The Crystal and Molecular Structure of 3-Benzyl-2,6-diphenyl-2*H*-thiopyran-5-carboxaldehyde

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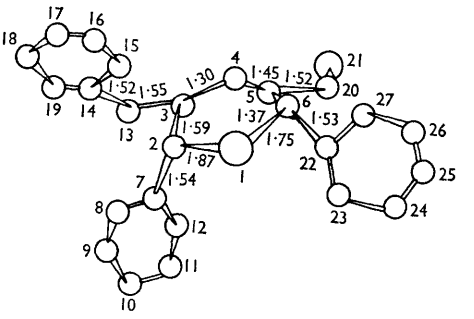
CHEMICAL, n.m.r., infrared, ultraviolet, and mass spectral data on a compound, $C_{25}H_{20}OS$, of unknown constitution suggested that several ring structures are possible. In the preceding Communication the synthesis and interpretation of these chemical and physical data are described.[1] An *X*-ray diffraction study of this compound shows that it is 3-benzyl-2,6-diphenyl-2*H*-thiopyran-5-carboxaldehyde.

The crystals are monoclinic with lattice constants, $a = 11{\cdot}004$, $b = 11{\cdot}062$, $c = 16{\cdot}855$ Å,

$\beta = 96{\cdot}5°$. The space group is $P2_1/n$ and there are four molecules in the unit cell. The intensities of 900 independent reflections were measured visually from Weissenberg photographs taken with Cu-K_α radiation. The crystal structure was solved from the Patterson analysis by location of the sulphur atom, and subsequent Fourier phases on the partial structure. Refinement by using Busing, Martin, and Levy's full-matrix least-squares programme has given an R of 16·4% refining positional and individual isotropic thermal parameters. The structure is given in the figure with pertinent bond distances. The thiopyran ring is nonplanar. The C(6)–S(1) distance of 1·75 Å indicates a partial double-bond character.



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[1] S. E. Cremer and A. V. Subbaratnam, preceding Communication.