

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 $H(P; T)$

Phase Boundary

Outline I

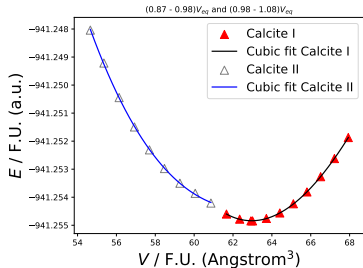
$F(V)$, $G(P)$ and pressure of intersection. Thermal evolution

Shapes of G , F , \mathcal{E}

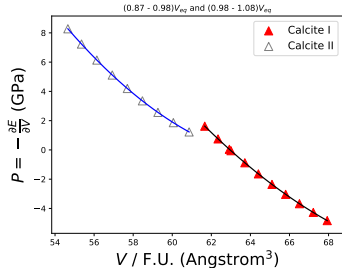
Shape of $H(P; T)$

Phase Boundary

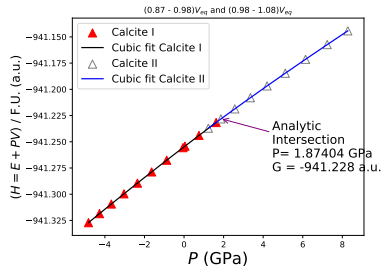
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



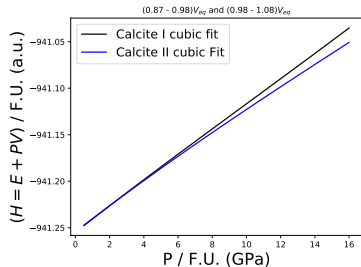
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



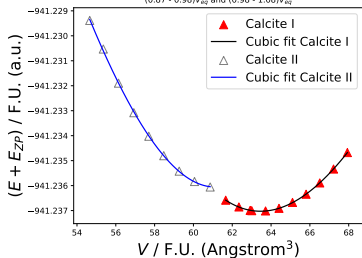
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



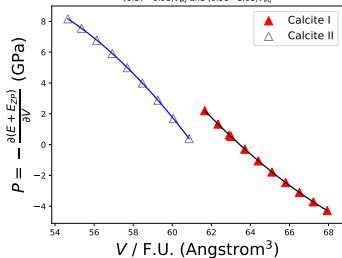
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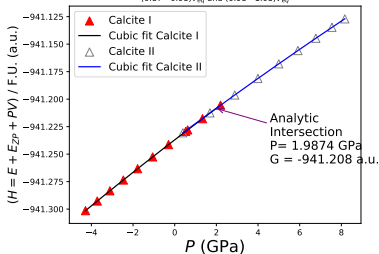
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98) V_{eq} and (0.98 - 1.08) V_{eq}



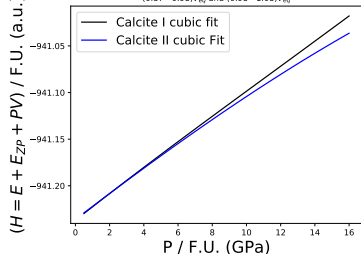
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
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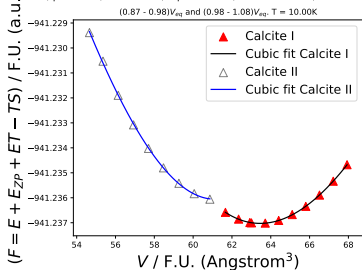


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98) V_{eq} and (0.98 - 1.08) V_{eq}

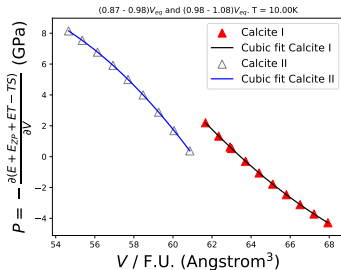


$T = 10.00K$

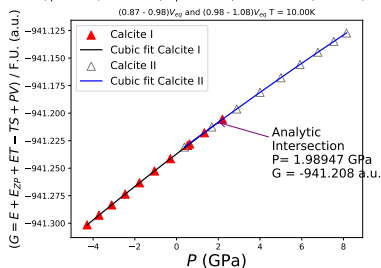
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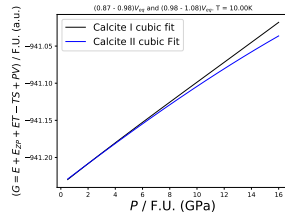
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



