

Research Article **NLO and NBO Analysis of Sarcosine-Maleic Acid by Using HF and B3LYP Calculations**

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We report a theoretical study on molecular structure, vibrational spectra, nonlinear optical (NLO), and natural bond orbital (NBO) analysis of sarcosine-maleic acid ($C_7H_{11}NO_6$) in the ground state calculated by using the Hartree-Fock (HF) and density functional method (DFT/B3LYP) with 6–31++G(d,p) basis set. We repeat NBO calculations with 6–31G(d,p) basis set so as to see the diffuse function impact on NBO analysis. Stability of the molecule arising from hyper conjugative interactions and charge delocalization has been analyzed using NBO analysis. NBO analysis shows that there is a O–H···O and N–H···O hydrogen bond in the title compound, which is consistent with the conclusion obtained by the analysis of molecular structure. The calculated HOMO and LUMO energies show that charge transfer occurs within the molecule. Also, these results are supported by the NLO parameters. Finally, the calculated results were applied to simulate infrared and Raman spectra of the title compound which showed good agreement with experimental ones.

1. Introduction

The development of organic NLO materials for device applications requires a multidisciplinary effort involving both theoretical and experimental studies in the fields of chemistry, physics, and engineering. Quantum-chemical calculations have made an important contribution to the understanding of the electronic polarization underlying the molecular NLO processes and the establishment of structure-property relationships [1, 2]. Reliable structure-property relationships, where property here refers to linear polarizability ($\langle \alpha \rangle$), and first-($\langle \beta \rangle$) are required for the rational design of optimized materials for photonic devices such as electrooptic modulators and all-optical switches.

Nonlinearity in organic chromophores can be synthetically modulated by varying the composition or length of conjugated π -systems, and by evaluating the effects of various electron-donor and -acceptor groups. However, the electron richness or deficiency of the aromatic rings cannot be predicted reliably on the basis of the calculated ring atom charge densities as these quantities are rather sensitive to the quality of the basis sets employed. Since the NLO properties depend on the extent of charge transfer (CT) interaction across the conjugative paths and the electron transfer ability of an aromatic ring depends primarily on its ionization potential (IP) and electron affinity (EA) which, in the framework of MO theory and Koopman's theorem, are, respectively, equal to the negative of HOMO and LUMO energies, a reliable trend of the electron releasing/withdrawing strengths of the heterocycles may be predicted on the basis of the calculated frontier orbital energies [3, 4].

Natural bond orbital (NBO) analysis [5] was originated as a technique for studying hybridization and covalency effects in polyatomic wave functions. The work of Foster and Weinhold was extended by Reed et al., who employed NBO analysis that exhibited particularly H-bonded and other strongly bound van der Waals complexes [6]. *Ab initio* wave functions transformed to NBO form are found to be in good agreement with Lewis structure concepts and with the basic Pauling-Slater-Coulson picture [7, 8] of bond hybridization and polarization. The filled NBOs σ of the "natural Lewis structure" are well adapted to describing covalency effects in molecules [6]. However, the general transformation to NBOs also leads to orbitals that are unoccupied in the formal Lewis structure and that may be used to describe noncovalent effects. The symbols σ and σ^* are used in a generic sense to refer to filled and unfilled orbitals of the formal Lewis structure, though the former orbitals may actually be core orbitals (*c*), lone pairs (*n*), σ or π bonds (σ , π), and so forth, and the latter may be σ or π antibonds (σ^* , π^*), extravalence-shell Rydberg (*r*) orbitals, and so forth, according to the specific case.

The antibonds represent unused valence-shell capacity, spanning portions of the atomic valence space that are formally unsaturated by covalent bond formation. The non-covalent delocalization effects are associated with $\sigma \rightarrow \sigma^*$ interactions between filled (donor) and unfilled (acceptor) orbitals, it is natural to describe them as being of "donor-acceptor", charge transfer, or generalized "Lewis base-Lewis acid" type.

