



Original Research Article

Molecular Structure, Optical Properties and Frontier Molecular Orbitals for Some of the 4-Substituted Cinnolines: *Ab initio* Calculations

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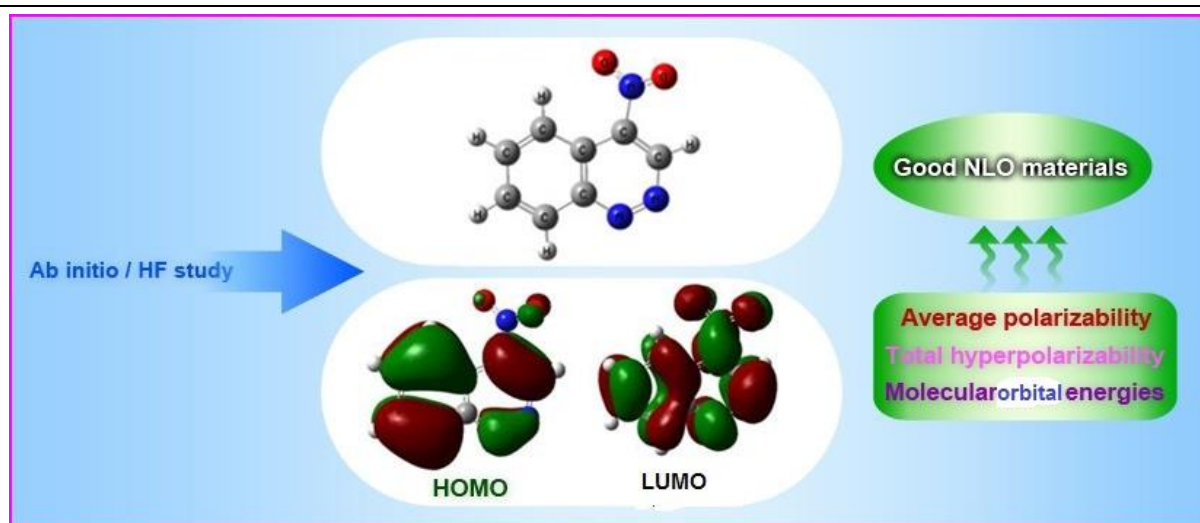
Nonlinear Optical (NLO) Materials

1, 2-Diazanaphthalene

ABSTRACT

In this paper, quantum chemical calculations were performed on urea, cinnoline, and some cinnoline derivatives (**1-8**) at *ab initio*/HF/6-311G (d, p) level of theory using Gaussian09 and Gussview05 programs. Calculated optimized molecular structure, dipole moment (μ), polarizability (α), molecular electrostatic potential (MEP), and the first order hyperpolarizability (β) for hetero-aromatics **1** to **8**, and urea (as a standard molecule) in three phases (gas phase, in presence of water and ethanol) were calculated. The effects of water and ethanol as solvents were taken into account with the aid of the polarizable continuum model (IEF-PCM). The optical properties of studied molecules are increasing in presence of solvents and their values have a direct relationship with the electric constants of solvents. There is a relationship between optical property and energy of the frontier molecular orbitals (FMOs), so these orbitals and the HOMO-LUMO energy gap (ΔE) were investigated. The nonlinear optical (NLO) materials are applied in optical devices, so they are very important. Since experimentally measurement of NLO property is hard, theoretical chemistry is useful in designing new NLO materials.

GRAPHICAL ABSTRACT



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Introduction

For almost half of a century, optical organic compounds have become very popular due to the fact that materials with nonlinear optical properties have potential utilization in the ground of optoelectronic such as dye-sensitized solar cells [1-6]. Many organic compounds have been considered with a large nonlinear optical property such as Schiff bases and their metal complexes [7, 8], aromatic compounds [9-11], charge transfer complexes [12, 13]. Among organo-compounds, the materials with delocalized and resonance electrons are good candidates for nonlinear optical molecules, such as hetero-aromatic rings.

