

B3LYP - AC

APOLAR CUBIC ICE
CRYSTAL

0 0 1

92

4.50 6.19

2

8 2.468239622677E-01 2.468239622677E-01 -5.964300890017E-21

1 -4.357720754002E-01 2.548938280386E-01 -1.617842002416E-01

ENDG