PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8  $(0.87 - 0.98) V_{eq} \text{ and } (0.98 - 1.08) V_{eq}. \, T = 70.30 K$ 