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

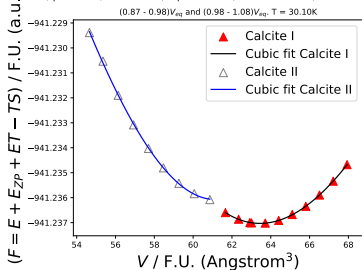


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

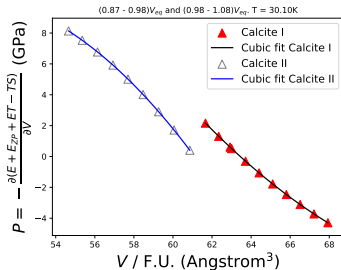


$$T = 30.10K$$

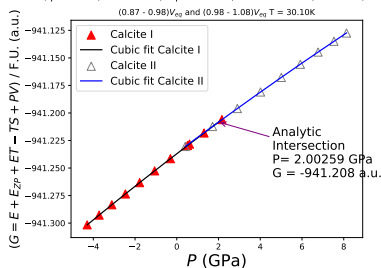
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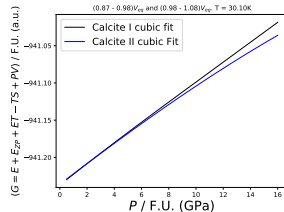
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PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

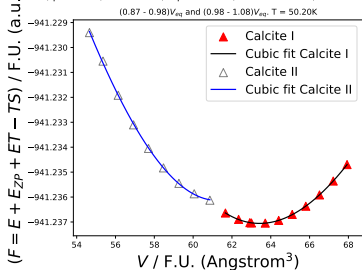


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

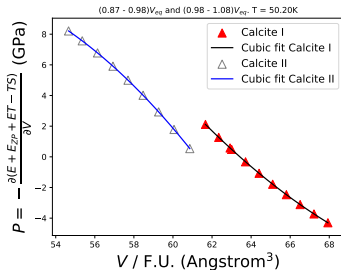


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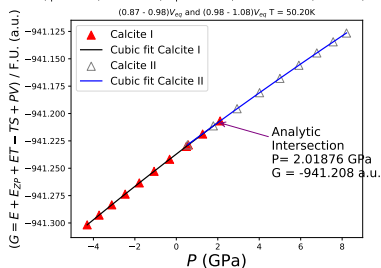
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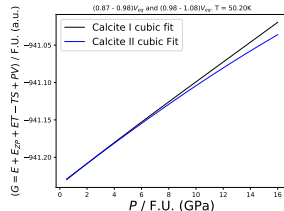
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PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

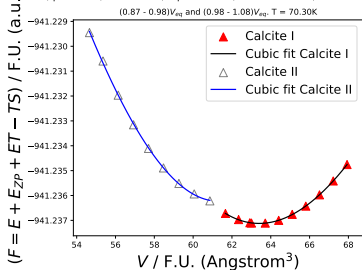


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

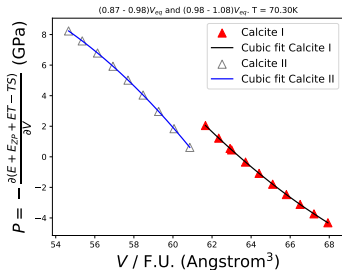


$$T = 70.30K$$

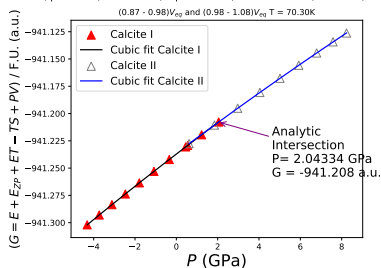
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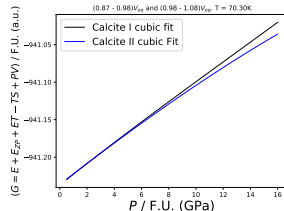
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PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

