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 = 190.91K ) -941. ) -941.175 -941.125 Calcite I Cubic fit Calcite I Calcite II Cubic fit Calcite II -941.200 · -941.225-941.250 --941.275 -941.300 · 60 64 54 56 58 62 66 68 V / F.U. (Angstrom<sup>3</sup>)