Solving the phase boundary between two solid phases

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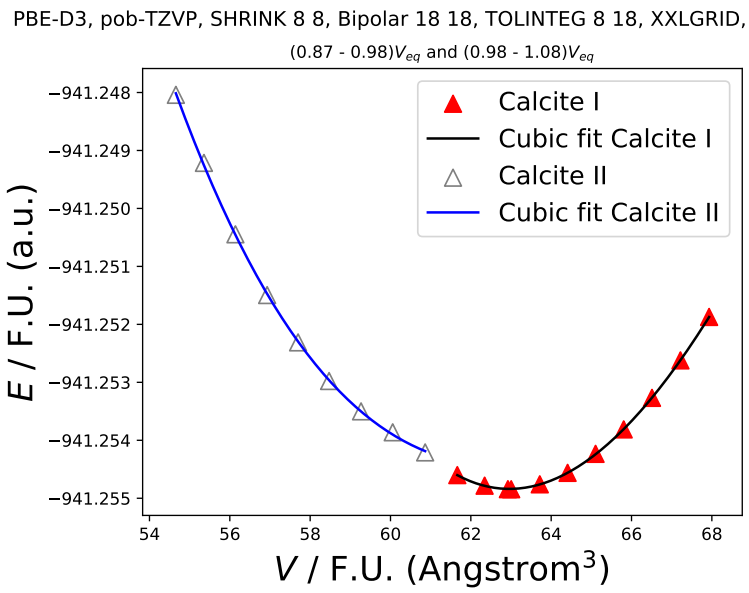
Outline

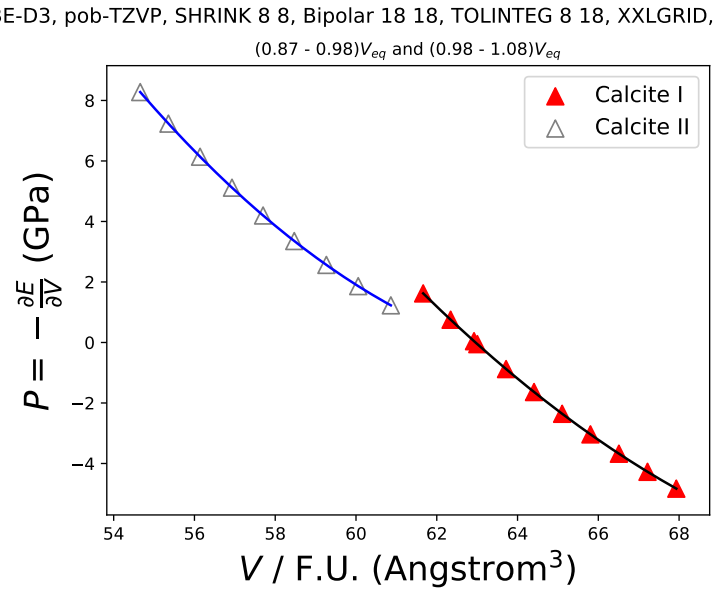
$F(V)$, $G(P)$ and pressure of intersection. Thermal evolution

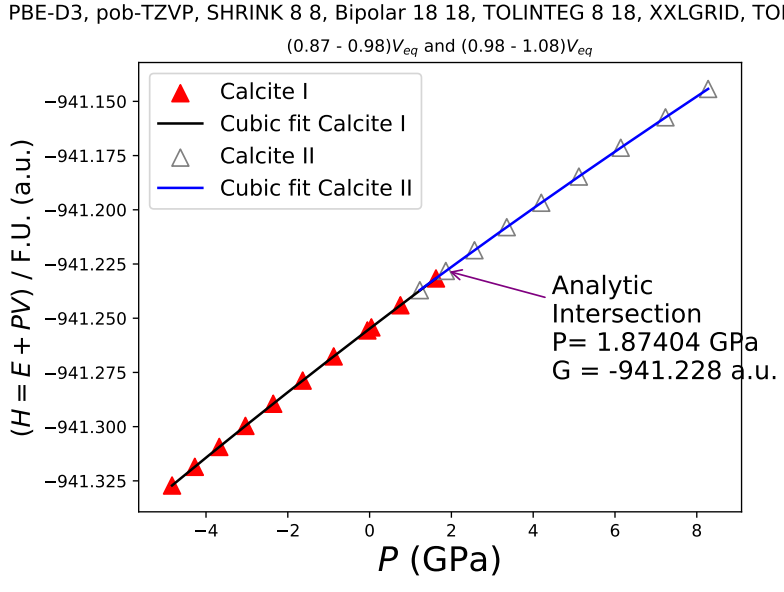
Shapes of G, F, $\mathcal{E}$

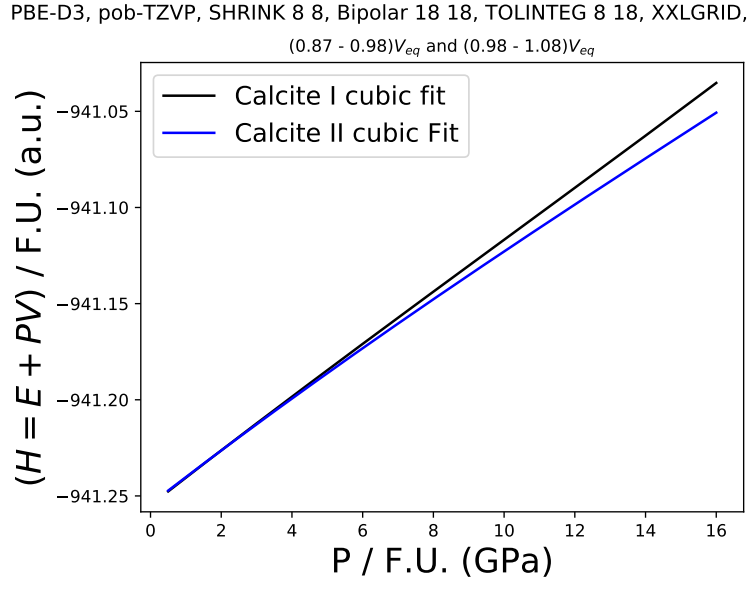
Shape of $H(P;T)$

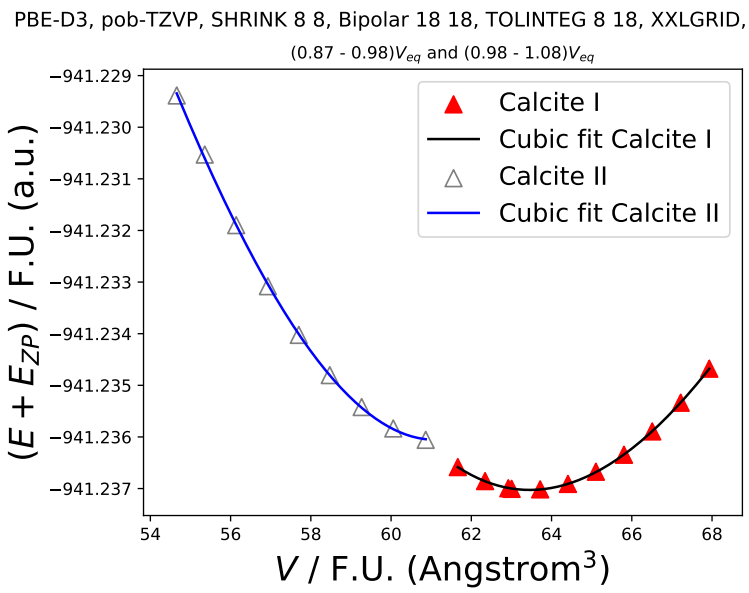
Outline I

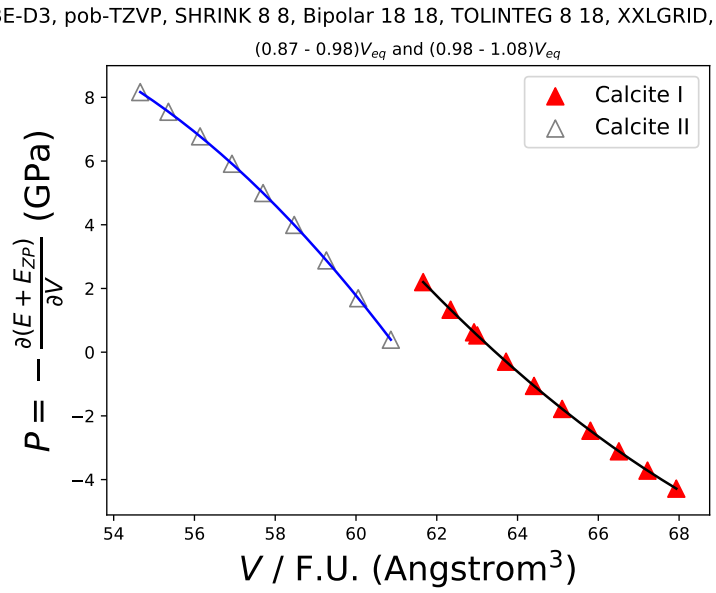

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
E / F.U. (a.u.)
V / F.U. (Angstrom^3)

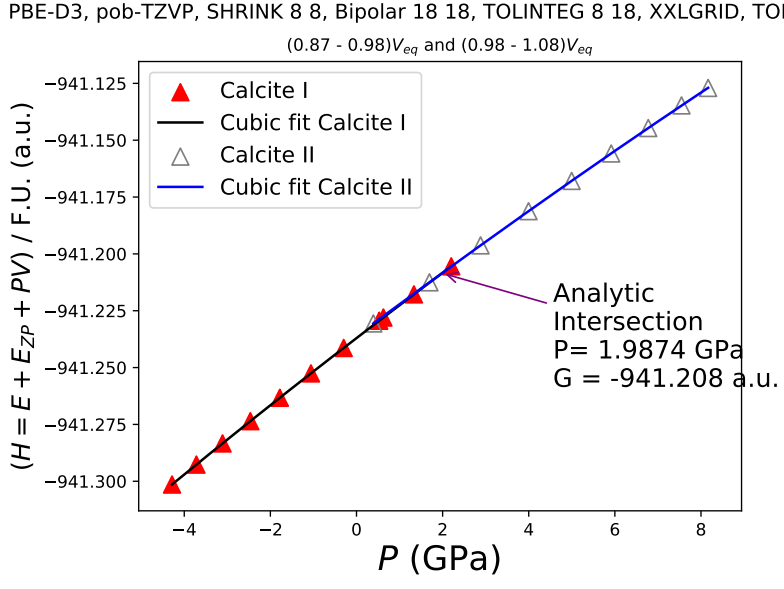

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}
Calcite I
Calcite II
$P = -\frac{\partial E}{\partial V}$ (GPa)
V / F.U. (Angstrom^3)

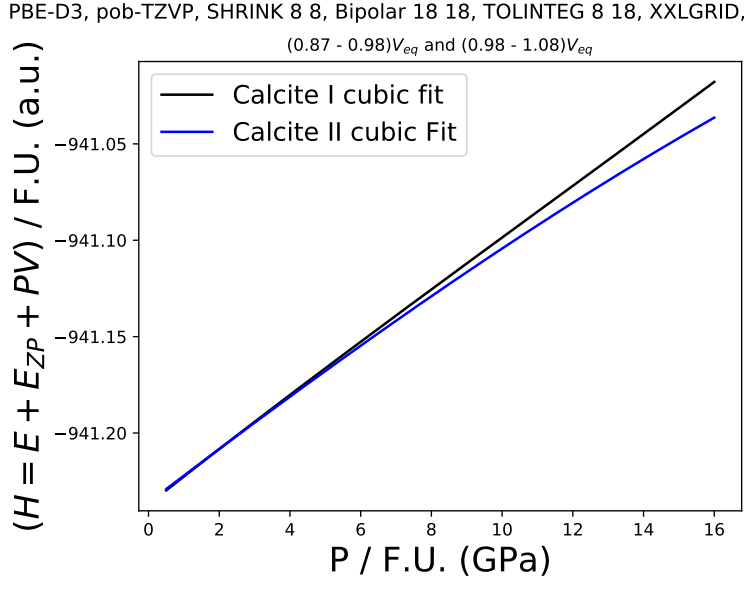

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
Analytic
Intersection
P= 1.87404 GPa
G = -941.228 a.u.
$(H = E + PV)$ / F.U. (a.u.)
P (GPa)


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 cubic fit
Calcite II cubic Fit
$(H = E + PV)$ / F.U. (a.u.)
P / F.U. (GPa)


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
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$(E + E_{ZP})$ / F.U. (a.u.)
V / F.U. (Angstrom^3)


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
Calcite II
$P = -\frac{\partial(E + E_{ZP})}{\partial V}$ (GPa)
V / F.U. (Angstrom^3)


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
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
Analytic
Intersection
P= 1.9874 GPa
G = -941.208 a.u.
$(H = E + E_{ZP} + PV)$ / F.U. (a.u.)
P (GPa)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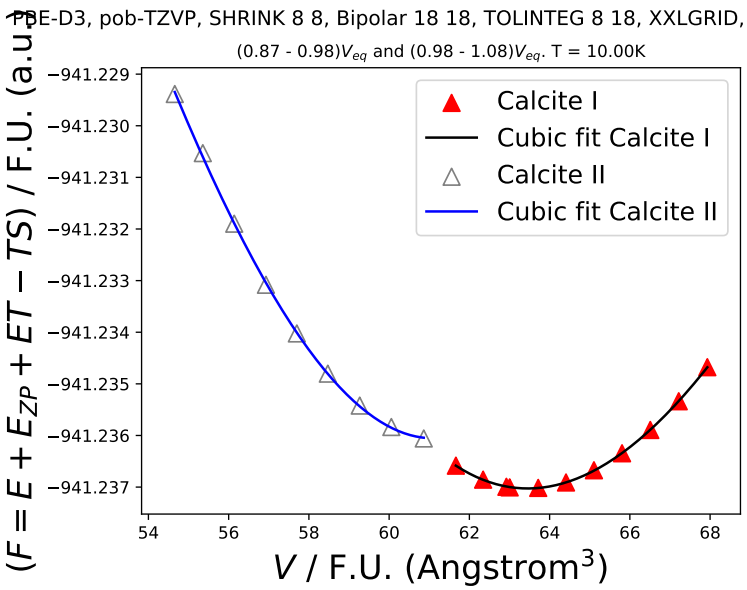
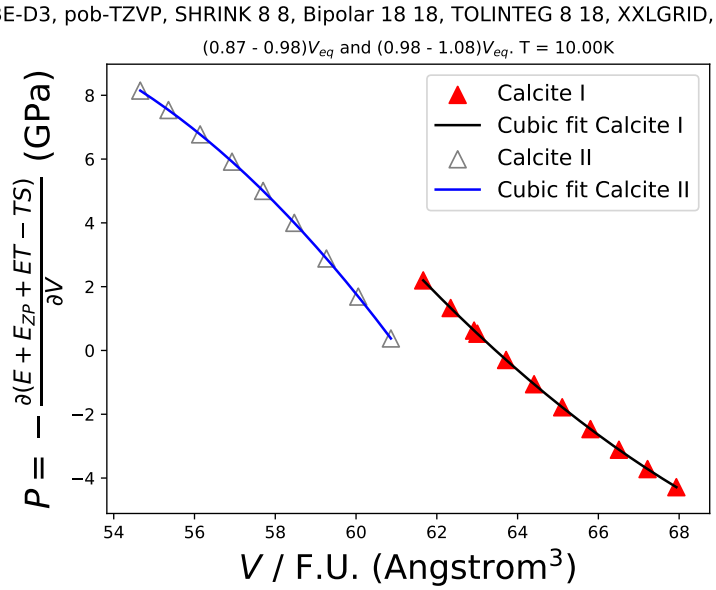
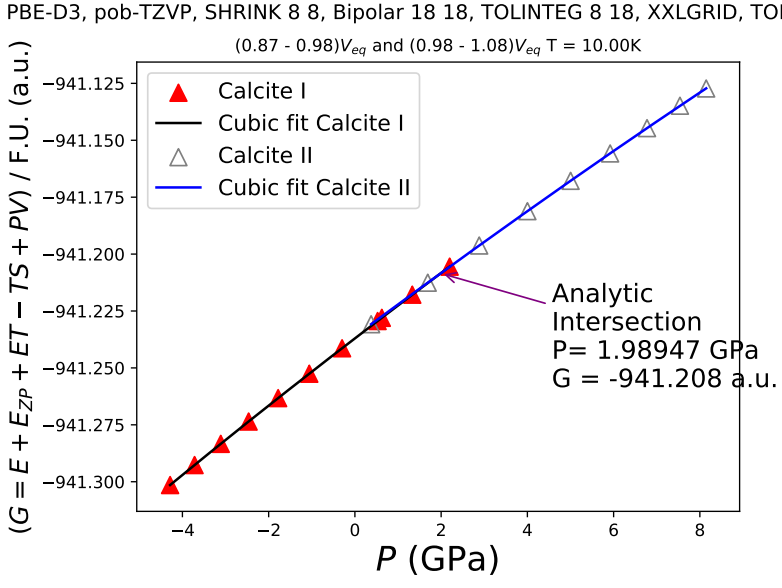
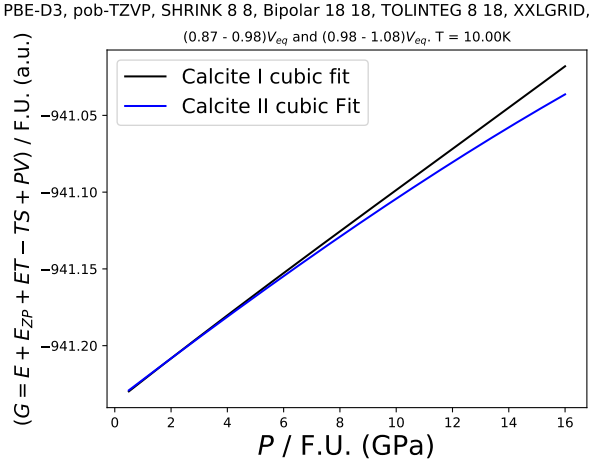
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}
Calcite I cubic fit
Calcite II cubic Fit
$(H = E + E_{ZP} + PV)$ / F.U. (a.u.)
P / F.U. (GPa)