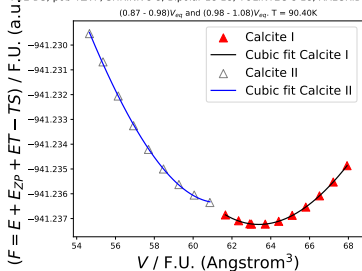


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

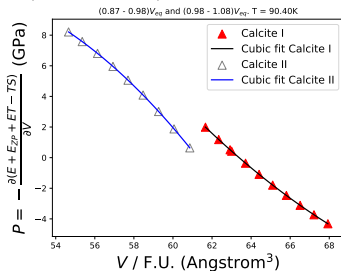


$$T = 90.40K$$

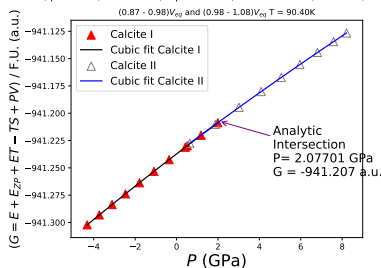
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



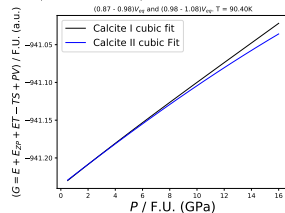
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PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

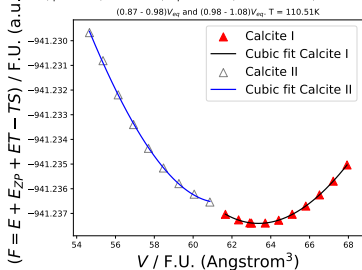


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

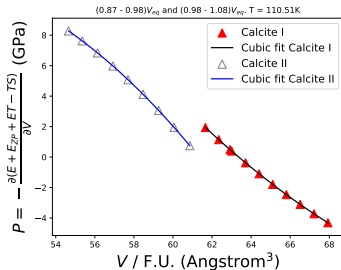


$T = 110.51K$

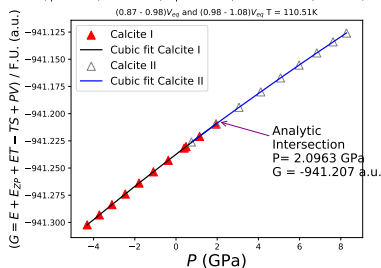
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



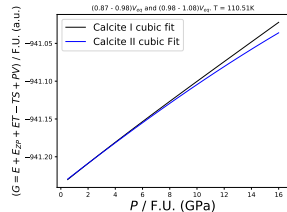
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PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

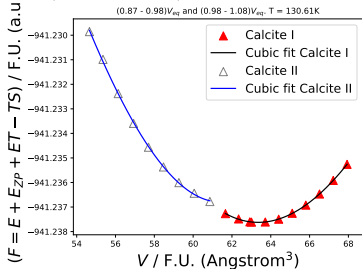


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

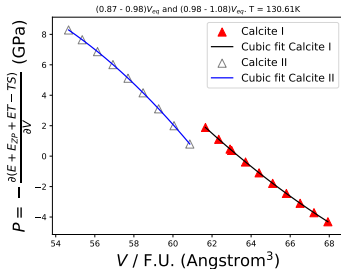


$T = 130.61\text{K}$

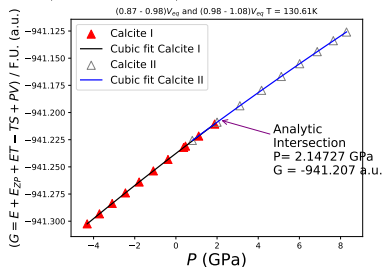
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



