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# THE CRYSTAL AND MOLECULAR STRUCTURE OF 3-MERCAPTO-1,3-DIPHENYLPROP-2-ENE-1-ONE

L.F. Power and K.E. Turner
James Cook University of North Queensland, Townsville, Australia

F.H. Moore
Australian Institute for Nuclear Science and Engineering,
Lucas Heights, Australia.

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Previous studies (1-4) of β-diketones have shown that these compounds exist, in the solid, in the enolic form with localisation of the enolic hydrogen. In view of the similarities between the β-diketones and the monothio-β-diketones it was felt appropriate to investigate a representative monothio-β-diketone in some detail.

Crystal data are as follows :

$C_{15}H_{12}SO$: $P2_{1/c}$ (No.14); a = 12.533(6), b = 7.435(7), c = 13.228(7),
β = 98.066(16), $D_m$ = 1.23; $D_c$ = 1.31; z = 4; $MoK_\alpha$ radiation.

Crystals were grown by slow evaporation from acetone. Two sets of equivalent reflections were collected on the A.A.E.C.'s computer controlled X-ray diffractometer employing a solid state detector, to yield a unique set of 1176 reflections. No absorption correction has yet been applied.

TABLE 1 - ATOMIC COORDINATES ($\times 10^4$)

| | x/a | y/b | z/c | | x/a | y/b | z/c |
|---|---|---|---|---|---|---|---|
| $C_1$ | 3138(5) | 3632(12) | 792(5) | O | 4852(4) | 4481(8) | 2181(3) |
| $C_2$ | 2265(6) | 3266(13) | 74(6) | S | 6968(2) | 4083(4) | 3257(2) |
| $C_3$ | 2394(6) | 2516(13) | -841(6) | $H_{SO}$ | 5480(48) | 4514(95) | 2733(47) |
| $C_4$ | 3408(6) | 2111(13) | -1056(5) | $HC_1$ | 3043(46) | 4019(90) | 1389(43) |
| $C_5$ | 4289(5) | 2428(11) | -323(5) | $HC_2$ | 1607(49) | 3549(94) | 250(46) |
| $C_6$ | 4166(5) | 3193(10) | 607(5) | $HC_3$ | 1760(52) | 2302(99) | -1349(48) |
| $C_7$ | 5092(5) | 3516(11) | 1416(5) | $HC_4$ | 3513(51) | 1527(94) | -1665(48) |
| $C_8$ | 6104(5) | 2852(10) | 1384(5) | $HC_5$ | 5008(46) | 2218(89) | -502(42) |
| $C_9$ | 7001(5) | 3017(10) | 2143(5) | $HC_8$ | 6195(42) | 2199(82) | 857(39) |
| $C_{10}$ | 8037(5) | 2242(10) | 1946(5) | $HC_{11}$ | 7884(46) | 2789(88) | 422(42) |
| $C_{11}$ | 8340(5) | 2275(11) | 982(5) | $HC_{12}$ | 9567(49) | 1860(94) | 137(47) |
| $C_{12}$ | 9328(6) | 1634(12) | 809(6) | $HC_{13}$ | 10657(48) | 545(92) | 1510(46) |
| $C_{13}$ | 10035(6) | 951(12) | 1591(6) | $HC_{14}$ | 10196(48) | 372(91) | 3136(44) |
| $C_{14}$ | 9737(6) | 841(12) | 2553(6) | $HC_{15}$ | 8564(49) | 1370(90) | 3395(45) |
| $C_{15}$ | 8765(6) | 1532(12) | 2730(5) | | | | |

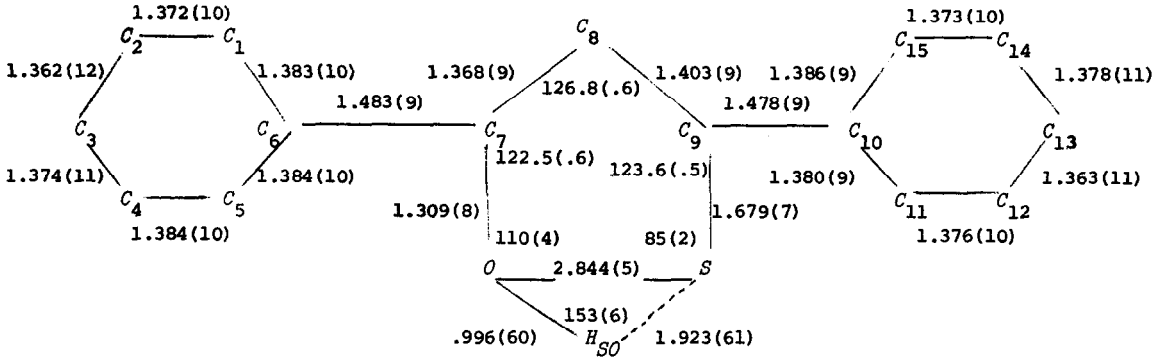


Fig.1 Bond Lengths and Angles

The structure was solved using the Symbolic Addition technique and all non-hydrogen atom positions located. Refinement, using block diagonal least squares and an empirical weighting scheme, proceeded smoothly and converged to an R(Fo) value of 11.5%. Phenyl hydrogen atoms were placed at calculated positions with individual isotropic thermal parameters of the atoms to which they were attached. The S - H - O hydrogen was located subsequently. Final cycles of least squares led to an R(Fo) = 7.8% and $R(Fo^2)$ = 6.8%. Positional parameters are listed in Table 1 while bond lengths and some angles are shown in Figure 1. For clarity C - H bond lengths and angles have been omitted from the figure.

As is the case for the β-diketones, the monothio-β-diketone ring exhibits an alternation of short-long bond lengths indicative of at least partial electron localisation. The S - H - O hydrogen is located on the oxygen atom, and the whole system exists in the enolic form in a manner analogous to the β-diketones.

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