Experimental electron density of \([\text{Cu}(2,2''\text{-bipyridine})\text{NO}_3]\text{NO}_3\)

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The electron density distribution of \([\text{Cu}(2,2''\text{-bipyridine})\text{NO}_3]\text{NO}_3\), obtained from high-resolution (0.5 Å) 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 Å, 110 K, R(F2,> 2s(F2)) = 0.035. Considering the herein defined local coordinate system for copper (see figure), orbitals \(dx^2-y^2\) (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 \(dz^2\). These results agree well to distances in the copper coordination sphere: two short bonds in the \(z\) direction, with \(d[\text{Cu} - \text{N1}] = 1.9878\) (6) Å and \(d[\text{Cu} - \text{N3}] = 1.9740\) (6) Å; and four longer \(\text{Cu}–\text{L}\) distances in plane \(XY\) (\(d[\text{Cu} - \text{N2}] = 2.1276\) (7) Å, \(d[\text{Cu} - \text{N4}] = 2.0114\) (6) Å, \(d[\text{Cu} - \text{O1}] = 2.1276\) (7) Å, and \(d[\text{Cu} - \text{O2}] = 2.596(7)\) Å). QTAIM (Bader, 1994) topological analysis shows differences in chemical bonds and atomic charges, depending on the \(\text{Cu} – \text{O}\) distances. QTAIM analysis in the aromatic rings shows distinct charges for different carbon atoms depending on their neighbors.


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