# Noncovalent Interactions of 1,4-Dithiafulvene and Nitroaromatics: A Combined DFT and Ab Initio Molecular Dynamics (AIMD) Study

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**Abstract**

The noncovalent interactions between a redox-active molecule, phenyl-substituted dithiafulvene (Ph-DTF), and ten commonly encountered nitroaromatic compounds (NACs) were systematically investigated by means of density functional theory (DFT) calculations and ab initio molecular dynamics (AIMD) simulations. Our modeling studies examined their 1:1 complexes in terms of equilibrium geometries, frontier molecular orbitals (FMOs), nature of noncovalent forces, intermolecular charge transfer (ICT), interaction energies and related energy decomposition analysis. The computational results indicate that Ph-DTF can form thermodynamically stable supramolecular complexes with trinitro-substituted benzenes (e.g., 2,4,6-trinisuchtrotoluene and picric acid), but its interactions with mono- and dinitrobenzenes do not exhibit such stability. The selective binding properties are further corroborated by AIMD simulations. Overall, this computational work establishes a comprehensive understanding of the nature of noncovalent interactions of Ph-DTF with various NACs, and the results can be used as theoretical guidance for the rational design of selective receptors and/or chemosensors for certain NACs that are of great concern in current industrial applications and environmental control.

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