Acta Cryst. (1958). **11**, 448

The unit cell and space group of hodgkinsonite.

By P. J. RENTZEPERIS,* *Department of Mineralogy, University of Thessaloniki, Greece*

(*Received* 10 *March* 1958)

Hodgkinsonite, $MnZn_2(OH)_2SiO_4$, a pneumatolytic silicate of the norbergite family, was discovered by H. Hodgkinson in association with franklinite and willemite at Franklin Furnace, New Jersey, and described by Palache & Schaller (1913). Its crystals, pink in colour, are usually pyramidal and belong to the monoclinic prismatic class. They show a perfect (001) cleavage and very easily yield thin plates or lamellae, a fact that renders their manipulation rather difficult.

Thin cleavage plates of hodgkinsonite were embedded in plexiglass and the directions of their a and b axes were found by observing the extinctions under the polarizing microscope. Parallel to these directions were cut small laths of almost equidimensional cross section. Using these laths and employing unfiltered Fe K radiation rotation and Weissenberg zero-layer and equi-inclination photographs were obtained. Precession diagrams were obtained with Mo $K\alpha$ radiation. The systematic absences found were: $h0l$ when h is odd and $0k0$ when k is odd. Thence it follows that the space group of hodgkinsonite is $P2_1/a$–C_{2h}^5.

Measurements of the unit-cell dimensions from oscillation and zero-layer Weissenberg photographs, in which high-order reflexions were considered ($\theta = 72°$–$83°$), led to the following lattice constants (Fe K radiation, $\lambda\alpha_1 = 1{\cdot}93593$ Å):

$$a_0 = 8{\cdot}17\pm0{\cdot}02,\quad b_0 = 5{\cdot}31\pm0{\cdot}005,\quad c_0 = 11{\cdot}76\pm0{\cdot}01\ \text{Å},$$
$$\beta = 95°\ 28'\pm15',\quad V = 507{\cdot}58\ \text{Å}^3.$$

The value of the angle β found from Weissenberg photographs is in good agreement with that given in the literature, $\beta = 95°\ 25'$ (Palache, 1914). The axial ratios calculated from the above lattice constants are:

$$a_0:b_0:c_0/_2 = 1{\cdot}538:1:1{\cdot}107$$

in excellent agreement with that given in the literature (Palache, 1914)

$$a:b:c = 1{\cdot}538:1:1{\cdot}1075.$$

For a unit cell content of four molecules $MnZn_2(OH)_2SiO_4$ a density of 4·08 g.cm.$^{-3}$ was deduced, whereas that given in the literature is 3·91 g.cm.$^{-3}$ (Palache & Schaller, 1913).

Determination of the structure of hodgkinsonite is in progress.

The author wishes to express his thanks to Prof. P. A. Kokkoros, Head of the Department, for suggesting the subject of this work.

References

PALACHE, C. (1914). *J. Wash. Acad. Sci.* **4**, 153.
PALACHE, C. & SCHALLER, W. T. (1913). *J. Wash. Acad. Sci.* **3**, 474.

* Now at: Mineralogisches Institut der Johann Wolfgang Goethe-Universität, Frankfurt a. M., Germany.

Acta Cryst. (1958). **11**, 448

Magnetic hydrogen bonds for molecular models*.

By LILLIAN CASLER and ROBERT B. COREY. *California Institute of Technology, Pasadena, California, U.S.A.*

(*Received* 5 *March* 1958)

Scale models designed for use in studies of molecular packing and configuration have been developed at the California Institute of Technology over a period of many years (Corey & Pauling, 1953). In one form, these models are built to the scale 1 inch = 2 Å and are cast from colored, rubber-like vinyl plastic; they are especially designed for use in studies of the structures of amino acids, peptides, and related compounds. The models are in many respects similar to the Stuart-type models that are available commercially; atoms are held one to another by means of snap fasteners and double-ended brass studs.

In crystals of amino acids and peptides and in structures containing polypeptide and polynucleotide chains, N–H · · · O, O–H · · · O, and N–H · · · N hydrogen bonds are of frequent occurrence and fundamental importance. To permit the construction of these hydrogen bonds, the models make use of a special hydrogen atom designed with a recess to receive the bonding oxygen or nitrogen atom. The radius of curvature of the recess corresponds to the van der Waals radius of an oxygen atom; the depth of the recess is such that the nitrogen and oxygen atoms of an N–H · · · O hydrogen bond are about 2·7 Å apart. Although this device for representing hydrogen bonds was satisfactory in many respects it had the disadvantage that it provided no means for holding the bonding oxygen or nitrogen atoms in place, so that the construction of complex hydrogen-bonded structures was often not practicable, and even simple structures of this sort were difficult to build and to maintain.

A very satisfactory solution of this problem has been found in the use of small permanent magnets. An alnico horseshoe magnet ground to the correct curvature is cast into the oxygen or nitrogen atom and the hydrogen atom is fitted with a recessed disk of stainless steel. Fig. 1 shows a cross-sectional view of a typical hydrogen atom (*a*) and of an oxygen atom (*b*) in which the magnet is

* Contribution No. 2322 from the Gates and Crellin Laboratories of Chemistry.