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A Density Functional Approach toward Structural Features and Properties of C_{20} and its Complexes with C_2X_4, C_2X_2 (X = H, F, Cl, Br) for Synthesis Application

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Abstract

The complexes between C_{20} and C_2X_4, C_2X_2 (X = H, F, Cl, Br) have been studied theoretically at the B3LYP/6-311G (d,p) level. The calculations include the optimized geometries, the interaction energies, aromaticity and thermodynamic. The interaction energies ranging from -60 to -101 kcal/mol and being ordered as: X = F> Cl > Br. Natural bond orbital (NBO) analysis has been performed on all geometries. The energy and oscillator strength calculated by Time-Dependent Density Functional Theory (TD-DFT) results, and indicate that, in all the molecules HOMO-1 → LUMO transition has the major contribution in the most intensity electronic transition.

Keywords: *C_{20} cages complexes, Alkenes, Alkynes, Interaction energy.*

Introduction

There have been extensive theoretical and experimental studies in the structure of the C_{20} molecule, particularly because it is potentially the smallest fullerene [1-6]. In 2000, the smallest possible fullerene C_{20} was generated and characterized in the gas phase [7]. Fullerenes are considered promising candidates for basic elements in nanoscale devices, and several examples of fullerene-based devices have been investigated both experimentally and theoretically [8-10]. Modification of C20 is a matter of general interest to experimentalist as well theoreticians to look into the structural as well as electronic properties. For example, structure and properties of fullerene C20 and its derivatives $C_{20}(C_2H_2)_n$ and $C_{20}(C_2H_4)_n$ (n=1–3) have been studied [11].

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In the present work, extensive ab initio and DFT calculations on fullerene C20 and their interactions with C_2X_2 and C_2X_4 (X=H, F, Cl, Br) have been performed. Structure, aromaticity, frontier orbital analysis and electronic transition have been explored.

Computational Methods

All calculations were carried out with the Gaussian 03 suite of program [12]. All molecules were described by the standard 6-311G (d,p) basis set [13-16]. Geometry optimization was performed using Becke's hybrid three-parameter exchange functional and the nonlocal correlation functional of Lee, Yang, and Parr (B3LYP) [17]. A vibrational analysis was performed at each stationary point which corresponds to an energy minimum.

Geometries were optimized at this level of theory without any symmetry constraints followed by the calculations of the first order hyperpolarizabilities. The total static first hyperpolarizability β was obtained from the relation:

$$\beta_{tot} = \sqrt{\beta_x^2 + \beta_y^2 + \beta_z^2}$$

upon calculating the individual static components:

$$\beta_i = \beta_{iii} + \frac{1}{3}\sum_{i\neq j}(\beta_{ijj} + \beta_{jij} + \beta_{jji})$$

Due to the Kleinman symmetry [18]:

$$\beta_{xyy} = \beta_{yxy} = \beta_{yyx};\ \beta_{yyz} = \beta_{yzy} = \beta_{zyy},\ldots$$

one finally obtains the equation that has been employed:

$$\beta_{tot}=[(\beta_{xxx}+\beta_{xyy}+\beta_{xzz})^2+(\beta_{yyy}+\beta_{yzz}+\beta_{yxx})^2+(\beta_{zzz}+\beta_{zxx}+\beta_{zyy})^2]^{1/2}$$

The electronic spectra for the studied compounds were calculated by TD-DFT [19] using the same hybrid functional and basis sets as used for the calculation of the hyperpolarizabilities. The 10 lowest excitation energies were computed.