$T = 10.00K$

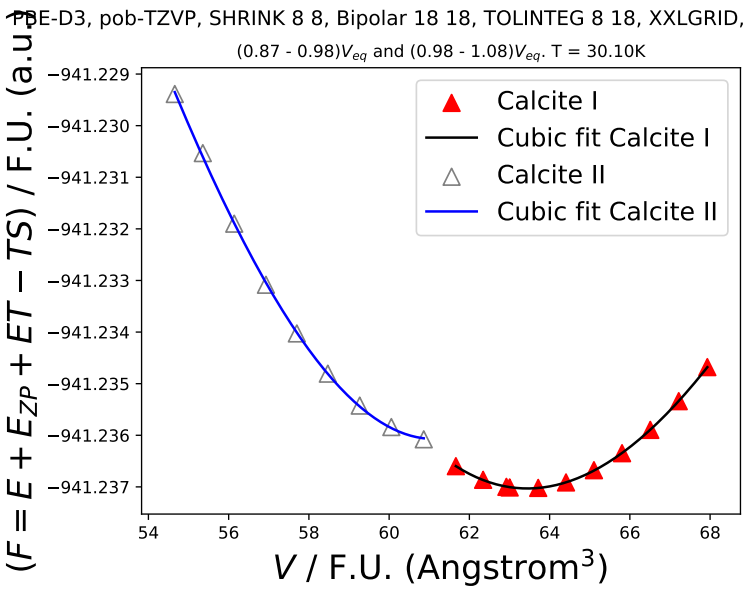

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 10.00K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$(F = E + E_{ZP} + ET - TS)$ / F.U. (a.u.)
V / F.U. (Angstrom^3)

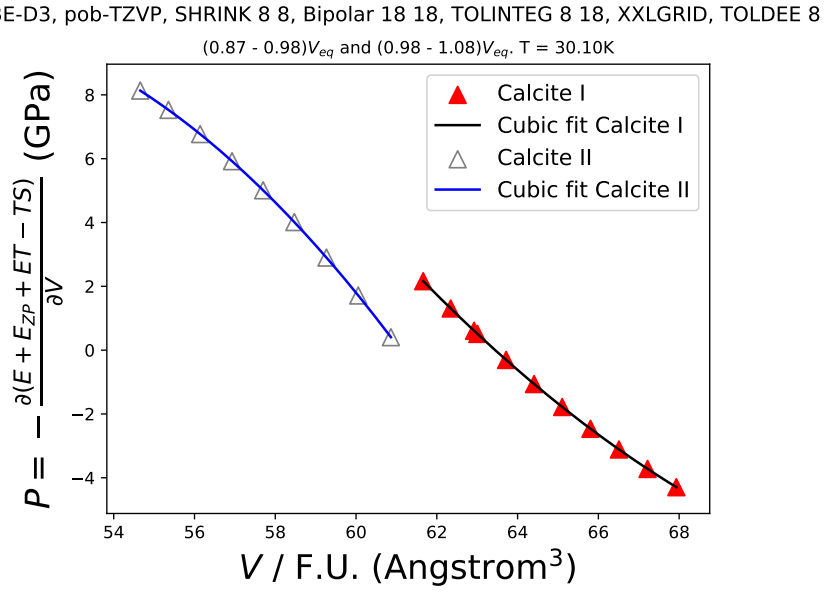

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 10.00K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$P = -\frac{\partial(E + E_{ZP} + ET - TS)}{\partial V}$ (GPa)
V / F.U. (Angstrom^3)

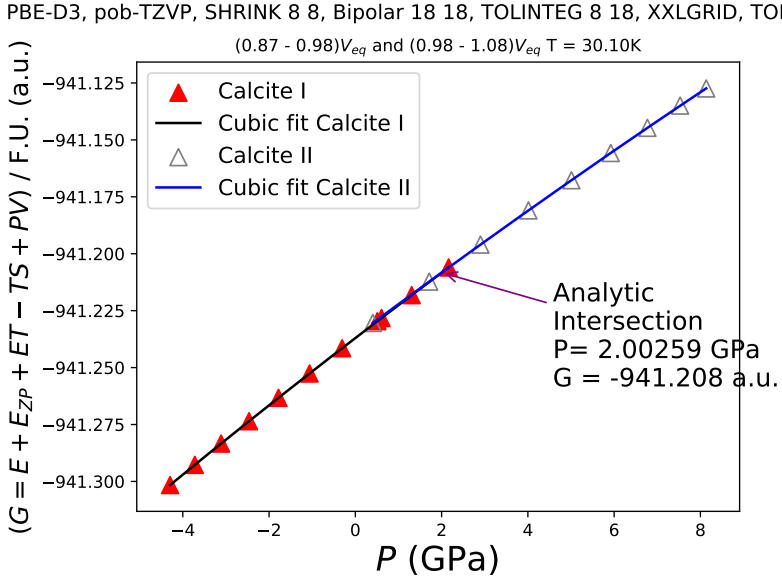

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq} T = 10.00K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
Analytic
Intersection
P= 1.98947 GPa
G = -941.208 a.u.
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P (GPa)

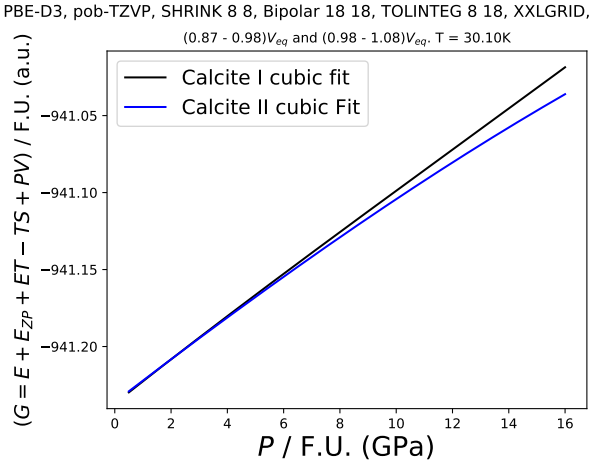

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 10.00K
Calcite I cubic fit
Calcite II cubic Fit
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P / F.U. (GPa)

$T = 30.10K$

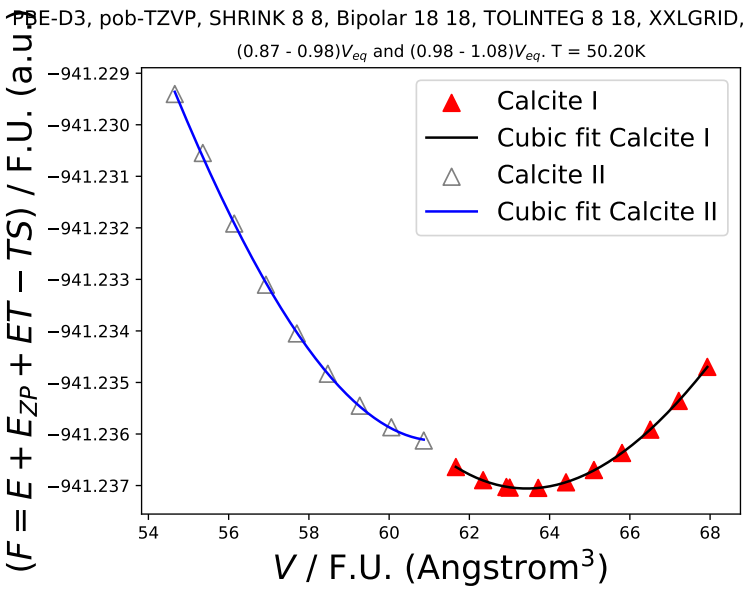

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 30.10K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$(F = E + E_{ZP} + ET - TS)$ / F.U. (a.u.)
V / F.U. (Angstrom^3)

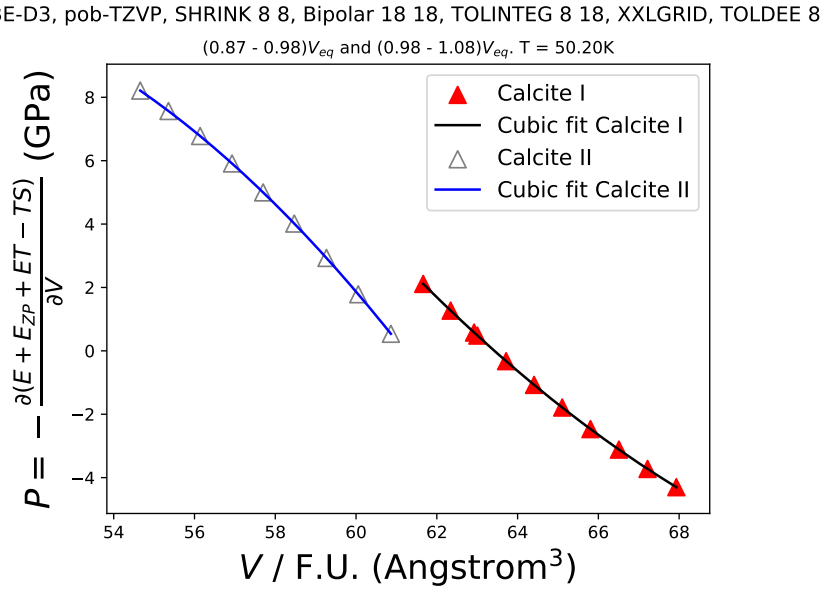

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 30.10K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$P = -\frac{\partial(E + E_{ZP} + ET - TS)}{\partial V}$ (GPa)
V / F.U. (Angstrom^3)

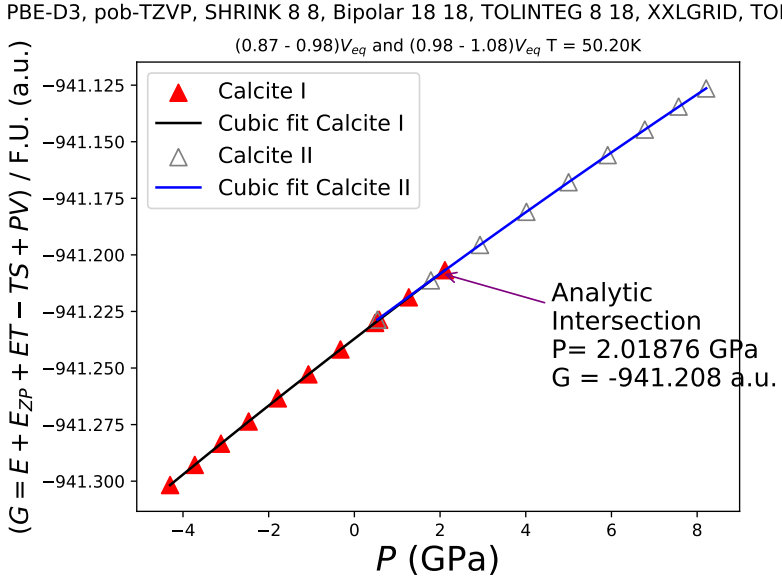

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq} T = 30.10K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
Analytic
Intersection
P= 2.00259 GPa
G = -941.208 a.u.
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P (GPa)

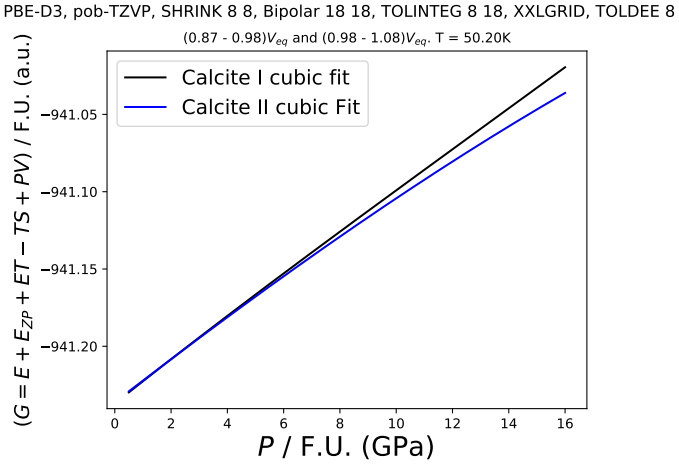

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 30.10K
Calcite I cubic fit
Calcite II cubic Fit
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P / F.U. (GPa)

$T = 50.20K$

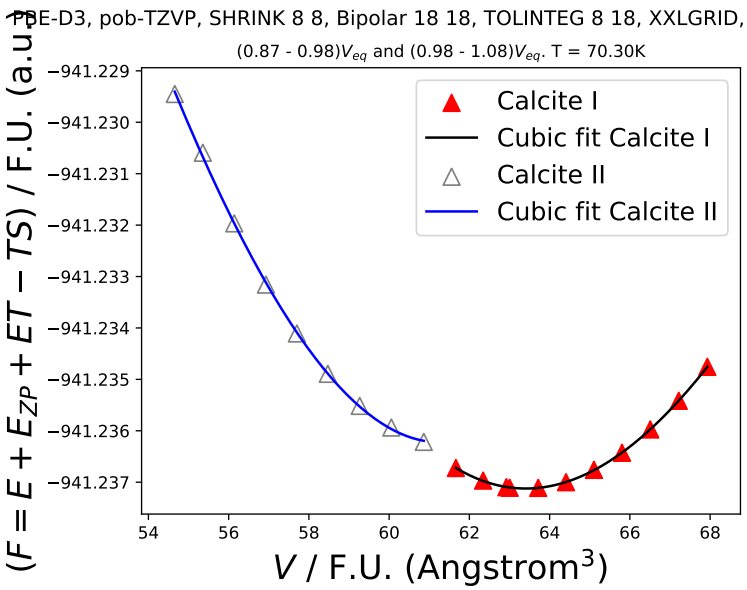

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 50.20K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$(F = E + E_{ZP} + ET - TS)$ / F.U. (a.u.)
V / F.U. (Angstrom^3)

