ison of the observed and calculated densities shows that there is one molecule in the asymmetric unit.

Isoacorone

The crystals are long orthorhombic needles with well developed {011} and {010} faces. The systematic absences are $00l$, l odd, $0k0$, k odd and $h00$, h odd. These determine the space group uniquely as $P2_12_12_1$. Comparison of observed and calculated densities again shows one molecule in the asymmetric unit.

Neoacorone

The crystals are also long orthorhombic needles with the {011} and {010} faces well developed. The systematic absences are the same as for isoacorone, again determining the space group uniquely as $P2_12_12_1$; it was, however,

found that the substances had two molecules in the asymmetric unit, by comparison of the observed and calculated densities.

The specimens studied were kindly supplied by Dr V. Herout of the Institute of Chemistry, Czechoslovak Academy of Science, Prague, who has recently advised us that Drs Línék and Novák of the same Institute have duplicated the above results for acorone and have begun a detailed study of two of its derivatives. In view of this, and the unpromising nature of the isomers described here, no further work on them is to be carried out in this laboratory.

The crystal structure of UN by neutron diffraction. By MELVIN H. MUELLER and HAROLD W. KNOTT,

Argonne National Laboratory, Lemont, Illinois, U.S.A.

UN and UC have been reported (Rundle, Baenziger, Wilson & McDonald, 1948) to be cubic with a NaCl rather than a ZnS type crystal structure. Although the contribution of the nitrogen or carbon to the diffracted X-ray intensity is small, sufficient differences of intensity were observed on powder patterns within several pairs of lines to support the NaCl type structure for UN and UC (Rundle *et al.*, 1948). Recently, additional X-ray and neutron diffraction data were obtained definitely confirming the NaCl type structure for UN.

The sample used for this study was obtained by two different methods. Part of the sample was made by the decomposition of UH_3 at 400 °C. with further heating at 1000 °C. under 1 atm. of purified nitrogen. Another part was made by heating massive uranium metal in a nitrogen atmosphere at 800 °C. followed by additional heating at 1200 °C.

The X-ray diffraction intensity data were obtained with an X-ray diffractometer using a finely powdered sample with a spinner. These intensities were found to be in better agreement for the NaCl rather than the ZnS type structure as evidenced by an R factor of 0·085 and 0·141, respectively, for these two structures. The R factor was determined according to the following relation, $R = \Sigma|I_o - I_c|/\Sigma I_o$. A lattice parameter of 4·890± 0·001 Å was obtained for this same material from a Debye–Scherrer powder pattern using a modified Cohen least-squares method.

In order to confirm the structure unequivocally a neutron diffraction pattern was obtained with the diffractometer described previously (Sidhu, Heaton & Zauberis, 1956). A relatively small sample of UN was used which filled a vanadium tube $\frac{1}{8}''$ in diameter $\times 1\frac{1}{2}''$ in length. A summary of the relative neutron intensities together with calculated values for the NaCl and ZnS type structures is given in Table 1. The value of $2B$ in the Debye–Waller temperature factor was determined from the slope of the plot of logarithm of I_o/I_c versus

Table 1. *Observed and calculated relative neutron diffraction intensities for* UN *with* $\lambda = 1{\cdot}088$ Å

hkl	Observed I/I_0	Calculated* NaCl type	Calculated* ZnS type
111	0·0	0·4	8·9
200	101·4	102·5	0·3
220	100·0	100·0	100·0
311	0·0	0·4	77·1
222	44·7	46·3	0·1
400	25·5	25·2	25·2
331	0·0	0·2	4·2
420	79·4	79·3	0·2
422	66·7	66·1	66·1
333, 511	0·0	0·2	12·9
440	20·4	24·3	24·3
531	0·0	0·2	45·7
442, 600	56·6	53·4	0·1
620	39·3	39·0	39·0

* $I \propto |F|^2 p (1/(\sin^2 \theta \cos \theta)) \exp (-2B \sin^2 \theta / \lambda^2)$.

$(\sin^2 \theta)/\lambda^2$, using only those reflections whose calculated intensity was the same for both structures. No correction was made for absorption since the μr value for the UN sample used was very small; namely, 0·035. There is considerable difference in the calculated relative intensities for many of the reflections for the two types of structure, and it is therefore apparent that the best agreement is with the NaCl type. The R factor for this type structure is 0·024.