Sarcosine, also known as *N*-methylglycine $(CH_3NH_2^+CH2OO)^-$, is a natural amino acid inhibiting two hydrogen atoms which are located at the nitrogen atom. There have been several reports investigating qualitatively the crystal structure of sarcosine in pure [9] and made on several crystalline complexes with organic and inorganic acids derivatives [10–17]. This amino acid is found naturally in starfish, sea urchins and in the antibiotic actinomycin [18], and is also used in certain cosmetics [19]. It is used in manufacturing biodegradable surfactants and toothpastes as well as in other applications.

Maleic acid ((Z)-Butenedionic acid) is an organic compound (sometimes named a dicarboxylic acid), a molecule with two carboxyl groups. Maleic acid is the cis isomer of butenedioic acid, whereas fumaric acid is the trans isomer of it [20]. It is mainly used as a precursor to fumaric acid, but unlike its parent maleic anhydride, maleic acid enjoys few applications. This acid is naturally present in honey and over the years has been subjected to extensive investigation by several researchers [21].

There are a number of quantum-chemical approaches for computing molecular nonlinearity and NBO analysis with different reliabilities [6, 22–31]. It has been demonstrated that the calculation results of these approaches are consistent with the experiments.

DFT methods, particularly hybrid functional methods, have evolved to powerful quantum chemical tool for the determination of the electronic structure of molecules [32– 34]. In the framework of DFT approach, different exchange and correlation functionals are routinely used. Among these, the B3LYP combination which is developed by modifying the exchange functional in the hybrid BLYP method is the most used since it proved its ability in reproducing various molecular properties, including vibrational spectra. The combined use of B3LYP functional and standard basis sets provide an excellent agreement between accuracy and computational efficiency of spectroscopic properties for large and medium size molecules.

The FT-IR, FT-Raman, and X-ray crystallography of sarcosine-maleic acid was discussed in detail [18]. In spite of its importance, mentioned above, there is not any theoretical calculation on the sarcosine-maleic acid. Therefore, we made a deep investigation and studied the structure, vibrational frequencies and frontier molecular orbital energies, NLO,

and NBO analysis of the title compound. The evaluations have been performed by means of the HF and DFT/B3LYP level of theory. Also, the chemical hardness (η) and softness (*S*) and electronegativity (χ) parameters have been obtained by using molecular frontier orbital energies.

2. Computational Details

The molecular structures of the title compound in the ground state are optimized HF and B3LYP with 6-31++G(d, p) basis set, then vibrational frequencies for optimized molecular structures have been calculated. The vibrational frequencies for these species are scaled by 0.9131 and 1.0013 for low-frequency vibrations and 0.8970 and 0.9614 for the rest of vibrations, respectively [35]. The RMS (root mean square) force criterion to 3×10^{-4} and the SCF convergence criteria set to RMSDP = 12×10^{-4} and MAXDP = 18×10^{-4} (the maximum absolute value change for individual density matrix elements between two successive SCF cycles). Also, the total static dipole moment (μ), (α), (β) values were calculated by using the following equations [28, 29, 31]:

$$\mu = \left(\mu_x^2 + \mu_y^2 + \mu_z^2\right)^{1/2},$$

$$\langle \alpha \rangle = \frac{1}{3} \left(\alpha_{xx} + \alpha_{yy} + \alpha_{zz}\right),$$

$$\Delta \alpha = \left(\frac{\left(\alpha_{xx} - \alpha_{yy}\right)^2 + \left(\alpha_{yy} - \alpha_{zz}\right)^2 + \left(\alpha_{zz} - \alpha_{xx}\right)^2}{2}\right)^{1/2},$$

$$\langle \beta \rangle = \left(\beta_x^2 + \beta_y^2 + \beta_z^2\right)^{1/2},$$
(1)

where

$$\beta_{x} = \beta_{xxx} + \beta_{xyy} + \beta_{xzz},$$

$$\beta_{y} = \beta_{yyy} + \beta_{xxy} + \beta_{yzz},$$

$$\beta_{z} = \beta_{zzz} + \beta_{xxz} + \beta_{yyz}.$$
(2)

By using HOMO and LUMO energy values for a molecule, electronegativity, and chemical hardness can be calculated as follows: $\chi = (I + A)/2$ (electronegativity), $\eta = (I - A)/2$ (chemical hardness), $S = 1/2\eta$ (chemical softness) where *I* and *A* are ionization potential and electron affinity, and $I = -E_{\text{HOMO}}$ and $A = -E_{\text{LUMO}}$, respectively [36, 37].

