# Molecular dynamics simulation of trivalent europium in aqueous solution: A study on the hydration shell structure



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| Résumé en anglais | As a prelude to a spectroscopic investigation of doped wet gels, we have made molecular dynamics simulations of a very dilute EuCl3 solution. The symmetry properties of the first hydration shell of Eu3+ have been determined. The 8 water molecules of this shell are roughly arranged according to the square antiprism D 4d pseudo-symmetry. Though the arrangement of oxygens is little distorted from regular positions, the orientation of the water molecules themselves is found to be not so well organized at room temperature. |
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**Liens**

[1] http://okina.univ-angers.fr/stephane.chaussedent/publications
[2] http://okina.univ-angers.fr/publications?f[author]=8745
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