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 = 592.93K -941.100*PV) /* F.U. (a.u.) Calcite I -941.125Cubic fit Calcite I Calcite II **-**941.150 -Cubic fit Calcite II <del>-</del>941.175 -941.200 $+E_{ZP}$  + -941.225 · -941.250Щ -941.275-941.30056 58 60 62 64 66 68 54 V / F.U. (Angstrom<sup>3</sup>)