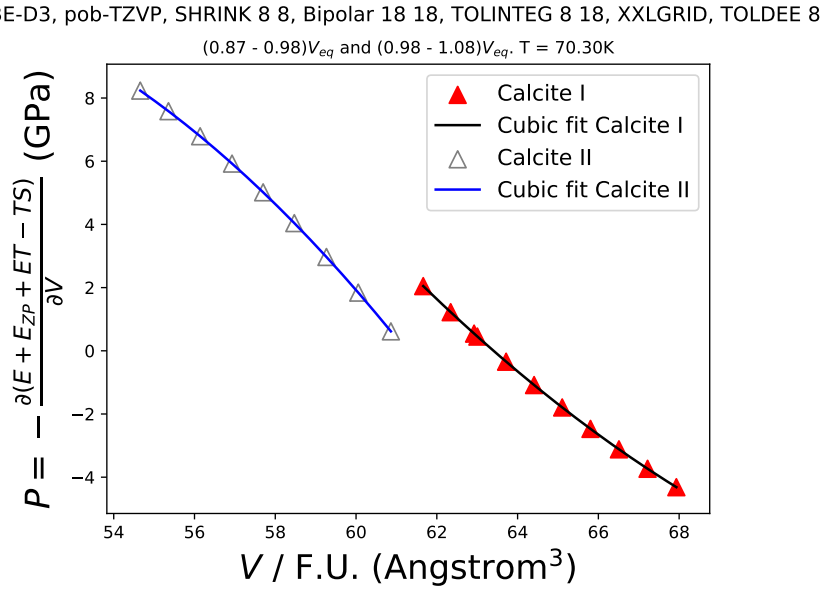

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 50.20K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$P = -\frac{\partial(E + E_{ZP} + ET - TS)}{\partial V}$ (GPa)
V / F.U. (Angstrom^3)

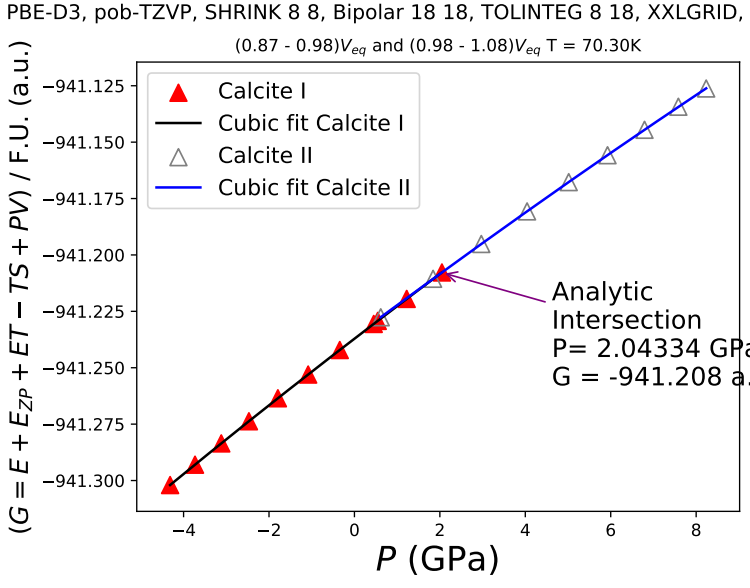

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq} T = 50.20K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
Analytic
Intersection
P= 2.01876 GPa
G = -941.208 a.u.
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P (GPa)

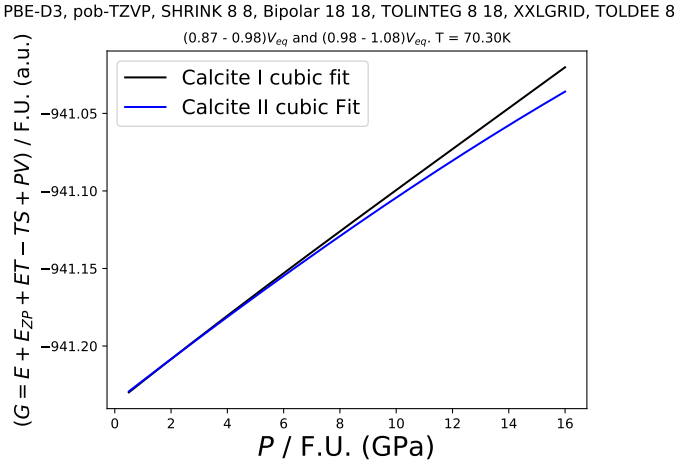

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 50.20K
Calcite I cubic fit
Calcite II cubic Fit
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P / F.U. (GPa)

$T = 70.30K$

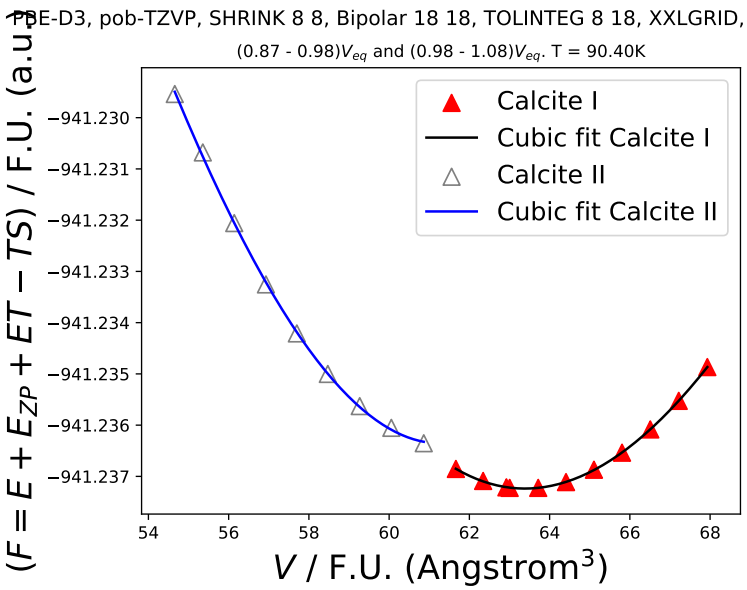

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 70.30K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$(F = E + E_{ZP} + ET - TS)$ / F.U. (a.u.)
V / F.U. (Angstrom^3)

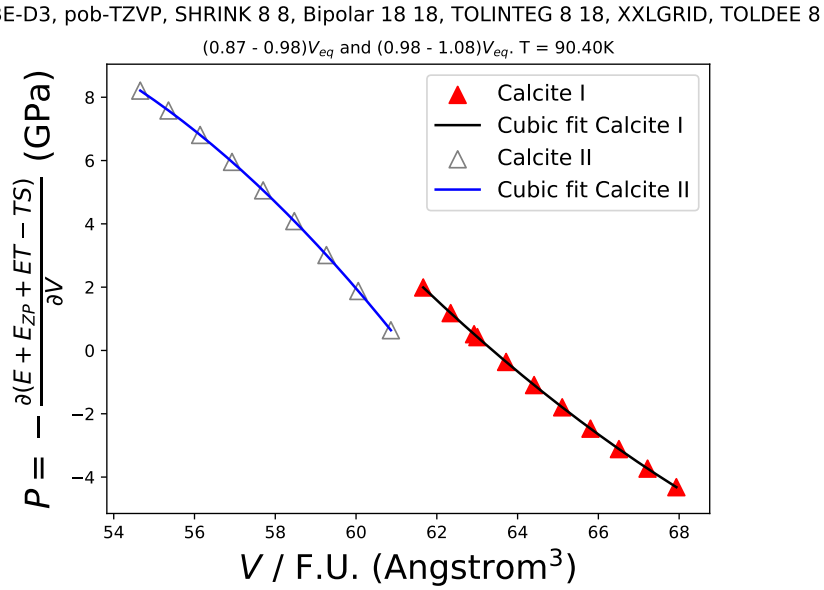

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 70.30K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$P = -\frac{\partial(E + E_{ZP} + ET - TS)}{\partial V}$ (GPa)
V / F.U. (Angstrom^3)


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
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
Analytic
Intersection
P= 2.04334 GPa
G = -941.208 a.u.
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P (GPa)


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
Calcite I cubic fit
Calcite II cubic Fit
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P / F.U. (GPa)

$T = 90.40K$


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 = 90.40K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$(F = E + E_{ZP} + ET - TS)$ / F.U. (a.u.)
V / F.U. (Angstrom^3)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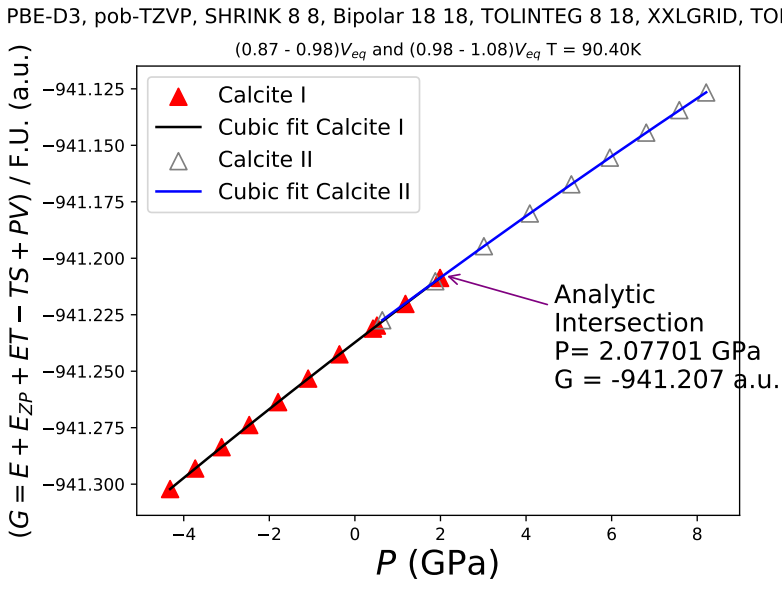
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 90.40K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$P = -\frac{\partial(E + E_{ZP} + ET - TS)}{\partial V}$ (GPa)
V / F.U. (Angstrom^3)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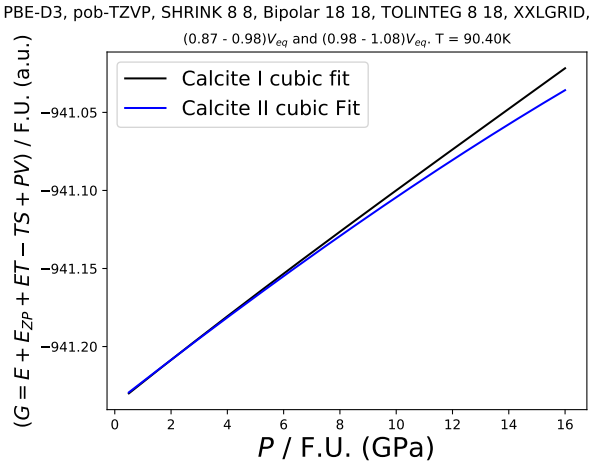
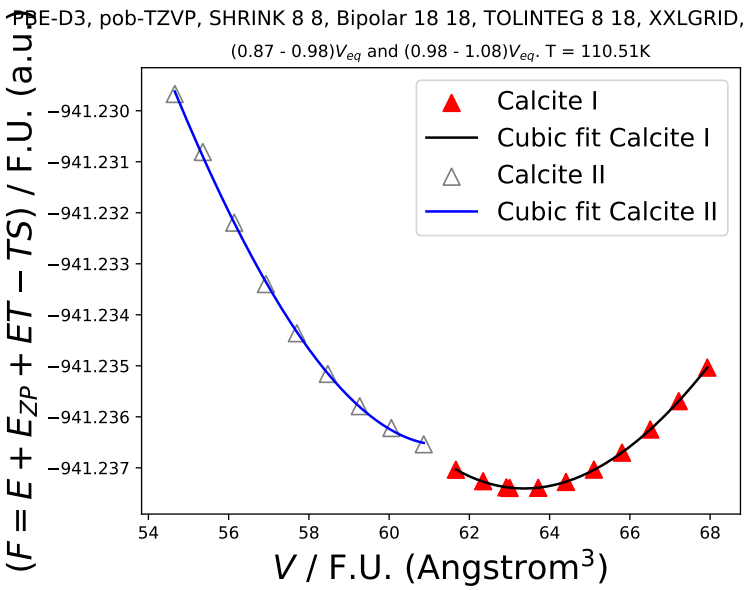
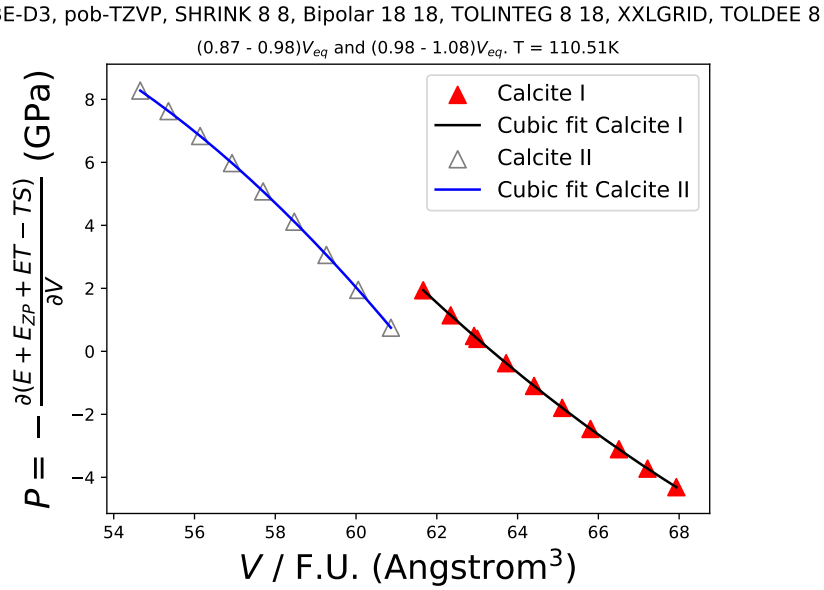
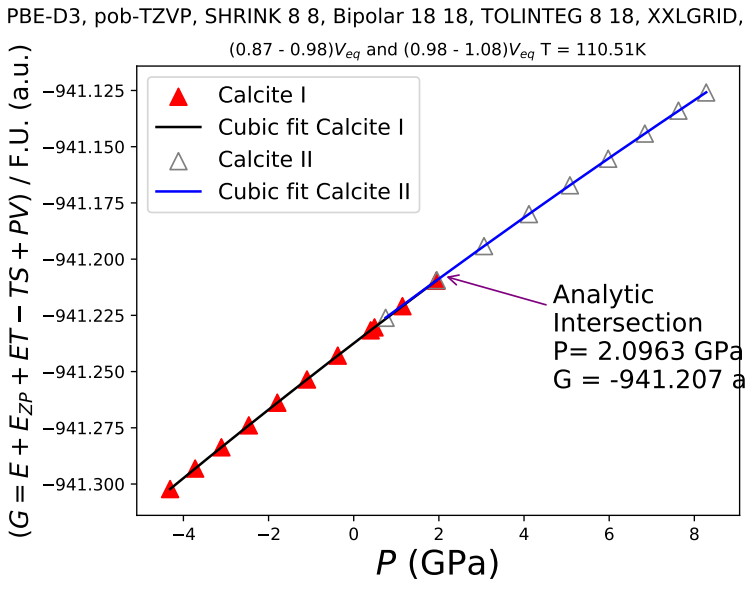
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq} T = 90.40K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
Analytic
Intersection
P= 2.07701 GPa
G = -941.207 a.u.
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P (GPa)

