Journal of Molecular Structure, 222 (1990) 401-414
Elsevier Science Publishers B.V., Amsterdam — Printed in The Netherlands

ROTATION AROUND (Y)C_{sp^2}–X BONDS (X=C, O; Y=C_{sp^2}, O) WITHIN THE FRAMEWORK OF THE MOLECULAR MECHANICS METHOD

ALEXANDER KH. PLYAMOVATYI*

A.E. Arbuzov Institute of Organic and Physical Chemistry, USSR Academy of Sciences, Kazan (U.S.S.R.)

RUSTAM SH. KHADIULLIN and RAUZA P. ARSHINOVA

A.M. Butlerov Scientific Research Chemical Institute, V.I. Ul'yanov-Lenine Kazan State University, Kazan (U.S.S.R.)

(Received 29 May 1989; in final form 28 July 1989)

ABSTRACT

Internal rotation around (Y)C_{sp^2}–X (X=C, O; Y=C_{sp^2}, O) bonds is considered. A calculation scheme, taking into account heteroatom lone pair interactions, is used. Wide literature information, concerning the rotation discussed here, is gathered and analysed. Rotation barrier uniform values are proposed on the basis of original simulations and their nature is discussed.

INTRODUCTION

The molecular mechanics method is a powerful representative of classical theoretical methods of investigation of the conformational behaviour of molecules. Its features are high speed calculations and no less reality than quantum chemical simulations. It is important that the cost of nonempirical (ab initio) calculations grows as the fourth power of atom number, whilst in molecular mechanics the value of this power is between two and three [1].

Briefly, the main idea of molecular mechanics is the following. The molecular mechanics model is based on the Born–Oppenheimer approximation. The molecule is constructed of interacting atoms [2]. One can build the potential energy surface as a function of independent geometrical parameters of the molecule, changing the mutual disposition of atoms. This surface has one or few minima with respect to one or a few stable conformations. It is assumed that the molecular energy is the certain sum

$$E=E_{\text{bon}}+E_{\text{ang}}+E_{\text{tor}}+E_{\text{nbon}}+E_{\text{q}}+E_{\text{hbon}} \quad (1)$$

*To whom correspondence should be addressed: Inst. Org. Phys. Chem., ul.Arbuzova 8, Kazan, 420083, U.S.S.R.

0022-2860/90/$03.50