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RESPONSES TO OUR PUBLICATIONS

DISCUSSION

NOT SILOCANES AND SILOCINS

BUT QUASISILATRANES

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In the 12th issue of the journal "Chemistry of Heterocyclic Compounds" for 2006 a review was published on "Metallocanes of group14 elements. 1. Derivatives of silicon and germanium" [1]. This name and the subsequent use of the terms "silocane" and "germocane" completely confuse the reader, since only derivatives of 1,3-dioxa-6-aza-2-silacyclooctane and their germanium analogs are examined in the review. According to IUPAC nomenclature [2], eight-membered saturated heterocycles not-containing a nitrogen atom are named ocanes (with the corresponding prefix indicating the endocyclic heterocycle). Silacyclooctane and germacyclooctane, corresponding to the general formula $H_2M(CH_2)_7$ where M = Si or Ge, are named silocane and germocane. Thus, their derivatives $Cl_2Si(CH_2)_7$ and $Me_2Ge(CH_2)_7$, for example, are named 1,1-dichlorosilocane and 1,1-dimethylgermocane respectively. The compounds examined in the review cannot even be called 1,3-dioxa-6-aza-2-metallocanes since they do not belong to the ocanes because they contain a nitrogen atom, and this is excluded by the IUPAC rules. At the same time, derivatives of 1,3,6-trioxa-2-silacyclooctane $R_2Si(OCH_2CH_2)_2O$ can be called 1,3,6,2-trioxasilocanes [2, 3].

In 1985 derivatives of 1,3-dioxa-6-aza-2-silacyclooctane were named 1,3,6,2-dioxazasilocines or even simply silocines [3], which is also unacceptable, since unsaturated eight-membered heterocycles containing silicon and nitrogen heteroatoms are named silocines [2]. In fact, according to IUPAC nomenclature, the compounds under discussion should be named 1,3,6,2-dioxazaperhydrosilocines. Two years later the heterocycle $H_2Si(OCH_2CH_2)_2NH$ was irregularly named a silocane [4]. Subsequently this unsubstantiated name has often been used in the chemical literature and particularly in reviews [1, 4].

We propose to call derivatives of 1,3-dioxa-6-aza-2-silacyclooctane, corresponding to the general formula $XYSi(OCH_2CH_2)_2NR$, quasisilatranes [5] since they can be regarded as silatranes [6-8] from the framework of which one OCH_2CH_2 edge substituted by substituents Y and R at the Si and N atoms respectively has been removed, while the intramolecular N→Si bond is retained. The similarity of the quasisilatranes to silatranes (the trigonal bipyramidal structure of the molecule, containing a transannular N→Si donor–acceptor bond) makes it necessary to use the widely accepted numbering of the atoms in silatranes when describing them. As an example we present the stereochemical structure of 1-fluoro-1-methylquasisilatrane with the corresponding numbering of the endocyclic atoms. Here the substituent X (F) is in the axial position while Y (Me) is in the equatorial position.

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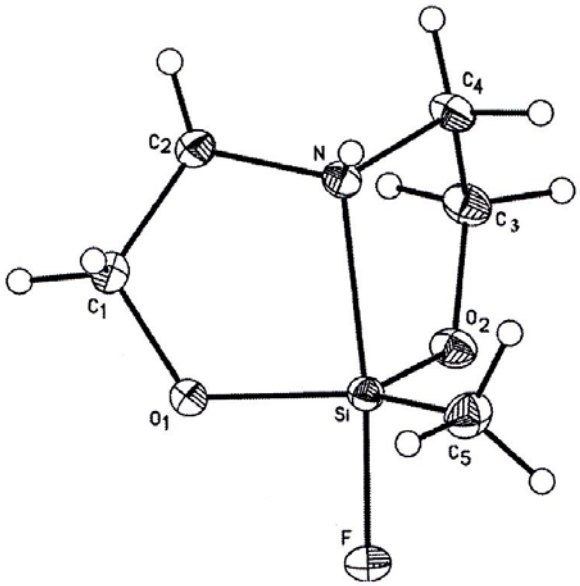
We synthesized the first representatives of quasisilatranes $Me_2Si(OCH_2CH_2)_2NR$, where R = H or Me, as far back as 1958 [9]. They were colorless liquids that readily distill under vacuum. In those years it was not possible even to imagine that they contained a transannular donor–acceptor N→Si bond. The absence of a clearly defined donor–acceptor N→Si bond in the above-mentioned quasisilatranes was confirmed in 1968 by dielcometric measurements [10]. Its presence in crystalline 1,1-diphenylquasisilatrane was first demonstrated by Daly in 1974 by X-ray diffraction [11]. In 1978 it was shown by ^{15}N and ^{29}Si NMR that the dative N→Si bond in the molecules of quasisilatranes containing at least one phenyl group at the silicon atom is retained in solution [12, 13].



Of course, all the foregoing can also be applied to quasigermatrane, which is isostructural with quasisilatranes.

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