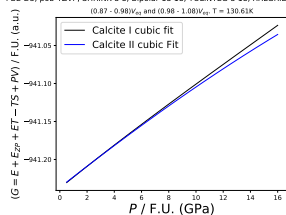
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PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

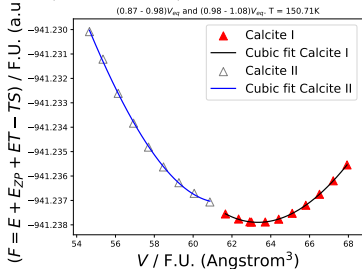


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

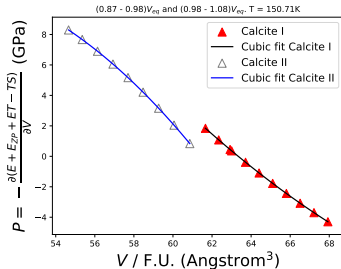


$$T = 150.71K$$

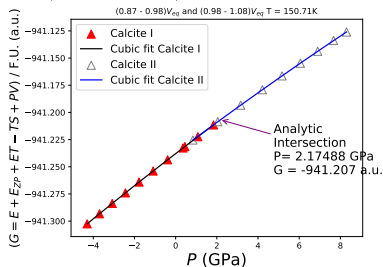
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



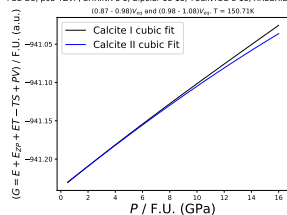
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PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

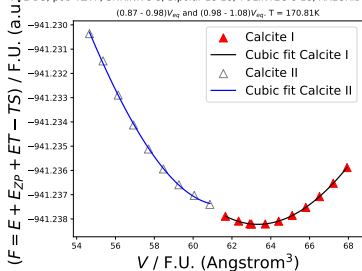


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

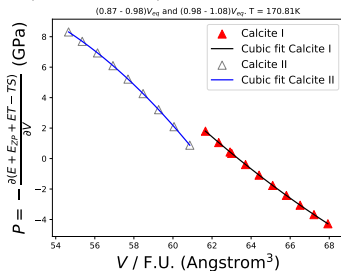


$$T = 170.81K$$

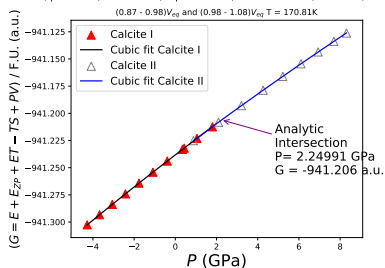
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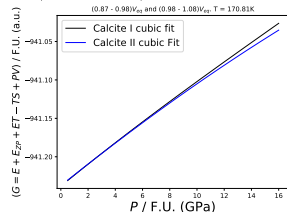
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PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

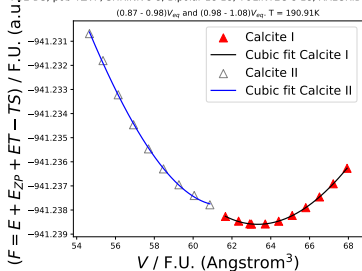


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

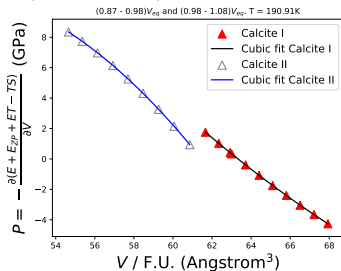


$$T = 190.91\text{K}$$

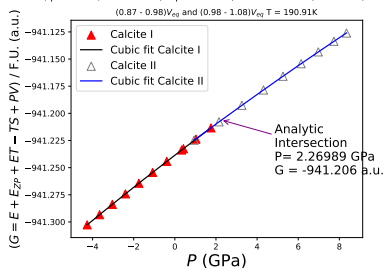
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