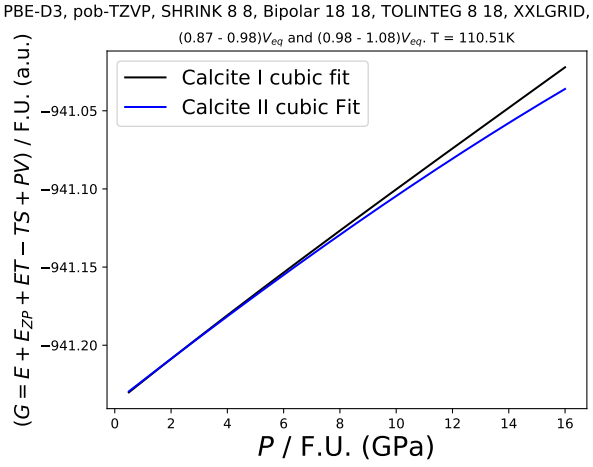

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 90.40K
Calcite I cubic fit
Calcite II cubic Fit
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P / F.U. (GPa)

$T = 110.51K$

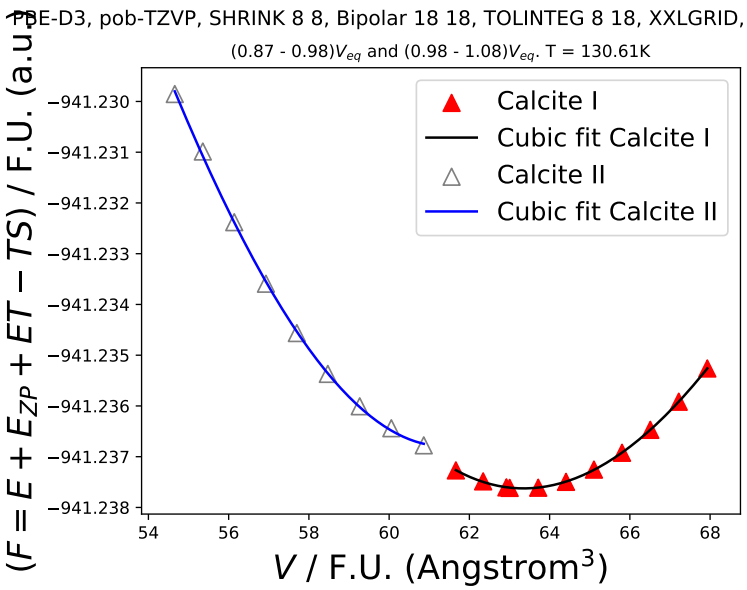

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 110.51K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$(F = E + E_{ZP} + ET - TS)$ / F.U. (a.u.)
V / F.U. (Angstrom^3)

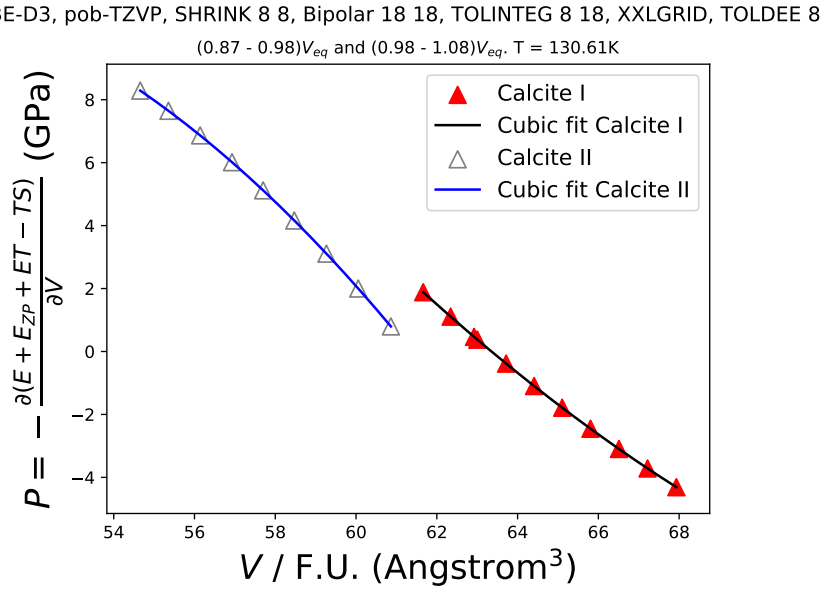

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 110.51K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$P = -\frac{\partial(E + E_{ZP} + ET - TS)}{\partial V}$ (GPa)
V / F.U. (Angstrom^3)

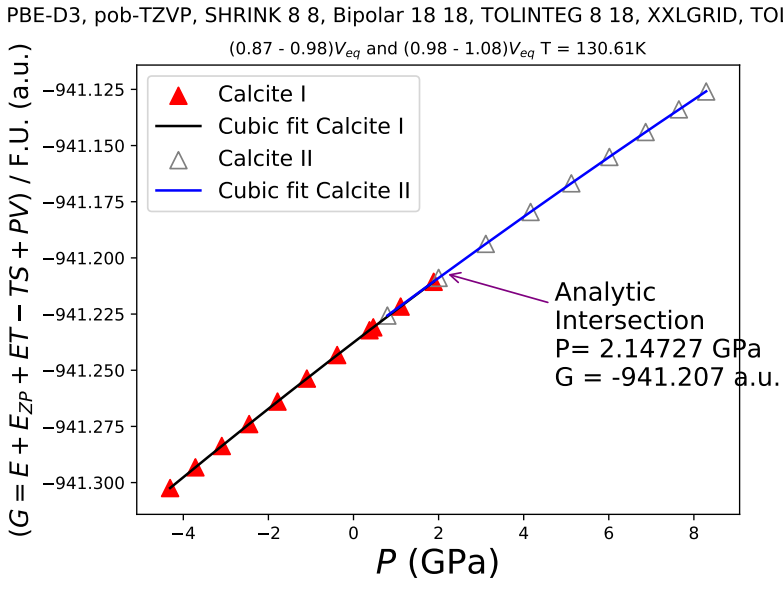

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq} T = 110.51K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
Analytic
Intersection
P= 2.0963 GPa
G = -941.207 a.u.
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P (GPa)

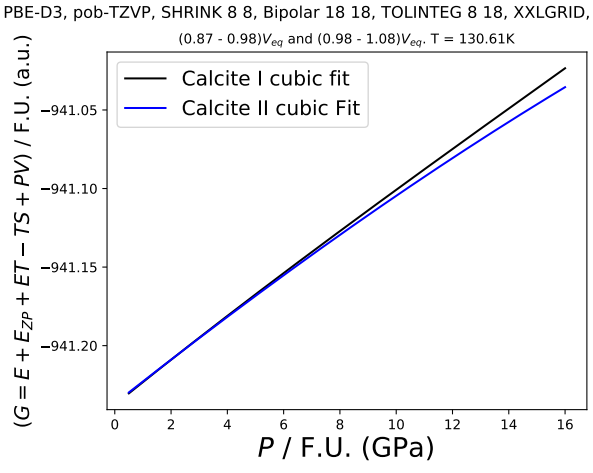

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 110.51K
Calcite I cubic fit
Calcite II cubic Fit
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P / F.U. (GPa)

$T = 130.61K$


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 = 130.61K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$(F = E + E_{ZP} + ET - TS)$ / F.U. (a.u.)
V / F.U. (Angstrom^3)

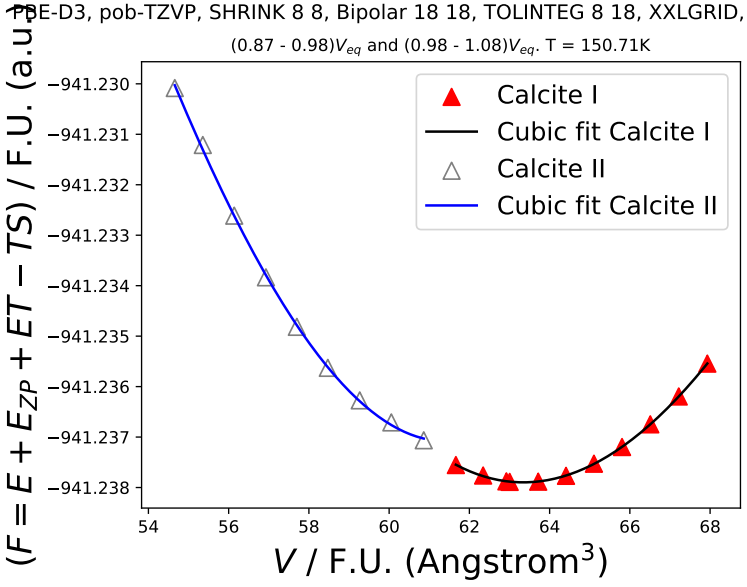

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 130.61K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$P = -\frac{\partial(E + E_{ZP} + ET - TS)}{\partial V}$ (GPa)
V / F.U. (Angstrom^3)


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 = 130.61K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
Analytic
Intersection
P= 2.14727 GPa
G = -941.207 a.u.
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P (GPa)

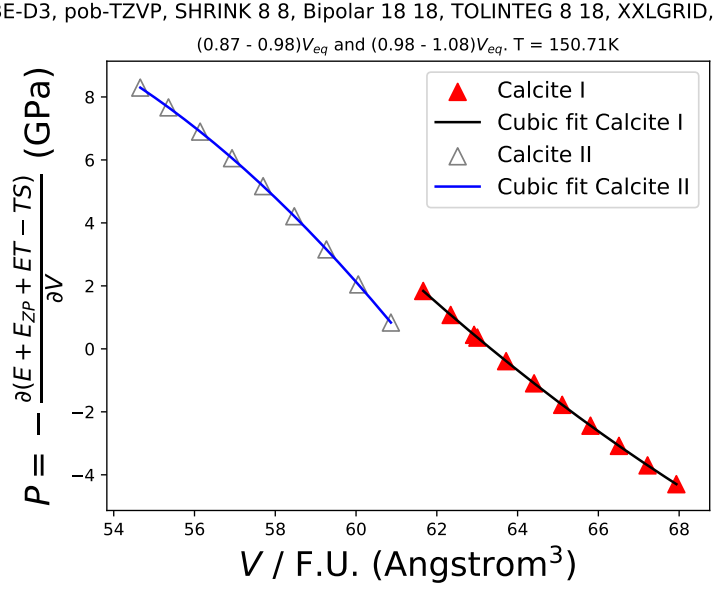

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 130.61K
Calcite I cubic fit
Calcite II cubic Fit
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P / F.U. (GPa)

$T = 150.71K$

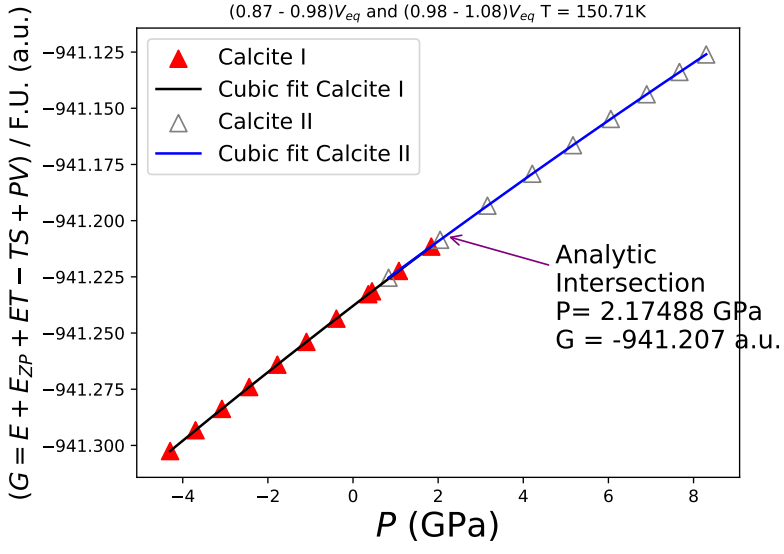
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



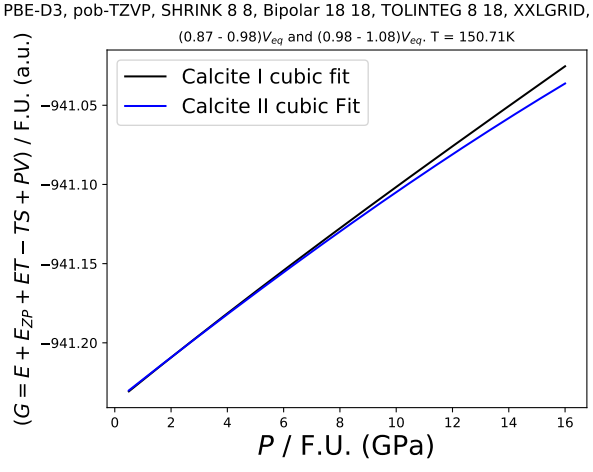
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



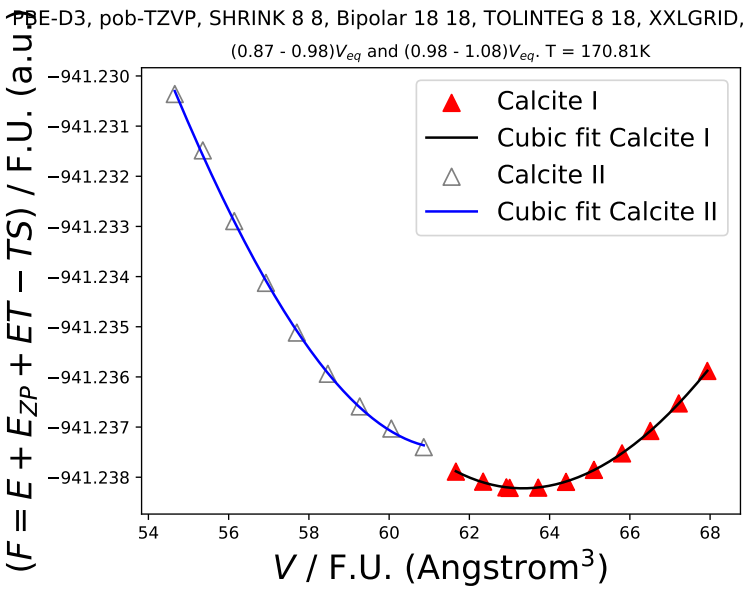
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

