

Supplementary Materials

In Search of an Efficient Complexing Agent for Oxalates and Phosphates: A Quantum Chemical Study

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Table S1. Gibbs free Formation energies for all complexes considered in the present study in kcal/mol. For lanthanum chloride, no stable complex was found.

	Acetate	Carbonate	Chloride	Citrate	Formate	Hydroxide	Oxalate	Phosphate	Sulphate
Li⁺	-14.3	-35.6	-13.5	-41.3	-12.4	-22.4	-26.4	-67.4	-24.7
Na⁺	-3.5	-18.8	-2.8	-15.9	2.5	-5.4	-9.7	-27.7	-10.3
Mg²⁺	-73.4	-70.8	-67.3	-223.8	-71.0	-78.6	-76.8	-248.4	-62.4
Ca²⁺	7.6	9.1	8.6	28.8	10.9	2.9	6.3	-10.3	8.1
Fe²⁺	-77.0	-72.9	-65.6	-215.2	-70.0	-77.9	-77.7	-242.9	-60.4
Cu²⁺	-44.2	-41.2	-39.6	-5.7	-33.0	-66.2	-42.2	-159.9	-31.7
Zn²⁺	-24.3	-25.1	-21.1	-67.4	-19.8	-40.3	-24.7	-121.4	-16.8
Al³⁺	-479.2	-996.3	-452.9	-459.3	-480.1	-522.3	-927.4	-491.3	-909.7
Fe³⁺	-186.4	-319.3	-167.7	-174.1	-184.5	-231.6	-267.9	-201.9	-255.1
La³⁺	23.2	33.3		38.0	26.9	17.6	51.0	20.4	64.1

The Gibbs free formation energy was estimated by calculating the Gibbs free formation energy of the complex at the smaller basis set (see computational methods) and correcting it using the formation energies as calculated in the main text at both the large and small basis sets:

$$G_{\text{formation}} = G_{\text{small}} - E_{\text{small}} + E_{\text{large}} \quad (\text{S1})$$