

**B3LYP - PH**

POLAR HEXAGONAL ICE  
CRYSTAL

0 0 0

36

4.42            7.85            7.23

5

8 5.000000000000E-01 1.572710170287E-01 6.025838419810E-02

8 1.707428504323E-18 3.282224651457E-01 -6.223548127703E-02

1 5.000000000000E-01 1.582759419883E-01 1.967939080283E-01

1 5.000000000000E-01 3.710761028766E-02 2.071454981782E-02

1 1.791350610615E-01 2.647598983009E-01 -1.876567538358E-02

ENDG