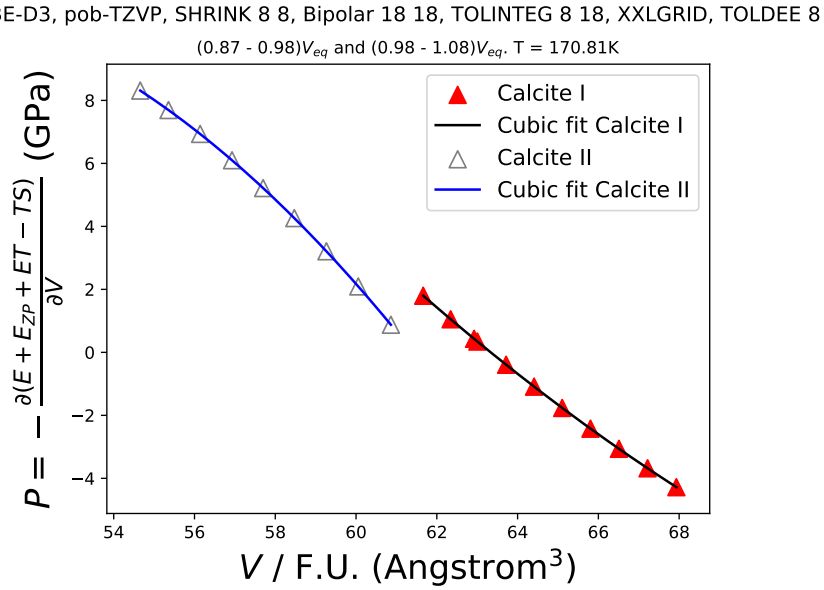


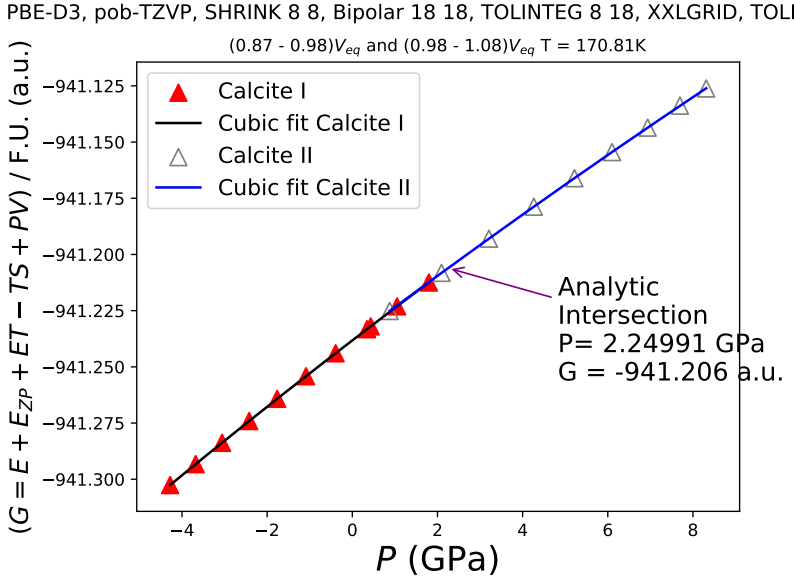
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

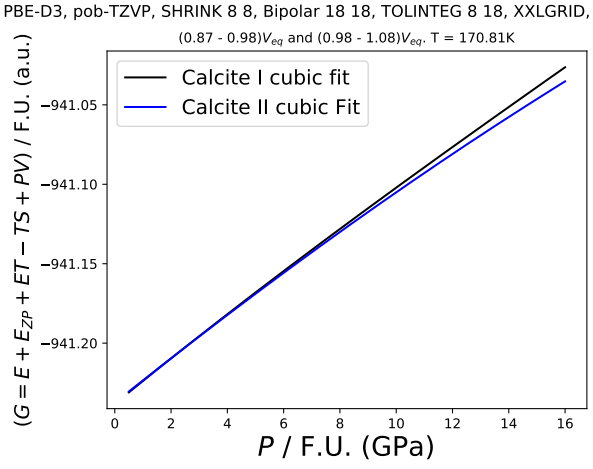


$T = 170.81K$

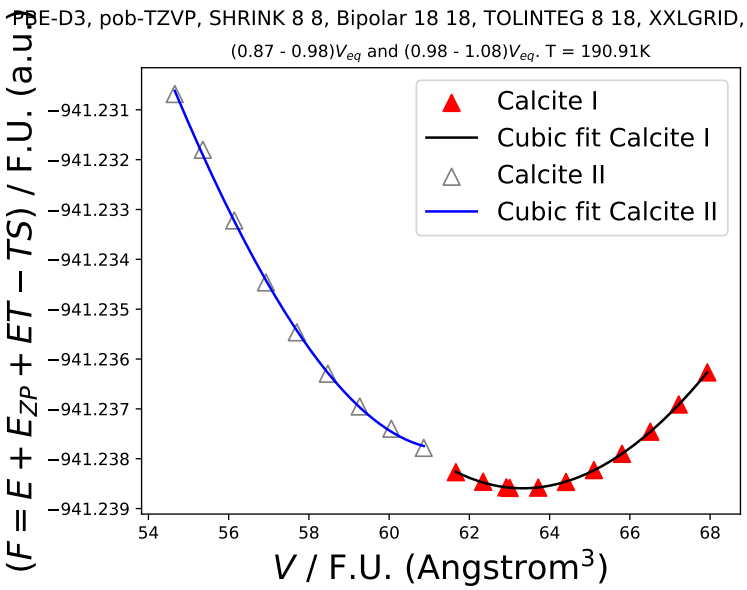

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 170.81K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$(F = E + E_{ZP} + ET - TS)$ / F.U. (a.u.)
V / F.U. (Angstrom^3)

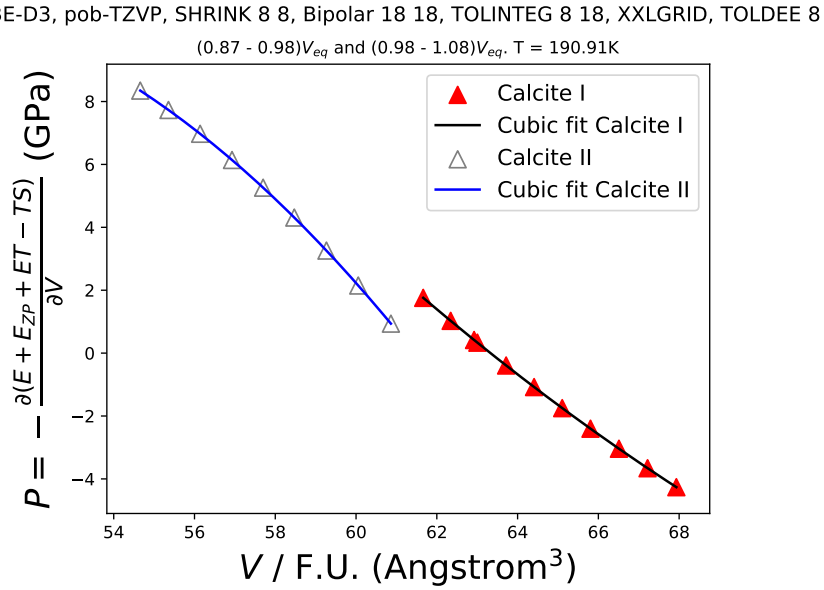

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 170.81K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$P = -\frac{\partial(E + E_{ZP} + ET - TS)}{\partial V}$ (GPa)
V / F.U. (Angstrom^3)

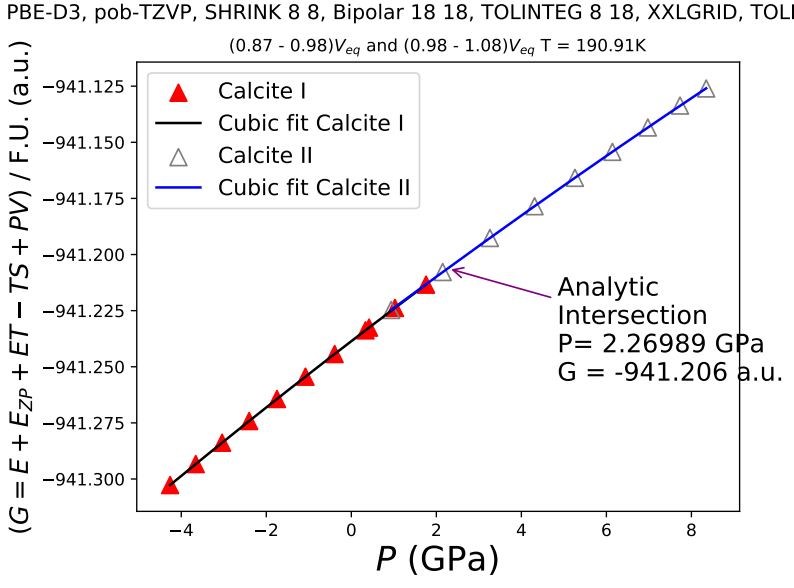

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq} T = 170.81K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
Analytic
Intersection
P= 2.24991 GPa
G = -941.206 a.u.
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P (GPa)

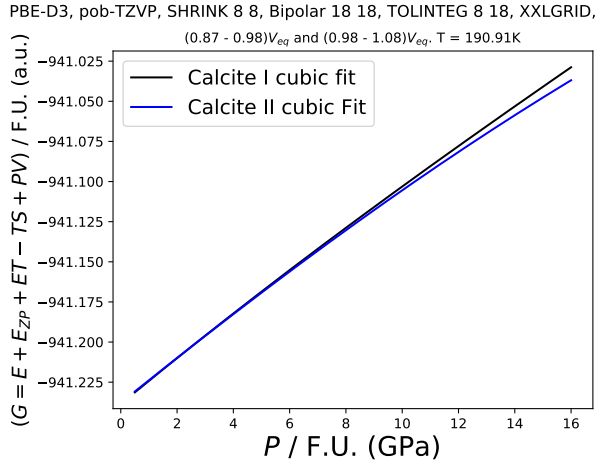

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 170.81K
Calcite I cubic fit
Calcite II cubic Fit
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P / F.U. (GPa)

$T = 190.91K$

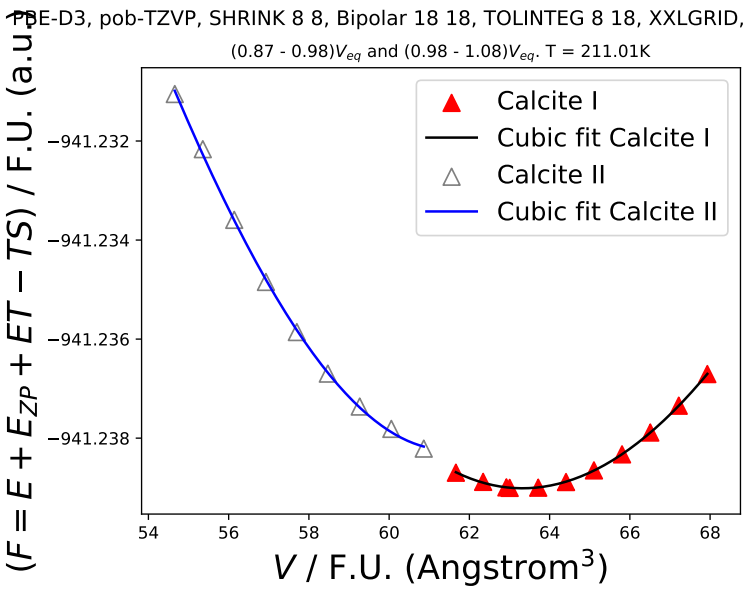

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 190.91K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$(F = E + E_{ZP} + ET - TS)$ / F.U. (a.u.)
V / F.U. (Angstrom^3)

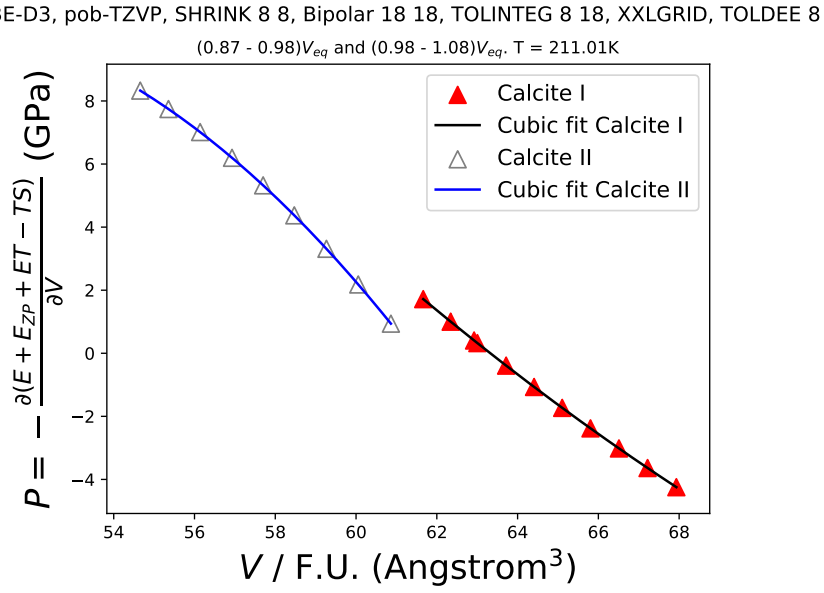

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 190.91K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$P = -\frac{\partial(E + E_{ZP} + ET - TS)}{\partial V}$ (GPa)
V / F.U. (Angstrom^3)

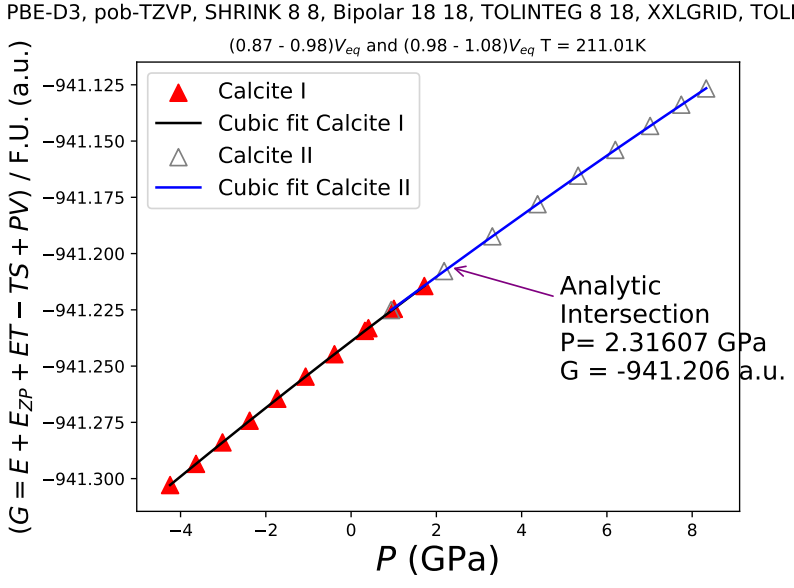

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq} T = 190.91K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
Analytic
Intersection
P= 2.26989 GPa
G = -941.206 a.u.
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P (GPa)

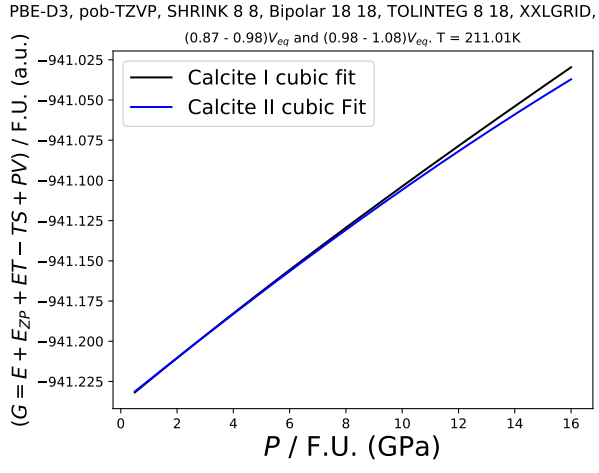

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 190.91K
Calcite I cubic fit
Calcite II cubic Fit
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P / F.U. (GPa)

$T = 211.01K$

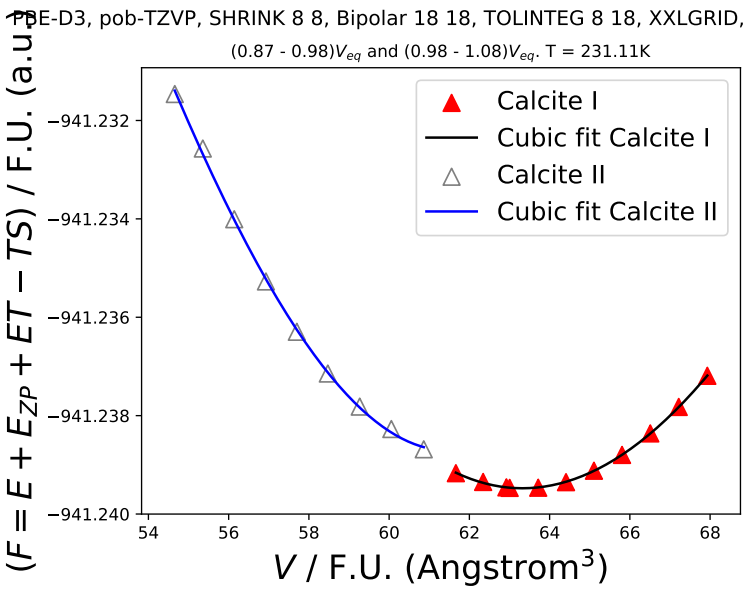

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 211.01K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$(F = E + E_{ZP} + ET - TS)$ / F.U. (a.u.)
V / F.U. (Angstrom^3)

