The Structure of the Adduct of Bisacetylacetonatocopper(II) with Quinoline

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THE extraction of co-ordinatively unsaturated metal chelates into organic solvents is enhanced by the addition of neutral molecules which can act as electron donors. It has been suggested that this increase in extraction, called synergism, is due to the formation of hydrophobic metal chelate adducts.[1] The structures of many metal chelate adducts have been predicted from the results of solvent-extraction experiments[2,3] and from spectral studies;[4] however, no *X*-ray structure determination of a metal chelate adduct has been published with the exception of a preliminary report on the crystal structure of diaquoacetylacetonatocopper(II) picrate.[4] We report here the results of a single-crystal *X*-ray structure determination of the adduct of bisacetylacetonatocopper(II) with quinoline.

The adduct was prepared by dissolving bisacetylacetonatocopper(II) in quinoline and allowing the solution to stand for several hours. The dark green crystals of the adduct that were formed were separated, but, on exposure to air, lost quinoline readily and reverted to the blue-grey bisacetylacetonatocopper(II) chelate. The *X*-ray studies were carried out with crystals of the adduct coated with paraffin wax. The compound forms triclinic crystals in the space group $P\bar{1}$, ($a = 14{\cdot}23$, $b = 8{\cdot}66$, $c = 8{\cdot}02$ Å, $\alpha = 94{\cdot}0°$, $\beta = 89{\cdot}4°$, $\gamma = 110{\cdot}8°$ and $Z = 2$).

The intensities of about 630 non-zero independent ($hk0$), ($h0l$), and ($0kl$) reflections were measured by the multiple film technique on Weissenberg photographs obtained with Cu-K_α radiation. No absorption corrections were made. Minimum functions of the projections down the y and z axes were synthesized graphically and the positions of all the atoms were located. The atomic co-ordinates were refined by successive Fourier and difference-Fourier syntheses until $R = 0{\cdot}14$, $0{\cdot}13$, and $0{\cdot}14$ for the ($hk0$), ($h0l$), and ($0kl$) reflections respectively. The overall temperature factors were, 4·2, 4·9, and 3·5Å^2 for the ($hk0$), ($h0l$), and ($0kl$) data. Absorption effects were partly responsible for the variation in these temperature factors.

The projection of the structure on a plane normal to the z-axis is shown in the Figure. The copper atom is penta-co-ordinated to the four oxygen atoms in the acetylacetone molecules, and to the nitrogen atom of the quinoline molecule. The four oxygen atoms are arranged in a square-planar configuration around the copper atom, which is located above the plane formed by the oxygen atoms. The planes of the acetylacetone molecules are bent away from the apical co-ordination site. It appears, therefore, that adduct formation has affected the planarity of the chelate rings and altered the symmetry of the molecule. This unexpected effect should have interesting consequences on the spectra of this compound.

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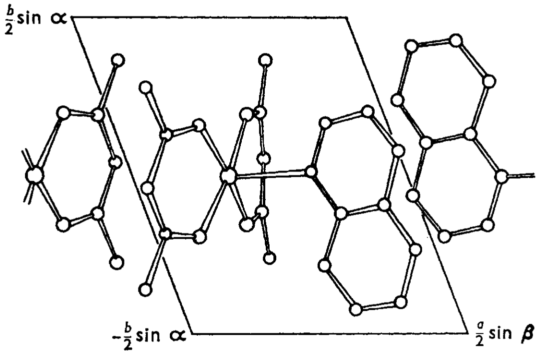

FIGURE

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