

Supplementary material

Gel–water partitioning of soil humics in DGT of their metal complexes

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Table S1. NICA–Donnan parameters used in equilibrium calculations

p is the width of the distribution; Q_{\max} is the binding site density; n_H is the non-ideality parameter for protons. For details see Benedetti et al.^[1]

	SRFA Specific parameters ^[1]		FSHA Specific parameters ^[2]	
	Carboxylic	Phenolic	Carboxylic	Phenolic
Q_{\max} (mol kg ⁻¹)	5.55	2.50	2.30	3.92
p	0.65	0.49	0.68	0.28
$\log K_H$	2.56	7.50	2.21	8.98
n_H	0.68	0.81	0.78	0.61
$\log K_{Cd}$	-3.17	–	-0.35	1.94
n_{Cd}	0.46	–	0.77	0.57

References

- [1] M. F. Benedetti, W. H. Van Riemsdijk, L. K. Koopal, D. G. Kinniburgh, D. C. Gooddy, C. J. Milne, Metal ion binding by natural organic matter: from the model to the field. *Geochim. Cosmochim. Acta* **1996**, *60*, 2503. doi:10.1016/0016-7037(96)00113-5
- [2] E. J. J. Kalis, L. P. Weng, F. Dousma, E. J. M. Temminghoff, W. H. Van Riemsdijk, Measuring free metal ion concentrations in situ in natural waters using the Donnan membrane technique. *Environ. Sci. Technol.* **2006**, *40*, 955. doi:10.1021/es051435v