Cu(H$_2$O)$_2$(en)SO$_4$ optical spectra comparison: experiment vs theory

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Cu(H$_2$O)$_2$(en)SO$_4$ was recently identified as a quasi-one-dimensional $S = 1/2$ antiferromagnetic insulator [1]. The structure possesses a monoclinic symmetry with the angle $\beta$ of 105.5$^\circ$. We measured the system’s optical functions in the range from 190 to 1700 nm and here compare these with results obtained from DFT-based (GGA+U) ab-initio calculations.

References: