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A Quantum Chemical Study on the Actinides Triflates An(OTf)n where (An= Th, U, Np, Pu, Am, Cm, Bk and No); n= (3, 4)

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The actinides triflates are formed from a central metal that relates to the ligands (CF3SO3-). The transition metal triflates (trifluoromethanesulfonates) are much considered as Lewis acid catalysts in a variety of organic reactions, as well as precursors in inorganic and organometallic synthesis. In coordination chemistry, the selective complexation of actinides (III) over lanthanides (III) with efficient extractant molecules is an important problem for both its fundamental aspects and its applications, in particular in the partitioning of spent nuclear fuels.

We carry out a quantum calculation based on the density functional theory (DFT) of the actinide triflates complexes. Our aim is to study the structural proprieties changes of these complexes geometries. Furthermore we report the computational study on An(OTf)n where (An= Th, U, Np, Pu, Am, Cm, Bk and No); n = (3, 4).

The quantum calculation DFT proved that the trigonal prismatic geometry is favored for all the studied actinide complexes of the general formula An(OTf)3 where (An= Th, U, Np, Pu, Am, Cm, Bk and No) so as by the lanthanide triflate complexes; where the trigonal prismatic geometry is most distorted in the case of triflate thorium Th(OTf)3 and almost perfect in the case of U(OTf)3. The OTf group is bonded to the central metal An as a bidentate ligand with a number of coordination equal to six.

For the An(OTF)4 where (An= Th, U and Pu), the optimized geometry results showed a dodecahedron geometry. Differences in the structural parameters (bond, lengths and angles) can be attributed partly to the nature of the metal atoms and the structural arrangement of the studied compounds.

Keywords: actinide- triflate- catalyst- DFT- trigonal prismatic.

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