
POP=NONE\ \Pagodane_(CH2)2Br_c2h4\ \0,1\C,-0.002251498,-1.27374638,2.35
06663936\C,0.002251498,-1.27374638,-2.3506663936\C,-0.002251498,1.2737
4638,2.3506663936\C,0.002251498,1.27374638,-2.3506663936\C,-0.73543832
55,-1.2900944099,-0.0124981067\C,0.7354383255,-1.2900944099,0.01249810
67\C,-0.7354383255,1.2900944099,-0.0124981067\C,0.7354383255,1.2900944
099,0.0124981067\C,-1.3043988982,1.2761370922,1.4339023389\C,1.3043988
982,1.2761370922,-1.4339023389\C,-1.3043988982,-1.2761370922,1.4339023
389\C,1.3043988982,-1.2761370922,-1.4339023389\C,-1.3153014117,-1.3137
383475,-1.4496997038\C,1.3153014117,-1.3137383475,1.4496997038\C,-1.31
53014117,1.3137383475,-1.4496997038\C,1.3153014117,1.3137383475,1.4496
997038\C,-2.163445273,0.,1.6486724182\C,2.163445273,0.,-1.6486724182\B
,-2.2959079842,0.,-1.7219102523\B,2.2959079842,0.,1.7219102523\C,-0.00
06875207,0.,3.2241444028\C,0.0006875207,0.,-3.2241444028\C,0.,0.,0.\H,
-1.9131175842,-2.1717133212,1.5806106387\H,1.9131175842,-2.1717133212,
-1.5806106387\H,-1.9131175842,2.1717133212,1.5806106387\H,1.9131175842
,2.1717133212,-1.5806106387\H,-1.8462969512,2.2646296537,-1.5635683705
\H,1.8462969512,2.2646296537,1.5635683705\H,-1.8462969512,-2.264629653
7,-1.5635683705\H,1.8462969512,-2.2646296537,1.5635683705\H,-2.5833222
398,0.,2.6565045486\H,2.5833222398,0.,-2.6565045486\H,-2.9973483698,0.
,0.9472884917\H,2.9973483698,0.,-0.9472884917\H,-3.2492983072,0.,-0.96
46694673\H,3.2492983072,0.,0.9646694673\H,-0.0244686435,2.1526220835,2
.997745778\H,0.0244686435,2.1526220835,-2.997745778\H,-0.0244686435,-2
```


.1526220835, 2.997745778\H, 0.0244686435, -2.1526220835, -2.997745778\H, -0.8644415216, 0., 3.8962581652\H, 0.8644415216, 0., -3.8962581652\H, -0.8909717044, 0., -3.8499754231\H, 0.8909717044, 0., 3.8499754231\H, 2.7403249608, 0., 2.8522513894\H, -2.7403249608, 0., -2.8522513894\\Version=x86-Linux-G98RevA.5\HF=-864.2744729\RMSD=6.388e-09\RMSF=4.795e-05\PG=C02H [O(C1),SGH(C4H12B2),X(C16H12)]\\@

12 (C₂₃B₂H₂₈, C_{2h})

1\1\ GINC-UGA-PVRS-PC18PVRS\FOpt\RB3LYP\6-311+G(d,p)\C23H28B2\ZXWANG\17-Mar-2002\0\#\ RB3LYP/6-311+G** OPT=RCFC NAME=ZXWANG POP=NONE GEOM=CHECK GUESS=READ SYM=L00SE\\OUT:cc4octch2brbh3dB6dd.out cc4octch2br_bh3d\\0,1\C,-0.8432650474,-1.260705456,2.2063639947\C,0.8432650474,-1.260705456,-2.2063639947\C,-0.8432650474,1.260705456,2.2063639947\C,0.8432650474,1.260705456,-2.2063639947\C,-0.6858166118,-1.2715448529,-0.2653403657\C,0.6858166118,-1.2715448529,0.2653403657\C,-0.6858166118,1.2715448529,-0.2653403657\C,0.6858166118,1.2715448529,0.2653403657\C,-1.7316330947,1.2735366505,0.8820068733\C,1.7316330947,1.2735366505,-0.8820068733\C,-1.7316330947,-1.2735366505,0.8820068733\C,1.7316330947,-1.2735366505,-0.8820068733\C,-0.7105950193,-1.2461957441,-1.8447120989\C,0.7105950193,-1.2461957441,1.8447120989\C,-0.7105950193,1.2461957441,-1.8447120989\C,0.7105950193,1.2461957441,1.8447120989\C,-2.6142078902,0.,0.7816968022\C,2.6142078902,0.,-0.7816968022\C,-1.4362965373,0.,-2.380724312\C,1.4362965373,0.,2.380724312\C,-1.1718739644,0.,3.0289344919\C,1.1718739644,0.,-3.0289344919\C,0.,0.,0.