Metal-substituted rubredoxin - theoretical prediction of the spin-spin coupling constants using ZORA

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The indirect nuclear spin-spin coupling constants between hydrogen atom in amid group in cysteine and metal cation in rubredoxin molecule have been calculated by means of density functional theory with zeroth order regular approximation Hamiltonian (DFT-ZORA). The mercury and the cadmium cations were chosen as metal cation -same as in the experimental work of Blake and coworkers [1].

The metal atom and four molecules of cysteine were selected as a model system - Figure 1.

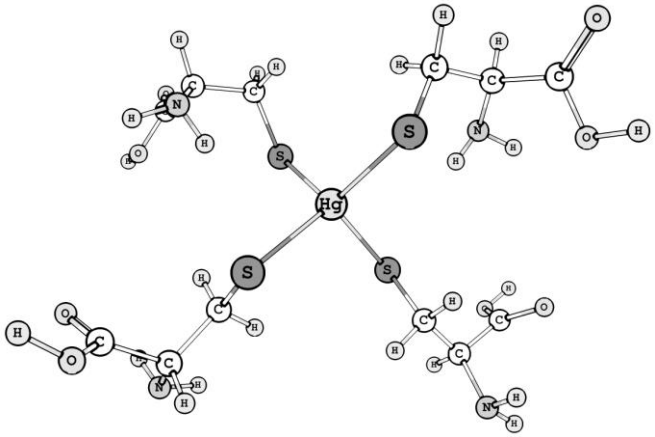

Figure 1. Model system of mercury substituted rubredoxin

Various functionals and basis sets have been tested on the model system. We have also checked how the predicted coupling constant value depends on the level of theory. It has been modeled how these values are affected by rotation of some groups in the model system.

The measured spin-spin coupling constants are in 0,29-0,56Hz range for Cd and in 0,57-2,20Hz range for Hg. The calculated values are in the similar range.

[1] Blake, P., Lee, B., Summers, M. and coworkers, *Journal of Biomolecular NMR*, 2:527-533, 1992.