

Supplementary Information

C. Mystrioti and N. Papassiopi,¹ Treatment of contaminated waters with heavy metals by supported green nZVI under flow conditions.

A) Effect of iminodiacetic acid ligands on the precipitation of Fe(III) and Cr(III) hydroxides

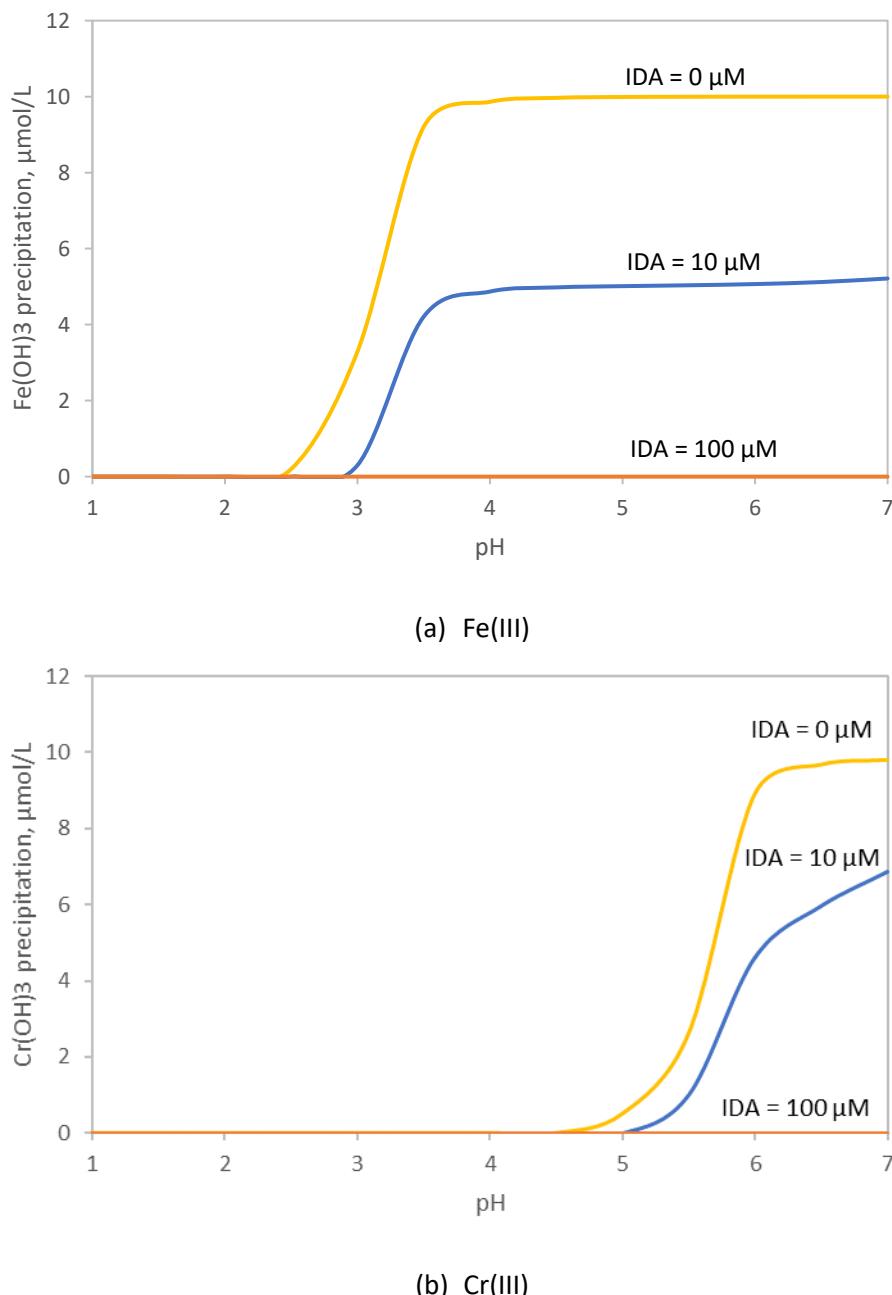


Figure S1. Precipitation of $\text{Fe}(\text{OH})_3$ and $\text{Cr}(\text{OH})_3$ as a function of pH from solutions containing 10 μM $\text{Fe}(\text{III})$ or $\text{Cr}(\text{III})$ and various concentrations of iminodiacetic acid (IDA), IDA=0, 10 and 100 μM .

