PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8 $(0.87 - 0.98)V_{eq}$ and $(0.98 - 1.08)V_{eq}$ Calcite I -941.150Cubic fit Calcite I -941.175 / F.U. (a.u.) Calcite II Cubic fit Calcite II -941.200 -941.225 Analytic Intersection -941.250 · P= 1.87404 GPa