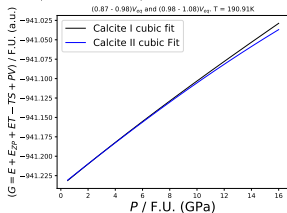
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PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

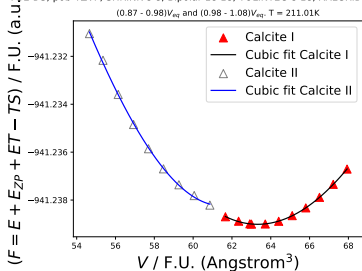


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

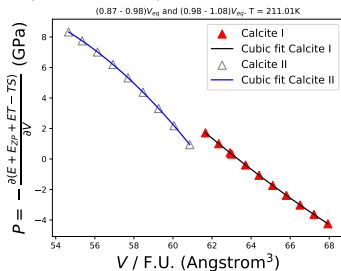


$$T = 211.01\text{K}$$

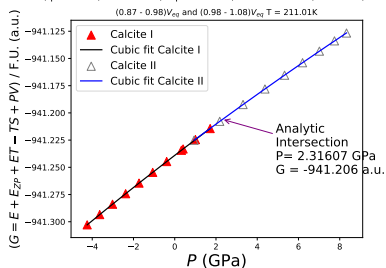
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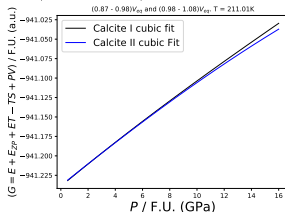
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PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

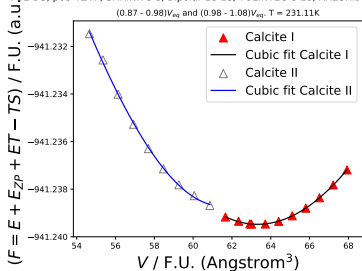


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

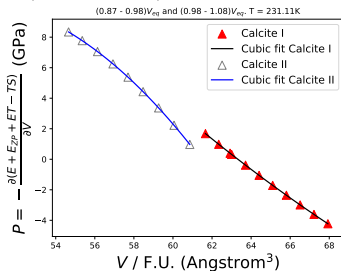


$$T = 231.11\text{K}$$

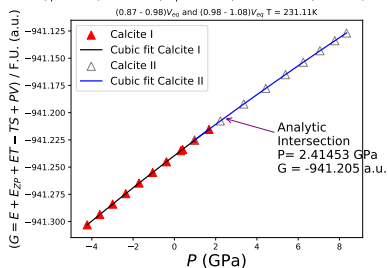
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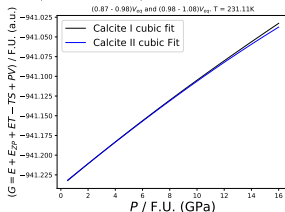
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PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

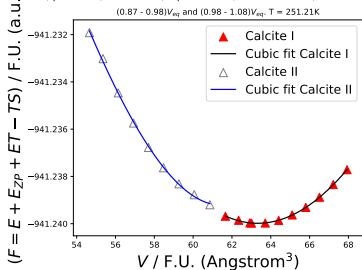


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

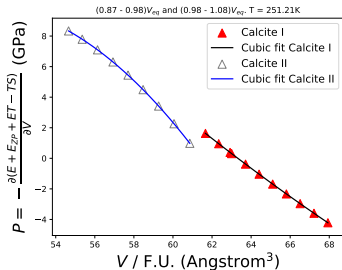


$$T = 251.21\text{K}$$

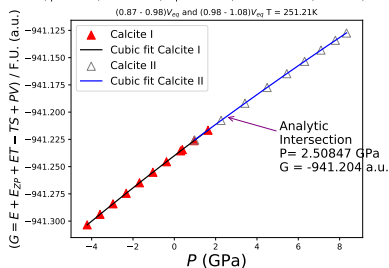
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



