The Atisane → Aconane Conversion: X-Ray Analysis of a Key Intermediate

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AN important intermediate in a synthetic scheme for the conversion of atisane into aconane is the olefinic ketone (VI)[1] produced on pyrolysis of the toluene-*p*-sulphonate (IV).[1] Because of the importance of (VI)[1] in the conversion scheme, and as a check on the chemistry leading to it, we have determined its structure and stereochemistry *via* a single-crystal *X*-ray analysis of the hydroiodide of (IX).[1] Our results are in complete agreement with the conclusions of the preceding Communication; the double bond is in the 8(15)-position in the derivative (IX)[1] examined. Part of

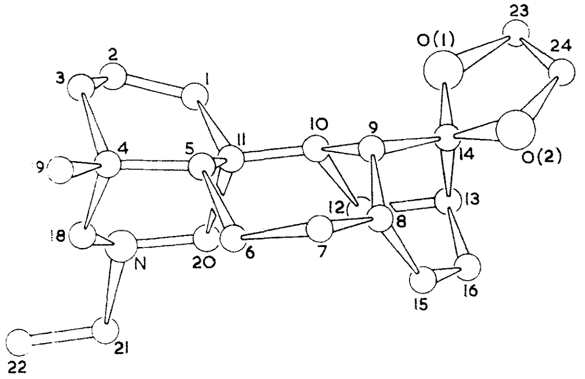

FIGURE. *The conformation of the* $C_{23}H_{36}NO_2^+$ *ion.*

the molecular framework constitutes an azabicyclo[3,3,1]-nonane system which in this instance adopts a flattened twin-chair arrangement with the *N*-ethyl group *exo*. The seven-membered ring adopts a chair conformation and, a view of the $C_{23}H_{36}NO_2^+$ ion is shown in the Figure.

The crystals are monoclinic, space group $P2_1$ with two molecules of $C_{23}H_{36}NO_2I$ in a unit cell: $a = 11{\cdot}20$, $b = 7{\cdot}81$, $c = 12{\cdot}92$ Å, $\beta = 107{\cdot}4°$. Some 1200 independent structure amplitudes were derived from equi-inclination Weissenberg photographs taken with a small crystal rotary about *b*. The structure was solved by the heavy-atom method and has been refined by electron-density calculations and least-squares methods. *R* is now 0·15.

(*Received, February 3rd,* 1969; *Com.* 148.)

J. P. Johnston and K. H. Overton, preceding communication.