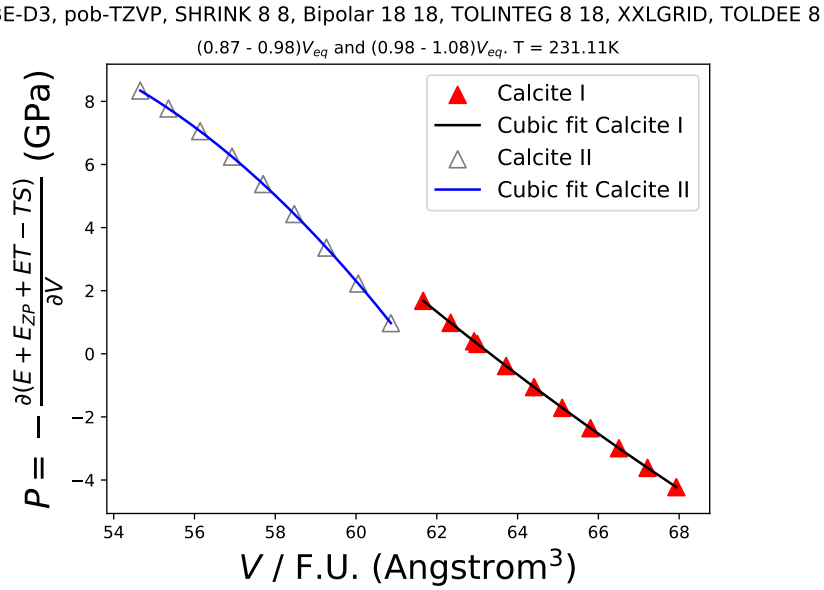

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 211.01K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$P = -\frac{\partial(E + E_{ZP} + ET - TS)}{\partial V}$ (GPa)
V / F.U. (Angstrom^3)

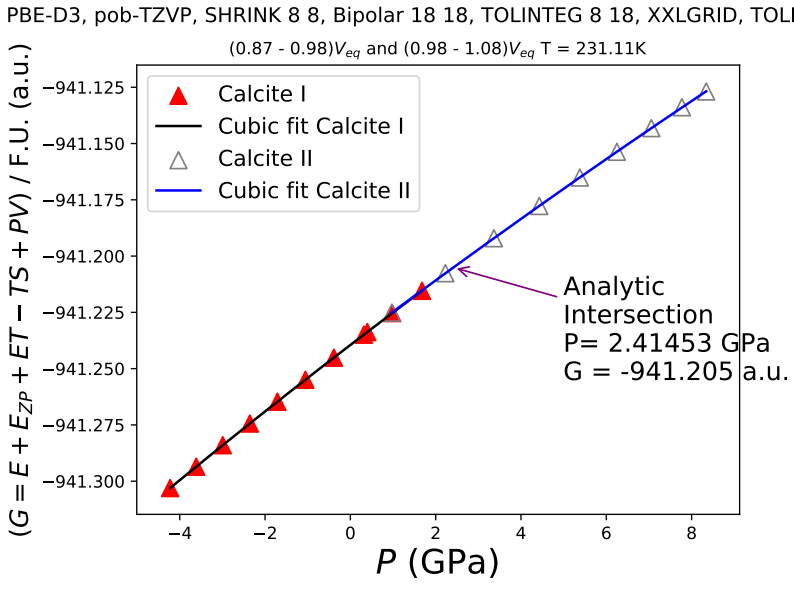

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq} T = 211.01K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
Analytic
Intersection
P= 2.31607 GPa
G = -941.206 a.u.
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P (GPa)

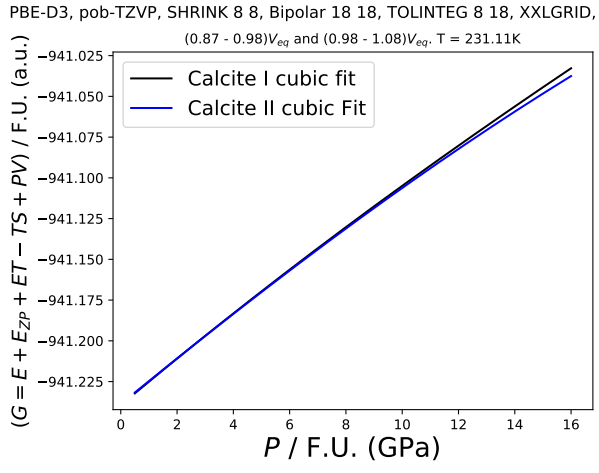

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 211.01K
Calcite I cubic fit
Calcite II cubic Fit
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P / F.U. (GPa)

$T = 231.11K$

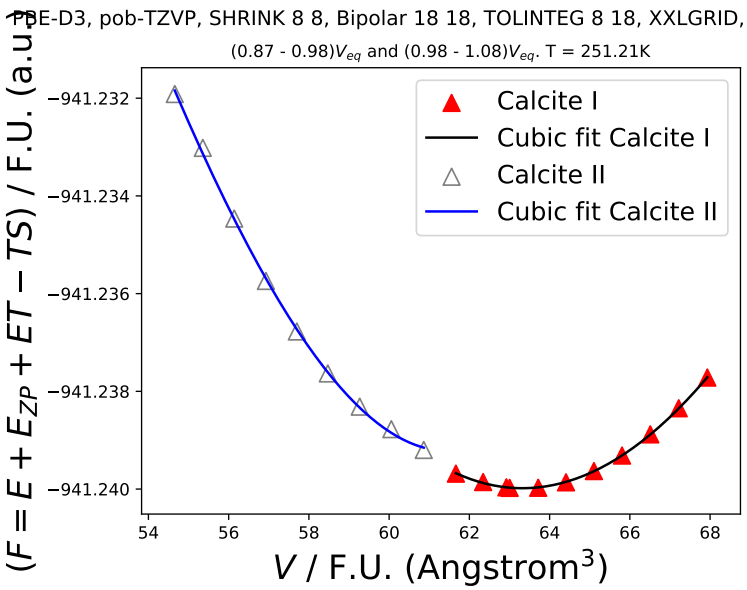

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 231.11K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$(F = E + E_{ZP} + ET - TS)$ / F.U. (a.u.)
V / F.U. (Angstrom^3)

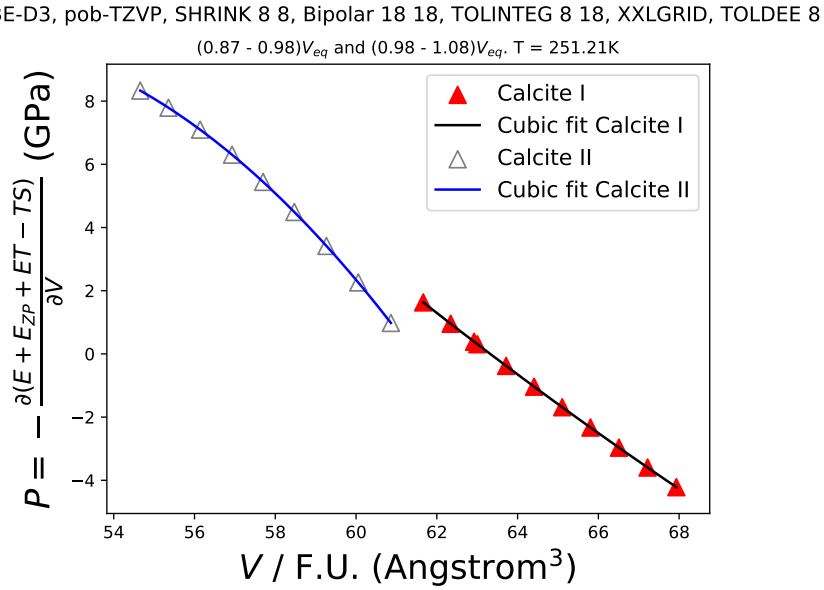

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 231.11K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$P = -\frac{\partial(E + E_{ZP} + ET - TS)}{\partial V}$ (GPa)
V / F.U. (Angstrom^3)

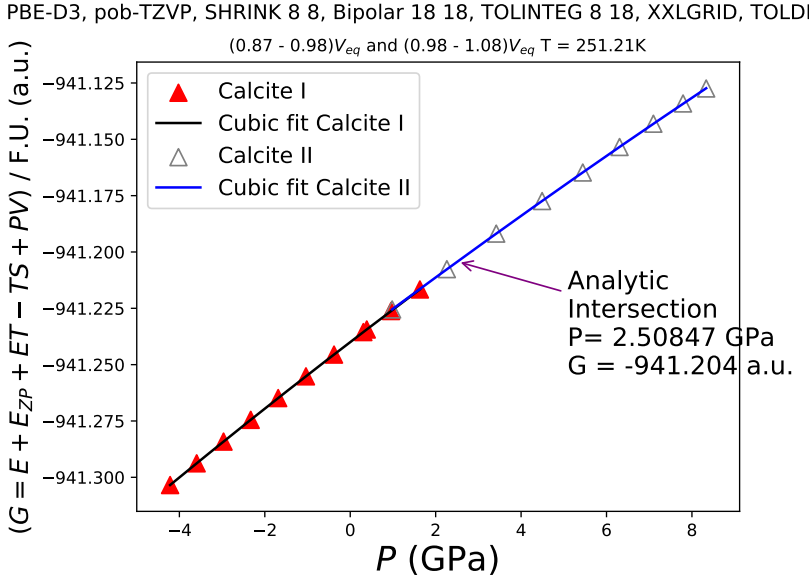

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq} T = 231.11K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
Analytic
Intersection
P= 2.41453 GPa
G = -941.205 a.u.
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P (GPa)

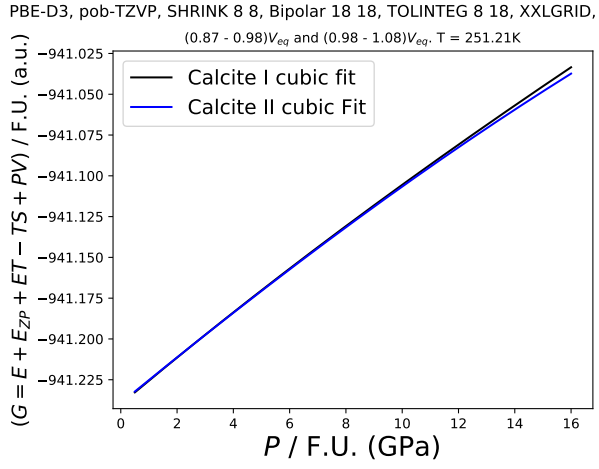

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 231.11K
Calcite I cubic fit
Calcite II cubic Fit
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P / F.U. (GPa)

$T = 251.21K$

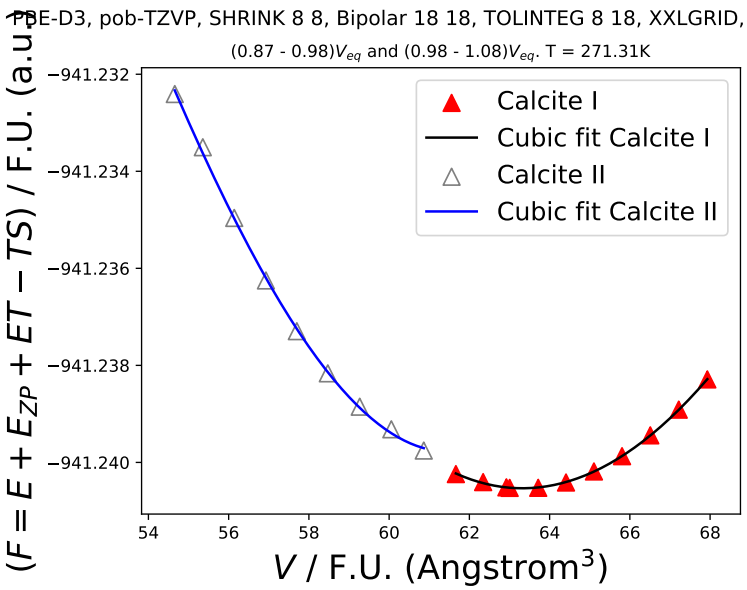

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 251.21K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$(F = E + E_{ZP} + ET - TS)$ / F.U. (a.u.)
V / F.U. (Angstrom^3)

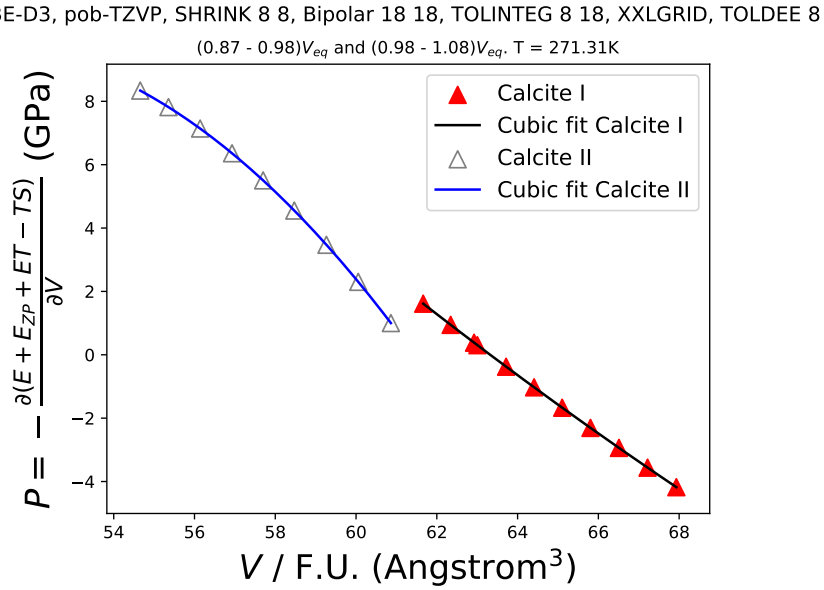

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 251.21K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$P = -\frac{\partial(E + E_{ZP} + ET - TS)}{\partial V}$ (GPa)
V / F.U. (Angstrom^3)

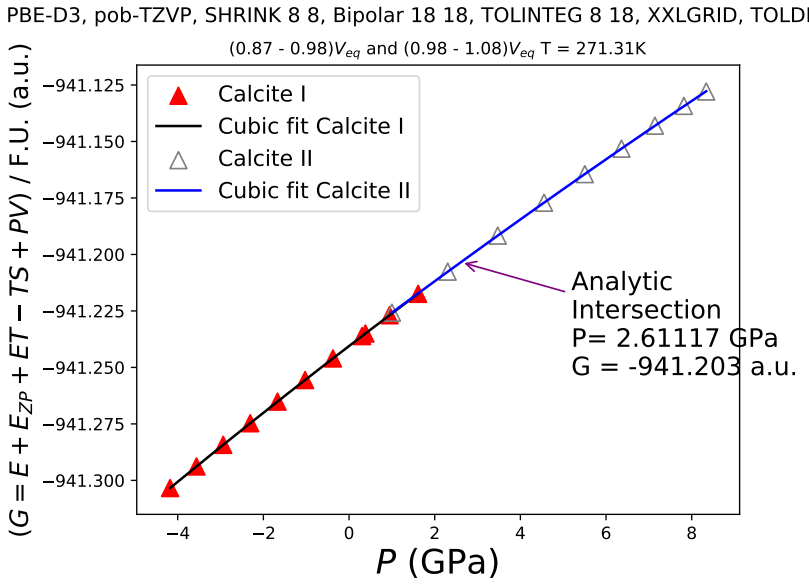

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq} T = 251.21K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
Analytic
Intersection
P= 2.50847 GPa
G = -941.204 a.u.
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P (GPa)

