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 = 70.30K

Legend:
- Calcite I (red filled triangles)
- Cubic fit Calcite I (black line)
- Calcite II (open triangles)
- Cubic fit Calcite II (blue line)

Axes:
- Y-axis: TS / F.U. (a.u.)
- X-axis: V / F.U. (Angstrom^3)