

# Contribution of Nitrogen Heteroatom to Anion- $\pi$ Interaction of N-heterocyclic Anthracene C14-2mH10-2mN2m ( $m = 1, 2$ , and $3$ ) with Chloride Anion

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## Abstract

N-heterocyclic aromatic in anion- $\pi$  interaction has been playing a crucial role in a host of chemical and biological processes. In the present contribution, several different complexes composed of N-heterocyclic anthracene C14-2mH10-2mN2m ( $m = 1, 2$ , and  $3$ ) and chloride anion are investigated at the atomic level. We find that anion- $\pi$  interactions are enhanced with the increasing number of N atoms. In addition, positions of nitrogen heteroatoms also have a significant effect on this interaction. Contributions of  $\alpha$ ,  $\beta$  and  $\gamma$  N atoms are in order of  $N\beta > N\gamma > N\alpha$ . Moreover, energy decomposition analysis indicates that electrostatic interactions are the dominant stabilizing forces when chloride anion locates above aromatic ring, while the influence of other terms becomes significant when chloride anion deviates from aromatic ring. It is worth noting that dispersion forces play an important role in those anion- $\pi$  interactions.

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