sodium 3,5-dibromobenzoate; it was recrystallized from propan-1-ol–water (2:3) and had m.p. 265° (decomp.). (Found: C, 30·4; H, 1·8; N, 5·0. $C_7H_6Br_2N_2$, $C_7H_4Br_2O_2$ requires C, 30·1; H, 1·8; N, 5·0%).

The crystals were columnar with marked striations along the [001] axis which is also the direction of elongation. Cleavage was perfect parallel to (100). Refractive index for polarized white light travelling along [010] was $1·615 \pm 5$ parallel to [001] and $1·750 \pm 5$ parallel to [100].

Orthorhombic

$a = 23·8$, $b = 32·1$, $c = 4·85$ Å, $U = 3705$ Å^3,
$D_m = 2·10$ g.cm.$^{-3}$, $Z = 8$, $D_x = 2·00$ g.cm.$^{-3}$.

S-Methylthiuronium benzoate
$CH_3S.C(:NH).NH_2$, $C_6H_5.CO_2H$

S-Methylthiuronium benzoate gave columnar crystals (Walker, 1949) with marked striations in the direction of elongation [001]. Cleavage was perfect parallel to (100).

Orthorhombic

$a = 9·52$, $b = 20·29$, $c = 5·61$ Å, $U = 1084$ Å^3,
$D_m = 1·28$ g.cm.$^{-3}$, $Z = 4$, $D_x = 1·30$ g.cm.$^{-3}$.

Space group $P2_12_12_1$. Absences observed: $h00$ when h odd, $0k0$ when k odd, $00l$ when l odd.

S-Methylthiuronium *p*-iodobenzoate
$CH_3S.C(:NH).NH_2$, $C_6H_4I.CO_2H$

S-Methylthiuronium *p*-iodobenzoate was obtained from S-methylthiuronium sulphate and sodium *p*-iodobenzoate; it was recrystallized from water and had m.p. 220° (decomp.). (Found: C, 32·1; H, 3·2; N, 8·2. $C_2H_6N_2S$, $C_7H_5IO_2$ requires C, 32·0; H, 3·3; N, 8·3%).

The crystals were prismatic or needle-shaped and cleavage was not pronounced. Interpenetrating twins were fairly common producing a pseudo-symmetry plane perpendicular to [100].

Monoclinic

$a = 9·40$, $b = 5·61$, $c = 23·55$ Å, $\beta = 101·5°$, $U = 1217$ Å^3,
$D_m = 1·82$ g.cm.$^{-3}$, $Z = 4$, $D_x = 1·85$ g.cm.$^{-3}$.

Space group $P2_1/c$ or $P2/c$. Absent reflexions: $h0l$ if l odd; $0k0$: only the second order observed.

S-Methylthiuronium *p*-bromobenzoate
$CH_3S.C(:NH).NH_2$, $C_6H_4Br.CO_2H$

S-Methylthiuronium *p*-bromobenzoate was similarly prepared from S-methylthiuronium sulphate and sodium *p*-bromobenzoate; it had m.p. 214° (decomp.). (Found: C, 37·3; H, 3·9; N, 9·5. $C_2H_6N_2S$, $C_7H_5BrO_2$ requires C, 37·2; H, 3·8; N, 9·6%).

The majority of crystals were tabular but a few prisms were also observed. Cleavage was imperfect parallel to (100). Frequent twinning as in isomorphous iodo-compound was observed.

Monoclinic

$a = 9·505 \pm 5$, $b = 5·61 \pm 1$, $c = 22·556 \pm 10$ Å,
$\beta = 103·22 \pm 5°$, $U = 1171$ Å^3, $D_m = 1·625$ g.cm.$^{-3}$,
$Z = 4$, $D_x = 1·651$ g.cm.$^{-3}$.

Space group $P2_1/c$ from systematic absences and from the appearance of the Patterson projection on $(0kl)$ which contained no prominent peaks related to a twofold axis.

S-Methylthiuronium *p*-chlorobenzoate
$CH_3S.C(:NH).NH_2$, $C_6H_4Cl.CO_2H$

S-Methylthiuronium *p*-chlorobenzoate was prepared in an analogous manner; it had m.p. 210–211° (decomp.). (Found: C, 44·1; H, 4·8; N, 11·2. $C_2H_6N_2S$, $C_7H_5ClO_2$ requires C, 43·8; H, 4·5; N, 11·4%).

It is isomorphous with the bromo-compound.

Monoclinic

$a = 9·505 \pm 5$, $b = 5·61 \pm 1$, $c = 22·176 \pm 10$ Å,
$\beta = 103·22 \pm 5°$, $U = 1151$ Å^3, $D_m = 1·41$ g.cm.$^{-3}$,
$Z = 4$, $D_x = 1·422$ g.cm.$^{-3}$.

Space group $P2_1/c$ from systematic absences.

References

KENNARD, O. & WALKER, J. (1954). *Acta Cryst.* **7**, 646.
KENNARD, O. & WALKER, J. (1961). (Forthcoming publication.)
LOW, B. W. & RICHARDS, F. M. (1952). *J. Amer. Chem. Soc.* **74**, 1660.
PINNER, A. (1892). *Die Imidoäther und ihre Derivate*, p. 158. Berlin: Oppenheim.
WALKER, J. (1949). *J. Chem. Soc.*, p. 1996.
WEISZ, O., COCHRAN, W. & COLE, W. F. (1948). *Acta Cryst.* **1**, 83.

Acta Cryst. (1961). **14**, 92

Données cristallographiques sur le diphényl méthane.

Par M. J. HOUSTY, *Laboratoire de Minéralogie et de Rayons X, Faculté des Sciences, Université de Bordeaux, France*

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Le diphényl méthane cristallise sous forme de cristaux monocliniques, incolores, allongés suivant la direction [010]. Ces cristaux sont obtenus par cristallisation à une température légèrement inférieure à la température de fusion (25 °C.) dans un bain thermostaté au 1/50ème de degré centigrade.

Le diphényl méthane étant volatil à la température ordinaire nous avons enfermé le cristal dans un tube de verre scellé.

L'étude radiocristallographique a été faite à l'aide d'une chambre de Bragg et d'un rétigraphe de de Jong, en utilisant la radiation Cu $K\alpha$. Nous avons ainsi déterminé les paramètres de la maille monoclinique:

$a = 8,95 \pm 0,04$, $b = 6,22 \pm 0,03$, $c = 20,50 \pm 0,05$ Å;
$\beta = 120° \pm 1°$.

Nombre de molécules par maille: 4.

La densité observée de 1,008 g.cm.$^{-3}$ est en bon accord avec celle calculée 1,017 g.cm.$^{-3}$ à partir des données cristallographiques.

Groupe spatial $P2_1/c$ ou $P2/c$.

Une étude plus poussée de cette structure est en cours.