NBO analysis was then performed by the NBO 3.1 program under Gaussian 2003 program package at the B3LYP level of theory [20]. The noncovalent bonding-antibonding interaction can be quantitatively described in terms of the NBO approach that is expressed by means of the second-order perturbation interaction energy (E(2)) [21-24]. This energy represents the estimate of the off-diagonal NBO Fock matrix elements. It can be deduced from the second-order perturbation approach [25]:

$$E^{(2)}=-q_i\frac{(F_{i,j})^2}{\varepsilon_j-\varepsilon_i}$$

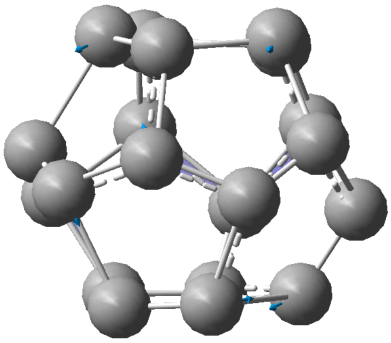
Where q_i is the ith donor orbital occupancy, ε_i, ε_i are diagonal elements (orbital energies) and F(i, j) is the off-diagonal NBO Fock matrix element.

Results and discussion

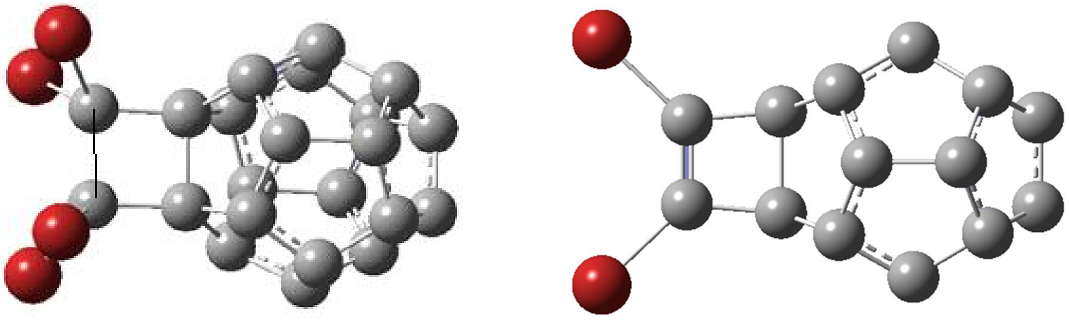
Energetic

Table 1 presents the computed absolute energies (E) of $C_{20}\ldots C_2X_4$, $C_{20}\ldots C_2X_2$, C_2X_4 and C_2X_2 (X=H, F, Cl, Br), interaction energies

(I.E) and the corrected interaction energies (I.E corrected) for the complexes (Figure 1). The interaction energies values show that interaction between alkyne species and C_{20} is stronger than alkene species. There is strongest interaction in the fluorinated species.



C_{20}



C_{20}...C_2F_4 **C_{20}...C_2X_4**

Figure1. Structures of C_{20}, C_{20}...C_2X_4, and C_{20}...C_2X_2 (X=F, Cl, Br) complexes.

Table 1. Calculated Energy (Hartree), interaction energy (kcal/mol), basis set super position error (BSSE, kcal/mol) and corrected interaction energy (kcal/mol), for C_{20}, C_{20}...C_2X_4, and C_{20}...C_2X_2 (X=F, Cl, Br) complexes by the method B3LYP with 6-311G(d, p) basis set.

Cage	E(cage)	E(C_2X_2)	IE	BSSE	$IE^{corrected}$
C_{20}	-761.59	-	-	-	-
C_{20}...C_2H_4	-840.30	-78.61	-60.58	0.00466	-57.65
C_{20}...C_2F_4	-1237.36	-475.65	-77.35	0.01198	-69.84
C_{20}...C_2Cl_4	-2678.76	-1917.08	-56.94	0.01215	-49.31
C_{20}...C_2Br_4	-11134.44	-10372.76	-53.06	0.00798	-48.05
C_{20}...C_2H_2	-839.06	-77.35	-69.01	0.00382	-66.61
C_{20}...C_2F_2	-1037.58	-275.83	-101.59	0.00711	-97.12
C_{20}...C_2Cl_2	-1758.30	-996.57	-86.30	0.00613	-82.45
C_{20}...C_2Br_2	-5986.15	-5224.42	-82.89	0.00676	-78.65

Structure

Table 2 reports the selected CC bond lengths. These values indicate CC bonds in C_2X_2 and C_2X_4 decrease in complexes. This decreasing is more for alkene than alkyne complexes. Furthermore, these distances are sensitive to the nature of X substituent, varying from 1.57 to 1.67 Å in alkene complexes, and

1.34 to 1.35 Å in alkyne complexes. On the other hand, $CC(C_{20})$ distances show a good correlation with interaction energies (Figure 2). In addition, our results indicate planar alkenes and alkynes distorted in complexes.