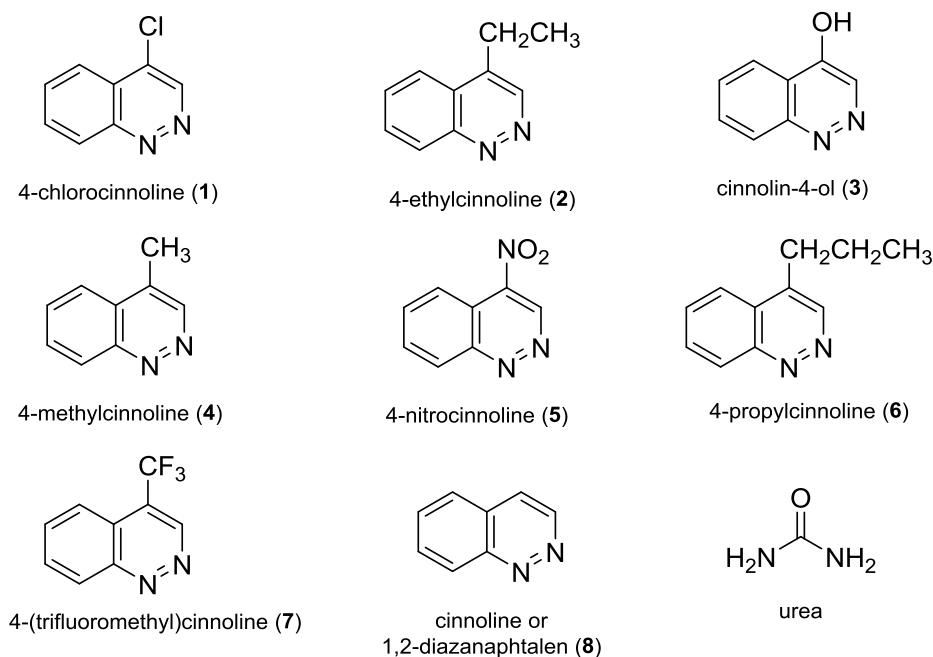
Cinnoline is an aromatic heterocyclic compound with the formula $C_8H_6N_2$. It is isomeric with quinoxaline, phthalazine, and quinazoline. This is a nitrogenous aromatic base and melts at 39 °C. Cinnolines have attracted considerable attention due to the variety of pharmacological activities such as anti-cancer, anti-microbial, anti-inflammatory, and anti-parasitic exhibited by these heterocycles. Other names for cinnoline are 1,2-diazanaphthalene and benzo [c]-1,2-diazine. 1, 2-diazanaphthalenes derivatives are hetero-aromatics, so I have studied these compounds. The aimed hetero-aromatics are shown in Scheme 1.

The NLO property of a compound is showing by the value of the first molecular hyperpolarizability (β), so theoretical calculations and practical measurements on NLO

property are key factors in designing the optical materials. The practical measurement of β is difficult, but theoretical methods resolve this problem. Mechanical quantum computations are helpful in consideration of the relationship between the structure and optical effects [14–20]. The HF theory applies the self-consistent field level and is thus very appropriate for computing many fields of chemistry, including optical properties.

In this inquiry, a computational study was performed about the linear and nonlinear optical properties of these hetero-aromatics in three phases, expressed as dipole moment (μ), average polarizability (α), total hyperpolarizability (β), and energy of HOMO-LUMO molecular orbitals. The geometries of molecules in their ground state were optimized using the HF method at *ab initio* level with a 6-311G (d, p) basis sets using the Gaussian09 software package. In order to study the solvation effect on the nonlinear and linear optical properties, all of calculations in water and ethanol were repeated.

The urea molecule is one of the favorite test molecules for the investigation of different aspects of the accuracy and computational methodology used in calculations of the nonlinear electric properties. Its static and dynamic electric properties have been studied in several papers at various levels of approximation. For comparison, the structural and optical properties of urea were calculated along with the aimed molecules.



Scheme 1. The 2 dimensional structures and IUPAC names of the aimed molecules

Theoretical Method

At first, all the molecules were drawn by Gussview05 [21] program for creating input files. All the ground state geometries of the molecules were optimized by Gaussian09 program [22] and “opt” keyword without imposing any symmetry constraint. The stationary points of all structures were found using “freq” keyword and standard analytical harmonic vibrational analysis. There are no imaginary (negative) frequencies so all the molecules are local structures with minima of potential energy. The dipole moment (μ value), polarizability (α value), first static hyperpolarizability (β value) and molecular orbitals of all the aimed molecules were obtained by “polar” keyword. Optimization and calculating the molecular orbitals and the optical properties were carried by Hartree-Fock theory along with 6-311G (d, p) basis sets. The solvent effects were taken into account with the aid of the polarizable continuum model IEF-PCM with the inclusion of solvent effects. Thus, all of the molecules have been studied in three states: In the gas phase, in presence of ethanol, and presence of water.

Results and Discussion

Molecular geometry optimization

The structure of 1,2-diazanaphthalenes (**8**), its 4-substituted derivatives (**1-7**), and urea have been optimized to study their electronic and optical properties. The equilibrium geometry optimization for all the molecules has been achieved by energy minimization, using *ab initio* method at the HF level of theory, employing the split valence basis sets 6-311G (d, p). The optimized geometries of all molecules under study are local true minima on potential energy surfaces.

