



Discovering Chemistry With Natural Bond Orbitals

Frank Weinhold

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This book explores chemical bonds, their intrinsic energies, and the corresponding dissociation energies which are relevant in reactivity problems. It offers the first book on conceptual quantum chemistry, a key area for understanding chemical principles and predicting chemical properties. It presents NBO mathematical algorithms embedded in a well-tested and widely used computer program (currently, NBO 5.9). While encouraging a "look under the hood" (Appendix A), this book mainly enables students to gain proficiency in using the NBO program to re-express complex wavefunctions in terms of intuitive chemical concepts and orbital imagery.

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