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Data Article

Electronic and optical absorption properties of the derivatives of 1,3,4-Oxadiazole

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ABSTRACT

The present data article report the electronic and optical properties such as ionization energy (IE), electron affinity (EA), energy gap between highest occupied and lowest unoccupied molecular orbitals ($\Delta E_{HOMO\text{-}LUMO}$) and maximum absorption wavelength (λ_{max}) for mono- and disubstituted derivatives of 1,3,4-oxadiazole with electron-donating and -withdrawing substituents. For the mono substituted derivatives studied, the pyrrole substituted oxadiazole has the least value of ionization energy and nitro substituted oxadiazole has the highest value of electron affinity. Among the various disubstituted derivatives of oxadiazole, the one with the substitution of pyrrole as a donor moiety and nitro as an acceptor moiety showed remarkable optical properties suggesting their use in optoelectronic devices.

Specifications table

Subject area	Computational Chemistry
Compounds	Derivatives of 1,3,4-oxadiazole
Data category	Computational simulations
Data acquisition format	Density functional theoretical method
Data type	Simulated
Procedure	Electronic structure calculations using the functional B3LYP, B3LYP-GD3 and M06-2X and 6–311++g(d,p) basis set
Data accessibility	Data is provided in article.

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Rationale

1,3,4-oxadiazole and its derivatives have taken wide attention due to their excellent charge injection ability, electron transport and hole blocking properties, absorption and emissive properties. Some of the recent theoretical and experimental studies of these compounds have been reported [1-10]. These studies revealed that the electronic and optical properties such as ionization energy, electron affinity, energy gap between the highest occupied and lowest unoccupied molecular orbitals (HOMO and LUMO) and the absorption wavelength of the derivatives of 1,3,4-oxadiazole depend on the substituents attached. Despite great advancement in the synthesis of the derivatives of 1,3,4-oxadiazole and their applications in various fields, a systematic study of substituent effects on the above properties is still not available, which motivated us to carry out further investigation in this direction. Taking a series of oxadiazole derivatives with electron-donating and –withdrawing substituents, we present a database of important parameters relevant to optoelectronic properties. To make the study more versatile, disubstituted derivatives of oxadiazole are also investigated.

Procedure

The geometry optimization of all the molecules considered in the present study were carried out using the hybrid density functional B3LYP [11], dispersion-corrected functional B3LYP-GD3 [12] and meta-hybrid functional M06-2X [13] in conjunction with 6–311 ++G** basis set. The frequency calculations were carried out for all the optimized geometries at the same level of theory to ensure that the optimized geometries belong to minima in the potential energy surface. The adiabatic ionization energy and the adiabatic electron affinity were calculated from the energies of the corresponding optimized geometries of the charged and neutral systems. The absorption wavelength and the oscillator strength of all the molecules were determined by means of time-dependent density functional theory (TD-DFT). All of the above calculations were done using the electronic structure program Gaussian 09 [14]. The optimized geometries and the molecular orbital diagrams were generated using the visualization program Gaussview 5 [15].

Data, value and validation

In order to validate the method used, we optimized the parent molecule 1,3,4-oxadiazole using higher level abinitio methods using the second order Møller-Plesset Perturbation (MP2) and Coupled Cluster Singles and Doubles (CCSD) methods. The ionization energy of 1,3,4-oxadiazole obtained using MP2 method was found to be 10.84 eV compared to the experimental value of 11.23 eV [16]. The ionization energy obtained using CCSD methods was 10.58 eV. The values of ionization energy obtained using the functional B3LYP, B3LYP-GD3 and M06-2X used in the present study are 10.79, 10.79 and 10.88 eV, respectively. Considering the computational cost and the accuracy of the results, further studies are limited to density functional methods only.

The various derivatives of oxadiazole considered in this study are categorized into three different sets as presented in scheme 1. The values of important parameters such as ionization energy, electron affinity, energy gap between HOMO and LUMO, the maximum absorption wavelength and the corresponding oscillator strength obtained for the molecules are listed in Table 1 of the present data article. The computed value of ionization energy and electron affinity of various mono- and disubstituted derivatives using B3LYP-GD3 functional are plotted as shown in figures S1-S4 of the supplementary information. The frontier molecular orbital diagrams of all the systems obtained using same functional are depicted in figure S5 of the supplementary information.

The following information is deduced from the results.

Among the monosubstituted derivatives of 1,3,4-oxadiazole, the one with pyrrole as the donor shows the lowest value of ionization energy and that with nitro group as the acceptor has highest electron affinity. For the disubstituted derivatives, the combination of pyrrole-nitro as donor-acceptor groups showed the least value of $\Delta E_{HOMO\text{-}LUMO,}$ which is in the range of values shown by the organic semiconducting materials. The frontier molecular orbital analysis supports strong intramolecu-