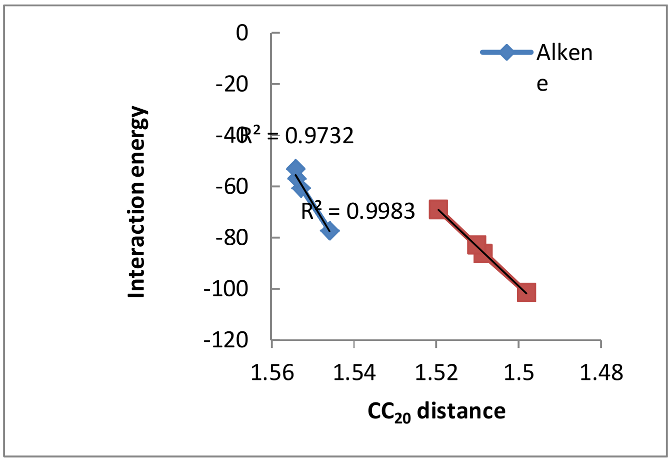


Figure 2. A linear correlation between interaction energy and CC_{20} distance.

Table 2. E-E bond distances for C_{20}, $C_{20}…C_2X_4$, and $C_{20}…C_2X_2$ (X=F, Cl, Br) complexes by the method B3LYP with 6-311G (d, p) basis set.

	CC	**Free ligand**	**Δr**	**$CC(C_{20})$**
$C_{20}…C_2H_4$	1.56665	1.32685	0.2398	1.55280
$C_{20}…C_2F_4$	1.58300	1.32197	0.26103	1.54586
$C_{20}…C_2Cl_4$	1.63378	1.34147	0.29231	1.55394
$C_{20}…C_2Br_4$	1.63536	1.34068	0.29468	1.55413
$C_{20}…C_2H_2$	1.34110	1.19805	0.14305	1.51947
$C_{20}…C_2F_2$	1.33829	1.18481	0.15348	1.49807
$C_{20}…C_2Cl_2$	1.34437	1.19970	0.14467	1.50872
$C_{20}…C_2Br_2$	1.34622	1.20373	0.14249	1.51012

Polarizability

Polarizabilities describe the response of a system in an applied electric field [26]. They determine not only the strength of molecular interactions (such as the long range intermolecular induction, dispersion forces, etc.) as well as the cross sections of different scattering and collision processes, but also the nonlinear optical properties of the system[27]. The isotropic polarizability <α> is calculated as the mean value as given in the following equation [28]:

$$\langle\alpha\rangle = \frac{(\alpha_{xx} + \alpha_{yy} + \alpha_{zz})}{3}$$

And anisotropic polarizability with:

$$\Delta\alpha = \left[\frac{(\alpha_{XX} - \alpha_{YY})^2 + (\alpha_{YY} - \alpha_{ZZ})^2 + (\alpha_{ZZ} - \alpha_{XX})^2}{2}\right]^{\frac{1}{2}}$$

The calculated isotropic and anisotropic polarizability values indicate these values increase in the complexes (Table 3). Also, these values show that isotropic polarizability of alkene complexes are more than alkyne complexes. But, anisotropic polarizability of alkene complexes is less than alkyne complexes. On the other hand, the calculated isotropic and anisotropic polarizability values increase in the halogenated species.

Table 3. Isotropic, anisotropic polarizability and NICS values in the center of cages values for C_{20}, $C_{20}\ldots C_2X_4$, and $C_{20}\ldots C_2X_2$ (X=F, Cl, Br) complexes by the method B3LYP with 6-311G (d, p) basis set.

