# QUANTUM CHEMICAL STUDY OF THE STRUCTURE OF THE CONFORMERS OF THE MOLECULES OF METHYLAMINE AND DIMETHYLAMINE 2-OXO-1,2-DIHYDROBENZO [CD]INDOLE-6-SULFONIC ACID

E. T. NUKHOVA

Ivanovo State University, Faculty of Biology and Chemistry, 1st year Master in Chemistry

## Annotation

***The aim*** of this work is to theoretically determine the geometric structure of the conformers of methylamine (A) and dimethylamide (B) molecules of 2-oxo-1,2-dihydro-benzo[cd]indole-6-sulfonic acid.

***The relevance*** of the studied topic is that on the basis of these compounds, antitumor drugs can be obtained, as well as substituted derivatives of naphthalene sulfonic acid act as intermediates, as a basis for the synthesis of new compounds.

***Research objectives***:

- Search for stable conformers of molecules;
- Investigation of the geometric structure of molecular conformers;
- Study of the effect of the substituent influence on the change in the geometric parameters of the indole core;
- The dependence of the energy of the molecules on the value of the torsion angles.

## Conclusions

Changes in the parameters characterizing the position and structure of sub-stituents in the studied molecules are studied.

The calculations performed showed that the studied molecules have several stable conformers that differ in the orientations of the sulfonamide and methyl groups relative to the naphthalene backbone.

The calculated structures show that the parameters of the indole island change slightly when one or two hydrogen atoms in the amide group are replaced by methyl groups. The greatest difference is observed in the values of the internuclear distances CC adjacent to the ipso-carbon atom in the conformer 1 of the dimethylamidamide molecule. The distance C1S increases even more noticeably, and S-N2 decreases. A noticeable increase in the C1-S-N2 valence angle in the 1 conformer of the dimethylamide molecule should be noted. In contrast, the Ipso angle C9-C1-C2 decreases when the hydrogen atoms are replaced by methyl groups, which is associated with an increase in the donor properties of the methylamide and dimethylamide groups.

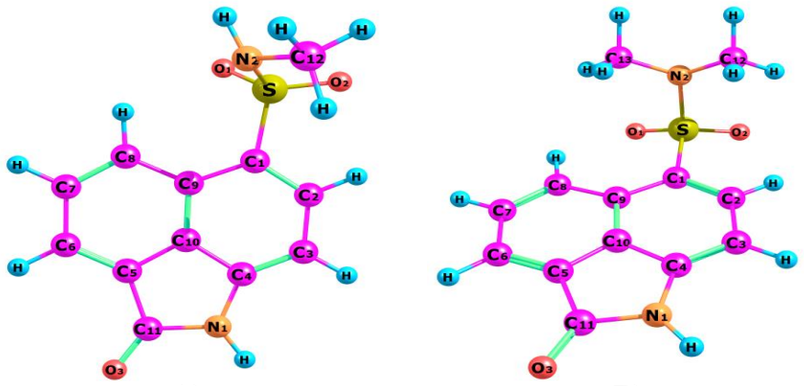
The geometry of molecules is one of the main characteristics of chemical compounds and is of fundamental importance for chemistry. A number of representatives of naphthalene sulfonic acid derivatives should be attributed to the compounds, the structure of which is currently poorly understood.

## Objects and methods

***Objects of research:***

- *methylamide* 2-oxo-1,2-dihydrobenzo[cd]indole-6-sulfonic acid;
- *dimethylamide* of 2-oxo-1,2-dihydrobenzo [cd]indole-6-sulfonic acid.

***Research methods:*** quantum chemical calculations using the GAUSSIAN-2009 computational complex, the B3LYP/cc-pVTZ DFT method.



A) B)

**Fig. 1**. Geometric structure of the most stable conformers of the studied molecules

## Results and discussion

A preliminary scan of the potential energy surface (PPE) corresponding to the change in the torsion angles with a step of 10° was performed, while all other parameters were independently varied (Figure 2). The conformational search was carried out on the basis of the analysis of the graphs of the PPE function. The energy minima indicate the presence of several stable conformers. Thus, it was found that the molecules of methylamine and dimethylamine have 5 and 4 stable conformers, respectively. The geometric structure of the most stable conformers of the studied molecules obtained as a result of calculations is shown in Figure 1.

**Table 1.** Structural parameters of the most stable conformers of the molecules of methylamine and dimethylamine 2-oxo-1,2-dihydro-benzo [cd]indole-6-sulfonic acid (the values of the internuclear distances are given in Å, the angles in deg)

| Parameters | Methylamide 1 conformer | Dimethylamide 1 conformer |
|---|---|---|
| $r_e$ $(C_{фен}\text{-}H)_{ср.}$ | 1.080 | 1.081 |
| $r_e$ (N2-C12) | 1.465 | 1.460 |
| $r_e$ (C1-C9) | 1.432 | 1.436 |
| $r_e$ (C1-S) | 1.785 | 1.798 |
| $r_e$ $(S\text{-}O)_{ср.}$ | 1.454 | 1.451 |
| $r_e$ (S-N2) | 1.680 | 1.676 |
| ∠ (C9-C1-C2) | 120.5 | 120.0 |
| ∠ (C9-C1-S) | 121.7 | 123.1 |
| ∠ (C1-S-N2) | 102.5 | 107.4 |
| ∠ C9-C1-S-N2 | 67.4 | 85.7 |
| ∠C1-S-N2-C12 | 83.5 | 70.3 |
| $\nu_1$ | 40.4 | 35.0 |

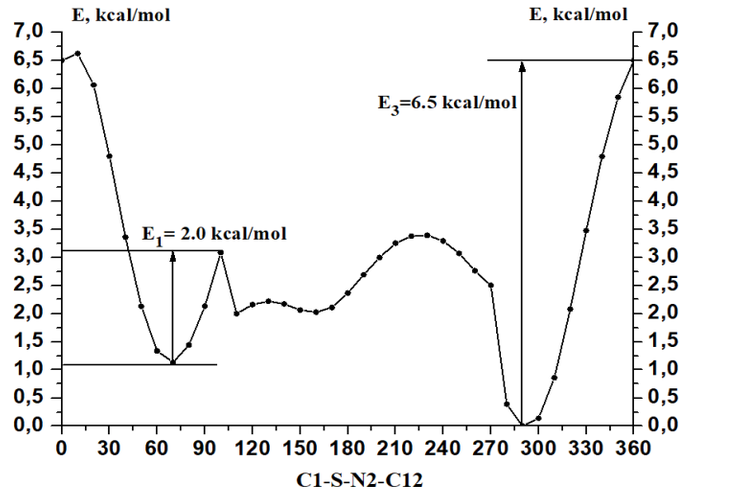



**Fig. 2**. Dependence of the total energy of the methylamino 2-oxo-1,2-dihydrobenzo[cd]indole-6-sulfonic acid molecule on the torsion angle C1-S-N2-C12, obtained by the B3LYP/cc-pVTZ method