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 = 492.42K Calcite I  $\mathcal{E} + PV$ ) / F.U. (a.u.) -941.125 Cubic fit Calcite I -941.150 -Calcite II Cubic fit Calcite II -941.175-941.200**-**941.225  $E + E_{ZP}$ **-941.250** · <del>-</del>941.275 -941.300 <sup>-</sup> 54 56 58 60 62 64 66 68 V / F.U. (Angstrom<sup>3</sup>)