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Photoelastic constants of magnesium oxide.

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The photoelastic behaviour of magnesium oxide was studied by West & Makas (1948), Burstein & Smith (1948) and Giardini & Poindexter (1958). These data show discrepancies with regard to the strain-optical constants p_{11} and p_{12}. Burstein & Smith reported that $p_{11} = -0{\cdot}32$ and $p_{12} = -0{\cdot}08$, whereas according to Giardini & Poindexter $p_{11} = -0{\cdot}21$ and $p_{12} = +0{\cdot}04$. Thus there is disagreement with regard even to the sign of p_{12}. Hence, in view of the interesting optical and photoelastic behaviour of magnesium oxide, it is thought desirable to redetermine the photoelastic constants and clear the discrepancy.

The experimental technique used in this investigation is the same as that reported earlier (Krishna Rao & Krishna Murty, 1961). The stress-optical constants $(q_{11} - q_{12})$ and q_{44} are determined by Filon's method and the ratio of the strain-optical constants, p_{12}/p_{11}, is obtained by Mueller's (1938) ultrasonic method. Combining these results, the absolute strain-optical constants p_{11} and p_{12} have been evaluated using the elastic constants reported by Susse (1961). The results obtained in the present investigation along with those reported earlier are shown in Table 1.

It can be seen from Table 1 that there is a good agreement between the values obtained by different investigators except for the constants q_{12} and p_{12}. The values of both the constants and the sign of p_{12} reported by Giardini & Poindexter differ from the values obtained in the present investigation as well as from those reported by Burstein & Smith. The value of q_{12} reported by Giardini & Poindexter is very large and as a consequence p_{12}, which is evaluated from q_{12}, becomes positive. The sign of p_{12}/p_{11}, obtained in the present investigation by the ultrasonic method, is positive, whereas it should be negative if p_{12} is positive. Hence, it may be concluded that the value of q_{12} reported by Giardini & Poindexter is in error.

The specimen used in this investigation is a flawless synthetic crystal kindly lent to us by Dr T. S. N. Murty of our Laboratory.

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Table 1. *Photoelastic constants of magnesium oxide*

	$(q_{11}-q_{12})$ (units of 10^{-13} C.G.S.)	q_{11}	q_{12}	$(p_{11}-p_{12})$	p_{12}/p_{11}	p_{11}	p_{12}	q_{44} (units of 10^{-13} C.G.S.)
West & Makas	−1·24	—	—	−0·25*	—	—	—	−0·62
Burstein & Smith	—	−1·11*	+0·09*	−0·24	—	−0·32	−0·08	—
Giardini & Poindexter	−1·25	−0·90	+0·30	−0·25	—	−0·21	+0·04	−0·66
Authors	−1·24	−1·12	+0·12	−0·25	+0·21	−0·31	−0·07	−0·68

* Calculated by the authors from the elastic constants reported by Susse.

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

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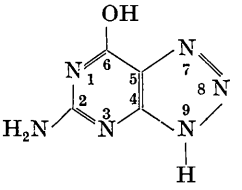
8-Azaguanine is a synthetic compound of considerable biological interest. It is known to be incorporated into nucleic acids *in vivo*, presumably in place of guanine. Such incorporation of 8-azaguanine is frequently fatal to the cell concerned (Brockman, Bennett, Simpson, Wilson, Thomson & Skipper, 1959).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

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