Some structural parameters for these molecules are indicated in Table 1. The studying of Φ_{GCCN} in these molecules shows that all of them are 180 degrees. This value represents the co-planarity of substituent (G) and ring. This co-planarity is necessary for resonance and electron delocalization occurrence in **1-7** structures. The molecules with more electron delocalization are good NLO materials.

The N=N bond lengths approximately are 1.26 angstrom in all the molecules; this parameter in literature is 1.279Å. There is good agreement between the calculated $r_{C=N}$ and its normal

experimental value. The r_{C-G} calculated and normal values are in good accordance with each other.

Table 1. The structural features obtained (bond lengths in Pico meter and angles in degrees) for the aimed molecules (**1 - 8**) in gas phase Φ_{GCCN}

Compound	$r_{N=N}$	Exp.	r_{C-G}	Exp.
1	126.36	128	173.31	176
2	125.98	128	151.33	(sp ³ -sp ²) 150
3	126.30	128	133.74	
4	126.20	128	150.50	(sp ³ -sp ²) 150
5	126.31	128	146.95	147
6	125.99	128	151.33	(sp ³ -sp ²) 150
7	125.98	128	150.47	(sp ³ -sp ²) 150
8	126.47	128	-	-

Electric moments

The polarity refers to the distribution of electric charge in a molecule or the degree to which a molecule has a dipole moment which relates to its inherent electric field. Polarity is a constant property of the molecule and does not change with the external field. The dipole moments result in the permanent charge separations through the distances and thus these significant molecular characters were principally applied for studying the interactions between molecules including dipole-dipole forces in polar molecules. The dipole moments of eight molecules and urea in Debye are given in Table 2. These molecules can be ordered on increasing polarity as follows:

In gas phase: **2** (4.63) > **6** (4.62) > **4** (4.58) > **8** (4.25) > **5** (4.02) > **urea** (3.89) > **3** (3.73) > **1** (3.53) > **7** (3.22)

In aqua phase: **2** (6.30) > **6** (6.26) > **4** (6.22) > **8** (5.75) > **urea** (5.24) > **3** (5.06) > **1** (4.73) > **7** (4.21) > **5** (3.96)

In ethanolic phase: **2** (6.21) > **6** (6.18) > **4** (6.13) > **8** (5.68) > **urea** (5.17) > **3** (4.99) > **1** (4.67) > **7** (4.17) > **5** (2.95)

The experimental dipole moment of urea is 4.56. The dipole moments of title molecules are approximately the same as of urea. The dipole moments for hetero-aromatics of **1** to **8** and urea have increased in the presence of a solvent and this increase is more in water.

Table 2. Calculated dipole moment (μ , in Debye) using HF/6-311G (d, p) method for molecules of **1-8** and urea

Compound	μ (gas phase)	μ (Ethanol)	μ (Water)
1 (Ar-Cl)	3.53	4.67	4.73
2 (Ar-Et)	4.63	6.21	6.30
3 (Ar-OH)	3.73	4.99	5.06
4 (Ar-Me)	4.58	6.13	6.22
5 (Ar-NO₂)	3.96	5.02	5.95
6 (Ar-Pr)	4.62	6.18	6.26
7 (Ar-CF₃)	3.22	4.17	4.21
8 (Ar-H)	4.25	5.68	5.75
urea	3.89	5.17	5.24

Polarizability

Due to the presence of an external electric field, the degree of the deformation in the electron clouds of the molecules or atoms is called polarizability. We can be aware of the forces between non-polar and electrically charged species by polarizability. The electron clouds can be deformed via an electric field. When the electron cloud is deformed, the molecule or atom gains an induced dipole moment. This has a correlation with polarizability and electric field strength according to the following formula:

$$\mu_{\text{ind}} = \alpha E$$

Polarizability is one of the properties of matter and determines the power of molecular interactions and NLO properties of the system [23, 24]. Polarizability was analytically calculated at HF/ 6-311G (d, p) level of theory using the keyword 'Polar'. The polarizability is displayed in the output file from Gaussian09w in this order as xx, yy, and zz tensors: α_{xx} , α_{xy} , α_{yy} , α_{xz} , α_{yz} , α_{zz} . The average polarizability (α_{ave}), is described as the following equation:

$$\alpha_{\text{ave}} = (\alpha_{xx} + \alpha_{yy} + \alpha_{zz}) / 3$$

The values of polarizability tensors on output files are shown in atomic unite (au), so the computed values (α_{ave}) were reformed as a standard unit namely electrostatic unit. (1 au

equals with 0.1482×10^{-24} esu) [25]. Table 3 presents the polarizability (α_{ave}) for all investigated molecules in different phases. A comparison between linear optical properties or average polarizability of aimed compounds in a gas phase and in presence of a solvent has been presented. The results showed the inclusion of solvent effects can increase polarizability (α_{ave}) in these compounds. The Polarizability (α_{ave}) values (in esu) can be ordered as follows:

