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 = 110.51K

Legend:
- Calcite I
- Cubic fit Calcite I
- Calcite II
- Cubic fit Calcite II

Y-axis: $(H = E + E_{ZP} + \mathcal{E} + PV)$ / F.U. (a.u.)

X-axis: V / F.U. (Angstrom^3)