The natural bonding orbitals (NBO) calculations [38] were performed using NBO 3.1 program [39] as implemented in the Gaussian 09 package [40] at the HF and DFT methods with 6-31++G(d,p) and 6-31G(d,p) levels. The second-order Fock matrix was used to evaluate the donor-acceptor interactions in the NBO basis [41]. The interactions result in a loss of occupancy from the localized NBO of the idealized Lewis structure into an empty non-Lewis orbital. For each

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Paramotors	Evr. [42]	Evn	Evp	Theoretica	al (6–31G++(d,p))
Parameters	Exp. [43]	Exp.	Exp.	HF	B3LYP
Bond lengths (Å)					
Sarcosine					
N_1-C_2	1.4818 (19)	1.481 (2) [9]	1.485 (3) [44]	1.474	1.469
$N_1 - C_3$	1.4973 (19)	1.484 (2) [9]	1.485 (3) [44]	1.477	1.475
$C_1 - C_2$	1.512 (2)	1.525 (2) [9]	1.497 (3) [44]	1.510	1.514
C_1-O_1	1.3099 (19)	1.271 (2) [9]	1.297 (3) [44]	1.310	1.346
C_1-O_2	1.2178 (18)	1.239 (2) [9]	1.297 (3) [44]	1.189	1.213
Maleic acid					
$C_4 - C_5$	1.500 (2)	1.473 (5) [45]	1.470 (5) [46]	1.507	1.507
C_4-O_3	1.2607 (19)	1.208 (6) [45]	1.217 (4) [46]	1.192	1.217
C_4-O_4	1.2640 (19)	1.303 (5) [45]	1.321 (5) [46]	1.309	1.335
O_4-O_5	—	2.427 (4) [45]	2.475 (4) [46]	2.583	2.625
$O_4 - H_{11}$	—	1.030 [45]	0.940 (5) [46]	0.966	0.986
$O_5 - H_{11}$	0.840	1.400 [45]	1.530 (5) [46]	1.627	1.652
$C_{5}-C_{6}$	1.338 (2)	1.318 (5) [45]	1.340 (5) [46]	1.329	1.348
$C_{6}-C_{7}$	1.497 (2)	1.480 (5) [45]	1.487 (5) [46]	1.505	1.489
$C_7 - O_5$	1.2913 (19)	1.258 (4) [45]	1.286 (4) [46]	1.271	1.336
C7-O6	1.2317 (18)	1.250 (4) [45]	1.220 (4) [46]	1.219	1.225
Bond Angles (°)					
Sarcosine					
$N_1 - C_2 - C_1$	110.66 (11)	111.40 (2) [9]	111.55 (18) [44]	108.71	110.01
$C_2 - C_1 - O_1$	112.39 (12)	115.20 (2) [9]	111.4 (2) [44]	112.07	111.78
$C_2 - C_1 - O_2$	121.80 (13)	118.70 (2) [9]	122.8 (2) [44]	122.65	124.45
$O_1 - C_1 - O_2$	125.80 (14)	126.10 (2) [9]	125.7 (2) [44]	125.12	123.74
$C_3 - N_1 - C_2$	111.86 (11)	112.90 (2) [9]	114.31 (18) [44]	114.74	113.10
Maleic acid					
$C_4 - C_5 - C_6$	129.39 (14)	131.5 (3) [45]	131.7 (4) [46]	133.53	134.81
$C_4 - O_4 - H_{11}$	—	108.0 [45]	107.0 (3) [46]	112.35	111.47
$C_5 - C_4 - O_3$	116.99 (13)	120.0 (4) [45]	119.3 (3) [46]	118.01	118.05
$C_5 - C_4 - O_4$	121.13 (14)	119.2 (4) [45]	120.4 (3) [46]	120.15	120.71
$C_5 - C_6 - C_7$	130.71 (14)	130.6 (3) [45]	131.7 (4) [46]	131.61	132.68
$C_6 - C_7 - O_5$	120.33 (13)	120.9 (3) [45]	118.8 (3) [46]	119.24	116.98
$C_6 - C_7 - O_6$	118.94 (13)	117.0 (3) [45]	118.4 (3) [46]	117.13	120.46
$O_3 - C_4 - O_4$	121.87 (14)	120.8 (4) [45]	120.3 (3) [46]	121.84	121.24
$O_5 - C_7 - O_6$	120.72 (14)	122.1 (3) [45]	122.8 (3) [46]	123.64	122.57
$C_7 - O_5 - H_{11}$	109.5	_	_	113.49	114.97

