Charge density study of $Cu_3(en)_2(CN)_4 \cdot H_2O$

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In our recent work we have studied distribution of the electron density in the model compounds for blue proteins. Two model compounds [1] representing the reduced and the oxidized form of the protein contains copper in state +1 and +2. The mixed-valence complex $Cu_3(en)_2(CN)_4.H_2O$ [2] contains copper atoms in both oxidation states, and so it should be possible to study electronic structure and particularly copper in both oxidation states not biased by different systematic errors. This provide us interesting comparison with our previous results.

Data were collected at at the beamline F1 at HASYLAB/DESY in Hamburg (T = 100 K, λ = 0.5604 Å). For corrections, integration and data reduction programs SAPRO, SAINT, and SORTAV were used. Multipole refinement was performed with XD software package.

[1] Flanagan S., Dong J., Haller K., Wang S., Scheidt W.R., Scott R.A., Webb T.R., Stanburry D.M., Wilson L.J., *J. Am. Chem. Soc.*, 1997, **119**, 8857. [2] Williams R. J., Larson A. C., Cromer D. T., *Acta Cryst.*, 1972, **B28**, 858.

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