



Computer Generated Physical Properties (Computer Modeling for Environmental Management)

Stan Bumble

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Computer Generated Physical Properties offers the environmental scientist a basis to predict the properties of molecules and reengineer them to remove those properties that are harmful to the environment. This technology is currently used in other fields and is now becoming popular in the environmental engineering field because of its pollution prevention and waste reduction capabilities.

This book, interdisciplinary in scope, treats the physical properties of matter as generated by computers. It covers a wide variety of topics pointing towards synthesizing new molecules to substitute for reactants, intermediaries, and products in industrial processes with better physical and environmental properties than the original. The author achieves this with a spreadsheet program called SYNPROPS that operates on a PC computer with optimization features. A radar type graph - one for each property - visually sorts the various groups in order of their contribution to the property, creating the necessity for a computer to obtain answers for the structure of the optimum molecules for substitution or synthesis.

The author discusses applications to biologically active molecules without side effects, including antineoplastic drugs. Additionally, he demonstrates model compounds and the applications of SYNPROPS' optimization and substitution. This book has everything you need to know about deriving properties and combinational chemistry from molecular structure.

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