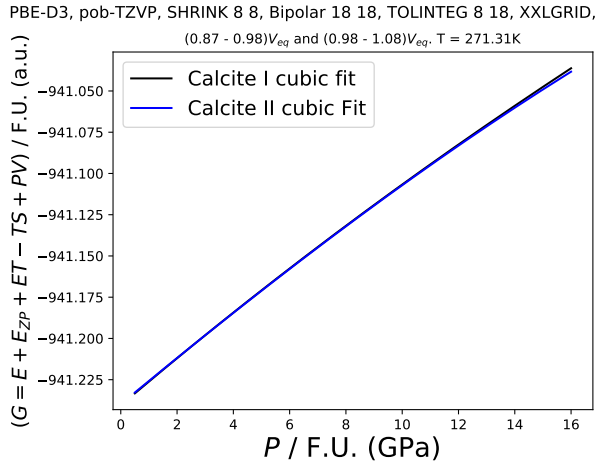

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 251.21K
Calcite I cubic fit
Calcite II cubic Fit
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P / F.U. (GPa)

$T = 271.31K$

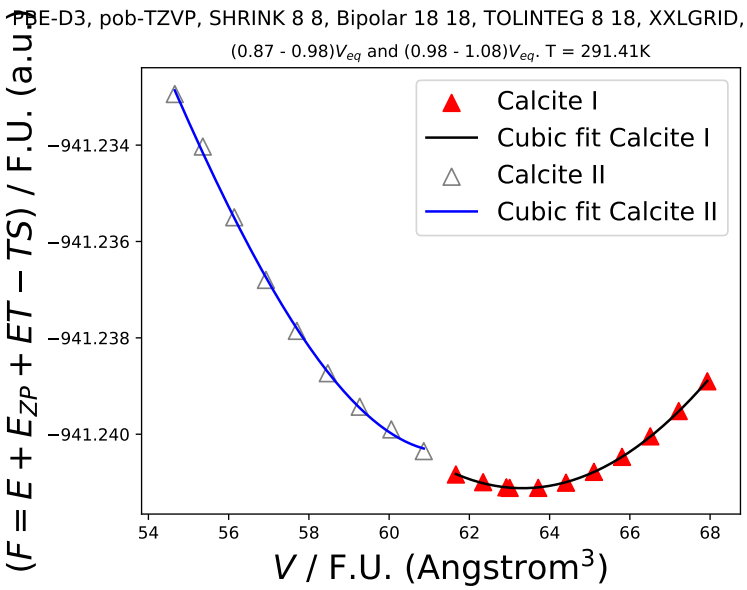

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 271.31K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$(F = E + E_{ZP} + ET - TS)$ / F.U. (a.u.)
V / F.U. (Angstrom^3)

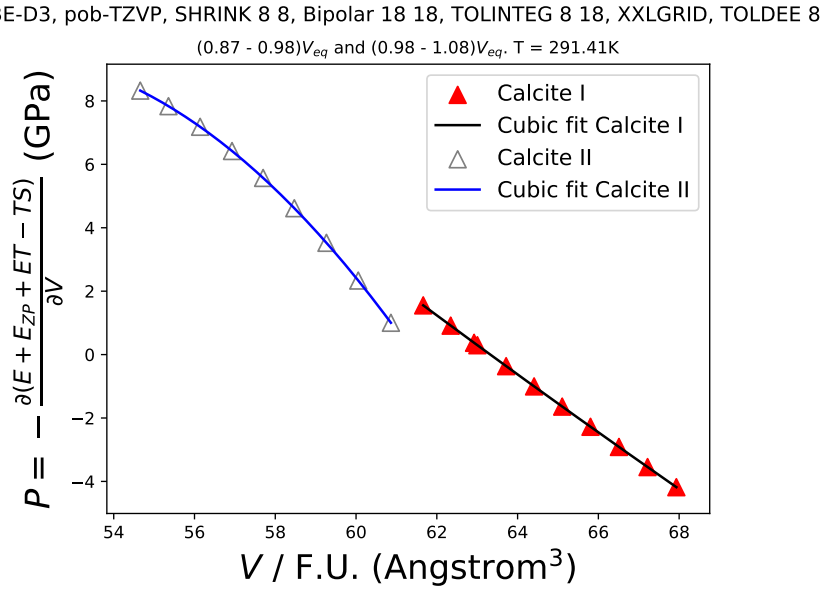

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 271.31K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$P = -\frac{\partial(E + E_{ZP} + ET - TS)}{\partial V}$ (GPa)
V / F.U. (Angstrom^3)

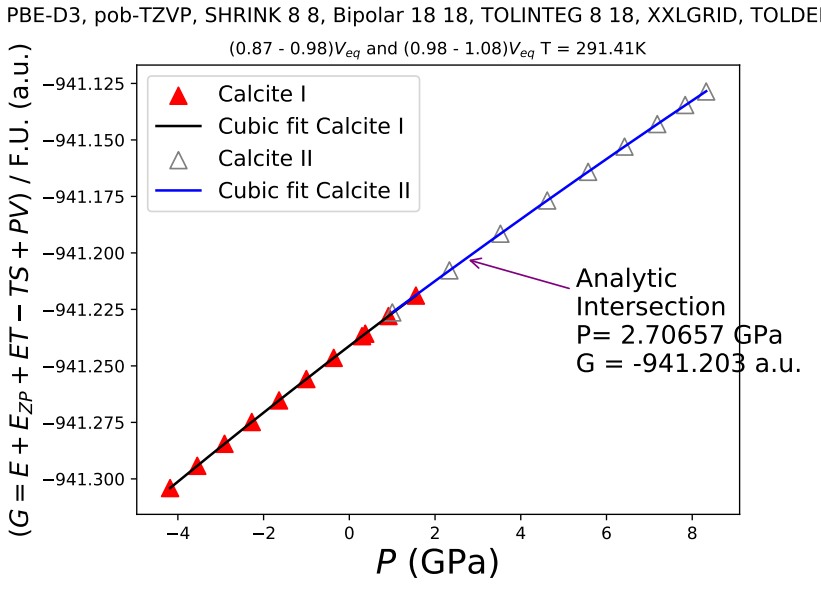

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq} T = 271.31K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
Analytic
Intersection
P= 2.61117 GPa
G = -941.203 a.u.
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P (GPa)

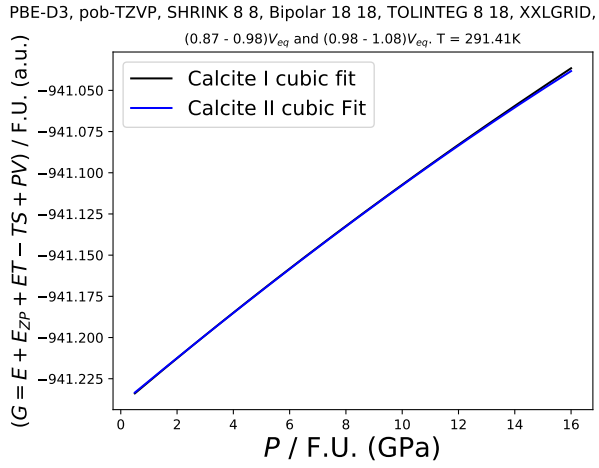

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 271.31K
Calcite I cubic fit
Calcite II cubic Fit
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P / F.U. (GPa)

$T = 291.41K$

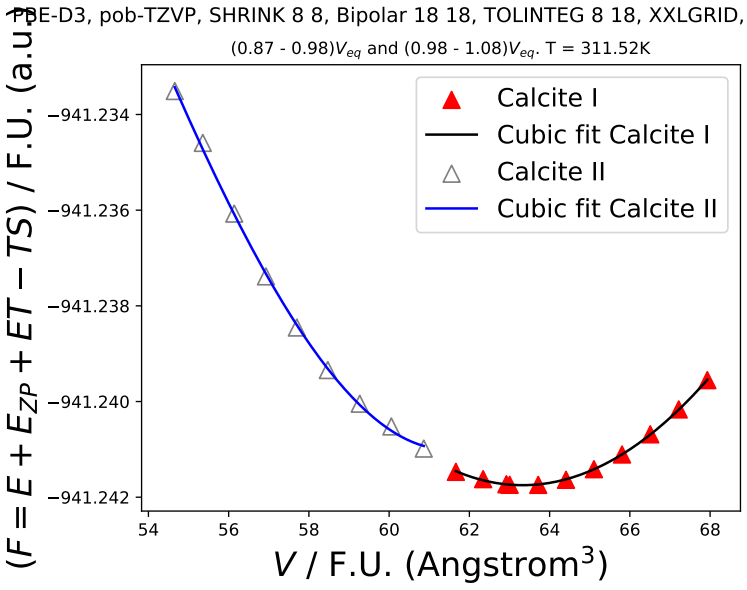

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 291.41K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$(F = E + E_{ZP} + ET - TS)$ / F.U. (a.u.)
V / F.U. (Angstrom^3)

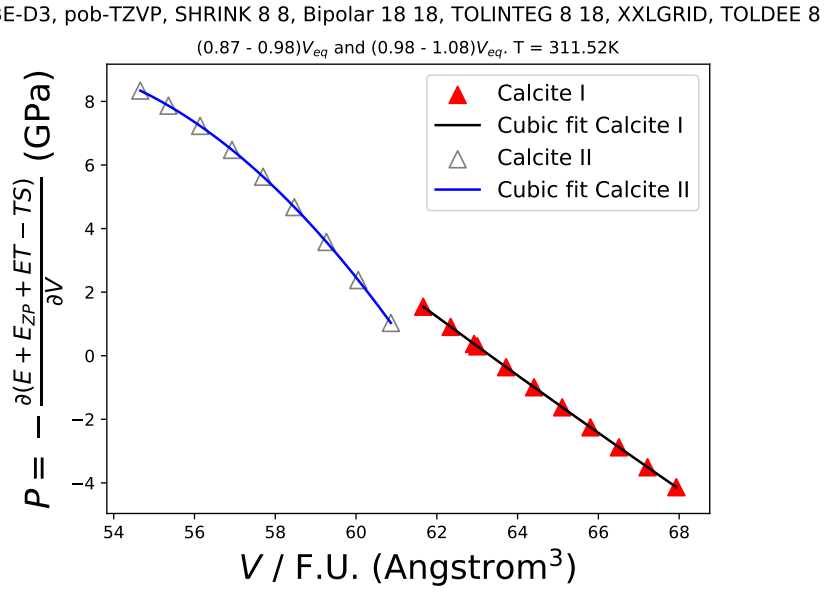

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 291.41K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$P = -\frac{\partial(E + E_{ZP} + ET - TS)}{\partial V}$ (GPa)
V / F.U. (Angstrom^3)

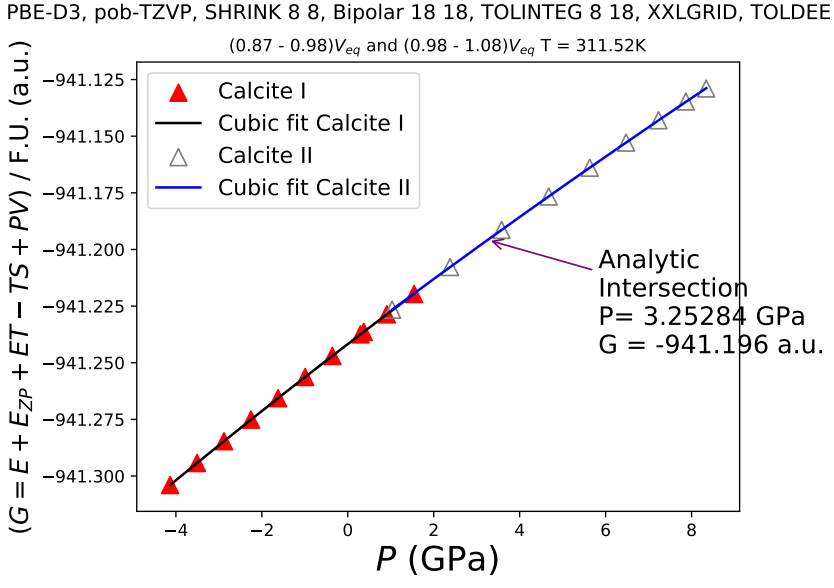

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq} T = 291.41K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
Analytic
Intersection
P= 2.70657 GPa
G = -941.203 a.u.
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P (GPa)

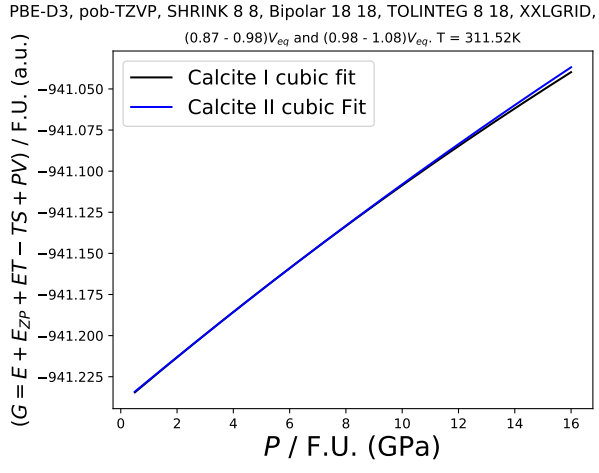

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 291.41K
Calcite I cubic fit
Calcite II cubic Fit
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P / F.U. (GPa)

$T = 311.52K$

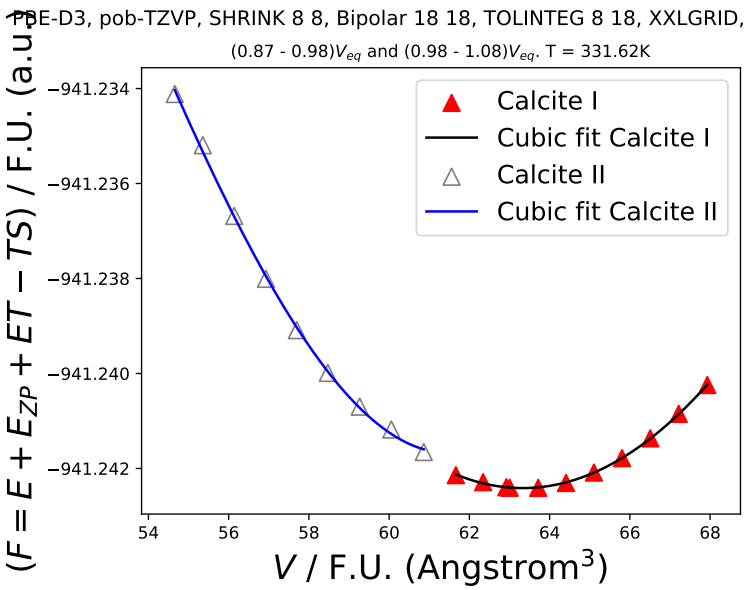

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 311.52K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$(F = E + E_{ZP} + ET - TS)$ / F.U. (a.u.)
V / F.U. (Angstrom^3)

