International Conference on Natural Products and Physiologically Active Substances (ICNPAS-2004)
September 12-17, 2004, Novosibirsk, Russia
Poster Presentation

Problems of Definition of Atomic Charges in Molecules of Alkaloids

M.G. Levkovich, N.V. Polyskalina

Institute of Chemistry of Plant Substances of ASUz
700170, Tashkent, Kh. Abdullaev st., 77
e-mail: m_levkovich@yahoo.com

The properties of each molecule must be formed by simple physical parameter set, which characterise the structure of molecule. The simplest parameter is the electric atomic charge. This notion is very wide-spread in chemistry, but still doesn't have any clear definition. It is impossible to measure it by experiment. Quantum calculation is also difficult.

The use of molecular modelling methods for definition of atomic charges shows an essential difference.

In this work we have calculated the atomic charges in cytizine molecule. This structure is a typical for alkaloids; moreover, there are two different nitrogen-atoms. We used six most modern methods: MPA, NPA, CHELP, CHELPG, Merz-Singh-Kollman and AIM.

The results show considerable dispersion from method of calculation. It is interesting, that not only heteroatoms were difficult for calculation, but some carbon atoms too. The choose of the optimal method for classic chemical purposes was made from comparison of our results concerning to typical properties of cytizine.

From our investigation we can do next conclusions. At first, it is important to differ the notion of atomic charge for typical physical or chemical purposes. For physical purposes the topologic distribution of electron density inside the molecule is more considerable. So the optimal method is AIM technology. For chemical problems the condition of external electrostatic fields has more importance. This is the case of chemical activity. In this case electrostatic methods gave the best result.

So for calculations of atomic charges in alkaloid molecules for typical chemical purposes we recommend the CHELPG-method as best.

Moreover, we have established, that it is better to calculate the hard-atomic charge as the sum of hard-atom charge and it's protons.