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Metal-humic binding models: Make them as simple as possible, but not simpler

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Humic substances, or natural organic matter in general, cannot be characterised by well-defined molecular structures, as small organic ligands are. We cannot define a "mole" of humic substance.

Defining conditional equilibrium constants for metal binding by small organic ligands is not always straightforward, as ambiguities can arise when different stoichiometries equally well describe experimental data. However, we always can start modelling with quantities like [mol / litre] or [mol / kg_{H2O}]. This is impossible in the case of humics and the problems already start with the question how to normalise experimental data concerning metal – humic binding with respect to a common basis [1].

Any model trying to describe metal – humic binding has to cope with this ambiguity by making assumptions about the structure of humics. These assumptions determine how simple or complicated the model and its parametrisation are, and ultimately limit the field of application of the humic binding model.

Two very simple metal – humic binding models with limited fields of applications, the 'conservative roof' model [2], and the 'local charge neutralisation' model [3], will be shortly discussed and set into perspective with more sophisticated models like 'Model VII' [4] and the 'NICA-Donnan' model [5].

References

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