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Lecture Notes in Chemistry

11

Franco A. Gianturco

The Transfer of Molecular Energies by Collision:

Recent Quantum Treatments

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"The abnihilisation of the etym by the grisning of the grosning of the grinder of the grunder of the first Lord of Hurtreford explodotonates through parsuralia with an ivanmorinthorrumble fragoromboasity amidwhiches general uttermosts confussion are perceivable moletons skaping with mulicules"

J. Joyce, Finnegan's wake

ABSTRACT

Volume 11: F.A. GIANTURCO

THE TRANSFER OF MOLECULAR ENERGIES BY COLLISION: RECENT QUANTUM TREATMENTS

17 figures, 327 pages, 1979

The aim of this study is to provide a summary of the currently used theoretical and computational techniques and a review of the most recent results that have dealt mainly with the simplest type of energy transfer in a molecular collision process, namely the conversion of the translational energy of a structureless atom in its ground electronic state into the internal rotational and vibrational energy of a diatomic molecule, also in its ground electronic state. This is probably one of the most common events in chemical processes and while the experimental data from molecular beam measurements have become increasingly more meaningful and reliable, only recent years have seen any thorough, ab initio approach to the various computational aspects of this problem. A brief résumé of potential scattering results is used as a preparation of the working formalism. The ab initio potential surface calculations are then examined and the various angular momentum coupling representations, those that yield the multichannel scattering formalism of vibrorotational inelastic cross sections in atom-molecule and molecule-molecule encounters, are discussed. Some of the numerical techniques that have lent themselves to the most recent applications are also reviewed together with the various decoupling schemes that are necessary when dealing with more complex cases. Finally, correlations of the state-to-state deexcitation cross sections with bulk measurements of relaxation times are also briefly presented. (498 References).

Contents: A résumé of quantum mechanical potential scattering. - Potential energy hypersurface calculations for simple systems. - Rotational and vibrational inelasticity in molecular encounters. - Dimensionality reduction methods for rotovibrational cross sections calculations.- Numerical methods for the coupled equations: a survey.- Rotovibrational relaxation models in simple gases.

FOREWORD

These Lecture Notes are intended as an introduction to the theoretical formulation and computational aspects of the molecular energy transfer processes which take place in an increasingly sophisticated range of molecular scattering experiments. They are directed to chemistry graduate students and emphasize the quantum mechanical approach, with little or no attention to classical and semi-classical treatments or to formal presentations.

Several Sections of the first Chapters are based on lectures given at the Graduate School of Physics of the University of Genoa a few years ago and I thank the students for their sense of duty in following to the end all those notation-filled blackboards and transparencies.

The kind patience of my wife Carolyn in reading the whole manuscript and improving its form is gratefully acknowledged.

Franco A. Gianturco

Bari, September 1978

CONTENTS