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 = 412.02K Calcite I / F.U. (a.u.) -941.125 Cubic fit Calcite I -941.150Calcite II Cubic fit Calcite II -941.175 -941.200 -941.225 -941.250**-**941.275 **-**941.300 -64 54 56 58 60 62 66 68 V / F.U. (Angstrom³)