In gas phase: **6** (18.36×10^{-24}) > **2** (16.66×10^{-24}) > **5** (15.27×10^{-24}) > **4** (15.00×10^{-24}) > **1** (14.85×10^{-24}) > **7** (14.60×10^{-24}) > **3** (13.75×10^{-24}) > **8** (13.29×10^{-24}) > **urea** (3.66×10^{-24})

In aqua phase: **6** (24.58×10^{-24}) > **2** (22.48×10^{-24}) > **4** (20.39×10^{-24}) > **1** (20.25×10^{-24}) > **7** (19.61×10^{-24}) > **3** (18.66×10^{-24}) > **8** (18.12×10^{-24}) > **5** (15.23×10^{-24}) > **urea** (4.26×10^{-24})

In ethanolic phase: **6** (24.24×10^{-24}) > **2** (22.17×10^{-24}) > **5** (20.44×10^{-24}) > **4** (20.11×10^{-24}) > **1** (19.97×10^{-24}) > **7** (19.35×10^{-24}) > **3** (18.40×10^{-24}) > **8** (17.87×10^{-24}) > **urea** (4.23×10^{-24})

The polarizability (α_{ave}) values show the linear optical property for **6** is the most and six times larger than the value of urea. This compound approximately is the most polar between aimed compounds.

Table 3. Calculated average polarizability (α_{ave}) using HF/6-311G (d, p) method for molecules of **1-8** and urea in three phases

Compound	Ethanol		Water		Gas phase	
	α_{ave} (in au)	α_{ave} (in esu) $\times 10^{-24}$	α_{ave} (in au)	α_{ave} (in esu) $\times 10^{-24}$	α_{ave} (in au)	α_{ave} (in esu) $\times 10^{-24}$
1 (Ar-Cl)	134.750	19.97	100.21	14.85	136.647	20.25
2 (Ar-Et)	149.585	22.17	112.40	16.66	151.682	22.48
3 (Ar-OH)	124.183	18.40	92.76	13.75	125.913	18.66
4 (Ar-Me)	135.677	20.11	101.18	20.39	137.595	20.39
5 (Ar-NO₂)	137.924	20.44	103.03	15.00	102.774	15.23
6 (Ar- Pr)	163.575	24.24	123.87	18.36	165.847	24.58
7 (Ar-CF₃)	130.541	19.35	98.52	14.60	132.325	19.61
8 (Ar-H)	120.579	17.87	89.64	13.29	122.290	18.12
urea	28.560	4.23	24.67	3.66	28.758	4.26

Hyperpolarizability

The first static hyperpolarizability or dipole hyperpolarizability can be considered as an indicator for nonlinear optical feature of the system, as it indicates the dipole moment's second-order reply to the applied electric field. It is very important of investigating the molecular NLO features because it plays a key role in information technologies as well as industrial applications. The hyperpolarizability is a third-order symmetric tensor that is elucidated by a $3 \times 3 \times 3$ matrix. The 27 constituents of this matrix are diminishing to 10 constituents as a consequence of the Kleinman symmetry [26]. The value of the total hyperpolarizability is computed by the following equations:

$$\beta_x = \beta_{xxx} + \beta_{xyy} + \beta_{xzz}$$

$$\beta_y = \beta_{yyy} + \beta_{yzz} + \beta_{yxx}$$

$$\beta_z = \beta_{zzz} + \beta_{zyy} + \beta_{zxx}$$

$$\beta_{\text{total}} = [(\beta_x^2 + \beta_y^2 + \beta_z^2)]^{1/2}$$

The first-order hyperpolarizability (β) of these molecular systems (**1-8**) and urea was calculated using HF level of theory with the standard 6-311G (d, p) basis sets. Since calculated values of the hyperpolarizability (β) are in atomic units (au.), these values have been converted into electrostatic unit (esu) ($1 \text{ au} = 8.6393 \times 10^{-33}$

esu). The results of hyperpolarizability for molecules **1** to **8** and urea are mentioned in Table 4, in which the total hyperpolarizability values have the following order:

In gas phase: **5** (0.68×10^{-30}) > **7** (0.67×10^{-30}) > **2** (0.64×10^{-30}) > **6** (0.63×10^{-30}) > **4** (0.57×10^{-30}) > **1** (0.54×10^{-30}) > **8** (0.53×10^{-30}) > **3** (0.50×10^{-30}) > **urea** (0.34×10^{-30})

In aqua phase: **5** (3.47×10^{-30}) > **7** (2.80×10^{-30}) > **8** (2.32×10^{-30}) > **1** (2.30×10^{-30}) > **3** (1.74×10^{-30}) > **2** (1.37×10^{-30}) > **6** (1.31×10^{-30}) > **4** (1.07×10^{-30}) > **urea** (0.43×10^{-30})

In ethanolic phase: **5** (3.26×10^{-30}) > **7** (2.64×10^{-30}) > **1** (2.17×10^{-30}) > **3** (1.64×10^{-30}) > **8** (1.43×10^{-30}) > **6** (1.23×10^{-30}) > **4** (1.09×10^{-30}) > **urea** (0.43×10^{-30}) > **2** (0.14×10^{-30})

The results show that 4-nitro-cinnoline (**5**) is the best material for NLO applications, and according to these data, it is clear cinnoline derivatives with electron-acceptor groups have more the nonlinear properties.

Urea is one of the prototypical molecules used for the NLO properties of the molecular systems for comparative purposes, so optical properties of urea were calculated at the same level of theory. Nevertheless, β_{tot} values of all these molecules are about 5 times more than that of urea.

Table 4. Calculated first hyperpolarizability using HF level of theory and 6-311G (d, p) basis sets for molecules of **1-8** and urea in three phases

h	Ethanol		Water		Gas phase	
	β_{total} (in au)	$\beta_{\text{total}} \times 10^{-30}$ (in esu)	β_{total} (in au)	$\beta_{\text{total}} \times 10^{-30}$ (in esu)	β_{total} (in au)	$\beta_{\text{total}} \times 10^{-30}$ (in esu)
1 (Ar-Cl)	250.77	2.167	266.52	2.30	62.09	0.54
2 (Ar-Et)	15.84	0.14	158.19	1.37	73.68	0.64
3 (Ar-OH)	189.93	1.64	200.86	1.74	57.69	0.50
4 (Ar-Me)	126.4	1.09	123.99	1.07	66.25	0.57
5 (Ar-NO₂)	377.4	3.26	401.3	3.47	78.3	0.68
6 (Ar-Pr)	142.76	1.23	151.66	1.31	72.55	0.63
7 (Ar-CF₃)	305.32	2.64	323.91	2.80	77.53	0.67
8 (Ar-H)	165.80	1.43	269.02	2.32	61.66	0.53
urea	49.38	0.43	49.69	0.43	39.74	0.34

Frontier molecular orbitals

The overlapping of two atomic or molecular orbitals produces two new molecular orbitals.

One of the new orbitals is higher in energy than the original ones named lowest unoccupied molecular orbital (LUMO) and one is lower, highest occupied molecular orbital (HOMO). The HOMO and LUMO are known as frontier molecular orbitals (FMOs) because they lie at the outermost boundaries of the electrons of a compound. These orbitals play an important role in evaluating molecular chemical stability, chemical reactivity and hardness-softness of the molecule [27]. These orbitals are a pair of orbitals in the compound, which allows them to interact most strongly.

To evaluate the relations between values of FMOs energy and the first static hyperpolarizability of the molecules, the calculated values of HOMO and LUMO energy, the energy gap (ΔE) of compounds **1-8** and urea using HF/6311G (d, p) method are listed in Table 5. It can be seen from this Table 5, the obtained values of β_{tot} for the similar compounds increase with decreasing values of the energy gap ,i.e., there is an inverse relationship between the β_{tot} and ΔE . The HOMO and LUMO energy help to use intramolecular charge transfer to explain the hyperpolarizability. The HOMO orbital acts as an electron donor, while the LUMO orbital is an electron acceptor. E_{HOMO} is often associated with the electron-donating ability of a molecule, whereas E_{HOMO} indicates its ability to accept electrons. The frontier molecular orbital figures of **4**, **5**, **8** and urea are shown in Figure 1.

