

Supplementary Material

Size evolution of Eu^{III}–fulvic acid complexes with pH, metal, and fulvic acid concentrations: implications for modelling of metal–humic substances interactions

Yasmine Kouhail^{A,B,C}, Pascal E. Reiller^A, Laurent Vio^{A,D} and Marc F. Benedetti^{B,}*

^AUniversité Paris-Saclay, CEA, Service de Physico-Chimie (SCP), F-91191 Gif-sur-Yvette, France

^BUniversité Paris Cité, Institut de Physique du Globe de Paris, CNRS, F-75005 Paris, France

^CPresent address: Karlsruher Institut für Technologie (KIT), Institut für Nukleare Entsorgung (INE), Hermann-von-Helmholtz Platz 1, D-76344 Eggenstein- Leopoldshafen, Germany

^DPresent address: CEA, DG/CEACAD/D3S/SPR/LANSE, Cadarache, Saint-Paul-lès-Durance Cedex, France

*Correspondence to: Email: benedetti@ipgp.fr

The supplementary data contains one figure and one table. The figure shows the simulation of the proportion of Eu^{III} bound to a generic fulvic acid for $C_{\text{Eu}^{\text{III}}}$ of 1 μM and 10 μM at pH 4, 6 and 7, using generic NICA–Donnan parameters. The table shows the hydrodynamic radii as function of C_{SRFA} for SRFA samples and Eu^{III} –SRFA complexes, for C_{Eu} of 1 and 10 μM , at pH 4, 6 and 7.

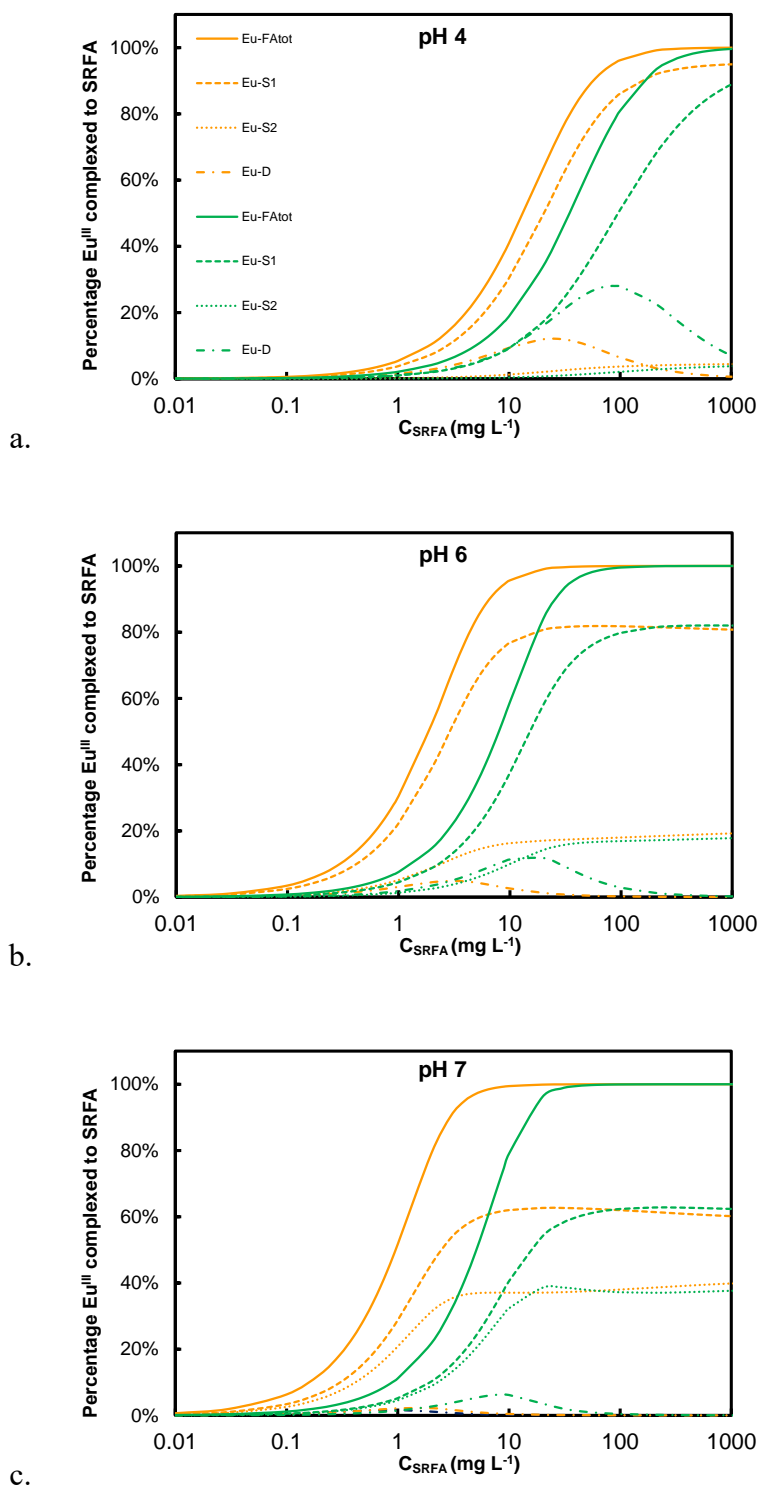


Fig. S1. Simulation of the proportion of Eu^{III} bound to a generic fulvic acid for $C_{\text{Eu}^{\text{III}}}$ of 1 μM (orange lines) and 10 μM (green lines) at pH 4 (a), 6 (b), and 7 (c). Simulation of Eu^{III} distribution on S₁ sites (dashed lines) and S₂ sites (dotted lines) of SRFA. Solid lines are the sum of S₁ and S₂ sites. Generic NICA–Donnan parameters are given in Table 1.

Table S1. Hydrodynamic radii (R_H) as function of C_{SRFA} for SRFA samples and Eu^{III} -SRFA complexes, for C_{Eu} of 1 and 10 μM , at pH 4, 6 and 7.

R_H (nm)

| | C_{SRFA} (mg L ⁻¹) | SRFA R_H (nm) | $Eu_{1 \mu M}$ -SRFA R_H (nm) | $Eu_{10 \mu M}$ -SRFA R_H (nm) |
|-------------|-------------------------------------|--------------------|------------------------------------|-------------------------------------|
| pH 4 | 30 | 0.91 | 0.92 | 0.78 |
| | 50 | 0.98 | 0.95 | 0.86 |
| | 100 | 0.98 | 0.88 | 0.90 |
| | 300 | 0.97 | 0.93 | 0.98 |
| | 500 | 0.92 | 0.91 | 0.90 |
| pH 6 | 30 | 0.99 | 1.01 | 0.80 |
| | 50 | 0.97 | 0.98 | 0.86 |
| | 100 | 0.98 | 0.99 | 0.91 |
| | 300 | 0.98 | 0.97 | 0.93 |
| | 500 | 0.92 | 0.92 | 0.89 |
| pH 7 | 30 | 1.01 | 0.99 | 0.83 |
| | 50 | 1.00 | 1.03 | 0.88 |
| | 100 | 0.98 | 1.00 | 0.91 |
| | 300 | 0.95 | 0.95 | 0.93 |
| | 500 | 0.88 | 0.90 | 0.89 |

Viscosity used for calculation is 0.00089 kg s⁻¹ m⁻¹.