



Volume 5

**ABSTRACT BOOK
IN 5 VOLUMES**

26–30 September, 2016
Ekaterinburg, Russia



MAKING SUBATOMIC ELECTRONIC DESCRIPTORS PREDICTIVE: THE CASE OF HALOGEN BONDS

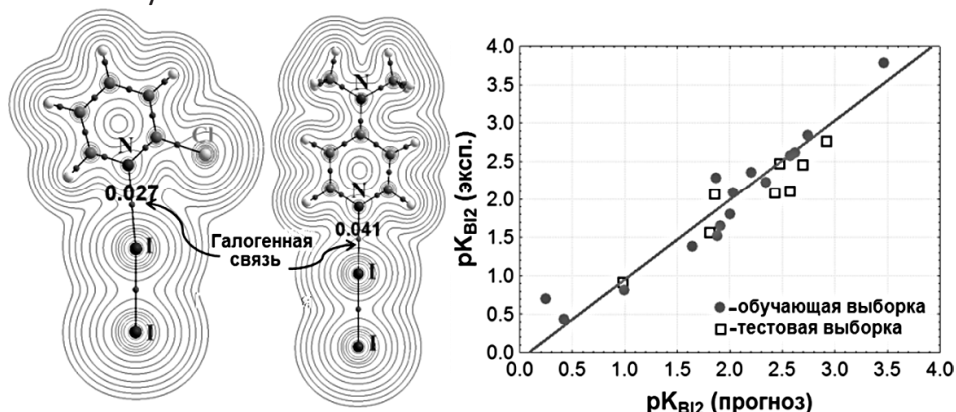
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Availability of the accurate electron density obtained from a wave function or from X-ray diffraction experiment allows to derive the structural descriptors at the subatomic level. Now, it is necessary to make possible the prediction of chemical binding properties by immersing these descriptors to the concept of structure-property relationships.

In this work we apply the combination of subatomic electron-density descriptors, as the delocalization indices^{1,2}, the source function^{2,3}, the interatomic energy calculated using Interacting Quantum Atom method^{2,4}, the atomic dipole moments as well as the energy characteristics at bond critical points of electron density to characterize a halogen bond. The N...I halogen bond features for the complexes of N-containing organic molecules with diiodine have been studied. In particular, we found that the delocalization indices of halogen N...I bond, $\delta(N, I)$, are well correlated⁵ with the basicity pK_{B12} according to the iodine basicity scale.



We have also tested the new approach considering the internal electronic pressure to look at the halogen bond from another perspective.

References

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This work was supported by Russian Foundation for Basic Research, grants 16-03-00057a and 14-03-00961.