\H,-2.3463571215,-2.1731338997,0.8080826239\H,2.3463571215,-2.1731338997,-0.8080826239\H,-2.3463571215,2.1731338997,0.8080826239\H,2.3463571215,2.1731338997,-0.8080826239\H,-1.212710775,2.1530752022,-2.1875402453\H,1.212710775,2.1530752022,2.1875402453\H,-1.212710775,-2.1530752022,-2.1875402453\H,1.212710775,-2.1530752022,2.1875402453\H,-3.3571387775,0.,1.5804237604\H,3.3571387775,0.,-1.5804237604\B,1.7497482605,0.,4.0599186958\B,-1.7497482605,0.,-4.0599186958\H,-3.1719904893,0.,-0.1556446474\H,3.1719904893,0.,0.1556446474\H,-2.4473582589,0.,-1.9674874888\H,2.4473582589,0.,1.9674874888\H,-1.0610143979,2.1530673664,2.7919032884\H,1.0610143979,2.1530673664,-2.7919032884\H,-1.0610143979,-2.1530673664,2.7919032884\H,1.0610143979,-2.1530673664,-2.7919032884\H,-2.2245966237,0.,3.3228248476\H,2.2245966237,0.,-3.3228248476\H,0.5767441761,0.,-3.9391074141\H,2.9550184357,0.,4.2257940965\H,-2.9550184357,0.,-4.2257940965\H,1.2551863891,1.001959117,4.5564747387\H,-1.2551863891,1.001959117,-4.5564747387\H,1.2551863891,-1.001959117,4.5564747387\H,-1.2551863891,-1.001959117,-4.5564747387\\Version=x86-Linux-G98RevA.5\HF=-942.8270054\RMSD=1.808e-09\RMSF=2.518e-05\PG=C02H [O(C1),SGH(C6H12B2),X(C16H16)]\\@

5⁺ (C₁₉B₂H₂₄, C_{2h})

1\1\ GINC-UGA-PVRS-PC19PVRS\FOpt\UB3LYP\6-311+G(d,p)\C19H24B2(1-,2)\ZXWANG\26-May-2002\0\#\ UB3LYP/6-311+G** OPT NAME=ZXWANG POP=NONE\\OUT:cc4octb2h4nrbDB6dd.out Octaplane + CC4 + (BH2)2\\-1,2\C,-0.7400348202,-1.3057086872,0.0207025669\C,0.7400348202,-1.3057086872,-0.0207025669\C,0.7400348202,1.3057086872,-0.0207025669\C,-0.7400348202,1.3057086872,0.0207025669\C,0.,0.,0.\C,1.2974841095,-1.3439598564,1.4125738461\C,1.2974841095,1.3439598564,1.4125738461\C,-1.2945925907,1.3905430275,1.4446627369\C,-1.2945925907,-1.3905430275,1.4446627369\C,1.2945925907,-1.

3905430275, -1.4446627369\C, 1.2945925907, 1.3905430275, -1.4446627369\C, -1.2974841095, 1.3439598564, -1.4125738461\C, -1.2974841095, -1.3439598564, -1.4125738461\C, 0.0207343906, -1.7086935849, 2.2577641066\C, 2.014744302, 0., 1.7822206639\C, 0.0207343906, 1.7086935849, 2.2577641066\B, -2.1272213278, 0., 1.8762462317\C, -0.0207343906, -1.7086935849, -2.2577641066\B, 2.1272213278, 0., -1.8762462317\C, -0.0207343906, 1.7086935849, -2.2577641066\C, -2.014744302, 0., -1.7822206639\H, -1.981437503, -2.2435136988, 1.5226343197\H, 2.0508338964, -2.1341770325, 1.51360268\H, 2.0508338964, 2.1341770325, 1.51360268\H, -1.981437503, 2.2435136987, 1.5226343197\H, -2.0508338964, -2.1341770325, -1.51360268\H, 1.981437503, -2.2435136987, -1.5226343197\H, 1.981437503, 2.2435136988, -1.5226343197\H, -2.0508338964, 2.1341770325, -1.51360268\H, 2.2234484476, 0., 2.8591203433\H, 0.0229323486, 1.1948843795, 3.2226137833\H, -2.3363066491, 0., 3.0881481363\H, 0.0229323486, -1.1948843795, 3.2226137833\H, 2.3363066491, 0., -3.0881481363\H, -0.0229323486, 1.1948843795, -3.2226137833\H, -2.2234484476, 0., -2.8591203433\H, -0.0229323486, -1.1948843795, -3.2226137833\H, 0.0645099955, -2.783300632, 2.4740984457\H, 2.9815543743, 0., 1.2682496682\H, 0.0645099955, 2.783300632, 2.4740984457\H, -3.2093585341, 0., 1.2842905579\H, -0.0645099955, -2.783300632, -2.4740984457\H, 3.2093585341, 0., -1.2842905579\H, -0.0645099955, 2.783300632, -2.4740984457\H, -2.9815543743, 0., -1.2682496682\Version=x86-Linux-G98RevA.5\HF=-788.1692543\S2=0.754926\S2-1=0.