

Supplement information:

IGLO-II basis sets for boron and hydrogen

-b 0

```
s 5 1.00
 2796.6035000 .12822290000E-02
 420.86799000 .97664082000E-02
 96.915866000 .47452550000E-01
 28.103058000 .16028625000
 9.3784384000 .36191858000
s 1 1.00
 3.4280972000 .42940014000
s 1 1.00
 1.3353938000 .14397325000
s 1 1.00
 .32384228000 -.55926315000
s 1 1.00
 .10202139000 -.56124151000
p 2 1.00
 11.290720000 .14449977000E-01
 2.4257124000 .88292042000E-01
p 1 1.00
 .68564974000 .30209882000
p 1 1.00
 .21569117000 .51644883000
p 1 1.00
 .70102360000E-01 .30983713000
d 1 1.00
 .70000000000 1.00000000000
```

-h 0

```
s 3 1.00
 33.6444000000 0.0061200000
 5.0579600000 0.0457500000
 1.1468000000 0.2057200000
s 1 1.00
 0.3211440000 1.0000000000
s 1 1.00
 0.1013090000 1.0000000000
p 1 1.00
 0.6500000000 1.0000000000
```

Cartesian coordinates of B₂₀H₁₆ computed at RMP2/6-31G* in a symmetry of D_{2d}

H 0.000000 2.503671 2.495619
H -2.458630 -1.639507 1.230503
B -0.880343 0.000000 2.656663
B -1.550149 0.881155 1.255379
H 0.000000 -2.503671 2.495619
H -2.458630 1.639507 1.230503
B 1.550149 -0.881155 1.255379
B 0.000000 1.193782 0.257358
B 0.000000 1.423440 2.003546
B 0.000000 -1.423440 2.003546
H 0.000000 1.475501 -3.683578
H 0.000000 -1.475501 -3.683578
B -1.550149 -0.881155 1.255379
H 2.458630 1.639507 1.230503
B 0.881155 1.550149 -1.255379
B 0.000000 -1.193782 0.257358
B 1.550149 0.881155 1.255379
H 1.475501 0.000000 3.683578
H 2.458630 -1.639507 1.230503
H -1.475501 0.000000 3.683578
B 0.880343 0.000000 2.656663
H 2.503671 0.000000 -2.495619
H -1.639507 -2.458630 -1.230503
B 0.000000 -0.880343 -2.656663
B 0.881155 -1.550149 -1.255379
H -2.503671 0.000000 -2.495619
H 1.639507 -2.458630 -1.230503
B -0.881155 1.550149 -1.255379
B 1.193782 0.000000 -0.257358
B 1.423440 0.000000 -2.003546
B -1.423440 0.000000 -2.003546
H -1.639507 2.458630 -1.230503
B 0.000000 0.880343 -2.656663
B -0.881155 -1.550149 -1.255379
H 1.639507 2.458630 -1.230503
B -1.193782 0.000000 -0.257358