

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

$(0.87 - 0.98)V_{eq}$ and $(0.98 - 1.08)V_{eq}$ $T = 271.31\text{K}$

