application of PCRA shows that the influence of the steric term was suppressed due to multicollinearity (set 2-2).
6. As is to be expected, the E_s (corr.) values given by Mager[16] are strongly related to the van der Waals radius r_v without any significant inductive or mesomeric contributions (set 3-1 and 3-2). This may be regarded as an additional proof for the usefulness of Charton's ν values[23] in both aromatic and aliphatic reactions.

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2 Acknowledgment. We would like to thank Prof. J.T. Webster, Department of Statistics, Southern Methodist University, Dallas, for sending us s computer program of latent root regression analysis. We also thank the referees whose insightful comments were most helpful in improving the presentation.
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Space-filling molecular models of oxiranes (epoxides)

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Summary. An oxirane unit was constructed from aluminium spheres to fit the popular CPK system of space-filling molecular models.

Molecular models are widely recognized as valuable tools for the study of stereochemical relationships in organic chemistry and biochemistry[2]. The 2 most popular and most frequently used sorts are the framework models of the Dreiding type[3] and the space-filling models of the CPK type[4]. Whereas the framework models are most suitable for the determination of distances between nonbonded atoms and of torsion angles, the space-filling type lends itself particularly well to the study of intra- and intermolecular steric interactions and to the estimation of the preferred conformations of molecules.
We recently started to investigate the conformation of a substituted bioxirane related to the anti-tumor antibiotic hedamycin[5], and wanted to use space-filling models for our studies. Since no CPK units are commercially available for 3-membered rings, we designed an oxirane unit compatible with the CPK models.

The model unit was devised to represent an average oxirane. Thus, the dimensions used for its construction were a compromise (fig. 1) between those measured for ethylene oxide itself[6], those of the standard Dreiding oxirane unit[7] and of the covalent and Van der Waals radii used in the CPK system[8].

The oxygen atom was cut from an aluminium sphere of radius 16.87 mm (corresponding to a Van der Waals radius of 1.35 Å at the scale of 12.5 mm/Å used in the CPK models). The covalent radii were adjusted to 0.66 Å. No provision was made for a socket, as the oxygen atom was to be glued to the carbons. The carbon atoms were made from aluminium spheres of radius 15.62 mm (1.25 Å), the size used for sp^3-hybridized carbons in the CPK models[8]. Covalent radii of 0.77 Å (towards oxygen), 0.735 Å (towards carbon) and 0.77 Å (towards hydrogen) were used.

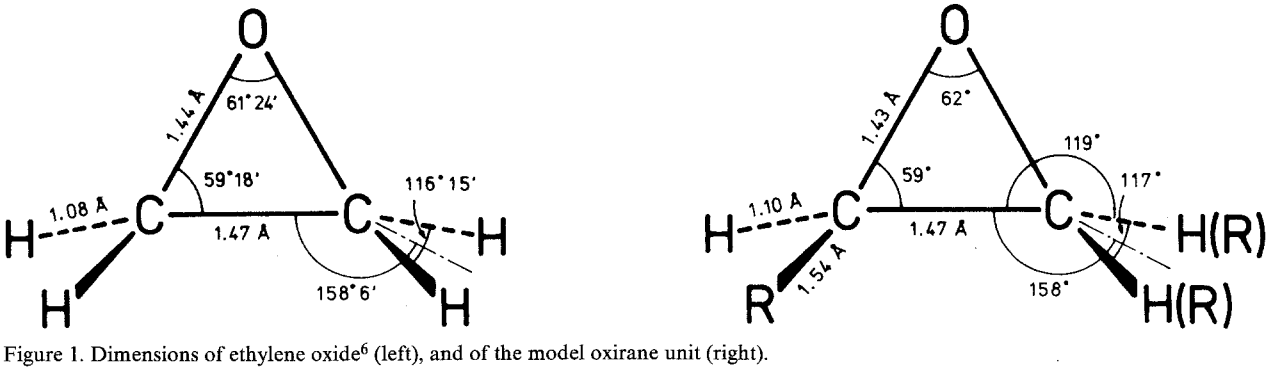

Figure 1. Dimensions of ethylene oxide[6] (left), and of the model oxirane unit (right).

The faces that were to carry the hydrogens (or other substituents) were cut 0.4 mm closer to the center of the sphere than corresponding to the above-mentioned covalent radius and were provided with a socket to allow the use of standard CPK connectors. The oxygen and carbon atoms were then anodized and colored red and black, respectively. Finally, they were cemented together with epoxy glue to give the oxirane unit shown in figure 2. We are sure that the oxirane model presented here will be a valuable tool for the investigation of steric interactions either within molecules containing epoxy groups or between such molecules and a wide variety of substances.