Calculations were carried out with Visual Minteq V3.2. Formation constants for Fe(III)-IDA chelates from Sanchiz et al., 1999, and for Cr(III)-IDA chelates from Mizuochi et al., 1970.

Table S1. IDA complexes as incorporated in VMinteq databases

Species	Reaction	log(K), log(β)	
			Sanchiz et al., 1999
HIDA ⁻¹	IDA ⁻² +H ⁺ → HIDA ⁻¹	9.25	
H ₂ IDA	IDA ⁻² +2H ⁺ → H ₂ IDA	11.79	
H ₃ IDA ⁺	IDA ⁻² +2H ⁺ → H ₃ IDA+1	13.46	
FeIDA ⁺	Fe ⁺³ +IDA ⁻² → FeIDA ⁺	10.90	
Fe(IDA) ₂ ⁻	Fe ⁺³ +2IDA ⁻² → Fe(IDA) ₂ ⁻	30.23	
Fe(OH)IDA	Fe ⁺³ +IDA ⁻² +H ₂ O→ Fe(OH)IDA+H ⁺	7.42	Sanchiz et al., 1999, VMinteq
Fe(OH) ₂ IDA ⁻	Fe ⁺³ +IDA ⁻² +2H ₂ O→ Fe(OH) ₂ IDA ⁻ +2H ⁺	3.85	>>
CrIDA ⁺	Cr ⁺³ +IDA ⁻² → CrIDA ⁺	10.90	Mizuochi et al., 1970
Cr(IDA) ₂ ⁻	Cr ⁺³ +2IDA ⁻² → Cr(IDA) ₂ ⁻	21.40	>>

Table S2. Complexes of N-Benzylamine-DA

Species	Reaction	LogK	
HBeDA ⁻¹	BeDA ⁻² +H ⁺ → HBeDA ⁻¹	8.96	Shtacher, 1966
H ₂ BeDA	BeDA ⁻² +2H ⁺ → H ₂ BeDA	11.05	
H ₃ BeDA ⁺	BeDA ⁻² +2H ⁺ → H ₃ BEDA ⁺¹	12.54	
CuBeDA+	Cu ⁺² +BeDA ⁻² → CuBeDA	10.51	Ando et al., 1966
NiBeDA+	Ni ⁺² +BeDA ⁻² → NiBeDA	7.98	
PbBeDA+	Pb ⁺² +BeDA ⁻² → PbBeDA	7.39	
ZnBeDA+	Zn ⁺² +BeDA ⁻² → ZnBeDA	6.97	
CaBeDA+	Ca ⁺² +BeDA ⁻² → CaBeDA	3.13	
MgBeDA+	Mg ⁺² +BeDA ⁻² → MgBeDA	2.63	

References

Sanchiz J., Esparza P., Dominguez S., Brito F., Mederos A., 1999. Solution studies of complexes of iron(III) with iminodiacetic, alkyl-substituted iminodiacetic and nitrilotriacetic acids by potentiometry and cyclic voltammetry. Inorganica Chimica Acta 291, 158–165. [https://doi.org/10.1016/S0020-1693\(99\)00125-5](https://doi.org/10.1016/S0020-1693(99)00125-5)

Marini L., Acconero M. 2007. Prediction of the thermodynamic properties of metal-arsenates and metal-arsenite aqueous complexes to high temperature and pressures and some geological consequences. Environmental Geology, 52, 1343-1363, <https://doi.org/10.1007/s00254-006-0578-5>