X-Ray Structural Characterization of the Aziridinylgallane Trimer

By W. HARRISON, A. STORR, and J. TROTTER*

(*Department of Chemistry, University of British Columbia, Vancouver 8, B.C., Canada*)

Summary Aziridinylgallane trimer, $[(CH_2)_2N,GaH_2]_3$, has been prepared and has been characterized by a single-crystal *X*-ray study.

THE reaction of aziridine with an equimolar amount of trimethylamine–gallane at room temperature yields the cyclogallazane $[(CH_2)_2N,GaH_2]_3$. Sublimation of this compound in sealed capillaries under low pressures of nitrogen gave colourless crystals suitable for an *X*-ray crystallographic study. The crystals are orthorhombic: a = 18·364(5), b = 10·823(3), c = 7·114(2) Å, space group *Pnma*; Z = 4 (trimeric units). The intensities of 732 (only 252 observed) reflexions with $2\theta \leqslant 40°$ were measured on a Datex-automated G.E. XRD 6 diffractometer with Mo-K_α radiation. The atomic positions were determined by Patterson and Fourier syntheses, and refined by full-matrix least-squares methods to R = 0·077 for the observed reflexions.

The six-membered $(Ga–N)_3$ ring is in the chair conformation (Figure), torsion angles 59—61°, and lies on a crystallographic mirror plane. The mean dimensions are Ga–N 1·97(2), N–C 1·54(4), C–C 1·55(5) Å, angles: N–Ga–N = 100(1), Ga–N–Ga 121(1), Ga–N–C 116(1)°, angles in three-membered rings close to 60°.

This structure is the first determined for a trimeric gallium compound and confirms earlier predictions on the configuration of this class of cyclogallazanes.[1,2] The mean Ga–N bond length of 1·97 Å is in good agreement with the Ga–N distances in the monomeric trimethylamine–gallane[3] and in gallium nitride,[4] and is also very close to the Al–N bond lengths in similar trimeric aluminum compounds $[MeNH,AlMe_2]_3$ [5] and $[(CH_2)_2N,AlMe_2]_3$,[6] which is to be expected since the two Group III atoms have almost identical covalent radii. The Ga···Ga and N···N non-bonded intramolecular distances of 3·40 and 3·01 Å respectively are also similar to the corresponding distances in the $[MeNH,AlMe_2]_3$ trimer.[5] The closest approach between axial carbon atoms of the aziridine methylene

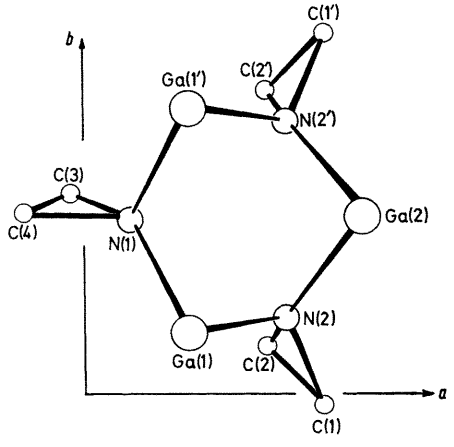

FIGURE. *Molecular structure of aziridinylgallane.*

groups in the molecule is 3 84 Å, which must lead to less severe non-bonded steric interactions in this molecule than in dimethylaminogallane, $[Me_2N,GaH_2]_2$, which is dimeric in solution [7]

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