

B3LYP - AH

APOLAR HEXAGONAL ICE
CRYSTAL

0 0 2

33

0 -12 0

7.27 7.66 4.50

6

8 6.247389835053E-02 -4.178299810252E-01 -2.497992058680E-04

8 -6.224284610300E-02 -8.207685002968E-02 1.067924424895E-04

1 1.982869995068E-01 -4.197707781257E-01 3.452723986389E-03

1 2.012989639073E-02 -4.779312104599E-01 1.810566206807E-01

1 -1.593068711755E-02 -2.031587373542E-01 -2.679988104915E-03

1 -1.602900802285E-02 -2.507711847002E-02 -1.816863597988E-01

ENDG