confirmed by the relatively large standard deviations in the coordinates of the Al atoms.

Statistical tests to distinguish between centrosymmetric and noncentrosymmetric structures seem inappropriate in this case. Any departures from a centrosymmetric arrangement must be small and to these the tests are relatively intensitive. The structures are also strongly layered, a feature which can significantly disturb the statistical distribution of intensities.

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## The unit-cell dimensions and space group of 2-(benzylthio)imidazoline and 2-(benzylthio)tetrahydropyrimidine hydrochlorides.

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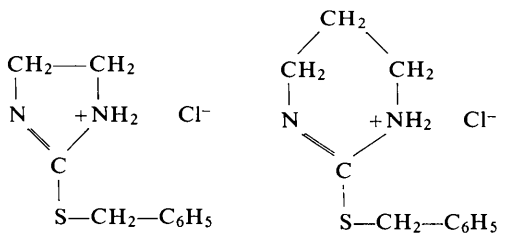
Crystals of 2-benzylthioimidazoline and of 2-benzylthiotetrahydropyrimidine hydrochlorides are isostructural. They crystallize in the orthorhombic system, space group $P2_12_12_1$, with $a=11{\cdot}06$, $b=10{\cdot}50$, $c=11{\cdot}25$ Å, $Z=4$, and $a=10{\cdot}93$, $b=11{\cdot}25$, $c=10{\cdot}17$ Å, $Z=4$, respectively.

In the course of investigations on the structure of thioamides, cyclic thioureines and related compounds (Piazzesi, Bardi, Mammi & Walter, 1964; Mammi, D'Angeli & Bezzi, 1965; Del Pra, D'Angeli & Di Bello, 1966) the hydrochlorides of 2-(benzylthio)imidazoline (I) and of 2-(benzylthio)tetrahydropyrimidine (II) (McKay & Hatton, 1956) have been examined by X-rays.




(I) (II)

The compounds were prepared by refluxing in ethanol for some hours the corresponding thioureines with benzyl chloride.

Single crystals were grown from ethanol solution as colourless prisms, with rectangular cross section, elongated along [100].

From Weissenberg and precession photographs of zero and upper layers, the crystal symmetry and the unit-cell dimensions of the two compounds were determined. The crystal densities were measured by flotation in carbon tetrachloride–benzene.

The physical and crystallographic data are reported in Table 1.

Table 1. *Crystallographic data*

| | (I) | (II) |
|---|---|---|
| | $C_{10}H_{13}SN_2Cl$ | $C_{11}H_{15}SN_2Cl$ |
| M.W. | 228·8 | 242·8 |
| m.p. (°C) | 170 | 183 |
| Crystal system | Orthorhombic | Orthorhombic |
| Space group | $P2_12_12_1$ | $P2_12_12_1$ |
| $a$ (Å) | 11·06 ± 0·01 | 10·93 ± 0·01 |
| $b$ (Å) | 10·50 ± 0·01 | 11·25 ± 0·01 |
| $c$ (Å) | 10·04 ± 0·01 | 10·17 ± 0·01 |
| $V$ (Å$^3$) | 1165·1 | 1252·0 |
| $D_x$ (g.cm$^{-3}$) | 1·303 | 1·288 |
| $D_m$ (g.cm$^{-3}$) | 1·310 | 1·281 |
| $Z$ | 4 | 4 |
| $F(000)$ (e) | 480 | 512 |
| $\mu_{CuK\alpha}$ (cm$^{-1}$) | 42·3 | 39·2 |
| $\mu_{MoK\alpha}$ (cm$^{-1}$) | 4·7 | 4·3 |

It was apparent both from these data and from a straightforward comparison of diffraction intensities that compounds (I) and (II) are isostructural.

No further work is contemplated.

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