KRISHNA RAO, K. V. & KRISHNA MURTY, V. G. (1961). *Naure, Lond.* **190**, 429.
MUELLER, H. (1938). *Z. Kristallogr.* A, **99**, 122.
SUSSE, C. (1961). *J. Rech.* **54**, 23.
WEST, C. D. & MAKAS, A. S. (1948). *J. Chem. Phys.* **16**, 427.

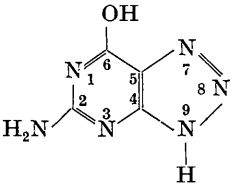
Acta Cryst. (1964). **17**, 789

Unit cell and space group of 8-azaguanine hydrochloride monohydrate.

By WALTER M. MACINTYRE and MANOUCHEHR ZIRAKZADEH,* *Chemistry Department, University of Colorado, Boulder, Colorado, U.S.A.*

(*Received* 22 *January* 1964)

8-Azaguanine is a synthetic compound of considerable biological interest. It is known to be incorporated into nucleic acids *in vivo*, presumably in place of guanine. Such incorporation of 8-azaguanine is frequently fatal to the cell concerned (Brockman, Bennett, Simpson, Wilson, Thomson & Skipper, 1959). The compound has the structural formula



and can be considered as being derived from guanine by replacement of a CH group by a N atom at the 8 position.

Structure analysis of this compound was initiated in order to determine the nature of the hydrogen bonding pattern exhibited in the crystal and to examine the effect on the molecular structure of substitution of N for CH.

The first crystals to be examined were those of 8-azaguanine hydrochloride monohydrate (AGHM). This derivative was chosen because of the remote possibility that it might be isomorphous with guanine hydrochloride monohydrate (GHM) whose crystal structure is known (Broomhead, 1951).

Crystals of the AGHM were prepared by cooling a warm concentrated solution of 8-azaguanine in 5*N* hydrochloric acid. The crystals grew as colorless, well-formed needles which extinguished perfectly when rotated between crossed polaroids.

Rotation and Weissenberg photographs were taken with the crystal rotating about the needle axis. A set of precession photographs was also taken with the crystal mounted in the same way. Examination of these photographs gave the following cell data:

System: monoclinic. Space group: $P2_1/a$.

$$a = 10{\cdot}94 \pm 0{\cdot}02,\ b = 12{\cdot}99 \pm 0{\cdot}02,\ c = 5{\cdot}56 \pm 0{\cdot}01\ \text{Å}$$
$$\beta = 93{\cdot}5° \pm 0{\cdot}2°.$$

The density of the crystals, as measured by flotation, was found to be 1·71 g.cm^{-3}. Assuming four units of AGHM per cell the density was calculated to be 1·72 g.cm^{-3}.

GHM likewise has space group $P2_1/a$ and four molecules per cell, but the cell dimensions are quite different from those above (Broomhead, 1951). Thus the two crystals are not isomorphous. This result is not too surprising since the presence of the N atom at position 8 in AGHM will provide additional possibilities for hydrogen bonding not available in GHM. The ratio of the cell volume of GHM to that of AGHM is 1·04. Thus the molecules in the AGHM crystals appear to be more tightly packed than those in the GHM crystals. This observation is also in accord with the more numerous hydrogen bonding possibilities available in the AGHM crystals.

Since the crystal structure of GHM could provide little assistance in solution of the structure of AGHM, the structure analysis was discontinued. We are currently completing a structure analysis of 8-azaguanine monohydrate, which will be reported later, and no further work on AGHM is contemplated in this laboratory.

It is a pleasure to record the support of this work by the National Cancer Institute of the National Institutes of Health, U.S.P.H.S., through their grant No. CA 0–4315.

References

BROCKMAN, R. W., BENNETT, L. L. JR., SIMPSON, M. S., WILSON, A. R., THOMSON, J. R. & SKIPPER, H. E. (1959). *Cancer Res.* **19**, 856.
BROOMHEAD, J. M. (1951). *Acta Cryst.* **4**, 92.

* Present address: 237 Braim, Abadan, Iran.