

Molecular Design: Chemical Structure Generation from the Properties of Pure Organic Compounds (Studies in Physical and Theoretical Chemistry)

A.L. Horvath



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This book is a systematic presentation of the methods that have been developed for the interpretation of molecular modeling to the design of new chemicals. The main feature of the compilation is the co-ordination of the various scientific disciplines required for the generation of new compounds.

The five chapters deal with such areas as structure and properties of organic compounds, relationships between structure and properties, and models for structure generation. The subject is covered in sufficient depth to provide readers with the necessary background to understand the modeling techniques. The book will be of value to chemists in industries involved in the manufacture of organic chemicals such as solvents refrigerants, blood substitutes, etc. It also serves as a reference work for researchers, academics, consultants, and students interested in molecular design.

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