PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8  $(0.87 - 0.98)V_{eq}$  and  $(0.98 - 1.08)V_{eq}$ Calcite I <del>-</del>941.230 Cubic fit Calcite I (a.u.) Calcite II Cubic fit Calcite II **-**941.232 Common tangent -941.234

