Prediction of the entropy for As - apatites based on lattice volume

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The structure of apatites, corresponding to the general chemical formula $M_{10}(AO_4)_6X_2$, is very flexible and allows for numerous substitutions. The substitutions result in systematic variations of entropy of formation S°_f. Close to ideal linear correlation of S°_f with the volume V of apatite lattice is observed for F^-, OH^-, Cl^-, and Br^- substitutions. The lines are parallel for Ca-Pb and P-As apatites. This was used for prediction of S°_f for arsenic-bearing apatites, for which the data are sparse.

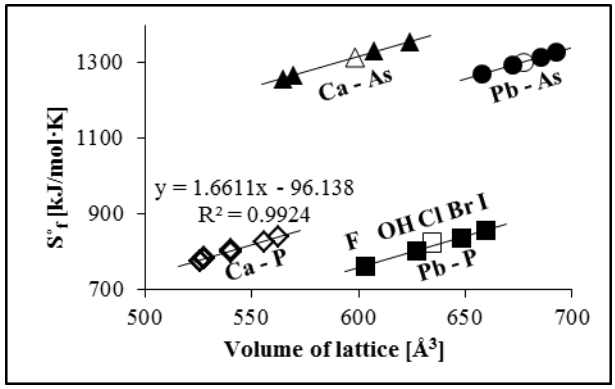

Figure 1. Linear variation of S°_f with the volume of lattice for selected apatites. Filled points mark predicted values.

As-apatites	S°_f [J/mol·K]		V [Å^3]	
	Ca	**Pb**	**Ca**	**Pb**
F	*1617*	*1509*	**570**	**658**
OH	*1651*	*1545*	**565**	**672**
Cl	**1314**	**1567**	**598**	**677**
Br	*1713*	*1598*	*608*	685
I	*320*	*176*	*624*	*692*

Table 1. An example of experimental (bold) and predicted (italic) S°_f and V for selected As – bearing apatites.

For the first time strong systematic variations of entropy of apatites and their constituents are observed and utilized for correlation, interpolation and extrapolation (Fig. 1.).