



Contribution ID: 137

Type: Verbal

## Speciation and thermodynamics of lanthanide and actinide ionic solutions described using the Mean Spherical Approximation (MSA)

A theoretical description of speciation and of the thermodynamic properties of lanthanide and actinide ionic solutions is proposed in the framework of the mean spherical approximation (MSA) [1-4]. In this model the ions are regarded as charged hard spheres immersed in a dielectric continuum representing the solvent (water). An interesting feature of the MSA is that it yields analytic expressions.

To account for complex formation, the multivalent cation (a lanthanide or an actinide ion) is assumed to possess a finite number of sites on its surface, on which anions can bind [5]. This property leads to the formation of 1:1, 1:2, 1:3,... complexes according to a stepwise complexation-equilibrium process. Explicit formulas are obtained for the speciation and the thermodynamic properties (osmotic and activity coefficients) within this model. They include the effects of complexation and electrostatic interactions.

The model is applied to the case of binary and ternary aqueous solutions of divalent, trivalent and tetravalent lanthanides and actinides.

### References

- [1] J.P. Simonin, L. Blum, P. Turq, J. Phys. Chem. 100 (1996) 7704.
- [2] J.P. Simonin, J. Phys. Chem. B, 101 (1997) 4313.
- [3] J.P. Simonin, O. Bernard, L. Blum, J. Phys. Chem. B 102, (1998) 4411.
- [4] A. Ruas, O. Bernard, B. Caniffi, J.P. Simonin, P. Turq, L. Blum, P. Moisy, J. Phys. Chem. B 110 (2006) 3435.
- [5] O. Bernard, L. Blum, J. Chem. Phys. 104 (1996) 4746.

**Primary author:** Prof. SIMONIN, Jean-Pierre (CNRS / Université P.M. Curie (Paris 6))

**Co-authors:** Dr RUAS, Alexandre (CEA Marcoule); Dr TORRES ARENAS, José (Universidad de Leon Guanajuato); Dr BERNARD, Olivier (CNRS / Université P.M. Curie (Paris 6)); Prof. MOISY, Philippe (CEA Marcoule)

**Presenter:** Prof. SIMONIN, Jean-Pierre (CNRS / Université P.M. Curie (Paris 6))

**Track Classification:** Separation Methods, Speciation