Analysis of charge density in nonaaquagadolinium(III) trifluoromethanesulfonate – insight into Gd^{III}—OH_2 bonding.

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The experimental charge-density distribution in $[Gd(H_2O)_9](CF_3SO_3)_3$ has been analysed and compared with the theoretical density functional theory calculations. Although the Gd—OH_2 bonds are mainly ionic, a covalent contribution is detectable when inspecting both the topological parameters of these bonds and the natural bond orbital results. This contribution originates from small electron transfer from the lone pairs of oxygen atoms to empty 5*d* and 6*s* spin orbitals of Gd^{3+}.

Słowa kluczowe

charge-density distribution, covalence, electronic structure, lanthanides

Adres publiczny

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