PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8  $(0.87 - 0.98)V_{eq} \text{ and } (0.98 - 1.08)V_{eq}. \text{ T} = 572.83K$ 