	αxx	αyy	αzz	$<\alpha>$	$\Delta\alpha$	**NICS**
C_{20}	167.14	167.64	162.49	165.76	4.92	-21.56
$C_{20}\ldots C_2H_4$	222.21	179.10	177.67	192.99	961.25	-37.94
$C_{20}\ldots C_2F_4$	213.84	176.54	177.60	189.33	676.40	-37.85
$C_{20}\ldots C_2Cl_4$	278.31	212.03	223.73	238.02	1877.40	-39.54
$C_{20}\ldots C_2Br_4$	315.29	236.25	249.00	266.85	2700.89	-40.73
$C_{20}\ldots C_2H_2$	217.84	178.21	170.56	188.87	965.86	-37.29
$C_{20}\ldots C_2F_2$	215.02	178.53	170.17	187.90	853.41	-37.37
$C_{20}\ldots C_2Cl_2$	265.77	207.64	175.42	216.28	3145.27	-36.36
$C_{20}\ldots C_2Br_2$	288.97	222.07	181.32	230.79	4430.46	-37.86

Frontier orbital energies and chemical hardness

The frontier orbital energies, HOMO-LUMO gap energy, hardness, chemical potential, and electrophilicity of all complexes computed are given in the Table 4. These values indicate the energy of HOMO decreases in complexes. LUMO energies increase in $C_{20}\ldots C_2H_4$ and C_{20}….C2H2comlxes, but these values decrease in halogenated substitution. Furthermore, alkene complexes are harder than alkyne complexes.

The hardness and chemical potential of these complexes calculated from the HOMO and LUMO orbital energies using the following approximate expression:

$$\mu=(\varepsilon_{HOMO} + \varepsilon_{LUMO})/2$$

$$\eta= (\varepsilon_{HOMO} - \varepsilon_{LUMO})/2$$

Where μ is the chemical potential (the negative of the electronegativity), and η is the hardness [29, 30].

The hardness values of in Table 4 indicate the increasing of these values in complexes.

The chemical potential were also evaluated for this set of molecules. The chemical potential characterizes the tendency of electrons to escape from the equilibrium system. The values of chemical potential show that the decreasing of these values in complexes (Table 4).

To evaluate the electrophilicity of these complexes, we have calculated the electrophilicity index,ω, for each complex measured according to Parr, Szentpaly, and Liu [31] using the expression:

$$\omega = \frac{\mu^2}{2\eta}$$

The values of electrophilicity index have been shown in Table 4. These values show that the electrophilicity decreases in complexes.

Table 4. Frontier orbital energies (Hartree), HOMO-LUMO gap energy (eV), hardness (eV), chemical potential (eV), and electrophilicity (ω) for C_{20}, $C_{20}...C_2X_4$, and $C_{20}...C_2X_2$ (X=F, Cl, Br) complexes by the method B3LYP with 6-311G(d, p) basis set.

	HOMO	LUMO	Gap	η	μ	ω
C_{20}	-0.200	-0.129	1.93	0.96	-4.48	10.41
$C_{20}...C_2H_4$	-0.208	-0.117	2.48	1.24	-4.42	7.86
$C_{20}...C_2F_4$	-0.228	-0.138	2.46	1.23	-4.99	10.10
$C_{20}...C_2Cl_4$	-0.230	-0.137	2.53	1.26	-5.00	9.89
$C_{20}...C_2Br_4$	-0.227	-0.134	2.53	1.27	-4.92	9.55
$C_{20}...C_2H_2$	-0.209	-0.119	2.45	1.23	-4.46	8.12
$C_{20}...C_2F_2$	-0.220	-0.130	2.45	1.22	-4.77	9.30
$C_{20}...C_2Cl_2$	-0.221	-0.131	2.44	1.22	-4.79	9.39
$C_{20}...C_2Br_2$	-0.220	-0.130	2.44	1.22	-4.77	9.30

Thermochemical Analysis

Thermochemical analysis is studied for all complexes. The values of ΔH, ΔS, ΔG and K are reported in Table 5 in which the individual terms are referred to a temperature of 298 K. The reaction can be considered as:

$$C_{20} + C_2X_m \rightarrow C_{20}\ C_2X_m \text{ (X=F, Cl, Br; m=2 or 4)}$$

As can be verified, the ΔS values are similar for all complexes. Since in this reaction two particles form one, ΔS should be a negative value. Although the relative difference of the ΔG is almost the same as the ΔH. The equilibrium constants of the all complexes are given in Table 5. These values show that complexation causes to increasing of the equilibrium constant in alkyne complexes. But, stability increases only in $C_{20}...C_2F_4$ complex. On the other hand, alkyne complexes have more stability than alkene complexes. The trend of stability in halogaenated species is: F>Cl>Br.

