The Crystal Structures of Acetyl Choline Bromide and Acetyl Choline Iodide

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Acetyl choline is known as a very powerful biological reactant showing special effects in the cholinergic nerve system. Chemically, acetyl choline belongs to the choline subgroup of the "onium" compounds or tetrasubstituted ammonium bases. In view of the chemical interest of "onium" compounds in general and the biological importance of this type of compounds in particular it appears worth while to investigate their crystal and molecular structure in detail.

The bromide and the iodide of acetyl choline are easily obtained in crystalline form. The bromide is the more stable compound, the iodide being to some extent decomposed by light. The chloride is more difficult to crystallize, and is furthermore very hygroscopic.

Crystals of acetyl choline bromide were prepared by recrystallization from absolute alcohol. The crystals are colourless, transparent, monoclinic prisms of cell edge ~1 mm or less. The most frequent limiting faces of the crystals are parallel to (010), (110), (1$\bar{1}$0) and (001). Faces parallel to (101), (120), (1$\bar{2}$0) and {111} have been observed, but are less frequent. (100) and (10$\bar{1}$) have not been found as external crystal faces. Cleavage is fairly good parallel to (010), less good along (101).

The crystallographic data for acetyl choline bromide obtained from X-ray diffraction photographs, using Cu$K\alpha$ radiation, are: $a = 10.55 \pm 0.05$ Å, $b = 13.67 \pm 0.05$ Å, $c = 7.18 \pm 0.02$ Å, $\beta = 70.0 \pm 0.03°$, $V = 1\,043$ Å^3, $d_x = 1.43$ g/cm^3 with $Z = 4$ molecules per unit cell. $0k0$ reflexions are absent when k is odd. Possible space groups are $P2_1$ and $P2_1/m$. A Patterson projection on (001) is incompatible with the holohedric space group.

Strictly, however, the unit cell thus described is apparently a pseudo-cell only, as fairly strong superstructure reflexions, indicating very long true repeats, are found in the X-ray photographs. This superstructure seems to be of some peculiar and hitherto unknown type, the superstructure reflexions being defined by:

1. $h0l$ reflexions for h odd integer are absent, but subsidiary reflexions occur slightly displaced from these points.
2. $k = 0$. Subsidiary reflexions occur close to principal reflexions when h even and l even but not for l odd and h even.
3. $k \gtrless 0$. Subsidiary reflexions occur close to principal reflexions for all values of h and l.
4. No subsidiary reflexions accompany the $h00$, $hk0$ reflexions.
5. In terms of the reciprocal lattice the displacement of the subsidiary reflexions from the points corresponding to integral values of hkl is largest near the plane through $0kl$ and decreases towards the plane through $hk0$. In the present case the subsidiary reflexions occur only on one side of the principal reflexions, and not as the more usual pairs of reflexions placed symmetrically to the principal ones.

It cannot be definitely excluded that these extra reflexions in some way may be due to a special sort of twinning. Further investigation on this problem is going on.

The structure of acetyl choline bromide has been solved by Patterson, Fourier and least squares methods, and a detailed report on this work will appear elsewhere.

Acetyl choline iodide crystallizes from alcohol-acetone in very thin, soft, colourless and partly transparent plates. X-Ray oscillation and Weissenberg photographs show that the crystals are pseudo-orthorhombic with axial lengths: $a = 8.32 \pm 0.05$ Å, $b = 16.44 \pm 0.05$ Å, $c = 31.80 \pm 0.1$ Å, $\beta \simeq 90°$, cell volume $V = 2\,172$ Å^3, $Z = 16$ and d_x calculated 1.67 g/cm^3. Reflexions $h00$ are absent when h odd, $0k0$ when k odd and hkl when $h + k$ odd. There is apparently no close similarity between the crystal structure of this compound and that of the bromide. No further structure determination is contemplated for the iodide of acetyl choline.

The crystals used in these investigations were prepared by Mr. G. Aksnes of this Institute.

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