

Acta Cryst. (1964). **17**, 209**Crystallographic data for DL-thiomalic acid, dihydrositsirikine *p*-bromobenzoate, and a methyl trichloro-trideoxy-hexoside.** By G. SMALL and J. TROTTER, *Department of Chemistry, University of British Columbia, Vancouver 8, B. C., Canada*

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Crystallographic data are given in Table 1 (λ , Cu $K\alpha$ = 1.5418 Å, λ , Mo $K\alpha$ = 0.7107 Å) for the three compounds.

Table 1. *Crystallographic data*

	DL-Thiomalic acid $C_4H_6O_4S$	Dihydro-sitsirikine <i>p</i> -bromobenzoate $C_{28}H_{31}N_2O_4Br$	Methyl trichloro-trideoxy-hexoside $C_7H_{11}O_3Cl_3$
<i>M</i>	150.2	539.5	249.5
Crystal system	Monoclinic	Orthorhombic	Monoclinic
<i>a</i>	5.23 ± 0.01 Å	37.79 ± 0.10 Å	7.87 ± 0.01 Å
<i>b</i>	14.19 ± 0.03	22.88 ± 0.07	5.42 ± 0.01
<i>c</i>	16.98 ± 0.03	16.09 ± 0.05	35.86 ± 0.05
β	96.6 ± 0.1°	—	119.9 ± 0.2°
<i>U</i>	1251 Å ³	13912 Å ³	1326 Å ³
<i>Z</i>	8	~20	4
<i>D_m</i>	~1.5 g.cm ⁻³	~1.25 g.cm ⁻³	1.25 g.cm ⁻³
<i>D_x</i>	1.59	1.29	1.25
Space group	<i>Cc</i> or <i>C2/c</i>	<i>P2₁2₁2₁</i>	<i>P2</i>

The DL-thiomalic acid crystals, HO₂C.CH(SH).CH₂.CO₂H, are colourless needles elongated along [100], and frequently twinned. The diffraction pattern exhibited a series of diffuse streaks parallel to *c**, through every reciprocal lattice point, and with occasional maxima of spacing about $\frac{1}{3}c^*$. These streaks probably correspond to a disordered structure with a partially ordered superlattice; no outstanding peaks corresponding to S-S vectors could be located on the *a*-axis Patterson projection. Crystals of dihydrositsirikine *p*-bromobenzoate are fine colourless needles elongated along [100]; the large unit cell, and large number of molecules in the cell, indicate a complex structure. Crystals of the hexoside are colourless needles elongated along [010]. Since the compound is optically active ($[\alpha]_D = +159^\circ$ in methanol), the alternative space groups, *Pm* and *P2/m*, are ruled out; there are two molecules in the asymmetric unit, so that structure analysis requires the initial location of six chlorine atoms.

As a result of these various complicating features no further work on these compounds is planned.

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Acta Cryst. (1964). **17**, 209**An X-ray powder investigation of ordered Au₃Mn.** By D. P. MORRIS and J. L. HUGHES, *Department of Physics, University College of North Wales, Bangor, Wales*

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The alloy Au₃Mn has been the subject of several recent investigations. Raub, Zwicker & Baur (1953) originally found that the high-temperature disordered f.c.c. solid solution of Mn in Au suffered a transformation at 645 °C into an ordered structure which was not determined. Resistance and magnetic measurements were made by Giansoldati & Linde (1955) and by Giansoldati, Linde & Borelius (1959). The knee observed in the resistance-temperature curve at 650 °C was characteristic of order-disorder, whilst that at -123 °C was attributed to a Néel point in the ordered alloy. Meyer (1957) carried out detailed magnetic measurements and observed a Néel point at 145 °K (-128 °C), and concluded that the ordered structure was a metamagnetic. The crystal structure has been investigated by Watanabe (1958, 1960) by electron diffraction on thin films and it was deduced that the structure can be thought of as formed from the fundamental face-centred orthorhombic lattice ($a_1 = 4.08$, $a_2 = 4.05$, $a_3 = 4.03$ Å) in which the atoms arrange themselves as in the ordered structure of Cu₃Au,

but the two kinds of step-shift, $\pm(a_2 \pm a_3)/2$ and $\pm(a_3 \pm a_1)/2$, occur at every M_1 and M_2 cells along the *x* and *y* directions respectively. M_1 and M_2 were found not to be integers but the idealized lattice of the ordered Au₃Mn was considered to have a unit cell of dimensions $2a_1, 4a_2, a_3$ (or a $2 \times 4 \times 1$ cell). The magnetic behaviour of disordered and ordered Au₃Mn has also been reported by Jacobs, Kouvel & Lawrence (1962) and by Sato, Hirone, Watanabe, Maeda & Adachi (1962). The former authors in their discussion assumed the ordered structure to be the idealized $2 \times 4 \times 1$ superlattice of Watanabe, whilst Sato *et al.* quote a table of observed and calculated lattice spacings and intensities based on a $2 \times 4 \times 1$ superlattice cell, but with a fundamental face-centred orthorhombic cell having $a = 4.08$, $b = 4.04$, $c = 4.01$ Å.

Morris & Hughes (1962) reported that a structure having a fundamental orthorhombic unit cell of dimensions $a = 4.0814$, $b = 4.0599$, $c = 4.0377$ Å, and referred to by them as the α'' phase, existed between about 21.0 and 22.2 at.% Mn after appropriate heat treatment.