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Determination of Structures and Binding Energies of Europium Complexes Bound to Biologically Relevant Analytes

Anion sensing is a crucial area of research due to its applications in medical diagnostics, environmental analysis and industry. Lanthanide complexes have been actively studied for anion sensing in biological media as they have a positively charged central cation that can provide strong electrostatic interactions with the anions. In addition, their unique photophysical properties such as high photoluminescence and quantum yield, and large stokes shift of about 200 nm, make them particularly useful to serve as biosensors.

Within this work, we investigate the geometries and binding energies of europium complexes bound to different biological anions using various computational methods. These results indicate that the composite r2SCAN-3c method produces highly accurate results at a low computational cost. Proceeding to a conformer analysis, we highlight how the investigated complexes possess a large number of conformers differing widely in terms of the energetic and structural features. Finally, we study binding energies considering computational methods, solvation as well as the effect of counterions and protonation states highlighting that these effects play a prominent role. We believe that this work will set a solid background for future investigations of luminescent europium complexes and their anion binding properties.

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