1·09 Å and free rotation of the methyl groups) are 2·33 Å.

Standard deviations

The standard deviations of the atomic positions were calculated from Cruickshank's formulae. From the *hk*0 data, $\sigma(x) = \sigma(y) = 0{\cdot}013$ Å for carbon, 0·011 Å for nitrogen and 0·010 Å for oxygen. The standard deviations of the individual bond lengths are 0·018 Å for C–C, 0·017 Å for C–N, and 0·015 Å for N–O.

Discussion

Within the limits of experimental error all the carbon atoms and the nitrogen atom lie in one plane, but since the *z*-coordinates have been determined with less accuracy than the *x* and *y* parameters it is possible that small deviations from strict planarity have not been detected. The oxygen atoms lie one above and one below the plane of the carbon and nitrogen atoms at distances of 0·95 Å, so that the nitro group is tilted out of the aromatic plane, the angle of tilt being 66·4°. This tilt is very similar to that found in 9:10-dinitroanthracene—63·7° (Trotter, 1959*c*).

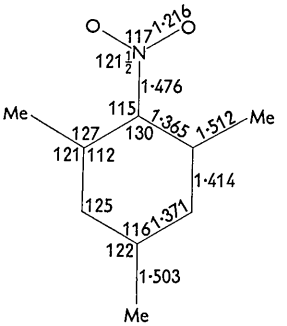

Fig. 3. Bond lengths and valency angles.

The molecular dimensions shown in Fig. 3 indicate that the repulsive forces between the oxygen atoms and the neighbouring methyl groups cause considerable distortions of the valency angles from the normal 120°, in addition to the large deviation of the nitro group from coplanarity with the aromatic ring. The mean bond lengths (with standard deviations) are

$$\begin{aligned} C_{ar}–C_{ar} &= 1{\cdot}383 \pm 0{\cdot}007 \text{ Å} \\ C_{ar}–C_{al} &= 1{\cdot}509 \pm 0{\cdot}010 \\ C_{ar}–N &= 1{\cdot}476 \pm 0{\cdot}017 \\ N–O &= 1{\cdot}216 \pm 0{\cdot}011 \end{aligned}$$

Intermolecular distances

All the intermolecular contacts correspond to normal van der Waals interactions. The shortest oxygen–oxygen distance is 3·66 Å between O_1 of the standard molecule and O_2 of the molecule with coordinates $(\bar{x}, 1-y, \frac{1}{2}+z)$. The shortest oxygen–carbon separation is between $O_2(x, y, z)$ and $C4(\bar{x}, \bar{y}, -\frac{1}{2}+z)$ where the distance is 3·29 Å, while the shortest carbon–carbon contact is 3·67 Å between $C3(x, y, z)$ and $C3(\bar{x}, \bar{y}, \frac{1}{2}+z)$. The shortest contact involving nitrogen is 4·12 Å. The perpendicular distance between the planes of the aromatic rings $= \frac{1}{2}c = 3{\cdot}63$ Å.

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Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 500 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible; and proofs will not generally be submitted to authors. Publication will be quicker if the contributions are without illustrations.

Acta Cryst. (1959). **12**, 607

The structure of Au_2Mn.

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The intermetallic compound Au_2Mn possesses interesting magnetic properties which seem to require an examination of its crystal structure. The first attempt to solve this was by Raub, Zwicker & Baur (1953) in the course of their study of the gold-manganese equilibrium diagram, but their tentative assignation of the lattice gives a fractional number of molecules per unit cell. The solution of the structure was taken up in this department during resistivity studies on the alloy, and a satisfactory determination of the space lattice by one of us has been quoted previously in the paper by Smith & Street (1957). It has now proved possible to solve the structure with reasonable accuracy from powder data alone.

