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On the crystal structure of kernite, $Na_2B_4O_7.4H_2O$.*

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As part of a program to correlate X-ray and nuclear magnetic resonance data on the structures of oxy-anions, it was found necessary to re-investigate the crystal structure of kernite. The results of this study indicate that the originally proposed space group and structure (Garrido, 1932; Minder, 1935; Amoros, 1945) are inconsistent with the results of nuclear magnetic resonance studies (Blood & Proctor, 1954; Waterman, 1954; Waterman & Volkoff, 1955; Das, 1957).

Synthetic crystals prepared by Dr W. T. Schaller, U.S. Geological Survey, were examined by the Weissenberg method using Cu $K\alpha$ and Mo $K\alpha$ radiation. The correct space group was found to be $P2_1/c$ not $P2/c$, owing to the presence of a screw axis since there were systematic extinctions of $0k0$ for $k \neq 2n$. The unit-cell dimensions, obtained from zero-layer line photographs of rotations about the a and b axes yielded the following values:

$$a = 7{\cdot}022,\ b = 9{\cdot}151 \pm 0{\cdot}002,\ c = 15{\cdot}676\ \text{Å};\quad \beta = 108^\circ\ 50' \pm 5'\ .$$

The originally proposed structure of kernite (Amoros) consisted of B_3O_6 rings of three $[BO_3]^{-3}$ triangles linked by halved B_2O_3 ions to form infinite chains along the b axial direction. The sodium atoms were proposed to lie in the two-fold special positions: (e) and (f) ($P2/c$). The original structure determination was found to give imperfect agreement between the observed and calculated intensities.

Waterman & Volkoff (1955) have determined from nuclear magnetic resonance analysis of single crystals of kernite that there are four non-equivalent sets of boron atoms per unit cell, all of which are in general positions. One-half of the boron atoms are tetrahedrally coordinated —the others triangularly coordinated to oxygen. The sodium atoms also were found to lie in general positions.

Preliminary X-ray analyses indicate that the basic structure of kernite is related to that of borax, $Na_2B_4O_7.10\,H_2O$ which consists of $[B_4O_5(OH)_4]^{-2}$ rings of tetrahedrally and triangularly coordinated boron (Morimoto, 1956). Christ & Clark (1957) have postulated that kernite is composed of infinite chains of composition $[B_4O_6(OH)_2]^{-2n}$ resulting from the polymerization of the $[B_4O_5(OH)_4]^{-2}$ rings of borax. X-ray three-dimensional data have been collected for kernite and refinement studies are being carried out in cooperation with the U.S. Geological Survey.

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Structure of *s*-triphenyltriazine.*

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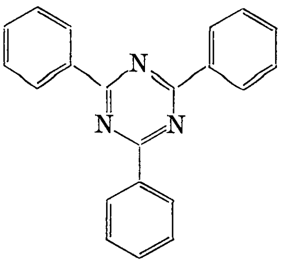
Recently great interest has been devoted to the study of molecular and electronic structure of conjugated heterocyclics containing nitrogen. Results of theoretical and experimental work (Bertinotti *et al.*, 1956; Hameka *et al.*, 1956; Herbstein *et al.*, 1955; Wheatley, 1955, 1957) have in particular indicated several interesting features of the structure of azines. We have therefore undertaken the X-ray structure determination of *s*–triphenyltriazine.

The unit-cell dimensions are:

$$a = 10{\cdot}94,\ b = 3{\cdot}91,\ c = 35{\cdot}84\ \text{Å};\quad \beta = 90^\circ\ 38',\ Z = 4;\ \text{space group}\ P2_1/c\ .$$



The Fourier transform method (Lipson & Cochran, 1953) was used in order to determine the orientation of the molecules with respect to the crystallographic axes from the weighted $h0l$ equatorial section.

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