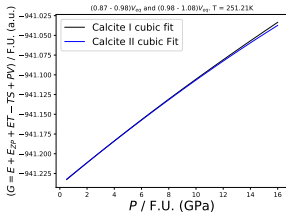
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



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

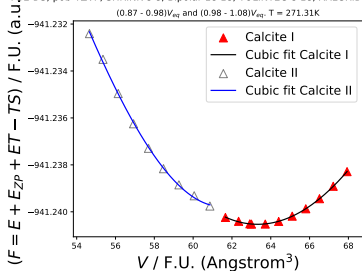


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

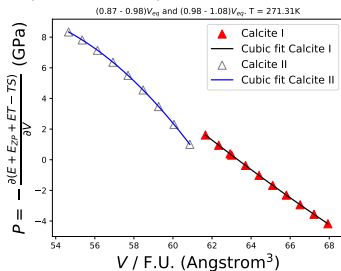


$$T = 271.31\text{K}$$

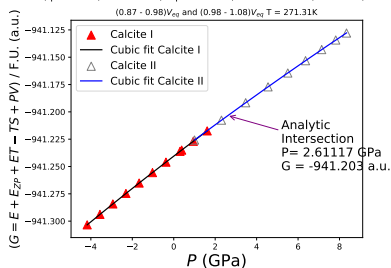
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



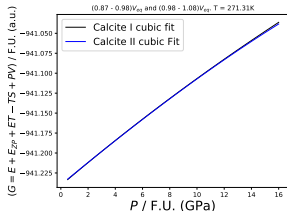
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PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

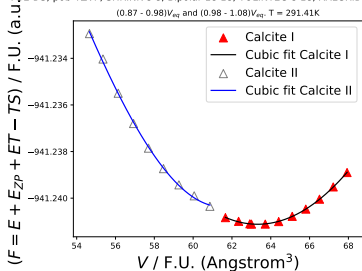


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

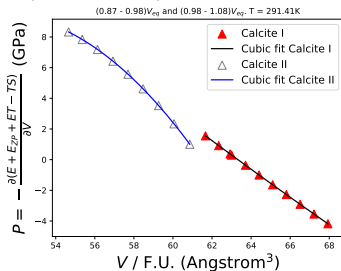


$$T = 291.41\text{K}$$

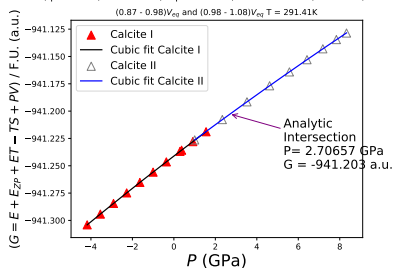
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



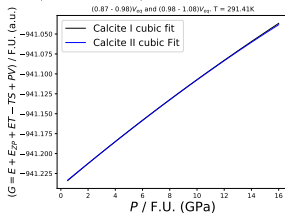
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



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

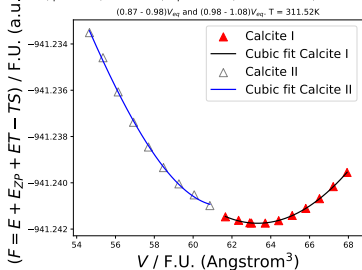


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

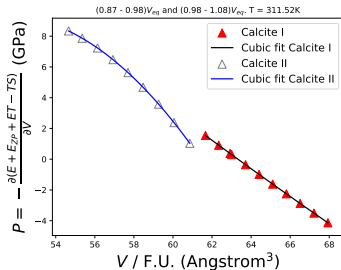


$$T = 311.52K$$

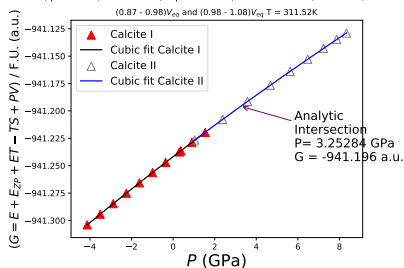
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



