On the Nomenclature of Cyclazines

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A modification of the cyclazine nomenclature introduced by Boekelheide is proposed. A procedure by which all types of cyclazine systems can be assigned unambiguous names is described.

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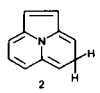
Cyclazines have been defined as tricyclic systems containing a completely conjugated perimeter of sp^2 hybridized carbon atoms held planar by a centrally lying nitrogen atom (1,2). A large number of similar compounds where one or more carbon atoms are substituted by nitrogen (3), sulphur (4), and/or selenium (5) atoms have been prepared. The original definition by Boekelheide, Gerson *et al.* (1,2), should therefore be extended to cover this type of compounds for which we now propose the name heterocyclazines. It should be noted that some of these systems, *e.g.*, the thia- and selenacyclazines and **6-8**, do not possess a completely conjugated periphery in the formal sense. However, peripheral, uninterrupted systems of π-electrons are also possible for these compounds since the sulphur, selenium, and bridgehead nitrogen atoms can each contribute two electrons. If the peripheral conjugation is interrupted, like in systems **1** (6) and **2**, it seems inappropriate to name them cyclazines.

1



2

At present two nomenclature systems for the cyclazines are in simultaneous use (7), one following the IUPAC rules (8) and one proposed by Boekelheide (1). *Chem. Abstr.* normally uses the IUPAC rules for fused heterocycles (Rule B-3) (8), but when these rules result in too complicated names, as for the last compound in Table I, the "a" nomenclature (Rule B-4) (8) is employed. The Boekelheide nomenclature system, using the name cyclazine as the base, expresses the combination of ring sizes with the number of peripheral atoms between the points of bonding to the central nitrogen atom. These numerals are placed in brackets and inserted in the base name, *e.g.* cycl[3.2.2]azine (1). A custom of arranging these numerals in decreasing order seems to have developed, although such a convention has never been formally proposed. Furthermore, the numbering of the atoms in the systems was designed to conform with the lowest possible numbers for substitution products (1).

The Boekelheide nomenclature is very simple, convenient, and widely accepted since the name makes the system immediately recognizable, which is not always the case when the IUPAC names are used. The annulenes (9), circulenes (10) or corannulenes (11), and cyclophanes (12) are other examples where special nomenclature systems have become popular.

In some cases, however, the Boekelheide nomenclature leads to ambiguous names as long as the order which the numerals in brackets should follow has not been specified. We, therefore, propose the following extension.

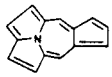
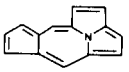
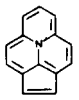
The tricyclic system should first be oriented and numbered according to the IUPAC rules for fused systems. (For an exception to this numbering, see below.) The bracket numerals are then arranged in the same order as the atoms from which these numerals are derived appear in the correctly numbered structure. If these additional requirements are not applied, the structures of *e.g.* the three isomeric 1-azacyclazines **3**, **4**, and **5** cannot be distinguished.

3

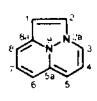
4

5

TABLE I

Orientation and name in original paper	Changed orientation and proposed name	Name in Chem. Abstr.
 cycl[3.2.2]azine[1]	 cycl[2.2.3]azine	pyrrolo[2,1,5-cd]indolizine
 1-azacycl[3.2.2]azine[3a]	 1-azacycl[2.2.3]azine	imidazo[5,1,2-cd]indolizine
 2-azacycl[3.2.2]azine[3e]	 1-azacycl[2.3.2]azine	imidazo[2,1,5-cd]indolizine
 5-azacycl[3.2.2]azine[3b]	 1-azacycl[3.2.2]azine	pyrimido[2,1,6-cd]pyrrolizine
 10-azacycl[3.3.2]azine[13]	 2a-azacycl[2.3.3]azine	
 6-azacycl[3.2.2]azine[3d]	 2-azacycl[3.2.2]azine	pyrazino[2,1,6-cd]pyrrolizine
 1,4-diazacycl[3.2.2]azine[3c]	 1,4-diazacycl[2.2.3]azine	1,4,7b-triazacyclopent[cd]indene
 cycl[4.3.2]azine[14]	 cycl[2.3.4]azine	azepino[2,1,7-cd]indolizine
 cyclopenta[h]cycl[4.2.2]azine[3d]	 cyclopenta[h]cycl[2.2.4]azine	cyclopent[4,5]azepino[2,1,7-cd]pyrrolizine
 Ref. 15	 cyclopenta[cd]cycl[3.3.3]azine	cyclopenta[ij]pyrido[2,1,6-de]quinolizine
 1,3,6-triazacycl[3.3.3]azine[16]		1,3,6,9b-tetraazaphenalene

If one or more heteroatoms appear at bridgehead positions, they are numbered in the same way as carbons in these positions, *cf.* **6**. This departure from the IUPAC numbering system is necessary in order to avoid ambiguity in naming *e.g.* **7** and **8**. However, so far no cyclazines of this type have been prepared.



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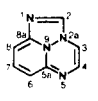

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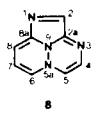

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If further rings are fused to the cyclazine system, the position of ring fusion is indicated as in the IUPAC system using the cyclazine as the base component, *cf.* Table I. In Table I we have summarized some examples of systems where the names and orientations originally proposed have been changed according to the above proposals.

REFERENCES

(1) R. J. Windgassen Jr., W. H. Saunders Jr. and V. Boekelheide, *J. Am. Chem. Soc.*, 81, 1459 (1959).

(2) F. Gerson, E. Heilbronner, N. Joop and H. Zimmermann, *Helv. Chim. Acta*, 46, 1940 (1963).

(3a) V. Boekelheide and A. Miller, *J. Org. Chem.*, 26, 431 (1961); (b) V. Boekelheide and S. Kertelj, *ibid.*, 28, 3212 (1963); (c) K. Valentin and A. Taurins, *Tetrahedron Letters*, 3621 (1966); (d) M. A. Jessep and D. Leaver, *Chem. Commun.*, 790 (1970); (e) O. Fuentes and W. W. Paudler, *J. Org. Chem.*, **40**, 1210 (1975).

(4) O. Ceder and B. Beijer, *Tetrahedron*, 30, 3657 (1974).

(5) O. Ceder and B. Beijer, *ibid.*, 32, 173 (1976).

(6) R. M. Acheson and R. S. Feinberg, *Chem. Commun.*, 342 (1965).

(7) D. Farquhar and D. Leaver, *ibid.*, 24 (1969).

(8) International Union of Pure and Applied Chemistry, Nomenclature of Organic Chemistry, Sections A & B, 2nd Ed., Butterworths, London, 1966.

(9) F. Sondheimer and R. Wolovsky, *J. Am. Chem. Soc.*, **84**, 260 (1962).

(10) J. H. Dopper and H. Wynberg, *Tetrahedron Letters*, 763 (1972).

(11) D. Hellwinkel, *Chem. Zg.*, **94**, 715 (1970).

(12) F. Vogtle and P. Neumann, *Tetrahedron Letters*, 5329 (1969).

(13) V. Boekelheide and N. A. Fedoruk, *J. Org. Chem.*, **33**, 2062 (1968).

(14) W. Flitsch, A. Gurke and B. Müter, *Chem. Ber.*, **108**, 2969 (1975).

(15) W. K. Gibson and D. Leaver, *Chem. Commun.*, 11 (1965).

(16) O. Ceder and J. E. Andersson, *Acta Chem. Scand.*, **26**, 596 (1972).