

## [PP1]

**Revealing the Common Trends for Non-Covalent Interactions  
with the Various Electrophilic Sites**Ekaterina V. Bartashevich<sup>1</sup>, Svetlana E. Muhitdinova<sup>1</sup>, Vladimir G. Tsirelson<sup>1,2</sup><sup>1</sup>South Ural State University, Chelyabinsk, Russia<sup>2</sup>D.I. Mendeleev University of Chemical Technology, Moscow, RussiaE-mail: [bartashevichev@susu.ru](mailto:bartashevichev@susu.ru)

Analysis of the quantitative relationships between the interaction energy,  $E_{\text{int}} = E_{\text{comp}} - [E(\text{NH}_3) + E(\text{AX})] + E_{\text{BSSE}}$ , in molecular complexes and the local properties at the bond critical points in electron density ( $\Gamma_{\text{bcp}}$ ) was performed for 55 complexes of ammonia interacted with substrates through the halogen (XB), chalcogen (ChB), and pnictogen (PnB) bonds ( $\text{XHal}\dots\text{NH}_3$ ,  $\text{X}_2\text{S}\dots\text{NH}_3$ ,  $\text{X}_2\text{Se}\dots\text{NH}_3$ ,  $\text{X}_3\text{P}\dots\text{NH}_3$ , where  $\text{X} = \text{H}, \text{Cl}, \text{F}, \text{Br}, \text{I}$ ). The level of calculations was M06-2X/aug-cc-pVDZ и B3LYP/6-311G\*\* with and without taking D3 correction into account. The one-factor regression analysis helped us to establish that the regular tendencies are observed even for the full sample containing the various types of non-covalent interactions.

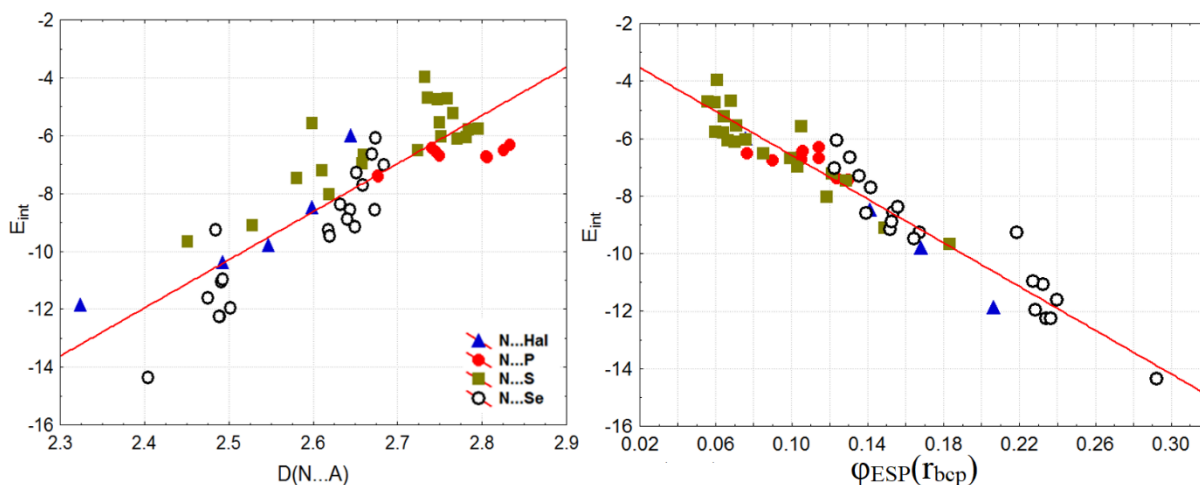


Figure 1: The relationships between interaction energy (kcal/mol) and interatomic distance  $D(\text{N}\dots\text{A})$  (Å) and electrostatic potential (a.u.) at bcp for XB, ChB, PnB in ammonia complexes.

We found the following links with the interaction energy:

$$E_{\text{int}} = -51.8 + 16.6 \cdot D(\text{N}\dots\text{A}), \quad R=0.86;$$

$$E_{\text{int}} = -2.7 - 38.1 \cdot \varphi_{\text{ESP}}(\Gamma_{\text{bcp}}), \quad R=0.96.$$

Here  $D(\text{N}\dots\text{A})$  is the interatomic distance;  $\varphi_{\text{ESP}}(\Gamma_{\text{bcp}})$  is the electrostatic potential at the bond critical point. The later showed the better relationship with the interaction energy. We can speculate that it reflects the role of electrostatics for the studied interactions, while the bond length is too oversimplified descriptor for them.

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