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Crystal structure of α -naphthol picrate. By R. P. RASTOGI and N. B. SINGH, *Department of Chemistry, University of Gorakhpur, Gorakhpur, U. P., India*

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The X-ray powder diagram of α -naphthol picrate has been indexed in terms of an orthorhombic unit cell with $a=9.64$, $b=12.84$, $c=6.70$ Å.

The solid-state reaction between picric acid and naphthols has recently been studied by Rastogi & Singh (1966, 1968). A knowledge of the structural chemistry of picrates is essential to an understanding of the mechanism of the interaction. Hence, the present study was undertaken.

α -Naphthol picrate was prepared by mixing the alcoholic solutions of α -naphthol and picric acid in equimolar proportions. The product was crystallized twice from alcohol. The X-ray diffraction pattern of the powdered substance was recorded with an X-ray diffractogram using Cu $K\alpha$ radiation. The lines of the diffraction pattern were indexed for the orthorhombic and tetragonal systems using the Hesse-Lipson method: the data fitted the orthorhombic system. The agreement between the observed and calculated $\sin^2 \theta(hkl)$ values is satisfactory (Table 1). The unit-cell dimensions are given in Table 2. For the sake of comparison the unit-cell dimensions of picric acid and α -naphthol are also given.

Table 1. Comparison of observed and calculated $\sin^2 \theta(hkl)$ for α -naphthol picrate

Line No.	hkl	$\sin^2 \theta$ (observed)	$\sin^2 \theta$ (calculated)
1	101	0.0194	0.0196
2	111	0.0223	0.0232
3	200	0.0261	0.0256
4	121	0.0331	0.0340
5	031	0.0460	0.0456
6	131	0.0502	0.0520
7	102 } 230 }	0.0585	0.0592
8	140	0.0644	0.0640
9	240	0.0825	0.0832
10	113	0.1284	0.1288
11	332	0.1415	0.1428
12	531	0.2061	0.2056
13	104 } 540 }	0.2175	0.2176
14	124	0.2321	0.2320

Table 1 (cont.)

		$\sin^2 \theta$	$\sin^2 \theta$
15	611	0.2470	0.2472
16	353	0.2652	0.2664
17	640	0.2886	0.2880
18	154	0.3078	0.3076
19	650	0.3208	0.3204
20	115	0.3404	0.3400
21	245	0.4131	0.4132
22	206	0.4999	0.5008
23	0,11,3	0.5539	0.5544
24	285	0.5867	0.5860
25	027	0.6611	0.6612

The density of the crystal as determined by pycnometer using distilled water as the displaced liquid was found to be 1.51 g.cm^{-3} at 19°C . The number of molecules per unit cell was found to be $2.01 \approx 2$. The density of the crystal, from X-ray data, is found to be 1.49 g.cm^{-3} .

A study of the hkl values shows that the crystal is neither body nor face-centred. More structural information will be necessary before the mechanism by which α -naphthol penetrates the lattice of picric acid to yield the corresponding picrate can be discussed.

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References

- RASTOGI, R. P. & SINGH, N. B. (1966). *J. Phys. Chem.* **70**, 3315.
 RASTOGI, R. P. & SINGH, N. B. (1968). *J. Phys. Chem.* **72**, 4446.
 KITAIGORODSKII, A. I. (1961). *Organic Chemical Crystallography*, p. 409. New York: Consultants Bureau.
 WINCHELL, A. N. (1954). *The Optical Properties of Organic Compounds*, p. 87. New York: Academic Press.

Table 2. Lattice parameters of α -naphthol, picric acid and α -naphthol picrate

Lattice parameter	α -Naphthol*	Picric acid†	α -Naphthol picrate
a	13.00	9.25	9.64
b	4.80	19.08	12.84
c	13.40	9.68	6.70
β	$117^\circ 10'$	—	—
Z	4	8	2
Space group	$C_{2h}^5 (P2_1/a)$	Pca	—
Type of crystal	Monoclinic	Orthorhombic	Orthorhombic

* Kitaigorodskii (1961).

† Winchell (1954).