Table 5. Calculated thermodynamic parameters: ΔG (kcal/mol), ΔH (kcal/mol), ΔS (kcal/mol.K), K for the for C_{20}, $C_{20}...C_2X_4$, and $C_{20}...C_2X_2$ (X=F, Cl, Br) complexes by the method B3LYP with 6-311G (d, p) basis set.

Cage	**ΔG**	**ΔH**	**ΔS**	**K**
$C_{20}...C_2H_4$	-41.56	-56.80	-0.0511	3.04E+30
$C_{20}...C_2F_4$	-58.42	-74.56	-0.0542	6.97E+42
$C_{20}...C_2Cl_4$	-37.65	-54.43	-0.0563	4.10E+27
$C_{20}...C_2Br_4$	-34.18	-50.60	-0.0551	1.17E+25
$C_{20}...C_2H_2$	-51.27	-65.28	-0.0470	3.96E+37
$C_{20}...C_2F_2$	-84.05	-98.71	-0.0492	4.39E+61
$C_{20}...C_2Cl_2$	-68.80	-83.55	-0.0495	2.87E+50
$C_{20}...C_2Br_2$	-65.31	-80.15	-0.0498	7.95E+47

Nucleus-independent chemical shift analysis (NICS)

The nucleus-independent chemical shift (NICS) method has been widely employed to characterize the aromaticity [32]. As an effort to discuss the use of NICS as a measure of aromaticity for cages, we have calculated NICS values in the center of the cage. See Table 5. From Table 5, it can be seen that all cages have large negative NICS values, indicating their enhanced aromatic properties. All these NICS values are mainly attribute to the delocalized π electrons current. These values show that complexation causes to increasing of aromaticty in cages. On the other hand, C_{20}… alkene complexes have more aromaticity than C_{20}…alkyne complexes. Also, aromaticity increase in halogen substituted complexes.

Natural bond orbital analysis (NBO)

Natural Bond Orbital (NBO) analysis was performed to investigate the charge populations and bonds properties of C_{20} and C_2X_4, C_2X_2 (X = H, F, Cl, Br) complexes.

Table 6 reports also the atomic charges of selected carbon atoms (C1, C2, C3, and C4) as computed from a natural population analysis of the B3LYP/6-311G(d,p) wavefunction. The natural charges of C1, and C2 of C_2H_2 and C_2H_4 are -0.221 and -0.359, respectively. As expected, upon replacement of H with halogen in alkene and alkyne the atomic charge of the C1 and C2 atoms increases. It is worth noticing that the atomic charge of the C1 and C2 atoms of C_2H_4 interacted to C_{20} substituents are slightly more negative than those of free C_2H_4. In other complexes, these charges are more positive than those of free alkyne and alkene. The C1 and C2 atoms of fluorinated species are the most positively charged amongst those tabulated.

Analyzing the hybridization of molecular orbitals (MOs) could help us to understand the chemical bond properties of the system. The hybridization of CC bond of alkenes and alkynes is analyzed as followings: there are two and three bond orbitals for free alkenes and alkynes, respectively three C–C bonds in alkenes (Table 6). But for C–C bonds in complexes, there are one and two bond orbitals. As seen from Table 6, the σ (C–C) bond is formed from a spn hybrid on carbon. As shown in Table 6 the contribution of p orbital increases in complexes.

Table 6. Charge of carbon, CC occupancy and hybridation in alkene or alkyne for C_{20}, $C_{20}…C_2X_4$, and $C_{20}…C_2X_2$ (X=F, Cl, Br) complexes in NBO basis.

