Poster Presentation

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Experimental electron density of [Cu(2,2'-bipyridine)NO_3]NO_3

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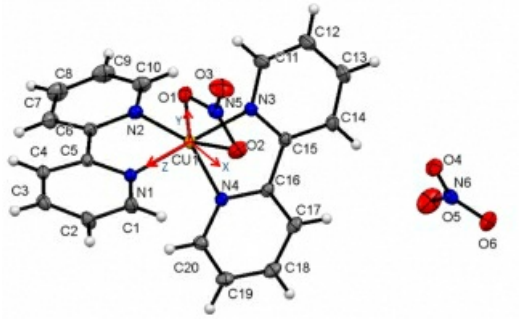
The electron density distribution of [Cu(2,2'-bipyridine)NO3]NO3, obtained from high-resolution (0.5 A) single-crystal X ray diffraction, using the Hansen-Coppens formalism, is herein described. N(meas) = 108763, N(ind) = 16999, N(obs, I>2sigma(I)) = 12848, Rint = 0.036, MoKa = 0.71073 A, 110 K, R(F2,> 2s(F2)) = 0.035. Considering the herein defined local coordinate system for copper (see figure), orbitals dx2-y2 (2.036 e) and dxy (2.204e) are the most occupied. The occupations of orbitals with z-components are considerably smaller: 1.788 e for dyz, 1.703 e for dxz and 1.499 e for dz2. These results agree well to distances in the copper coordination sphere: two short bonds in the z direction, with d[Cu -N1] = 1.9878 (6) A and d[Cu-N3] = 1.9740 (6) A); and four longer Cu–L distances in plane XY (d[Cu-N2]=2.1276 (7) A, d[Cu-N4] = 2.0114 (6) A, d[Cu-O1] = 2.1276 (7) A, and d[Cu-O2] = 2,596(7) A). QTAIM (Bader, 1994) topological analysis shows differences in chemical bonds and atomic charges, depending on the Cu – O distances. QTAIM analysis in the aromatic rings shows distinct charges for different carbon atoms depending on their neighbors.
Bader, R. F. W. (1994) Atoms in Molecules: A Quantum Theory - Oxford University Press



Keywords: charge density, copper complex, Bader topological analysis.