$Cu(H_2O)_2(en)SO_4$ optical spectra comparison: experiment *vs* theory

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$Cu(H_2O)_2(en)SO_4$ was recently identified as a quasi-one-dimensional $S = 1/2$ antiferromagnetic insulator [1]. The structure possesses a monoclinic symmetry with the angle β of 105.5 °. 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:

[1] J. Appl. Phys. **115**, 17B305 (2014)