The energy gap (ΔE) represents the chemical reactivity of compounds and is an important stability index. For a system, lower value of ΔE makes it more reactive or low kinetic stability. The more ΔE makes the material more stable for optical devices such as a solar cell. As depicted in the following order, compound **3** has the largest energy gap:

In gas phase: urea (15.16 eV) > **3** (10.67 eV) > **8** (10.61 eV) > **6** (10.57 eV) > **2** (10.56 eV) > **4** (10.55 eV) > **7** (10.50 eV) > **1** (10.46 eV) > **5** (10.02 eV)

In aqua phase: urea (15.78 eV) > **3** (10.55 eV) > **8** (10.49 eV) > **6** (10.45 eV) = **2** (10.45 eV) > **4** (10.43 eV) > **7** (10.37 eV) > **1** (10.35 eV) > **5** (9.89 eV)

In ethanolic phase: urea (15.81 eV) > **8** (10.60 eV) > **3** (10.54 eV) > **6** (10.46 eV) > **2** (10.45 eV) > **4** (10.44 eV) > **7** (10.38 eV) > **1** (10.35 eV) > **5** (9.90 eV).

Molecular electrostatic potential surface

The molecular electrostatic potential (MEP) at a given point p (x, y, z) in the vicinity of a molecule is the force acting on a positive test charge (a proton) located at p through the electrical charge cloud generated by the molecules, electrons, and nuclei [28]. The molecular charge distribution remains unperturbed through the external test charge (no polarization occurs). The electrostatic potential of a molecule is a good guide in assessing the reactivity of the molecule towards electrophilic or nucleophilic reactants.

The MEP surfaces or electrostatic potential energy maps are very useful tools for simultaneously displaying shape, size, and charge density distribution in the three-dimensional space of a molecule. This may be a method for predicting relationships of physicochemical properties with the molecular structure.

These maps are calculated using quantum methods or experimental methods. The MEP is typically visualized by mapping its values onto the surface reflecting the molecules' boundaries. To calculate the MEP of the molecules, first molecular geometries were optimized at the HF/6-31G (d, p) level of theory. Then, the maps of the studied compounds were drawn by Gussview05 program (Fig. 2). Red and blue colors in the MEP structure point to more electron-rich and electron-poor regions, respectively. The blue zone is the region where the charge density is positive or has a positive electrostatic potential and forms the positive pole of the molecule. The more negative electronegative and positive electrostatic potential sites are more favorable for the attraction of nucleophilic and electrophilic species.

Table 5. The obtained molecular orbital energies (in eV) using HF/6-311G (d, p) method for molecules of **1-8** and urea in three phases

Compound	Gas phase				Ethanol				Water			
	E _{LUMO} (au)	E _{HOMO} (au)	ΔE _t (au)	ΔE _t [*] (eV)	E _{LUMO} (au)	E _{HOMO} (au)	ΔE _t (au)	ΔE _t (eV)	E _{LUMO} (au)	E _{HOMO} (au)	ΔE _t (au)	ΔE _t (eV)
1 (Ar-Cl)	0.0494	-0.3351	0.3846	10.46	0.0476	-0.3329	0.3805	10.35	0.0474	-0.3329	0.3803	10.35
2 (Ar-Et)	0.0660	-0.3222	0.3882	10.56	0.0602	-0.3240	0.3842	10.45	0.0598	-0.3242	0.3840	10.45
3 (Ar-OH)	0.0722	-0.3198	0.3920	10.67	0.0666	-0.3209	0.3875	10.54	0.0663	-0.3210	0.3872	10.55
4 (Ar-Me)	0.0647	-0.3228	0.3875	10.55	0.0596	-0.3239	0.3835	10.44	0.0593	-0.3240	0.3833	10.43
5 (Ar-NO₂)	0.0163	-0.3517	0.3680	10.02	0.01961	-0.3441	0.3637	9.90	0.0197	-0.3438	0.3635	9.89
6 (Ar- Pr)	0.0666	-0.3218	0.3883	10.57	0.0604	-0.3240	0.3844	10.46	0.0601	-0.3241	0.3842	10.45
7 (Ar-CF₃)	0.0420	-0.3440	0.3860	10.50	0.0416	-0.3397	0.3813	10.38	0.0416	-0.3395	0.3811	10.37
8 (Ar-H)	0.0624	-0.3274	0.3897	10.61	0.0624	-0.3274	0.3897	10.60	0.0581	-0.3273	0.3854	10.49
urea	0.1404	-0.4168	0.5572	15.16	0.1569	-0.4229	0.5798	15.78	0.1577	-0.4232	0.5809	15.81