\S2A=0.750017\RMSD=9.973e-09\RMSF=3.204e-05\PG=C02H [O(C1),SGH(C2H8B2),X(C16H16)]\@\

7. (C₂₁B₂H₂₈, C_{2h})

1\1\ GINC-UGA-PVRS-PC20PVRS\FOpt\UB3LYP\6-311+G(d,p)\C21H28B2(1-,2)\ZXWANG\26-May-2002\0\#\ UB3LYP/6-311+G** OPT=RCFC NAME=ZXWANG POP=NONE GEOM=CHECK GUESS=READ\OUT:cc4octbh3-1DB6dd.out Octaplane + CC4 + exo-(BH3)2\ -1,2\C, -0.6669462783, -1.2937606182, 0.3230041887\C, -0.6669462783, 1.2937606182, 0.3230041887\C, 0.6669462783, -1.2937606182, -0.3230041887\C, 0.6669462783, 1.2937606182, -0.3230041887\C, 0., 0., 0.\C, 1.7745399405, -1.3346728302, 0.7440997958\C, 1.7745399405, 1.3346728302, 0.7440997958\C, -1.7745399405, -1.3346728302, -0.7440997958\C, -1.7745399405, 1.3346728302, -0.7440997958\C, -0.55624213, 1.3192367555, 1.8619276227\C, -0.55624213, -1.3192367555, 1.8619276227\C, 0.55624213, 1.3192367555, -1.8619276227\C, 0.9658271652, -1.6679428524, 2.0479866381\C, 0.9658271652, 1.6679428524, 2.0479866381\C, -0.9658271652, -1.6679428524, -2.0479866381\C, -0.9658271652, 1.6679428524, -2.0479866381\C, 2.5903357297, 0., -0.7666371678\C, -2.5903357297, 0., -0.7666371678\C, -1.0649492673, 0., 2.5422569549\C, 1.0649492673, 0., -2.5422569549\H, -1.1623887237, -2.1260760379, 2.2835955649\H, -1.1623887237, 2.1260760379, 2.2835955649\H, 1.1623887237, -2.1260760379, -2.2835955649\H, 1.1623887237, 2.1260760379, -2.2835955649\H, 2.4870781099, -2.139118344, 0.5324162946\H, 2.4870781099, 2.139118344, 0.5324162946\H, -2.4870781099, -2.139118344, -0.5324162946\H, -2.4870781099, 2.139118344, -0.5324162946\H, 3.2349893388, 0., 1.652170481\H, -3.2349893388, 0., -1.652170481\H, 1.3639834181, 1.1688478007, 2.9313735954\H, 1.3639834181, -1.1688478007, 2.9313735954\H, -1.3639834181, 1.1688478007, -2.9313735954\H, -1.3639834181, -1.1688478007, -2.9313735954\B, -0.8774295715, 0., 4.1870458585\B, 0.8774295715, 0., -4.1870458585\H, 1.0500944627, -2.7443123749, 2.2246742769\H, 1.0500944627, 2.7443123749, 2.2246742769\H, -1.0500944627, -2.7443123749, -2.2246742769\H, -1.0500944627, 2.7443123749, -2.2246742769\H, 3.2543135172, 0., -0.1049541713\H, -3.2543135172, 0., 0.1049541713\H, -2.1532427419, 0., 2.3667164767\H, 2.1532427419, 0., -2.3667164767\H, -1.4118336131, -1.0064371811, 4.6537112633\H, -1.4118336131, 1.0064371811, 4.6537112633\H, 1.4118336131, -1.0064371811, -4.6537112633\H, 1.41183

36131,1.0064371811,-4.6537112633\H,0.3121201674,0.,4.5147650673\H,-0.3
121201674,0.,-4.5147650673\\Version=x86-Linux-G98RevA.5\HF=-866.770127
3\S2=0.754734\S2-1=0.\S2A=0.750016\RMSD=8.260e-09\RMSF=3.484e-06\PG=C0
2H [O(C1),SGH(C4H8B2),X(C16H20)]\\@