Reply to "A Supplement to the Historical Origins of Stereochemical Line and Wedge Symbolism"

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I would like to thank Andrew Dicks for calling attention to the official IUPAC recommendations with regard to stereochemical line and wedge symbolism (1), which I failed to mention in my brief historical survey of this subject (2). My communication uncovered two separate methods of indicating out-of-plane bonds: (i) the use of various kinds of lines (thickened, hatched, dashed, etc.); and (ii) the use of solid wedges and the laws of perspective. At the end of my survey I criticized several textbooks for either intermixing these two methods or incorrectly applying them and also indicated my preference for systems that consistently used either one or the other.

Based on these criteria, I rejected both structures 1 and 2 given by Dicks and would—had I been aware of them—also have rejected the two IUPAC structures. The earliest of these (structure 4) intermixes the two notations, using line type for receding bonds and wedge direction for projecting bonds, whereas the most recent (structure 3) does the same but adds on the further defect of subverting the laws of perspective, which was the historical reason for the introduction of wedges instead of lines in the first place, as may be readily verified by consulting the well-known books by Gillespie (3) and Wells (4).

Indeed, these problems highlight the fact that the IUPAC recommendations seem to be based solely on the parochial needs of organic chemists and are best applied to selected sites within a complex molecule rather than to the structure of the molecule as a whole. The limitations of the earlier proposal in this regard are particularly apparent when it is applied to the overall structures of the cage, cluster, and infinitely extended species typical of inorganic chemistry or, for that matter, to such organic species as tetrahedrane, where the result is an unattractive welter of thickened hatched lines. The coopting of wedge direction in the later proposal for the purpose of highlighting stereogenic centers, rather than projecting and receding bonds, further overlooks the fact that vast numbers of molecules are lacking such centers. In short, both IUPAC proposals fail as general notations for drawing complete 2D projections of 3D structures on paper that would be equally applicable to all molecules and nonmolecular solids, whether organic or inorganic in nature, and both violate already well-established historical precedents for the use of wedge notation.

References and Notes

1. A. P. Dicks, "A Supplement to the 'Historical Origins of Stereochemical Line and Wedge Symbolism,'" *J. Chem. Educ.* **2013**, *90*; 1109.

2. W. B. Jensen, "The Historical Origins of Stereochemical Line and Wedge Symbolism," *J. Chem. Educ.* **2013**, *90*, 676-677.

3. R. J. Gillespie, I. Hargatti, *The VSEPR Model of Molecular Geometry;* Allyn & Bacon: Boston, MA, 1991.

4. A. F. Wells, *Structural Inorganic Chemistry,* 5th ed.; Clarendon: Oxford, 1984.