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 = 50.20K <del>-</del>941.125 Calcite I Cubic fit Calcite I **-**941.150 · Calcite II **-941.175** Cubic fit Calcite II -941.200 --941.225  $E_{ZP}$  + -941.250 · -941.275-941.300-941.32564 56 58 60 62 66 68 54 V / F.U. (Angstrom<sup>3</sup>)