The B value of 0·51 Å² as obtained above was also used to calculate $\bar{\mu}$, the root-mean-square displacement of an average lattice point in a direction perpendicular to the reflecting plane, and Θ_M the characteristic temperature, according to the following given relation (James, 1948):

$$B = M/(\sin \theta/\lambda)^2 = 8\pi^2 \overline{\mu^2} = \{6h^2 T/(mk\Theta_M^2)\} \times \{\Phi(x) + x/4\} .$$

A $\bar{\mu}$ of 0·080 Å and a Θ_M of 232 °K. were obtained for UN from the above expression.

The writers wish to thank Ralph Kraft, formerly with the Ceramics group, for the UN samples, Dr Stanley Flikkema for the use of his sample spinner and Dr LeRoy Heaton for helpful suggestions. This work was performed under the auspices of the U.S. Atomic Energy Commission.

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Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. Copy should be sent direct to the Editor (P. P. Ewald, Polytechnic Institute of Brooklyn, 333 Jay Street, Brooklyn 1, N.Y., U.S.A.) or to the Technical Editor (R. W. Asmussen, Chemical Laboratory B of the Technical University of Denmark, Sølvgade 83, Copenhagen K, Denmark)

Pittsburgh Diffraction Conference

The annual Pittsburgh Diffraction Conference will meet at Mellon Institute, Pittsburgh, Pennsylvania on November 5 through 7, 1958. Submitted papers will be presented in the fields of X-ray, neutron, and electron diffraction. In addition invited speakers will include

J. Bardeen (Recent Developments in the Theory of Superconductivity),
R. D. Heidenreich (Electron Micro Probe Analysis),
A. N. J. Heyn (X-ray Studies of Fibrous Polymers), and
W. B. Pearson (Intermetallic Compounds).

For programs or further information write J. R. Townsend, Physics Department, University of Pittsburgh, Pittsburgh 13, Pennsylvania, U.S.A.

Preliminary Single-Crystal X-ray and Optical Study of Nor-Harman, $C_{11}H_8N_2$

Errors occur in the above article by Lilabati Ray (*Acta Cryst.* (1957), **10**, 707). The refractive indices published are: $\alpha = 1·758$, $\beta = 1·759$ and $\gamma = 1·806$. These values should be replaced by: $\alpha = 1·753$, $\beta = 1·764$ and $\gamma = 1·783$.

The Interpretation of Difference Maps

Errors occur in the above paper by Yuen C. Leung, Richard E. Marsh and Verner Schomaker (*Acta Cryst.* (1957), **10**, 650). Equations (2·7) and (2·8) should be written as approximate equalities, and a minus sign should precede the $4\pi^2$ in both. The signs of the left-hand members of (2·9), (2·10), (2·11), and (3·7), as well as the expressions for Δx, Δy and Δz just before the beginning of section 3, should be changed to minus, and likewise for the argument $\frac{1}{4}(\Delta B_1 h_1^2 + \Delta B_2 h_2^2 + \Delta B_3 h_3^2)$ in (3·1), (3·2), (3·4), and (3·8). The sign of the second term of the right-hand side of (3·9) should be plus. The derivatives expressed by $\dfrac{\delta \varrho_c(0)}{\delta B_i}$ in (3·5) and (3·7), should be written $\dfrac{\delta \varrho_c(0)}{\delta \Delta B_i}$ instead. The respective symbols f and T should be replaced throughout by f_0 and T_0.

Book Reviews

Works intended for notice in this column should be sent direct to the Editor (P. P. Ewald, Polytechnic Institute of Brooklyn, 333, Jay Street, Brooklyn 1, N.Y., U.S.A.). As far as practicable books will be reviewed in a country different from that of publication.

X-ray Crystal Structure. By D. MCLACHLAN, Jr. Pp. xiii+416 with many figs. New York; Toronto; London: McGraw-Hill. 1957. Price $15·00; £5.16.6.

In the preface to this book which is largely based on lecture notes used at the University of Utah, the author writes 'Although the lone investigator is borne in mind throughout the book, it has been hoped that the book may also be use as a university text in a two-quarter course in structure analysis'. The author, who has a long and varied experience in his subject, declares that the book is intended to bridge the gap which exists between books on X-ray crystallography written in a *popular* style and those written with *rigor*. It is the reviewer's opinion that the book fails to achieve its purpose; few lecturers would be prepared to recommend it in its present form and the lone investigator would quickly run into difficulties.

The reviewer makes two major criticisms. The first is concerned with the presentation. Too much of the material, including some of the fundamental ideas in crystallography, is treated sketchily or is badly organized and presents unnecessary problems to newcomers to the subject. One wishes that basic concepts had been ex-