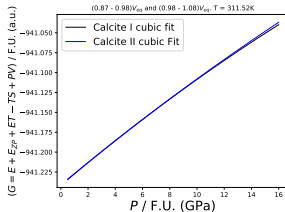
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



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

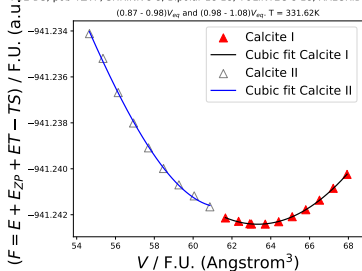


PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8

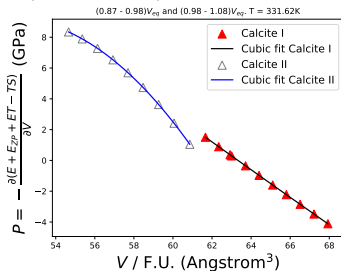


$$T = 331.62K$$

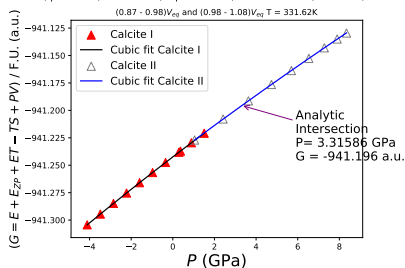
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



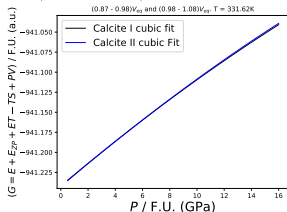
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



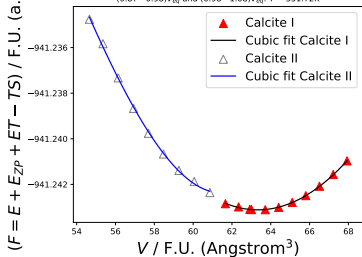
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



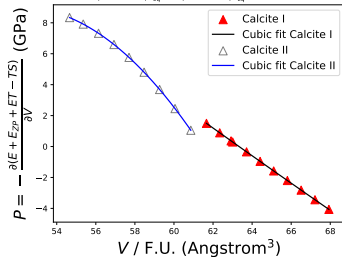
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8



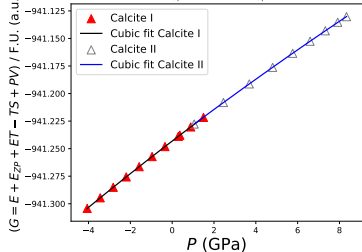
PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8
(0.87 - 0.98) V_{eq} and (0.98 - 1.08) V_{eq} , T = 351.72K



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 = 351.72K



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 = 351.72K



Outline I

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

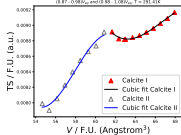
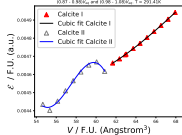
Shapes of G , F , \mathcal{E}

Shape of $H(P; T)$

Phase Boundary

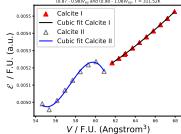
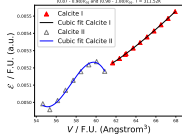
T = 291.41K:

PBE-O3, pbe-TZVP, SHRINK 8 8, Bipolar 18 18, TOLNTEG 8 18, XGLGRID, TOLDEE 8
 (0.87, 0.886 ϵ_{∞} and 0.96, 1.086 ϵ_{∞} , T = 291.41K) PBE-O3, pbe-TZVP, SHRINK 8 8, Bipolar 18 18, TOLNTEG 8 18, XGLGRID, TOLDEE 8
 (0.87, 0.886 ϵ_{∞} and 0.96, 1.086 ϵ_{∞} , T = 291.41K)



