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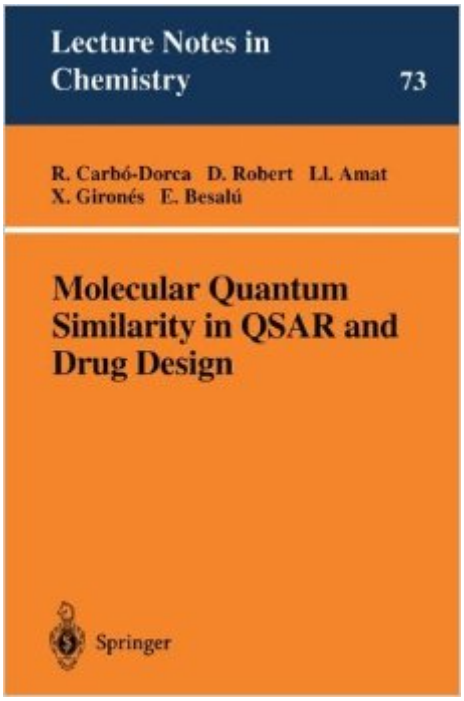

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Synopsis

The authors introduce the concept of Molecular Quantum Similarity, developed in their laboratory, in a didactic form. The basis of the concept combines quantum theoretical calculations with molecular structure and properties even for large molecules. They give definitions and procedures to compute similarities molecules and provide graphical tools for visualization of sets of molecules as n-dimensional point charts.

Book Information

Series: Lecture Notes in Chemistry (Book 73)

Paperback: 123 pages

Publisher: Springer; Softcover reprint of the original 1st ed. 2000 edition (October 4, 2013)

Language: English

ISBN-10: 3540675817

ISBN-13: 978-3540675815

Product Dimensions: 6.1 x 0.3 x 9.2 inches

Shipping Weight: 7 ounces (View shipping rates and policies)

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