



www.uni.lodz.pl/concepts

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

F. A. Bogomolov

Courant Institute of Mathematical Studies

New York University

It is an interesting article which touches a serious difficulty in the systematic application of quantum theory to chemistry. It must be said that Schroedinger equation looks deceptively simple, but there are many caveats in its applications to concrete systems. One of the general difficult problems is that we are forced to deal with time dependent potential H which variation depends on the configuration of the system. Since the parameters of the system are now described by function the operator H itself has also be considered in a similar manner and we have to apply to H a Schroedinger type operator equation for a ψ function of H . Thus we have to deal with a "distribution of operators" I dont think it is possible to perform this procedure effectively in any concrete system, unless we assume that the variation of H is guided by parameters subjected to nonquantum laws. It is therefore almost impossible to consider potentials substantially depending on the positions of individual particles involved.

There is an approach based on the treatment of isomers as differ-

Comment

ent states of the same "molecule". In this approach the ground states of the "molecule" are actually not the individual isomers, but their weighted combinations. This approach provides an explanation for some interesting phenomena. However the parameters of the individual isomers and the corresponding space configurations are treated within the classical framework and quantum effects are calculated via perturbation theory only.