

TO THE PROBLEM OF FORMULATION OF BASIC PRINCIPLES IN THE THEORY OF MOLECULAR STRUCTURE AND DYNAMICS

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(Received 22 August 2007; accepted 8 December 2007)

Abstract

In this contribution some basic problems of practical applications of quantum mechanics to the functioning of microsystems have been discussed. In particular, it has been shown that starting from fundamental principles one cannot calculate 3D-configurations of atoms in molecules. In order to get meaningful results in these calculations, the empirical information about the configuration of molecule is necessary. The problem of variables separation in quantum chemistry was discussed. It has been shown that the separation of electronic and

nuclear parts in nuclear-electronic problem of quantum chemistry can be performed in the adiabatic approximation only. The Schroedinger equation with the stationary operator H , common for all isomers of any molecule, cannot be written as well.