

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

$(0.87 - 0.98)V_{eq}$  and  $(0.98 - 1.08)V_{eq}$ .  $T = 130.61\text{K}$

