Experimental Electron Density of [Cu(phen)₂Cl](NO₃)(H₂O)

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The electron density of the title complex was obtained from a high resolution (0.55Å) X-ray diffraction experiment at 100 K, with a KappaCCD diffractometer. Experimental data were collected with MoK α radiation. 11199 independent reflections were used in the refinements. The charge density model was obtained from the Hansen-Coppens formalism. R(F)=0.0368, wR(F)=0.0406.

The copper ion presents coordination between trigonal bipyramidal and square pyramidal. The chlorine atom and one phenantroline nitrogen are in the equatorial plane. Deformation density maps around the copper ion and its d-orbital occupations can be explained in terms of crystal field theory and the π -donating effect of chlorine. Two hydrogen bonds with the water oxygen stabilize the crystalline complex: [Cl···H1–O(w) and O(w)–H2···O(nitrate)].

Bader's¹ topological analysis of the electron density was performed. (3,-1) critical points were found in all chemical bonds. This analysis shows that the Cu–N and Cu–Cl bonds are ionic, and that the hydrogen bonds are electrostatic. The C–C, C–N and C–H bonds, on the other hand, are covalent. (3,+1) critical points are present approximately in the center of each phenantroline ring, as well as in the center of the rings containing the copper atom.

[1] Bader R. F. W., *Atoms in Molecules – A Quantum Theory*, Oxford University Press, Oxford, 1994.

Keywords: copper compounds, crystal field theory, multipole refinements