

# Density Functional Theory Studies of Bonding in Complexes $\text{H}_3\text{N}\cdots\text{XY}$ of Ammonia and Dihalogen Molecules: A Comparison with Experimental Results from Rotational Spectroscopy

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The electron density and nuclear quadrupole coupling constants (NQCC) of the  $\text{H}_3\text{N}\cdots\text{XY}$  ( $n\sigma$  type in Mulliken notation) complexes, ( $\text{X}, \text{Y} = \text{F}, \text{Cl}, \text{Br}$  and  $\text{I}$ ), are analyzed with the aid of density functional calculations. To demonstrate the quality of the calculations, various bond lengths and NQCCs obtained by using the hybrid Becke-Lee-Perdew-Yang functional are compared with the corresponding experimental values determined from rotational spectroscopy. An analysis of the NQCC values and various quantities derived from the natural bond orbital approach reveals that the molecular interaction is mainly electrostatic, with probably only a small extent of intermolecular electric charge redistribution on complex formation.

*Key words:* DFT; Quadrupole Coupling Constants;  $n\sigma$  complexes.