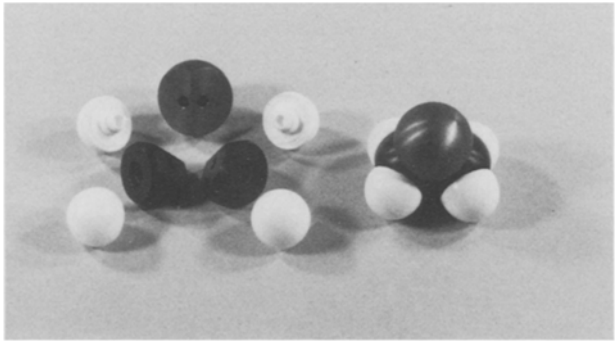

Figure 2. Oxygen and carbon atoms made from aluminium and standard plastic CPK hydrogens (left); fully assembled model of ethylene oxide (right).

1 The author thanks W. Arnold and F. Stehlin of the Institut für Organische Chemie for their careful machining of the aluminium models. Financial support by the Swiss National Science Foundation (project No. 2.837-0.80) is gratefully acknowledged.
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Inhibition of cytosolic rat hepatic glutathione S-transferase activities by bromosulfophthaleins

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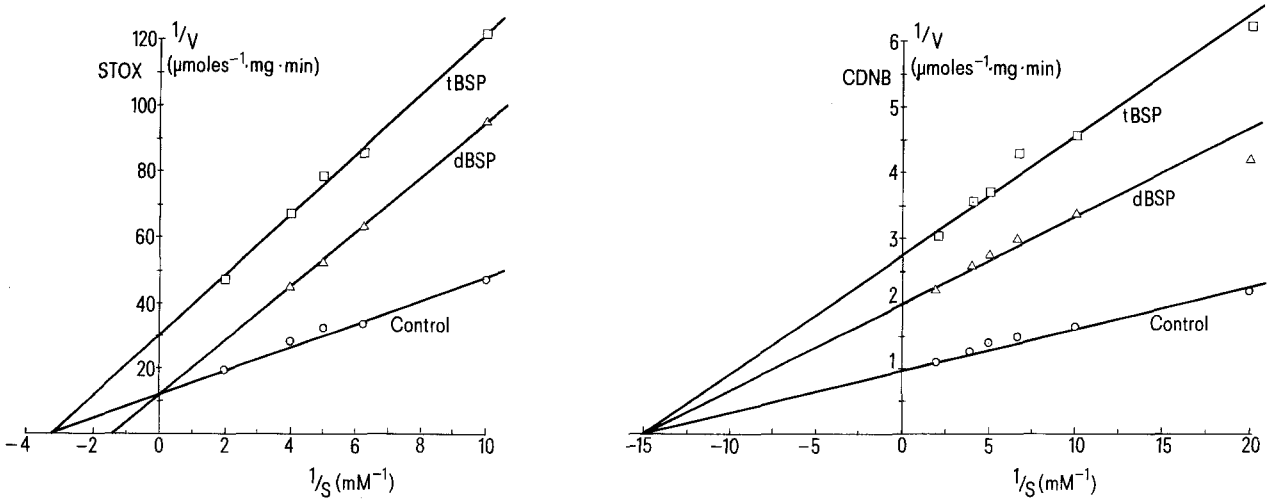
Summary. The enzymatically catalyzed conjugation of glutathione with 1-chloro-2,4-dinitrobenzene and styrene-7,8-oxide is inhibited by tetrabromosulfophthalein in a non-competetive way, although tetrabromosulfophthalein itself is a substrate for glutathione S-transferases. Dibromosulfophthalein, which is not a substrate for glutathione S-transferases, inhibits the 1-chloro-2,4-dinitrobenzene conjugation competetively and the styrene-7,8-oxide conjugation non-competetively.

Conjugation with glutathione (GSH), an important phase II reaction in the metabolism of electrophilic xenobiotics, is catalyzed by the GSH S-transferases (E.C.2.5.1.18), a family of enzymes located mainly in the cytoplasm[1]. Bromosulfophthaleins are known to interact with GSH S-transferases: 3,4,5,6-tetrabromosulfophthalein (tBSP) was shown to be a substrate[2], while 3,6-dibromosulfophthalein (dBSP) is not a substrate but was characterized as an inhibitor[3]. The bulk of enzyme activity towards tBSP and 1-chloro-2,4-dinitrobenzene (CDNB) is associated with trans-



Inhibition of rat hepatic glutathione S-transferase activities (control: ○) by dibromosulfophthalein (0.25 mM dBSP: △) and tetrabromosulfophthalein (0.05 mM tBSP: □), using 0.5 mM glutathione as the 1st substrate and styrene-7,8-oxide (STOX, left panel) or 1-chloro-2,4-dinitrobenzene (CDNB, right panel) as the electrophilic 2nd substrate, respectively.