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British Books in Print ,1967 Theoretical Treatments of Hydrogen Bonding Dušan Hadži,1997-12-29 Hydrogen bonding is crucial in many chemical and biochemical reactions as well as in determining material properties A good insight into the theoretical methods of treating hydrogen bonding is essential for those wishing to model its effects computationally in a wide range of fields involving hydrogen bonding as well as those wishing to extract the maximal amount of information from experimental data Theoretical Treatments of Hydrogen Bonding presents the reader with the state of the art of the key theoretical approaches to hydrogen bonding and considers the hydrogen bond from the various aspects The first five chapters are devoted to the methods used for treating the electronic basis of hydrogen bonding including a consideration of the electrostatic model density functional theory and molecular orbital methods Later chapters consider the dynamics of hydrogen bonds with particular attention to the treatment of proton transfer manifestations of dynamics as reflected in infrared spectra and nuclear magnetic relaxation are also considered Hydrogen bonding in liquids and solids such as ferroelectrics are included The book concludes with an epilogue which discusses the likely development of hydrogen bond computations in very large chemical systems Theoretical Treatments of Hydrogen Bonding offers the reader a comprehensive

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