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The structures of two bromo-β-hydroxy-*cyclo*heptatrienones.

By T. R. R. McDonald, *Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England*

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The α-hydroxy-*cyclo*heptatrienones (α-hydroxy-tropones, tropolones) have been known for several years, and have been extensively studied. X-ray results confirm a seven-membered ring structure (Robertson, 1951; Sasada, Osaki & Nitta, 1954). β-Hydroxy-tropones have recently been prepared (Johnson & Johns, 1954). The crystal structures of the 2-bromo and 7-bromo derivatives of β-hydroxy-tropone are reported here. The chemical configurations are confirmed. Both structures are being refined in view of the interest which attaches to the fine structure of the seven-membered ring system.

2-Bromo-3-hydroxy-tropone, $C_7O_2H_5Br$

Molecular weight 201·0; brown needles; space group $P2_12_12_1$;

$a = 13{\cdot}3$, $b = 12{\cdot}8$, $c = 4{\cdot}00$ Å, all ±1%;
$V = 681$ Å^3; $Z = 4$; $\varrho_c = 1{\cdot}96$ g.cm.$^{-3}$.

Fig. 1(*a*) shows the electron density projected down the *c* axis. The agreement index $R(hk0) = \Sigma||F_o|-|F_c|| \div \Sigma|F_o|$ is 0·15 at the present stage of the refinement. The molecules appear to be held together by hydrogen bonds between the hydroxyl and carbonyl oxygen atoms. The refinement has proceeded far enough to show that the bond lengths in the ring are not all equal.

7-Bromo-3-hydroxy-tropone

Yellow needles; space group $P2_12_12_1$;

$a = 14{\cdot}0$, $b = 12{\cdot}3$, $c = 4{\cdot}00$ Å, all ±1%;
$V = 689$ Å^3; $Z = 4$; $\varrho_c = 1{\cdot}94$ g.cm.$^{-3}$.

The *c*-axis projection of the electron density is shown in Fig. 1(*b*). For this zone, $R = 0{\cdot}25$. The two structures are very similar as regards atomic positions in the unit cell, but in this case the hydrogen bonding appears to lead to dimer or chain formation about the screw axes. It is to be noted that, at the present stage of the analysis, the results for this compound are equally consistent with the 4-bromo configuration, the carbonyl and hydroxyl oxygen atoms being indistinguishable.

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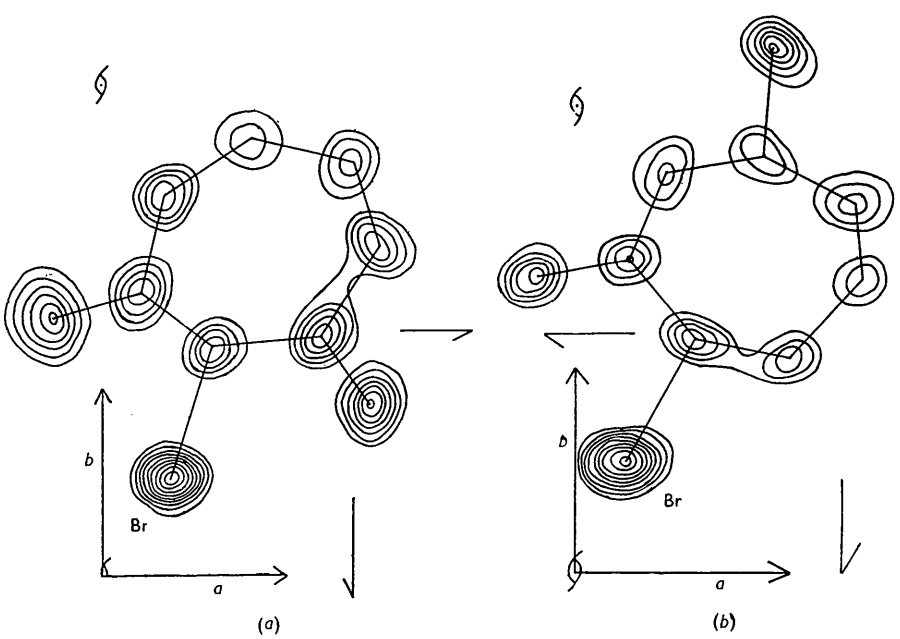

Fig. 1. (*a*) 2-Bromo-3-hydroxy-tropone: *c*-axis projection. Contours at an interval of approximately 2 e.Å^{-2} for carbon and oxygen, and 10 e.Å^{-2} for bromine. (*b*) 7-Bromo-3-hydroxy-tropone: *c*-axis projection. Contours as for (*a*).