Samples of Au_2Mn powder were heat-treated at 660 °C. for 24 hours and quenched, and diffraction photographs taken using a Unicam evacuable 9 cm. camera and filtered Cu or Fe $K\alpha$ radiation. From the measured

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d values, the lines were identified with Bunn charts, and the parameters so obsained were corrected for absorption using the method of Taylor & Floyd (1950). These measurements gave the lattice as tetragonal, $a_0 = 3{\cdot}363$ Å, $c/a = 2{\cdot}555$—values which differ slightly from those previously published. The X-ray density with 2 molecules per unit cell, is 15·33 g.cm.$^{-3}$, compared with an experimentally determined value of 15·1 g.cm.$^{-3}$.

The characteristic absences with $h+k+l$ odd immediately identified the lattice as body-centred, and a study of the space-group tables revealed that only two were possible:

$I\bar{4}m2$: Mn at 0, 0, 0; $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$; Au at $0, \frac{1}{2}, z$; $\frac{1}{2}, 0, \bar{z}$;

$I4/mmm$: Mn at 0, 0, 0; $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$; Au at $0, 0, z$; $0, 0, \bar{z}$.

The former was, however, excluded, as the {112} line was not detected, and $|F_c|$ cannot be made zero for this line in this space group, whatever the value of z. On the other hand, the latter group gives $|F_c| = 0$ for the {112} line with $z \simeq \frac{3}{8}$.

Values of F_0 were therefore determined for each line after microdensitometry of the film. Standard tables were used, but the introduction of the absorption factor, which includes an unknown packing fraction for the powder, of necessity introduces errors which, with the radiation used, may be appreciable. Graphs of $|F_c|$ were made for seven selected lines for values of z between $\frac{1}{4}$ and $\frac{3}{8}$. A comparison of F_0 and $|F_c|$ then allowed the value of z to be chosen for best fit as $z = (0{\cdot}35 \pm 0{\cdot}01)$; the agreement with the other lines then appears satisfactory, as can be seen from Table 1. A scale drawing of the structure, taken on the (110) plane containing the 2 manganese atoms, is shown in Fig. 1. The Mn–Mn separation is thus 4·91 Å, and each Mn atom is surrounded by gold atoms at a distance of either 2·64 Å or 3·01 Å. Coupling between the manganese atoms must therefore take place *via* two gold atoms.

After this work was completed, our attention was drawn to a paper by Herpin, Meriel & Meyer (1958) who had independently solved the structure by neutron diffraction. Their accuracy was however lower, and gave $z \simeq \frac{1}{3}$.

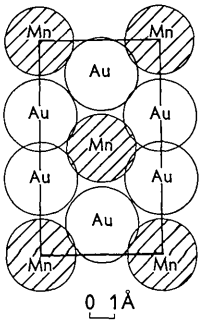

Fig. 1. Scale model of Au_2Mn. Atomic diameter of Au and Mn 3·0 and 2·6 Å respectively. $a_0 = 3{\cdot}364$ and $c_0 = 8{\cdot}596$ Å. Distance between centres of a Mn atom and either of its two Au atoms = $0{\cdot}35c_0$. Section is (110) face.

Table 1. *Table of d values, F_o and $|F_c|$ for observed and possible reflexions from* Au_2Mn

hkl	*d*	F_o	$\lvert F_c\rvert$
101	3·1265	130	132
110	2·3652	280	280
103	2·1914	250	259
112	—	—	45
200	1·6762	264	258
114	1·6021	138	138
105	—	—	28
202	—	—	35
211	1·4774	138	99
006	1·4519	242	230
213, 204	1·3325	138	140
116	1·2405	240	172
220	1·1867	232	220
107	1·1676	138	151
222	—	—	60
301	—	—	124
206	1·0995	138	162
008	—	—	20
310	1·0625	134	204
224, 303	1·0463	134	127
312	—	—	66
118	—	—	40
217, 314	0·9584	90	132
305	—	—	21
109	0·9332	102	90
226	0·9207	130	147
208	—	—	23
323	0·8872	100	147
0,0,10, 316	0·8592	130	140

Additional calculated values

hkl	'*d*'	$\lvert F_c\rvert$
105	1·5282	28
222	1·1392	60
301	1·1097	124
008	1·0695	20
312	1·0263	66
305	0·9347	21
208	0·90227	23

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