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 = 532.63K ε + PV) / F.U. (a.u.) Calcite I -941.125 Cubic fit Calcite I Calcite II -941.150Cubic fit Calcite II -941.175-941.200 -941.225 $+ E_{ZP}$ -941.250Ш **-**941.275 -941.300 54 56 58 60 62 64 66 68 V / F.U. (Angstrom³)