

# Directional Long Range Secondary Forces: A Key Player in Regulating Electrostatics Dominated Noncovalent Interactions

Mrityunjay Kumar Tiwari and Kumar Vanka

Email: [mk.tiwari@ncl.res.in](mailto:mk.tiwari@ncl.res.in)

There has been a conscious effort in recent times to exploit noncovalent interactions in order to achieve specifically designed goals. Noncovalent interactions that have obtained biggest attentions so far are dominated by electrostatic contributions, *e.g.*, H-bonding,  $\sigma$ -hole bonding, interactions between ion-pairs and so on. A recent review by Clark, Politzer and Murray states that the polarization and the covalent factors that contribute significantly to noncovalent interactions are electrostatic in nature.<sup>1</sup> According to the Feynman interpretation, even the dispersion interaction is electrostatic in origin.<sup>2</sup> Existing literature also signifies that electrostatic interactions are long range interactions<sup>3</sup> as they decrease with distance less quickly than  $r^{-d}$ , where  $d$  is the dimensionality of the system. Herein, we have proposed a method based on electrostatic force calculations that emphasizes upon the significance and directional nature of long range secondary electrostatic interactions.<sup>4</sup> The basic theme of our work has been explained by a simple model shown in Fig. 1. If all of the individual distances between the charges on the smaller and the larger subunit in Fig. 1 are equal in the two complexes, the intermolecular electrostatic potential of both the systems would be the same. However, the electrostatic force of interaction will vary: the structure on the right

will be more tightly held. One can also see from Fig. 1 that the line of approach of the two interacting species is of significance. We have further shown that our method can also be exploited in designing new superior systems of diverse binding by designing new molecules of association constant up to 15 orders of magnitude higher than the best reported hydrogen bonded complexes in which goal of researchers is to obtain as strong a binding as possible; and by further designing an anion which has 6 order of magnitude lower association tendency with cation than the best reported example in Contact-ion pair case where researchers aim to design anions with as weaker binding as possible.

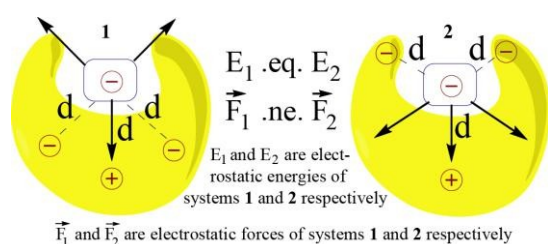


Figure 1. The representation of electrostatic forces between two molecular

partners bonded by noncovalent interactions and having different charge distributions in three-dimensional space;  $d$  is the distance between the two charges. This model considers both primary and secondary interactions.

## References:

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