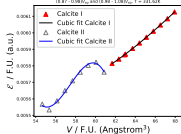
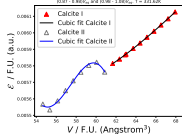
T = 311.52K:

PBE-O3, pbe-TZVP, SHRINK 8 8, Bipolar 18 18, TOLNTEG 8 18, XGLGRID, TOLDEE 8
 (0.87, 0.886 ϵ_{∞} and 0.96, 1.086 ϵ_{∞} , T = 311.52K) PBE-O3, pbe-TZVP, SHRINK 8 8, Bipolar 18 18, TOLNTEG 8 18, XGLGRID, TOLDEE 8
 (0.87, 0.886 ϵ_{∞} and 0.96, 1.086 ϵ_{∞} , T = 311.52K)



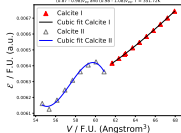
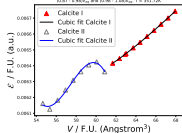
T = 331.62K:

PBE-O3, pbe-TZVP, SHRINK 8 8, Bipolar 18 18, TOLNTEG 8 18, XGLGRID, TOLDEE 8
 (0.87, 0.886 ϵ_{∞} and 0.96, 1.086 ϵ_{∞} , T = 331.62K) PBE-O3, pbe-TZVP, SHRINK 8 8, Bipolar 18 18, TOLNTEG 8 18, XGLGRID, TOLDEE 8
 (0.87, 0.886 ϵ_{∞} and 0.96, 1.086 ϵ_{∞} , T = 331.62K)



T = 351.72K:

PBE-O3, pbe-TZVP, SHRINK 8 8, Bipolar 18 18, TOLNTEG 8 18, XGLGRID, TOLDEE 8
 (0.87, 0.886 ϵ_{∞} and 0.96, 1.086 ϵ_{∞} , T = 351.72K) PBE-O3, pbe-TZVP, SHRINK 8 8, Bipolar 18 18, TOLNTEG 8 18, XGLGRID, TOLDEE 8
 (0.87, 0.886 ϵ_{∞} and 0.96, 1.086 ϵ_{∞} , T = 351.72K)



Outline I

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

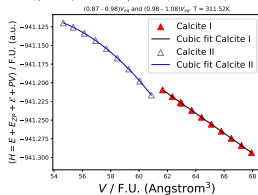
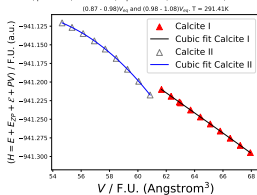
Shapes of G , F , \mathcal{E}

Shape of $H(P; T)$

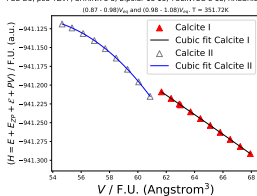
Phase Boundary

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



Outline I

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

Shapes of G , F , \mathcal{E}

Shape of $H(P; T)$

Phase Boundary

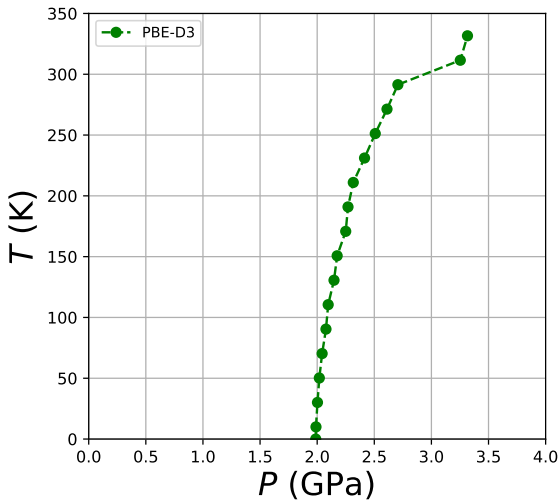


Figure 1: Pressure-temperature phase boundary