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Theoretical Chemistry Study of Uranyl (VI)-Sulphate complex species

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This theoretical study of several possible complex species of the general formula ([$UO_2(H_2O)_a(\eta^1$-$SO_4)_b(\eta^2$-$SO_4)_c]^{2-2(b+c)}$, 0 $b+c$ 4, 5 $a+b+2c$ 6, $[UO\_2(H\_2O)\_2(\eta\hat{}1-SO\_4)(\eta\hat{}2-SO\_4)]\hat{}\{2-\}depictedattheFig.1.)aspirestothetheoVISabsorption, excitationandemission/fluorescencespectrawerecalculatedaswell.Ourstudyisalsothefirststeptowardsthedynamicalstudysearchingseekingforanotherapproachtopredict\DeltaG°,\DeltaH°andlog\beta$° and, more importantly, to predict the fluorescence lifetimes (or more generaly - the TRLFS spectra) and their dependance on the temperature and ionic strength (or, more generaly - the solution composition).
The comparison of all of the ab initio predicted and experimentally obtained quantities is included.
Both, the purely ab initio methods based on the Dirac(-Breit) equation (DHF, MCDHF, KRCI, CCSD) and the density functional methods (DFT (b3-lyp/def-SVP), TDDFT (bh-lyp/def-SVP)) were used.
This work tries to reproduce and further develop the study of uranyl-sulfates done by Jakub Šebera [1].

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