Acta Cryst. (1957). **10**, 128

An X-ray Analysis of Bivalent Silver Nicotinate

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(*Received* 22 *August* 1956 *and in revised form* 26 *October* 1956)

Bivalent silver nicotinate is tetragonal with $a = b = 6{\cdot}98$, $c = 12{\cdot}68$ Å; $Z = 2$.

The molecular formula of bivalent silver nicotinate, which is chocolate-red in colour, is $Ag[C_6H_4NO_2]_2$. The molecular formula was established by oxidimetric and gravimetric tests, and the bipositive nature of silver was proved from the measurement of magnetic susceptibility. The full details of the preparation and properties of the substance have been given by Banerjee & Rây (1955).

Table 1. *Intensities and observed and calculated* $\sin^2\theta$ *values for hkl planes*

I	$(\sin^2\theta)_{obs.}$	$(\sin^2\theta)_{calc.}$	hkl
vs	0·0121	0·0122	100
vw	0·0150	0·0148	002
w	0·0241	0·0244	110
s	0·0331	0·0333	003
ms	0·0394	0·0392	112
ms	0·0487	0·0488	200
m	0·0596	0·0592	004
s	0·0656	0·0647	211
m	0·0837	0·0836	114
m	0·0940	0·0943	213
mw	0·1115	0·1124	222
vs	0·1222	0·1220	310
w	0·1335	0·1332	006
m	0·1438	0·1431	303
s	0·1542	0·1535	215
		0·1553	313
vw	0·1635	0·1623	321
w	0·1736	0·1734	322
mw	0·1890	0·1901	225
w	0·2044	0·2057	117
m	0·2294	0·2301	207
mw	0·2397	0·2407	413
w	0·2514	0·2511	325
w	0·2887	0·2877	405
w	0·3014	0·2999	415
		0·2997	009
w	0·3237	0·3241	119
w	0·3366	0·3365	425
w	0·3582	0·3588	318
		0·3575	521
w	0·3752	0·3765	407
		0·3764	514
vw	0·4126	0·4130	524
vw	0·4532	0·4540	602
vw	0·4683	0·4676	2,2,10
vw	0·5077	0·5073	535
vw	0·5198	0·5213	623
vw	0·5338	0·5335	543
vw	0·5467	0·5480	536
		0·5450	1,0,12
w	0·5634	0·5638	632
w	0·5949	0·5961	537

As the substance was available only in powder form, the analysis was carried out by the powder method, using Cu $K\alpha$ radiation. A preliminary investigation on the spacing and intensity of each line was reported by Chackraburtty & Banerjee (1955). A redetermination of the θ values was carried out and the 37 q values ($q = (\sin^2\theta)_{obs.}$) are tabulated in Table 1. By means of the methods suggested by Hesse (1948) and Stosick (1949), and within the experimental measurements of the θ's, the following relations were obtained from the analysis of the first 9 q's, namely

$$q_6 = 2q_3;\ q_3 = 2q_1;\ q_3+q_7 = q_9;\ q_2+q_3 = q_5;\ q_7 = 4q_2.$$

From the relations $q_6 = 2q_3 = 4q_1$, the system appears to be tetragonal with $A = 0{\cdot}0121/M_1$, where $M_1 = (h^2+k^2)$. From the relation $q_7 = 4q_2$ and $q_7+q_3 = q_9$, $Cl^2 = 0{\cdot}0596$. Also from the data it was evident that $q_2/4 = q_4/9 = q_7/16$; therefore $C = 0{\cdot}0596/16 = 0{\cdot}003725$. For indexing all the lines, particularly the lines at large $\sin^2\theta$ values, it was found that $M_1 = 1$; therefore $A = 0{\cdot}0121$. After some modification of the constants A was taken as 0·0122 and C as 0·00370. With these values of A and C all the lines were satisfactorily indexed and no better fit with a smaller unit cell could be found. The values of A and C give

$$a=b=6{\cdot}98,\quad c=12{\cdot}68\ \text{Å}\quad (\text{with}\ \lambda(\text{Cu}K\alpha)=1{\cdot}5418\ \text{Å}).$$

The *hkl* values of the lines are shown in Table 1.

The observed density is 1·897 g.cm.$^{-3}$. From the axial lengths of the substance the calculated density is 1·894 g.cm.$^{-3}$. The number of molecules per unit cell is 2. No definite space group is assigned for this substance. Further work is in progress.

The author expresses his thanks to Prof. B. N. Srivastava for his keen interest in the work.

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