Crust to Core workshop: An introduction to Perple_X

Part 3: What data is Perple_X actually using?

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Perple_X finds an optimum set of pseudo-compounds for the *P, T, X* conditions of interest. This is based on available information on the *H, S, V* of end-members, combining these into solution-phases.

Ignoring some complexity (e.g.*X*), we could write a simple equilibria that we could solve by hand

Kyanite = Al_2SiO_5 = Sillimanite

$$-TS_{\text{Kyanite}} + PV_{\text{Kyanite}} = -TS_{\text{Sillimanite}} + PV_{\text{Sillimanite}}$$

It is univariant, so each *P* has one unique *T* at which this occurs, we just need *S* and *V* for each phase…

Extract of THERMOCALC molar thermodynamic properties, Table 5 of Holland & Powell, 1998

	H	sd(*H*)	*S*	*V*	*a*	*b*	*c*	*d*	aū	κ	T_c	S_{max}	V_{max}
Kyanite	-2593.13	0.7	83.5	4.414	0.2794	-0.7124	-2055.6	-2.2894	4.04	1590			
Sillimanite	-2585.89	0.7	95.5	4.986	0.2802	-0.69	-1375.7	-2.3994	2.21	1320	2200	4	0.035

But these are the values for *V*, *S* (and *H*) at 25 ˚C, atmospheric pressure!

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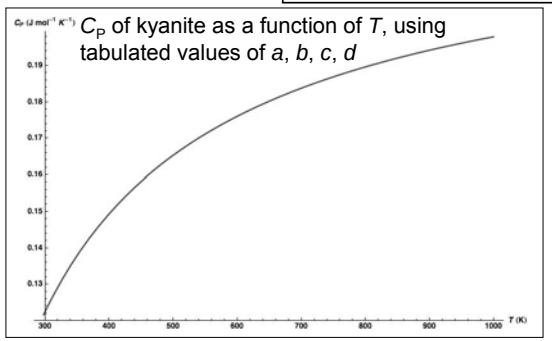
$$C_p = a + bT + cT^{-2} + dT^{-1/2}$$

C_P = J mol^{-1} K^{-1}



C_P of kyanite as a function of *T*, using tabulated values of *a*, *b*, *c*, *d*

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$$S_T = S_0 + (S_{Max}/1000)Q_{298}^2 + \left[a\ln\left(\frac{T}{298}\right)\right] + [b(T-298)] - \frac{c}{2}\left(\frac{1}{T^2} - \frac{1}{298^2}\right) - 2d\left(\frac{1}{\sqrt{T}} - \frac{1}{\sqrt{298}}\right)$$

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V at 25 ˚C, 1 atm

Thermal expansivity, K^{-1}

$$V_{1,T} = (V_0 + V_{Max}Q_{298}^2)\left[1 + a^\circ(T - 298) - 20a^\circ\left(\sqrt{T} - \sqrt{298}\right)\right]$$

V at *T* of interest, 1 atm

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Bulk modulus (degree of incompressibility)

V at *T* of interest, 1 atm

Volume at the *P* and *T* of interest
(based on the Murnaghan EoS)

$$\int_1^P V\,dP = \frac{V_{1,T}\kappa_T}{3}\left[\left(1 + \frac{4P}{\kappa_T}\right)^{3/4} - 1\right]$$

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We can thus use the tabulated data, with the correct set of equations, to extrapolate the thermodynamic properties (*V*, *S* & *H*) to the *P* and *T* of interest - this is *part of* what THERMOCALC does.

This handling of data is explained more fully in:

HOLLAND, T. J. B. & POWELL, R. (1998), *J. Metamorphic Geology*, **v16**, 309-343.