PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8 $(0.87 - 0.98)V_{eq}$ and $(0.98 - 1.08)V_{eq}$ -941.229Calcite I -941.230 Cubic fit Calcite I (a.u.) Calcite II -941.231Cubic fit Calcite II **-**941.232