TABLE 1: Selected experimental and theoretical bond lengths and angles for sarcosine-maleic acid.

donor (*i*) and acceptor (*j*), the stabilization energy E(2) associated with the delocalization $i \rightarrow j$ is estimated as

$$E(2) = \Delta E_{ij} = q_i \frac{F(i,j)^2}{\varepsilon_j - \varepsilon'_i},$$
(3)

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

All the calculations are performed by using Gauss-View molecular visualization program [42] and Gaussian 09 program package [40].

The conversion factors for α , β , γ , and HOMO and LUMO energies in atomic and cgs units: 1 atomic unit

(a.u.) = 0.1482×10^{-24} electrostatic unit (esu) for polarizability; 1 a.u. = 8.6393×10^{-33} esu for first hyperpolarizability; 1 a.u. = 27.2116 eV (electron volt) for HOMO and LUMO energies.

3. Results and Discussion

3.1. Geometric Structure. Sarcosine-maleic acid is chemically related to C₇H₁₁NO₆ empirical formula. The molecule is monoclinic with the cell parameters of a = 22.754(5) Å, $\alpha = 90^{\circ}$, b = 5.8830(10) Å, $\beta = 96.56(3)^{\circ}$, c = 13.628(3) Å, and $\gamma = 90^{\circ}$ [18]. The optimized geometric parameters (bond lengths and angles) by using HF and B3LYP method

	Experim	nental (cm^{-1}) [18]	Theoretical with 6-31G++(d,p) basis set			
Assignments	IR	R	HF	B3LYP		
ν(O-H)	3428	_	3744	3603		
v(N-H)	3189	3190	3369	3361		
v(O-H)	2764	2787	3333	3283		
ν(C-H)	3059	3058	3077	_		
ν(C-H)	2849	_	3068	_		
$v_{a}(C-H_{2})$	2963	2965	3050	3084		
$v_{a}(C-H_{3})$	3015	3014	3041	_		
$v_{a}(C-H_{3})$	2924	_	3031	_		
$v_{a}(C-H_{2})$	2982	_	2958	3024		
$v_{\rm s}(\rm C-H_3)$	2887	2909	2949	2989		
$v_{\rm s}(\rm C-H_2)$		2816	_	2980		
v(O-H)	2420	2420	2292	1899		
v(C=O)	1719	_	1835	1743		
ν (C=O)	1692	1694	1826	1717		
ν (C=O), ν s(C=C), δ (N-H ₂)	1613	1610	1717	1656		
$v_{\rm s}(\rm C=C), \delta(\rm N-H_2)$	_	_	_	1605		
$\delta(N-H_2)$	_	_	_	_		
v (C=O), v_s (C=C), v (N-H ₂)	_	_	1662	_		
ν (N-H ₂), (C=O)	1574	_	1589	1527		
$\rho(C-H), \gamma(C-H_2), t(N-H_2), \rho(O-H)$	1491	1494	1497			
δ(C-H ₃)	1464	1466	1461	1457		
$\delta(C-H_3)$	1448	1456	1452	1449		
$\delta(C-H_2), \nu(COO)$	1433	-	1424	1432		
$\delta(C-H_2)$	1418	1420	1379	1423		
$\delta(C-H_3)$	1397	1394	1297	1397		
$\delta(C-H_3), \rho(C-H), \rho(O-H), \gamma(C-C)$	_	_	_	_		
$\rho(C-H), \gamma(C-H_2), t(N-H_2)$	_	_	1287	_		
$\rho(C-H), \rho(O-H)$		_	_	_		
$t(N-H_2) \rho(O-H) \nu(C-H_2)$	1369	1370	1224	1354		
$t(C-H_2), \rho(0-H_2)$	1340	_	_	1302		
$\rho(C-H)$	1273	1267	_			
$v(C-OH), v(C-H_2), v(N-H_2)$	1296	1286	1214	1267		
$v(C-C), o(O-H), v(C-H_2)$	_	_	1205	1250		
$t(C-H_2), v(N-H_2)$	_	_	_	1224		
$t(C-H_2), \rho(N-H_2)$	_	_	_	_		
р(С-H)	1208	1206	_	1172		
$t(C-H_2), v(C-H_3)$	1142	1150	1178	1163		
$t(C-H_2), v(C-H_3)$	_	_	_	1129		
v(C-N-C)	_	_	1077	1077		
$t(C-H_2), v(C-H_3), v(N-H_2)$	1048	1047	_	1013		
v(C-N)	1192	_	_	_		
t(C-H)	1180	1176	1050	986		
$\rho(C-H), \gamma(N-H_2), \gamma(C-H_3)$	_	_	_	_		
v(C-N-C)	_	_	_	_		
ν (C-C), ρ (C-H)	_	_	_	_		
ρ(N-H)	_	_	_	_		

