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 = 10.00K Calcite I 0.000004 Cubic fit Calcite I Calcite II 0.000003 Cubic fit Calcite II

