ABSTRACT

PROGNOSTICATION OF DENSITY OF ORGANIC SUBSTANCES WITHIN THE NEW APPROACH ANSAB

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In the present study we have offered a new approach to spatial representation of molecular systems, in which each molecule-forming atom doesn't have spherical symmetry. The corresponding computer program has been called "ANSAB".

The set of the Cartesian coordinates for all atoms forming the molecular system under consideration serves as initial information. It is possible to get these data in various ways. However, in our opinion, the PM3 method of calculation of atomic coordinates is the simplest.

In the same way, as in "DENSON" model, which is based on spherical symmetry of atomic radii, a particular atomic radius r^0 is attributed to each chemical element. Thus, zero radius for the hydrogen atom ($r^0(H)$) is considered equal to 0,3325 angstroms; for the carbon atom $r^0(C)$ = 0,6500, and so on. Then, as the result of interaction between atoms, deformation of the initial sphere takes place. Amount of deformation Δr is determined by known formulas. The practical realization of the new model within ANSAB program is carried out as follows. On the initial spherical surface of an atom N points are placed. Each point is described by its own coordinates. Then the values of these coordinates change depending on the environment of the given atom. In order to develop the new geometric approach to the atomic volume, ellipsoidal approximation has been chosen, that is, on the straight line of interaction between atoms the spherical form of an atom is transformed into the elliptical one, to the Δr value. Considering all possible interactions for the chosen atom, we calculate the new coordinates for all surface points. As the result, the overview of the atom changes, with one, two or several elliptical parts. The algorithm described above is used for every atom in a molecule. In the earlier spherical description the molecular volume was calculated as the sum of atomic volumes, not overlapping, but in the case of non–spherical approximation such summation wouldn't be perfectly correct. In order to find the volume of a complicated figure, it is possible to use a simple sequence: it is necessary to construct a parallelogram according to molecular geometric dimensions, to divide it by definite steps in three coordinates, and check the points obtained on the parallelogram in this way, whether they come inside one atom at least. Multiplying the number of points by elementary volume, we determine the final volume of the molecule.

The density of a substance can be calculated according to the known formula. The experimental values (d^{20}_4) and calculated values (d_1) of relative density can be compared; in the present case we have studied non–cyclic hydrocarbons. The average deviation (Δd) in the sample has amounted to 0,00323 for 31 compounds studied.

The correlation of theory and experiment may be considered good enough. As any model, "ANSAB" has been tried for simple, though various, molecular systems. As the result, the new view of atoms and a molecule as a whole has been obtained, which shows influence of the kind of interaction and its force on spatial forms more precisely.

Key words: density of substances, “ANSAB” model, non-spherical symmetry
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