

# Lecture Notes in Chemistry

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István Hargittai

## Sulphone Molecular Structures

Conformation and Geometry from Electron Diffraction  
and Microwave Spectroscopy; Structural Variations



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## Foreword

Recently, the molecular structures of a relatively large number of sulphone compounds have been elucidated in the vapour phase by electron diffraction and microwave spectroscopy. The main purpose of these studies is the determination of the sulphur bond configuration and the conformational properties. This leads to the observation and correlation of characteristic structural variations as various ligands are attached to the  $\text{SO}_2$  group and as comparisons are made with related molecules.

Today it may be said that the structure of sulphone molecules is relatively well studied, and it appeared necessary to systematize the accumulated experimental data after critical considerations. This is done in the first part of this monograph. The second part presents the observed characteristic structural variations. Attempts are made to interpret these variations by valence shell electron pair repulsions and non-bonded interactions. Correlation relationships between geometric and vibrational parameters are also presented.

It is the metrical aspects of the molecular structure which are primarily considered. Since they correlate with other aspects of the molecular structure, e.g. electronic, it is hoped that the experimental information on the molecular geometry provides stimulus for further experimental, and, in particular, theoretical work on sulphones and related systems.

#### IV

It is attempted to cover all electron diffraction and microwave spectroscopic investigations on sulphone molecules to date. Admittedly, however, relatively larger weight is given to the electron diffraction studies originating from the author's own laboratory.

The core of this work was presented as an invited lecture to the IV European Microwave Spectroscopy Conference organized under the chairmanship of Professor Werner Zeil (Tübingen) as Conference on Determination of Molecular Structure by Microwave Spectroscopy and Electron Diffraction, Tübingen, March 21-25, 1977. It was then Professor Zeil who suggested to put together this volume.

I would like to give here some words of appreciation. Professor Lev V. Vilkov (Moscow) first turned my attention to the structural problems of sulphones. Professor Sándor Lengyel made invaluable contribution to creating the Budapest electron diffraction laboratory. Professor János Holló gave us support and encouraged us at decisive moments in the studies of sulphur stereochemistry.

Numerous colleagues and co-workers have participated in our studies on sulphone structures. I have shared interest and work in this field for years with Dr. Jon Brunvoll (Trondheim). Especially significant contributions were made also by Dr. Magdolna Hargittai, Mr. József Hernádi (deceased), Mrs. Mária Kolonits and

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Typing this monograph was a special task performed by Mrs. Julia Simon with care and patience. Most of the Figures were drawn by Mrs. Judit Szilágyi.

Budapest, May 23, 1977

*Hargittai Iván*

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