Cage	q_C	occupancy	CC hydridation
C_2H_4	-0.35907	1.99484	0.7071* C sp 1.42 + 0.7071* C sp 1.42
		1.99929	0.7071* C p 1.00 + 0.7071* C p 1.00
C_2F_4	0.62766	1.99837	0.7071* C sp 1.20 + 0.7071* C sp 1.20
		1.99724	0.7071* C sp 1.00 + 0.7071* C p 1.00
C_2Cl_4	-0.14885	1.99459	0.7071* C sp 1.20 + 0.7071* C sp 1.20
		1.98181	0.7071* C p 1.00 + 0.7071* C p 1.00
C_2Br_4	-0.30695	1.99616	0.7071* C sp 1.14+ 0.7071* C sp 1.14
		1.98643	0.7071* C p 1.00+ 0.7071* C p 1.00
C_2H_2	-0.22107	1.99164	0.7071* C sp 0.90 + 0.7071* C sp 0.90
		1.99957	0.7071* C p 1.00+ 0.7071* C p1.00
		1.99957	0.7071* C p 1.00+ 0.7071* C p 1.00
C_2F_2	0.26566	1.99105	0.7071* C sp 0.62 + 0.7071* C sp 0.62
		1.99779	0.7071* C p 1.00+ 0.7071* C p 1.00
		1.99779	0.7071* C p 1.00 + 0.7071* C p 1.00
C_2Cl_2	-0.12848	1.99087	0.7071* C sp 0.72 + 0.7071* C sp 0.72
		1.98970	0.7071* C p 1.00 + 0.7071* C p 1.00
		1.98970	0.7071* C p 1.00 +0.7071* C p 1.00
C_2Br_2	-0.20644	1.99282	0.7071* C sp 0.73+ 0.7071* C sp 0.73
		1.99135	0.7071* C p 1.00 +0.7071* C p 1.00
		1.99135	0.7071* C p 1.00+ 0.7071* C p 1.00
$C_{20}…C_2H_4$	-0.37105	1.98095	σ: 0.7071* C sp 2.93+ 0.7071* C 22 sp 2.93
$C_{20}…C_2F_4$	0.75760	1.98269	σ: 0.7071* C sp 2.79+ 0.7071* C sp 2.79
$C_{20}…C_2Cl_4$	-0.07519	1.97636	σ: 0.7071* C sp 2.67+0.7071* C 22 sp 2.67
$C_{20}…C_2Br_4$	-0.22208	1.97891	σ: 0.7071* C sp 2.47+ 0.7071* C 22 sp 2.47
$C_{20}…C_2H_2$	-0.14621	1.98131	σ: 0.7071* C sp 1.73 + 0.7071* C sp 1.73
		1.91652	π: 0.7071* C p 1.00+ 0.7071* C p 1.00
$C_{20}…C_2F_2$	0.37066	1.98480	σ: 0.7071* C sp 1.53+ 0.7071* C sp 1.53
		1.90195	π: 0.7071* C p 1.00+ 0.7071* C p 1.00
$C_{20}…C_2Cl_2$	-0.04537	1.98074	σ: 0.7071* C sp 1.53 + 0.7071* C sp 1.53
		1.91311	π: 0.7071* C p 1.00 + 0.7071* C p 1.00
$C_{20}…C_2Br_2$	-0.11735	1.98174	σ: 0.7071* C sp 1.50 + 0.7071* C sp 1.50
		1.91605	π: 0.7071* C p 1.00+ 0.7071* C p 1.00

Electronic spectra

We found the most intense electronic transition (λ_{max}) of molecules. The wavelength, oscillator strength and the composition of the transitions obtained by TD-DFT calculations are given in Table 7.

The energies of the most intensity transition (λ_{max}) show that these values increase in the complexes. λ_{max} values of alkyne complexes are more than alkene complexes.

Theoretical calculations indicate that, in all the molecules HOMO-1 → LUMO transition makes the major contribution in this electronic transition.