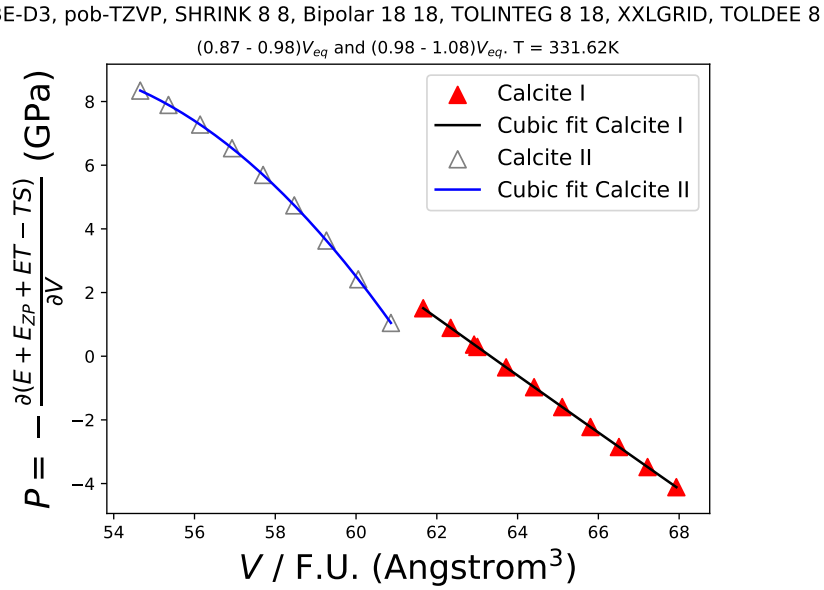

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 311.52K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$P = -\frac{\partial(E + E_{ZP} + ET - TS)}{\partial V}$ (GPa)
V / F.U. (Angstrom^3)

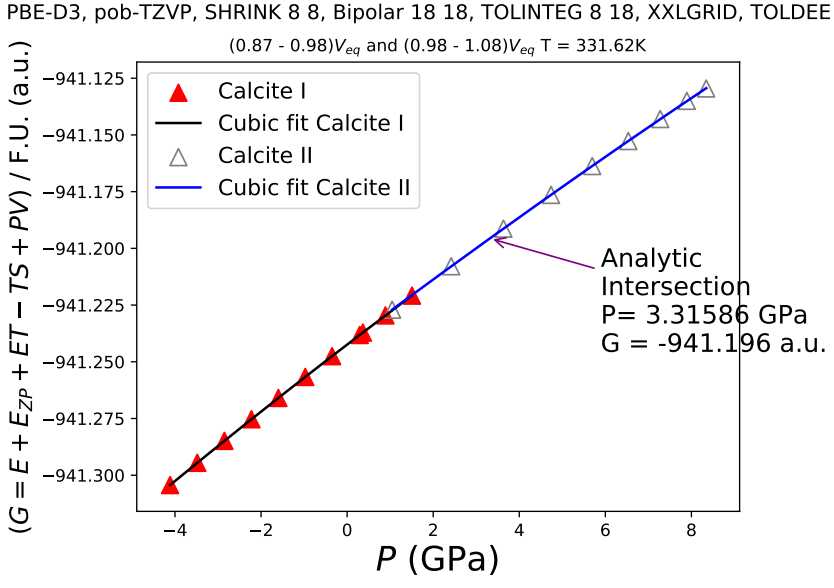

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq} T = 311.52K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
Analytic
Intersection
P= 3.25284 GPa
G = -941.196 a.u.
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P (GPa)

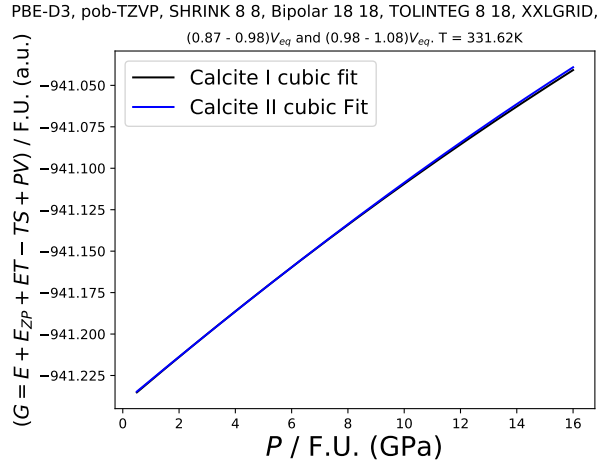

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 311.52K
Calcite I cubic fit
Calcite II cubic Fit
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P / F.U. (GPa)

$T = 331.62K$


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 = 331.62K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$(F = E + E_{ZP} + ET - TS)$ / F.U. (a.u.)
V / F.U. (Angstrom^3)

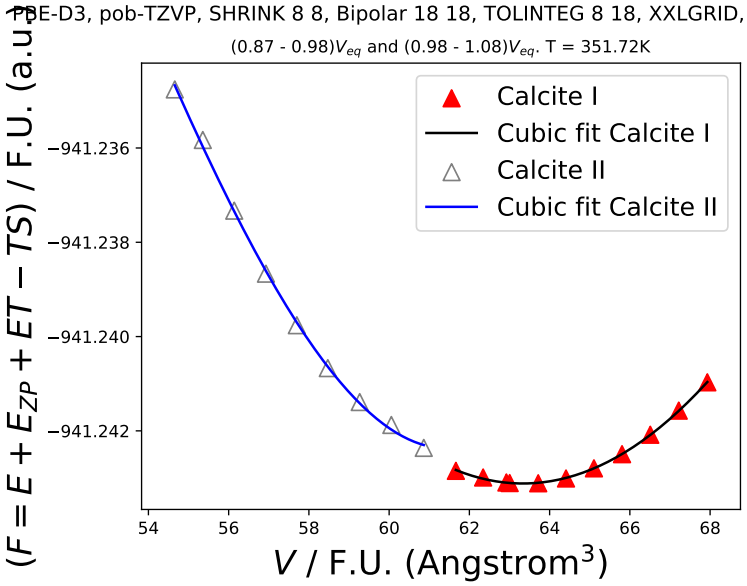

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 331.62K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
$P = -\frac{\partial(E + E_{ZP} + ET - TS)}{\partial V}$ (GPa)
V / F.U. (Angstrom^3)


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 = 331.62K
Calcite I
Cubic fit Calcite I
Calcite II
Cubic fit Calcite II
Analytic
Intersection
P= 3.31586 GPa
G = -941.196 a.u.
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P (GPa)

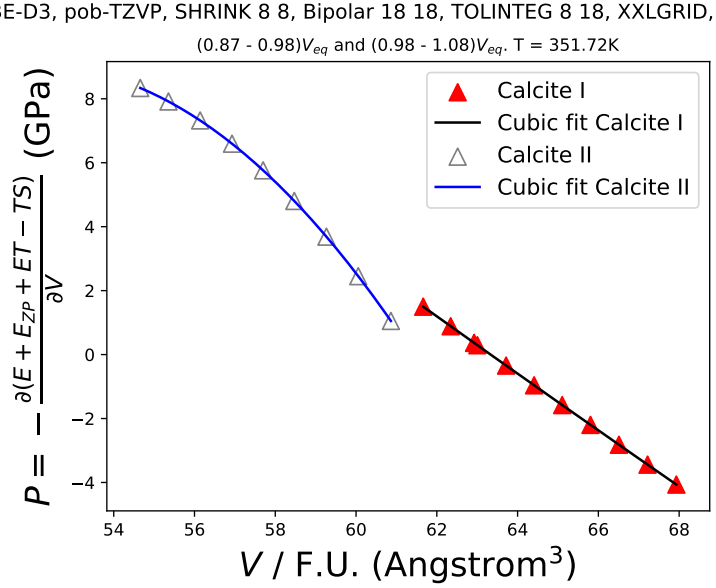

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98)V_{eq} and (0.98 - 1.08)V_{eq}. T = 331.62K
Calcite I cubic fit
Calcite II cubic Fit
$(G = E + E_{ZP} + ET - TS + PV)$ / F.U. (a.u.)
P / F.U. (GPa)

$T = 351.72K$

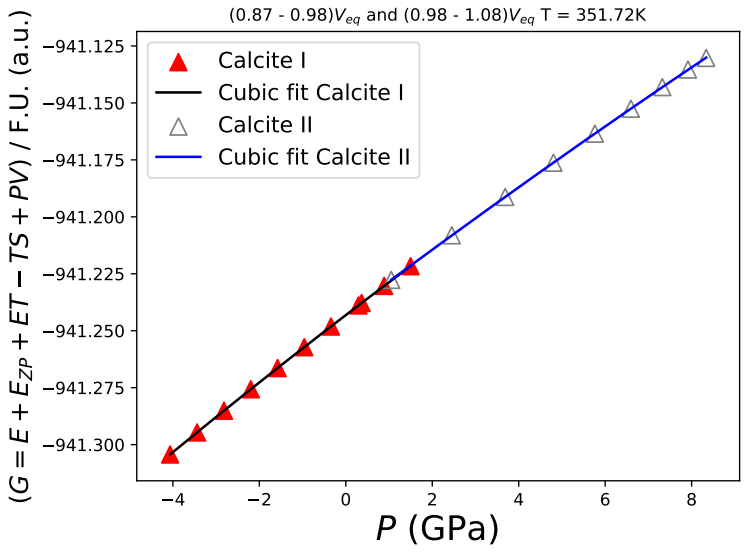
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



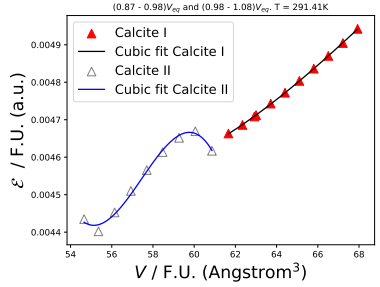
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



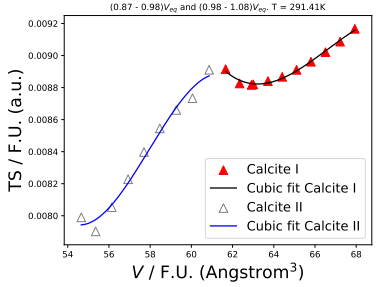
Outline I

T = 291.41K:

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

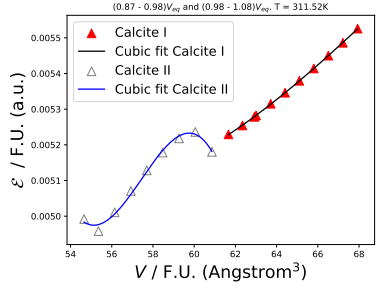


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

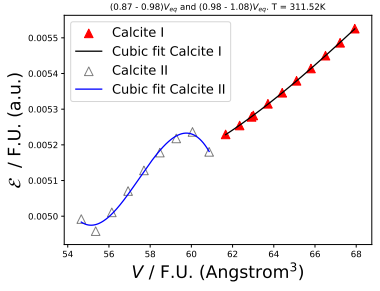


T = 311.52K:

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

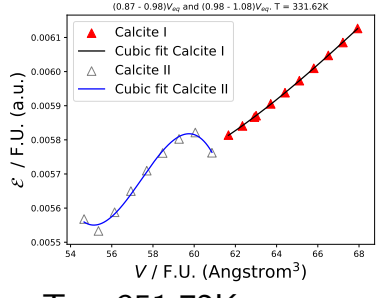


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

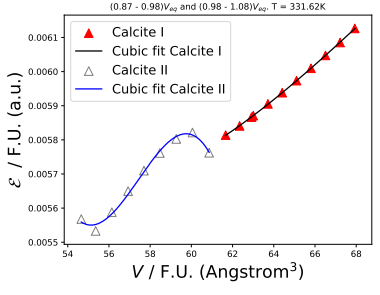


T = 331.62K:

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

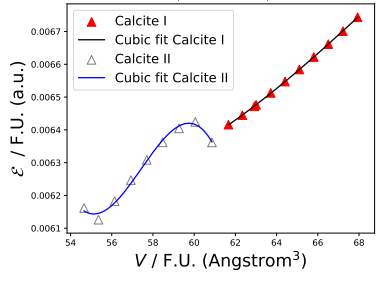


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

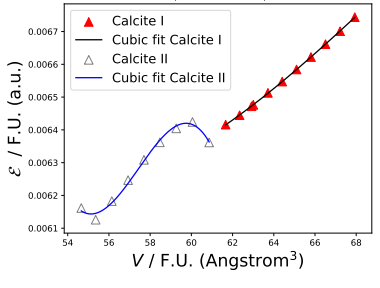


T = 351.72K:

PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



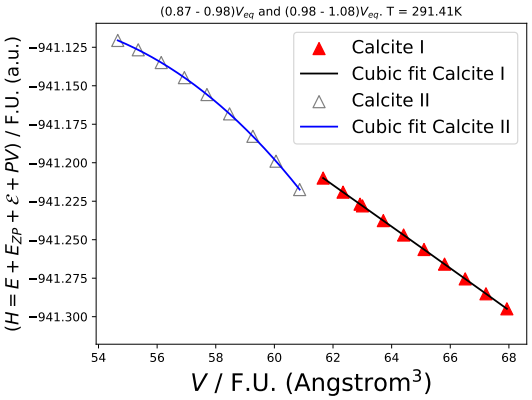
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



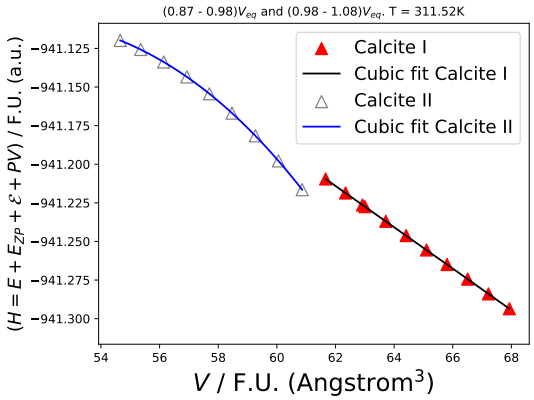
Outline I

When $H(P;T) = E + E_{ZP} + \mathcal{E}(T) + PV$:

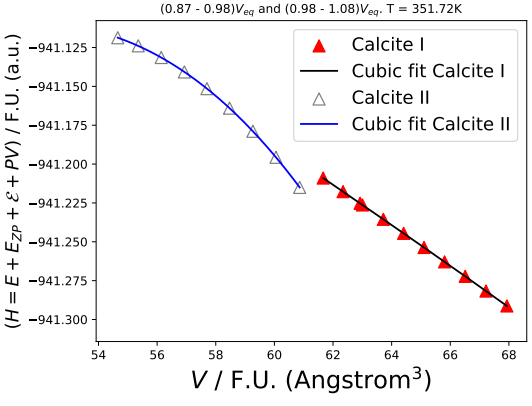
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



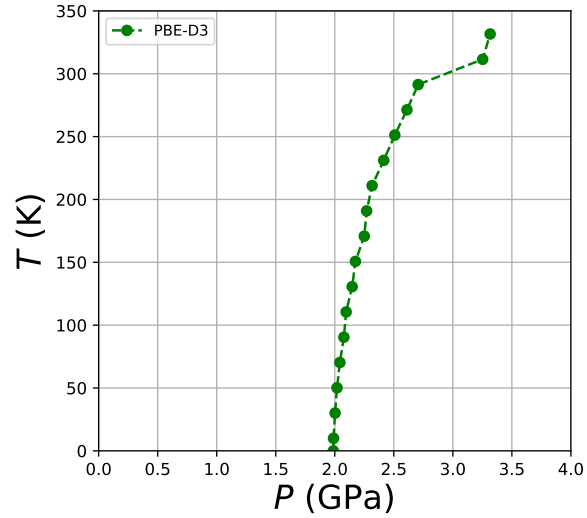


Figure 1: Pressure-temperature phase boundary