

AUTHORS' REPLY

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Dear Colleagues!

In reply to the brief communication "Not silocanes and silocins but quasisilatrane" sent to the editors of the journal "Chemistry of Heterocyclic Compounds" we consider it necessary to make the following comments.

In our review "Metallocanes of group 14 elements. 1. Derivatives of silicon and germanium" [1] we considered it right to use the terms "silocanes" and "germocanes" primarily because these names have been used in most of the publications of recent times on the class of compounds under discussion, including papers of review type [2, 3].

In 1964 the creator of the chemistry of silicon derivatives based on trialkanolamines Academician M. G. Voronkov introduced the term "silatrane" to describe compounds with the general formula $N(CH_2CH_2O)_3SiX$ containing intramolecular $Si \leftarrow N$ coordination interaction. In spite of the fact that this name is trivial, the appearance of this term was accepted enthusiastically by the scientific community. Since that time the word "atranes" has become entrenched in the literature in so far as its use substantially simplifies the naming and perception of the names of the compounds, replacing the cumbersome 2,8,9-trioxa-5-aza-1-silabicyclo[3.3.3.0]undecane.

Similarly, the term "silocanes" was first introduced with the aim of simplifying the notation of the specific class of compounds and simplifying to some extent the naming of the compounds according to substitutive nomenclature (based on silocane instead of silacyclooctane). Actually the original name of the heterocycle $HN(CH_2CH_2O)_2SiH_2$ silocane probably occurred to us in an "irregular" way and was trivial since it did not conform to the IUPAC rules of 1979 [4]. At the present time, however, the basic term "ocane" corresponds fully to the present-day recommendations of IUPAC. According to the IUPAC nomenclature, for heterocyclic systems containing more than 10 atoms in the ring naming according the Hantzsch–Widman system can be used in addition to substitutive nomenclature. Since IUPAC nomenclature has been called upon to systematize names that already exist in the literature (i.e., start from practise) and not create rules and arrangements disconnected from reality, in 1983 the Hantzsch–Widman system was re-examined. According to the last edition of the "IUPAC Recommendations" [5] the single ending "ocane" is accepted for all eight-membered saturated heterocycles regardless of the nature of the heteroatoms in the ring. Examples of names of compounds according to the IUPAC nomenclature containing various heteroatoms in the eight-membered ring are given in Table 1.

Concerning M. G. Voronkov's proposal to use the term "quasisilatrane" for compounds with the general formula $RN(CH_2CH_2O)_2SiX_2$, we are unable to agree with this proposal for several reasons. First, this term has already been used in the literature but for other purposes. Thus, J. Verkade in his review "Main group atranes: chemical and structural features" [6] calls compounds in which there is only weak transannular element–nitrogen interaction "quasiatranes". An example of such a compound is $N(CH_2CH_2O)_3SiPt(PMe_2Ph)_2Cl$, in which the length of the $S \leftarrow N$ bond amounts to 2.89 Å. However, weak interaction is nevertheless present in this

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TABLE 1. IUPAC Nomenclature Containing Various Heteroatoms in the Eight-membered Ring

Silocane	Name in the Hantzsch–Widman system	Name according to IUPAC substitutive nomenclature
MeN(CH ₂ CH ₂ O) ₂ SiH ₂	6-Methyl-1,3,6,2-dioxasilocane	6-Methyl-1,3-dioxa-6-aza-2-silacyclooctane
MeN(CH ₂ CH ₂ S) ₂ SiH ₂	6-Methyl-1,3,6,2-dithiasilocane	6-Methyl-1,3-dithia-6-aza-2-silacyclooctane
S(CH ₂ CH ₂ S) ₂ SiH ₂	1,3,6,2-Trithiasilocane	1,3,6-Trithia-2-silacyclooctane
O(CH ₂ CH ₂ O) ₂ SiH ₂	1,3,6,2-Trioxasilocane	1,3,6-Trioxo-2-silacyclooctane
MeN(CH ₂ CH ₂ NMe) ₂ SiH ₂	1,3,6-Trimethyl-1,3,6,2-triazasilocane	1,3,6-Trimethyl-1,3,6-triaza-2-silacyclooctane

compound as demonstrated by: a) the displacement of the nitrogen atom toward the silicon atom from the plane formed by the three carbon atoms; b) the Si←N is shorter than the sum of the van der Waals radii of these elements. A compound in which the interaction is absent and which, according to Verkade's classification, can be called a "proatrane" has also been described in the silatrane series. This is N(CH₂CH₂O)₃SiOs(η²-S₂CNMe₂)(CO)(PPh₃)₂. The bond length in this compound (3.18 Å) is close to the van der Waals radii of the silicon and nitrogen atoms, while the nitrogen atom is displaced from the plane formed by the three carbon atoms toward the *opposite* side from the silicon atom [7].

Second, the name "quasisilatrane" [8, 9] is at the present time even more trivial than "silatrane" since the numbering of the ring atoms in this case does not conform either to the Hantzsch-Widman system or to IUPAC substitutive nomenclature.

Furthermore, in the opinion of M. G. Voronkov the name "quasisilatrane" must refer only to compounds containing strong intramolecular Si←N interaction. However, silicon derivatives of dialkanolamines, such as PhN(CH₂CH₂O)₂SiMe₂, in which this bond is absent have been described in the literature [10]. Consequently, this compound cannot be called a "quasisilatrane", and we suppose that compounds belonging to one type must be named according to one principle.

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