Table 7. The most intensity electronic transition, wave length and oscillator strength for C_{20}, $C_{20}...C_2X_4$, and $C_{20}...C_2X_2$ (X=F, Cl, Br) complexes.

	Transition	λ_{max}	**f**
C_{20}	HOMO-1 -> LUMO	413.60	0.0033
$C_{20}...C_2H_4$	HOMO-1 -> LUMO	468.37	0.0124
$C_{20}...C_2F_4$	HOMO-1 -> LUMO	464.37	0.0122
$C_{20}...C_2Cl_4$	HOMO-1 -> LUMO	460.22	0.0100
$C_{20}...C_2Br_4$	HOMO-1 -> LUMO	460.76	0.0094
$C_{20}...C_2H_2$	HOMO-1 -> LUMO	468.59	0.0130
$C_{20}...C_2F_2$	HOMO-1 -> LUMO	463.55	0.0125
$C_{20}...C_2Cl_2$	HOMO-1 -> LUMO	464.87	0.0124
$C_{20}...C_2Br_2$	HOMO-1 -> LUMO	465.29	0.0123

Hyperpolarizability

The first static hyperpolarizability (β_{tot}) values for the molecules are shown in Table 8. The results show that the magnitude of the first hyperpolarizability tensor increases in all complexes. These values are rather moderate.

Table 8. β components and β_{tot} values (10^{-30} esu) of C_{20}, $C_{20}...C_2X_4$, and $C_{20}...C_2X_2$ (X=F, Cl, Br) complexes.

	C_2H_4	**C_2F_4**	**C_2Cl_4**	**C_2Br_4**	**C_2H_2**	**C_2F_2**	**C_2Cl_2**	**C_2Br_2**	**C_{20}**
β_{XXX}	409.17	-83.09	112.14	-106.07	-298.93	94.27	54.42	-538.52	0.00
β_{XXY}	7.57	1.65	3.92	51.85	-2.92	-2.19	4.73	1.03	0.00
β_{XYY}	91.53	-23.56	22.03	-11.81	-82.06	33.56	-10.77	-10.85	0.00
β_{YYY}	-0.13	-7.18	-2.86	159.14	-1.87	-2.24	-1.89	-0.37	0.00
β_{XXZ}	-11.10	6.94	2.73	-41.85	-0.95	-3.82	5.19	-4.97	0.00
β_{XYZ}	-1.81	-5.13	-4.39	8.35	-9.20	-1.01	3.13	6.91	0.00
β_{YYZ}	-2.05	10.53	-0.52	-12.61	7.64	-3.90	5.49	6.38	0.00
β_{XZZ}	135.27	10.11	74.35	-48.30	-41.27	-44.10	12.66	-20.96	0.00
β_{YZZ}	2.25	-12.02	2.58	30.21	-5.29	-6.30	-9.89	-11.20	0.00
β_{ZZZ}	11.93	24.80	-4.90	-69.46	-13.36	-2.46	8.45	9.16	0.00
β_{tot}	5.50E-30	9.23E-31	1.80E-30	2.75E-30	3.65E-30	7.35E-31	5.17E-31	4.93E-30	3.36E-35
$\beta_{tot}\times10^{-30}$	5.50	0.92	1.8	2.75	3.65	0.73	0.52	4.93	0

Conclusion

In this present work, we have performed the theoretical structure and properties analysis of fullerene C_{20} and its interaction with C_2X_4, C_2X_2 (X = H, F, Cl, Br). The molecular geometry, frontier orbital analysis, electronic transitions, aromaticity and non-linear optical properties of the molecule in the ground state have been calculated by using ab initio DFT (B3LYP) methods with 6-311G(d,p) basis set. The computed geometries show changes in the bond lengths caused by the presence of interaction. The molecular Gibbs's free energy, the reaction enthalpy and several thermo dynamical parameters were also being found with the ab initio and DFT methods with the same basis set. The predicted first hyperpolarizability shows that the molecule might have a reasonably moderate nonlinear optical (NLO) behaviour. The HOMO–LUMO energy gap reflects the chemical reactivity of the molecule. Predicted NICS values indicate that C20, and its complexes are of aromaticity.

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