*1 Hartree (au)=27.2116 eV

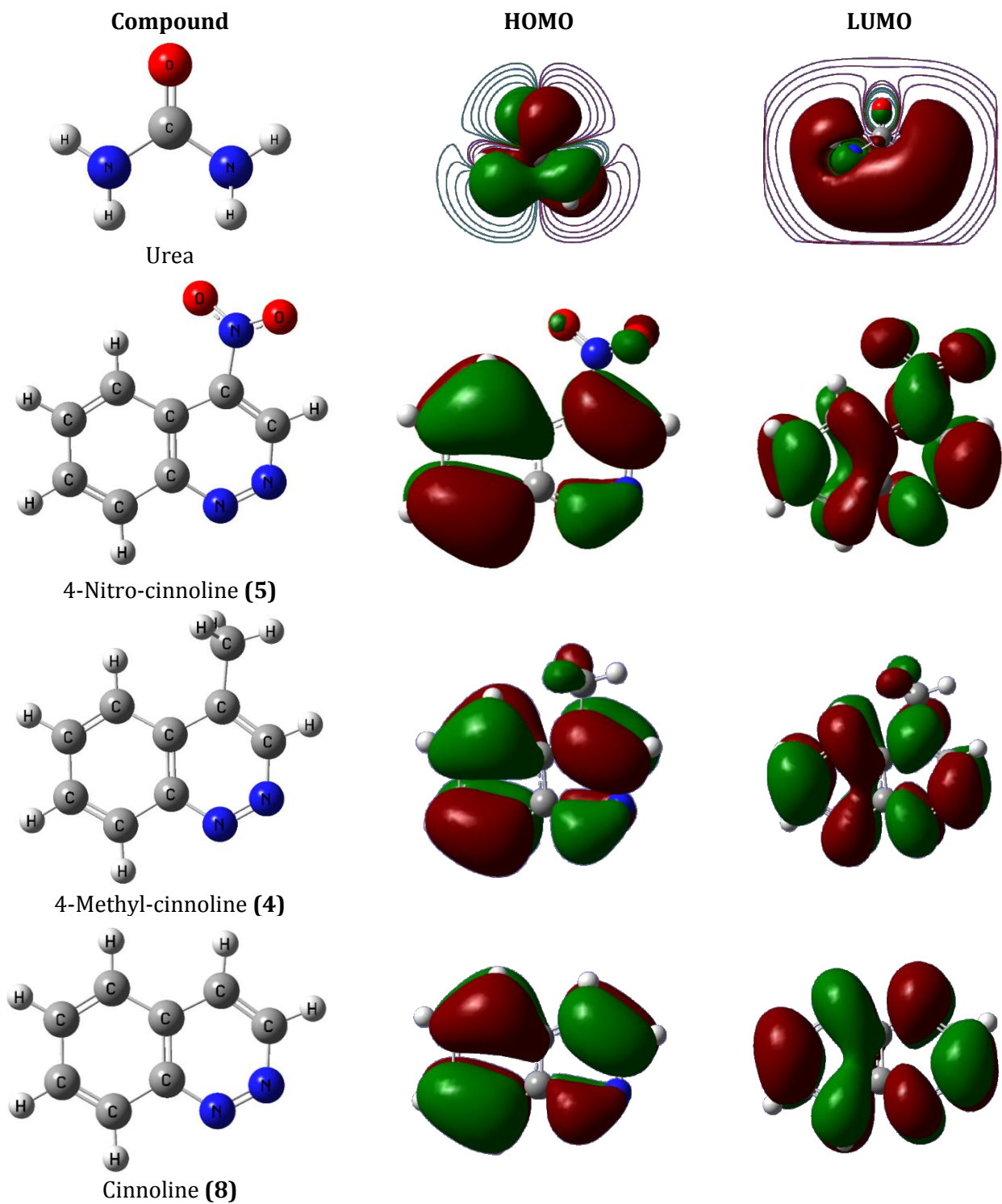


Figure 1. The frontier molecular orbital figures of 4, 5, 8 and urea

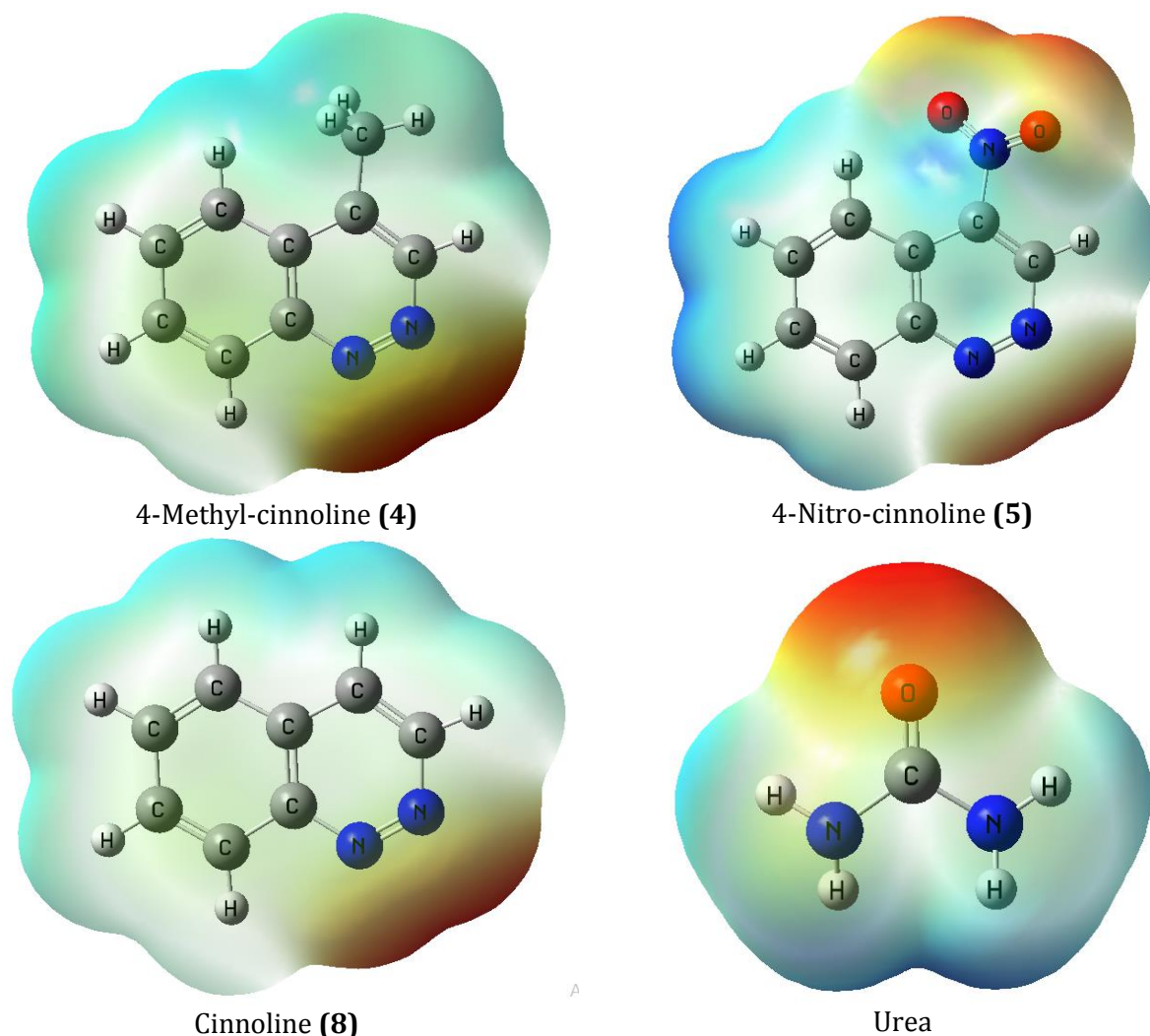


Figure 2. Molecular electrostatic potential surfaces of **4**, **5**, **8** and urea

Conclusion

Theoretical calculations provide another method to research the essential properties of organic compounds. Since practically measurement of NLO property such as Z-scan is hard, theoretically chemistry provides a useful way.

The molecular structures of 4-substituted cinnolines (**1-7**) were studied using HF level of theory and 6-311G (d, p) basis sets. Linear and NLO features of compounds **1-8** and urea were obtained by calculating the dipole moment, the average polarizability and the first static hyperpolarizability with this method. This

research showed that the investigated 4-substituted cinnolines (**1-7**) are good candidates for non-linear optical materials. Especially 4-nitro-cinnoline (**5**) has larger the first hyperpolarizability β values (β for **5** is 5 times more than β for urea), which makes these compounds attractive objects for future studies of nonlinear optics.

Also, frontier molecular orbitals energies (E_{HOMO} and E_{LUMO}), a HOMO-LUMO energy gap (ΔE) of compounds **1 to 8** using the same method were calculated. The frontier orbitals energy gap is one of the important stability indexes. The energy gap (ΔE) represents the chemical reactivity of compounds and is an important stability index.

ΔE and reactivity or kinetic stability of a structure have an inverse relation. The more ΔE makes the material more stable for optical devices. The molecules **3** and **8** have the largest energy gap so they show higher stability in optical applications including solar cells. The significant requirements for becoming a high-quality NLO material include a high optical coefficient, high thermal and chemical stability, and good transparency that the studied molecules have these characters.

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Disclosure statement

No potential conflict of interest was reported by the author.

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