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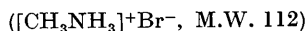
The crystal structure of methyl ammonium bromide. By E. J. GABE*, *Pure Physics Division, National Research Council, Ottawa, Canada*

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The crystal structures of the methyl ammonium halides were first investigated by Hendricks (1928), and the structure of the chloride was later redetermined by Hughes & Lipscomb (1946). The present investigation was undertaken at the suggestion of Prof. C. Sandorfy of the University of Montreal, who is working on the infra-red spectra of these substances, with particular interest in a hydrogen bond of the type $N^+-H \cdots Br^-$.

Crystal data

The crystals of methyl ammonium bromide



are extremely thin, irregularly shaped, soft plates, tabular on (001). The space group ($P4/nmm$) and axial lengths ($a=4.81$, $c=8.74$ Å) were determined from precession photographs. The observed density is 1.78 g.cm.^{-3} ; the density calculated for $Z=2$ is 1.84 g.cm.^{-3} . Hendricks found $a=5.09$ and $c=8.75$ Å.

Structure determination

With $Z=2$ the molecules must be in special positions, but the only systematic absences were those characteristic of the space group. Hence the molecules must occupy positions, $0, \frac{1}{2}, z$ and $\frac{1}{2}, 0, \bar{z}$ and only the z parameters remain undetermined.

The $0kl$ intensity data were collected from Weissenberg photographs; 51 reflections of a possible 60 within the Cu circle were recorded. The Br coordinate was determined as 0.810 from the $00l$ Patterson synthesis (Hendricks gives a value of 0.815), and bromine structure factors were calculated with an assumed $B=4.5$ Å². The F_o data were placed on an approximately absolute scale by comparison with $F_{c(Br)}$ and a correction of $\Delta B = +0.3$ Å² was also derived from this comparison. R_{0kl} was 23.1% at this stage. The $0kl$ Fourier map gave the positions of the two light atoms, though it was not possible to distinguish between them. Two cycles of Fourier and difference map refinement brought the R value down to 8.9%. It was still not possible to resolve the ambiguity of the light atom positions and it seems unlikely that this could be done even with three-dimensional data, both because of the dominance of the Br atom and the poor shape of the crystals for accurate data collection.

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Cell dimensions and space group of magnesium nitrate hexahydrate. By R. L. MOZZI and W. R. BEKEBÉDE, *Research Division, Raytheon Company, Waltham, Massachusetts, U.S.A.*

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Precession camera data were obtained on single crystals of $Mg(NO_3)_2 \cdot 6H_2O$ grown from aqueous solution and encapsulated in thin-walled glass capillaries to prevent

The fractional coordinates are

	x	y	z
Br	0	0.500	0.817
C	0	0.500	0.196
N	0	0.500	0.365

The light-atom positions were assigned on the basis of a slight difference of peak height in the final Fourier map.

Discussion

With these parameters $N-C=1.48$ Å, the distance from the C atom to the Br at $0, \frac{1}{2}, -0.193$ is 3.31 Å and to the Br at $\frac{1}{2}, 0, 0.193$ is 3.40 Å. The distance from the N atom to the Br at $0, \frac{1}{2}, 0.817$ is 3.95 Å. If we consider the ionic radius of Br^- to be 1.95 Å and use the values for the van der Waal radius of the methyl group (2.0 Å) and the ionic radius of the $NH_4^+(CH_3-NH_3^+)$ group (1.4 Å), as given by Hughes & Lipscomb (1946), $N-Br^- = 3.35$ Å and $C-Br^- = 3.95$ Å. Therefore it seems likely that the C and N parameters as given above need to be interchanged. The observed non-bonded distances then agree very well with the calculated values and the results are in good agreement with those for the chloride. It is also of interest to note that when this is done the N, H and Br atoms are almost in a straight line if we assume a tetrahedral C-H-N angle.

The light atoms occupy the same pair of special positions as they do in the chloride, which has the same space group but is not isomorphous. Hence the remarks in the earlier paper about the rotation of the CH_3 and NH_3^+ groups also apply here, but no attempt has been made to allow for this rotation. However, some photographs were taken at approximately -120 °C. but no change in the diffraction pattern could be detected. The crystals tended to shatter at this temperature and because of their poor quality no structure work was attempted.

I wish to thank Prof. C. Sandorfy for suggesting the problem and supplying the crystals, Dr W. H. Barnes and Dr A. W. Hanson for their interest in the work, and the referee for some helpful suggestions.

References

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