Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible. Publication will be quicker if the contributions are without illustrations.*

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Crystallographic and optical data for *N*-methyl-2,4,6-trinitroacetanilide.*

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Crystallographic and optical data are recorded.

In connection with n.m.r. work conducted in this laboratory, Weissenberg and precession photographs with Cu $K\alpha$ radiation were taken of *N*-methyl-2,4,6-trinitroacetanilide, recrystallized from ethanol, to determine the symmetry and unit-cell size. The crystals were thin, colorless, transparent square plates laying on the (001) face. Cleavage was parallel to the plate. These plates yielded an almost centered Bx_0 figure. A second recrystallization from ethanol yielded large polyhedra. Both morphological forms gave the same crystallographic cells. The cell parameters were determined by least-squaring 19 high angle reflections obtained from a precision Weissenberg camera. The density was determined by flotation methods. Although agreement between calculated and observed density indicated that the unit cell contained no solvent molecules, microscopic examination indicated that the polyhedral form had inclusions of solvent. The systematic absences observed were $0k0$, $k=2n+1$ and $00l$, $l=2n+1$.

Table 1. *Crystallographic data*

a	$=7{\cdot}813\pm0{\cdot}002$
b	$=8{\cdot}666\pm0{\cdot}002$
c	$=17{\cdot}990\pm0{\cdot}001$
β	$=100{\cdot}521\pm0{\cdot}006°$
U	$=1197{\cdot}71$ Å^3
D_m	$=1{\cdot}56$ g.cm^{-3}
D	$=1{\cdot}60$ g.cm^{-3}
Z	$=4$

Space group $P2_1/m$ or $P2_1$

Table 2. *Optical data*

Biaxial(−)
$\alpha=1{\cdot}528\pm0{\cdot}003$
$\beta=1{\cdot}645\pm0{\cdot}003$
$\gamma=1{\cdot}718\pm0{\cdot}003$
$x=1{\cdot}718\pm0{\cdot}003$
$x=\mathbf{b}$
$Z\wedge[001]=74°$
$2V_\alpha=67{\cdot}2°$

* Based on work performed under the auspices of the U.S. Atomic Energy Commission.

† Student aide.

We wish to thank John Weil for supplying the crystals.

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Sur deux déterminations indépendantes de la structure cristalline de la 1,5-dihydroxyanthraquinone.

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(*Reçu le* 24 *février* 1967)

Two independent determinations by X-ray diffraction of the crystal structure of anthrarufin are compared. The discrepancies between the results are given with the r.m.s. from the two refinement methods. The latter are underestimated, as seems to be most frequently the case in structure refinements.

La structure cristalline de l'anthrarufine a fait l'objet d'une note aux *Comptes Rendus de l'Académie des Sciences* (Guilhem, 1964) (Deux projections), et d'une communication aux *Journées de Chimie Organique de la Société Chimique de France*, le 24 septembre 1965 (Structure tridimensionnelle affinée). La publication de la structure complète, faisant partie d'un travail de thèse, a été différée (Guilhem, 1967).

Hall & Nobbs (1966) ont publié une étude analogue. Il semble intéressant de comparer des résultats obtenus de manière entièrement indépendante.

Pour simplifier, nous désignerons par HN le travail de Hall & Nobbs, et par JG celui de l'auteur. Nous adopterons la convention généralement admise $a<c$ (JG). Par contre, la numérotation atomique sera celle de HN.

Nous donnerons dans chaque cas les résultats avec leurs écarts-types, la différence entre les deux résultats, et l'écart-type, calculé à partir de la moyenne des variances.

Maille élémentaire

	HN	JG	δ	σ
a	6,003 (0,005)	6,02 (0,01)	0,017	0,008
b	5,308 (0,005)	5,31 (0,01)	0,002	0,008
c	15,755 (0,010)	15,74 (0,01)	0,015	0,010
	93,62 (0,08)	94,0 (0,1)	0,38	0,09
V	501,0	502 (2)		
D_m	1,570	1,592		
D_c	1,595	1,589 (0,007)		