EVALUATION OF POINT GROUP SYMMETRY IN COORDINATION COMPLEXES

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Molecular structure dictates physical properties, and symmetry plays a defining role in determining electronic structure. Group theory therefore provides a powerful framework for understanding and predicting molecular behavior. In inorganic chemistry, coordination geometries are often approximated as idealized high-symmetry polyhedra, enabling predictive models through ligand field theory. However, real molecular systems rarely exhibit ideal symmetry. While continuous shape measures can quantify deviations from reference polyhedra, these approaches often fail for lanthanide(III) complexes, which commonly feature high coordination numbers, ambiguous principal axes, and no obvious choice of reference structure.

In this talk, I will present an algorithmic method that systematically orients a molecular structure with respect to the symmetry elements of any chosen point group and computes its deviation from ideal symmetry. [1, 2] This approach enables a quantitative and unbiased symmetry analysis, even for highly coordinated and geometrically complex systems. Using this framework, we evaluate a range of coordination complexes, with particular emphasis on lanthanide systems, and discuss how refined symmetry analysis provides deeper insight into their electronic structure and structure–property relationships. [3]

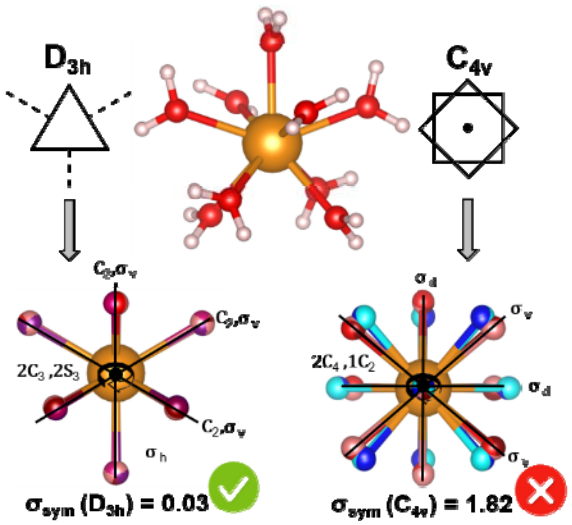

Figure: A nine coordinated lanthanide(III) aqua complex is evaluated with two different point group symmetries.

[1] Nielsen, V. R. M.; Le Guennic, B.; Sørensen, T. J. J. Phys. Chem. A 2024, 128, 28, 5740–5751

[2] Nielsen, V. R. M, B.; Sørensen, T. J. Nat. Comm. 2025, 16, 11122

[3] Nielsen, V. R. M., Grasser, M.; Le Guennic, B.; Sørensen, T. J., J. Inorg. Chem. 2025, 64, 7, 3463-3475