Predictions of thermodynamic properties of As-bearing apatites from linear trends in existing data

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Systematic variations of thermodynamic properties with isomorphic cationic and anionic substitutions in the apatite structure are commonly observed. We determined close to ideal linear correlation of ΔG°_f, ΔH°_f and S°_f with 1) the type of additional anion (F^-, OH^-, Cl^-, Br^-); or 2) the electronegativity of bivalent cations (Ca^{2+}, Pb^{2+}, Ba^{2+}, Sr^{2+}, Mg^{2+}, Zn^{2+}, Cd^{2+}, Cu^{2+}). This was used for prediction of thermodynamic properties of arsenic-bearing apatites, for which the values are still missing.

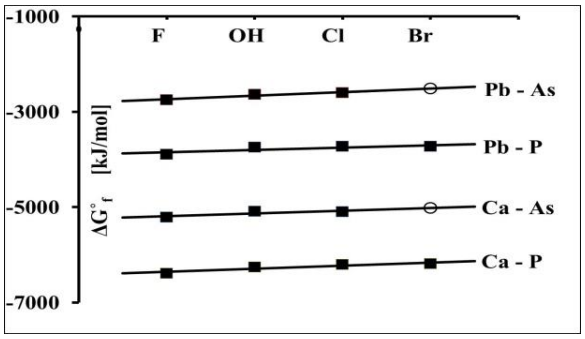

Figure 1. Linear variation of ΔG°_f and the type of additional anion for selected apatites. Empty circles mark predicted values.

ΔG°_f [kJ/mol]	F	OH	Cl	Br
Pb – As	-2749	-2634	-2600	*-2512*±55
Pb – P	-3891	-3741	-3729	-3730
Ca – As	-5210	-5090	-5095	*-5017±86*
Ca - P	-6390	-6255	-6209	-6191

Table 1. An example of experimental and predicted ΔG°_f for selected apatites. Predicted values in italics with an error calculated form the standard errors of linear correlation coefficients.