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 = 512.53K Calcite I $\mathcal{E} + PV$ / F.U. (a.u.) -941.125 Cubic fit Calcite I -941.150Calcite II Cubic fit Calcite II -941.175 -941.200-941.225 $+ E_{ZP}$ -941.250Ш -941.275-941.30054 56 58 60 62 64 66 68 V / F.U. (Angstrom³)