ON THE DETERMINATION OF UNIT CELL DIMENSIONS FROM POWDER DIFFRACTION DATA OF COMPLEX SILVER LUTIDINE NITRATE

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ABSTRACT. Debye Scherrer pattern of Silver Lutidine Nitrate has been photographed using a Rigaku camera at room temperature. The analysis showed that the crystal belongs to the orthorhombic system with $a = 13.7$ Å; $b = 16.8$ Å and $C = 7.12$ Å; The unit cell contained four molecules. The space group P222 or Pmm2 can be assigned to the crystal.

INTRODUCTION

Silver Lutidine Nitrate, $Ag(C_7H_9N)_2NO_3$ is a white microcrystatlline substance whose dia-magnetic properties are of special interest. The crystallographic data was obtained from powder diffraction data.

EXPERIMENTAL

A Machlett A-2 X-ray diffraction tube with copper target running at 30 K.V. and 20 m.A. supplied the *X*-rays. The radiation was made monochromatic by using a Ni filter. The specimen, finely powdered, was contained in a Lindamann glass capillary tube of 0.5 mm dimeter and of 0.01mm wall thickness. The Debye Scherrer pattern was obtained in four hours over a photographic film in a Rigaku camera of 9 cm diameter.

The interplanar distances were calculated accurately after measurements on the diffraction pattern and attempts were made to index the powder lines in terms of cubic, tetragonal and hexagonal systems. Since the data did not fit in with any of these systems, Lipson's method (Lipson, 1949) was tried.

The values of $\mathrm{Sin}^2\theta$ for the rings in the powder pattern are given in the table. With these values the difference diagram was drawn according to Lipson's method. The frequently occurring values 0.00315, 0.00206 and 0.01175 were taken as the constants A, B and C respectively.

$$\left(A = \frac{\lambda^2}{4a^2} ; \quad B = \frac{\lambda^2}{4b^2} ; \quad C = \frac{\lambda^2}{4c^2} \right)$$

Using the equation $\text{Sin}^2\theta = Ah^2+Bk^2+Cl^2$ and the above values of A, B and C, all the rings were indexed quite satisfactorily.

The axial lengths calculated from the values of A, B, C are $a = 13.7$Å, $b = 16.8$Å $c = 7.12$Å.

The values of $\text{Sin}^2\theta$, calculated with these axial lengths, the intensities of the lines on the Debye Scherrer pattern and the corresponding d spacing values are given in the table.

As there have been no systematic absences the space group $P222$ or $Pmm2$ can be assigned to the crystal. It contains four molecules per unit cell. The observed density 1.5645gms./c.c. is in good agreement with the calculated density of 1.5535gms/c.c.

TABLE I

No. of lines	Intensity	dÅ observed	Values of Sin $^2\theta$		Indices
			Observed	Calculated	
1.	w	14.188	0.00295	0.00315	100
2.	s	7.384	0.01090	0.01139	120
3.	s	7.018	0.01207	0 01175	001
				0.01260	200
4.	s	6.510	0.01402	0 01381	011
5.	vs	6.010	0.01645	0 01696	111
6.	vvw	5.409	0.02031	0.01999	021
				0.02084	220
7.	w	4.273	0.03255	0.03259	221
				0.03296	040
8.	m	4.088	0.03556	0.03611	140
9.	w	4.004	0.03709	0.03659	320
10.	ms	3.806	0.03998	0.04010	301
11.	s	3.702	0.04334	0.04289	231
12.	vs	3.537	0.04749	0.04700	002
				0.04786	141
				0.04689	330
13.	w	3.387	0.05174	0.05150	050
				0.05221	112
14.	vw	3.222	0.05725	0.05731	241
15.	vw	3.083	0.06253	0.06215	401
16.	vw	2.969	0.06742	0.06784	222
17.	vw	2.896	0.07086	0.07039	421
18.	w	2.744	0.07817	0.07875	500
				0.07741	312
				0.07814	232

TABLE I—(*contd*).

No. of lines	Intensity	dÅ observed	Values of $\sin^2\theta$		Indices
			Observed	Calculated	
19.	s	2.705	0.08124	0.08081	510
				0.08069	431
20.	s	2.645	0.08570	0.08591	061
21.	s	2.581	0.08922	0.08906	161
22.	ms	2.461	0 09813	0.09850	052
				0.09851	261
				0.09874	521
23.	ms	2.347	0.1079	0.10781	013
				0.1083	342
24.	w	2.254	0.1170	0.11714	123
25.	ms	2.182	0.1248	0.12456	460
				0.12415	601
				0.12429	033
				0.12431	162
26.	w	2.091	0.1359	0.1363	461
				0.1362	313
27.	vw	2.042	0.1425	0.1420	551
				0.1423	323
28.	w	2.001	0.1484	0.1489	452
29.	w	1.913	0.1625	0.1625	612
30.	vw	1.867	0.1704	0.1699	253
31.	vw	1.823	0.1785	0.1789	632
32.	w	1.790	0.1854	0.1856	353
33.	vw	1.750	0.1939	0.1934	642
34.	vw	1.724	0.2000	0.2006	204
				0.1999	562
35.	vvw	1.7098	0.2033	0.2030	533
36.	vw	1.658	0.2161	0.2164	304
37.	w	1.618	0.2269	0.2274	623
38.	vw	1.584	0.2363	0.2360	553
39.	vw	1.564	0.2431	0.2427	154
40.	vw	1.540	0.2516	0.2521	254
				0.2521	643
41.	vvw	1.507	0.2618	0.2622	064
42.	vw	1.469	0.2755	0.2750	524
43.	vw	1.444	0.2849	0.2853	534
44.	vw	1.429	0.2909	0.2905	364
45.	vvw	1.396	0.3047	0.3051	125
46.	vw	1.355	0.3238	0.3242	315
47.	vw	1.332	0.3349	0.3344	644
48.	vvw	1.307	0.3480	0.3484	155
49.	vvw	1.288	0.3583	0.3579	255

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