



Molecular dynamics simulation of Eu³⁺ in aqueous solution comparison with experimental luminescence spectra

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Auteur	Chaussement, Stéphane [1], Monteil, André [2], Ferrari, Maurizio [3]
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Résumé en anglais	Using molecular dynamics simulations, we have studied the environment of Eu ³⁺ salts in aqueous solution. In the case of hydration number of 8, the symmetry of the first hydration shell is found to be very close to the D _{4d} . We have therefrom calculated the ligand field parameters according to the point charge model. The luminescence spectra were reconstructed from this set of computed B _{kq} , and finally compared with experimental spectra.
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- [1] <http://okina.univ-angers.fr/stephane.chaussement/publications>
- [2] [http://okina.univ-angers.fr/publications?f\[author\]=8745](http://okina.univ-angers.fr/publications?f[author]=8745)
- [3] [http://okina.univ-angers.fr/publications?f\[author\]=8790](http://okina.univ-angers.fr/publications?f[author]=8790)
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