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An Introduction to Physical Chemistry
The Structural Approach

This textbook starts from molecular structure, molecular shape, size and conformation, and proceeds to derive the basic formulas of quantum chemistry and molecular orbital theory for the calculation of quantized molecular energies. Thermodynamic functions U, S, and G are then derived through a synthetic approach to statistical mechanics, and internal energy is also introduced via the modern modeling techniques of Molecular Dynamics. The results of this Boltzmann-Schrödinger approach are then collated with the traditional Joule-Clausius approach to the two laws of thermodynamics. Chapters on the formal presentation of thermochemistry and equilibria follow, with exercises based on real data from the literature and solutions worked out in every detail. Further chapters deal with metastability and descriptive kinetics, based on real experiments and literature material. The text is tailored to a semester of 70-100 teaching hours for second-year students of nearly all courses in chemical, physical or natural sciences. Formal mathematical derivation is largely avoided in favor of textual description of the key points (the “read this formula in words” approach). The examples, exercises and discussion sections take about one half of the total size of the book.

Angelo Gavezzotti received his degree in Chemistry in 1968, and spent post-degree research terms in France and the US. Since 1987) he is Professor of Physical Chemistry at the University of Milano. He is author of about 150 research papers in major Journals and of a book on Molecular Aggregation (Oxford University Press, 2007). He has been keynote speaker at a many international meetings and has given lectures in Universities and major Chemical Companies worldwide. He has been on the Editorial Board of several international Journals and Co-Editor of Acta Crystallographica. He is a Fellow of the Royal Society of Chemistry and in 2007 he has been awarded the Trueblood Prize of the American Crystallographic Association. His research interests are presently in the field of the structural physical chemistry of organic condensed phases.

ISBN 978-88-548-xxxx-x

STUDIO BG

euro 19,00

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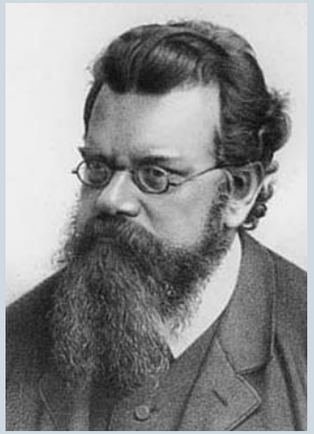
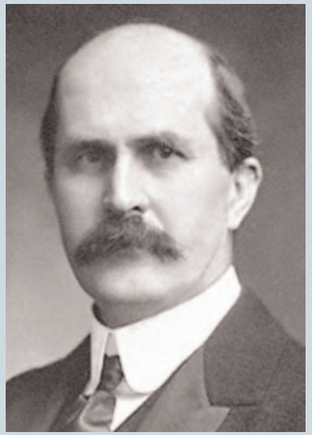
The Structural Approach

Schrödinger



Boltzmann

Maxwell



Bragg