 TABLE 2: Comparison of the observed and calculated vibrational spectra for sarcosine-maleic acid.

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Assignments	Experin	nental (cm ⁻¹) [18]	Theoretical	with 6-31G++(d,p) basis set
Assignments	IR	R	HF	B3LYP
γ(C-H ₃), γ(N-H ₂)	_	_	_	_
γ(C-H ₂), γ(O-H)	961	962	1004	—
$t(C-H_3), \gamma(N-H_2)$	—	—	—	—
v(C-C)	916	915	940	878
γ (N-H ₂), ρ (C-H)	—	—	—	—
γ(C-C)	885	889	813	842
γ(C-H)	876	876	—	—
$W(N-H_2), \rho(C-H)$	868	—	—	—
ν (C–C), ρ (N–H)	—	—	—	—
ρ(O-H)	—	—	—	824
(C–C), ρ (N–H)	—	—	—	—
<i>t</i> (C=C), γ(O–H)	—	—	—	788
ρ (C–H ₂), ρ (N–H), γ (COO)	655	654	594	—
γ(O-H)	—	—	—	779
$\delta(\text{COO})$	—	—	—	—
$\delta(\text{COO})$	600	600	584	—
δ (COO), ρ (C–H)	588	590	—	—
δ (COO), ρ (C–H)	—	—	—	—
γ(C-H)	—	—	—	—
ho(C-H ₂)	—	—	447	590
ρ (C-H ₂)	_	—	438	527

TABLE 2: Continued.

Vibrational modes: v: stretching; a: asymmetric; s: symmetric; ρ : rocking; δ : scissoring; w: wagging; t: twisting; γ : in-plane deformation.



FIGURE 1: (a) The experimental structure of the sarcosine-maleic acid crystal and the atoms numbering scheme [18]. (b) The calculated geometric structure of the sarcosine-maleic acid.

with 6-31++G(d, p) basis set are listed in Table 1 and are compared with the experimental data of the title compound. Figures 1(a) and 1(b) depict the experimental and theoretical structure of sarcosine-maleic acid.

The crystal structure of a complex of sarcosine with maleic acid have already been reported [43]. Also, the bond lengths and angles for the sarcosine were taken from the work of Mostad and Natarajan [9] and Krishnakumar et al. [44] and for the maleic acid were taken from Franklin and Balasubramanian [45] and Zhang et al. [46]. O–H bond lengths (0.940 and 1.530 Å) in the maleic acid were taken from the work of Zhang et al. [46]. For the title molecule, the O–H···O bond lengths predicted by HF/6-31++G(d, p) method are 0.966 and 1.627 Å and there are 0.986 and

TABLE 3: (a) Selected NBO results showing formation of Lewis and non-Lewis orbitals for sarcosine-maleic acid by using the HF method with 6-31++G(d,p) and 6-31G(d,p) basis sets. (b) Selected NBO results showing formation of Lewis and non-Lewis orbitals for sarcosine-maleic acid by using the B3LYP method with 6-31++G(d,p) and 6-31G(d,p) basis sets.

						(a)						
				HF	/6-31++G(d	,p)			H	F/6-31G(d,r)	
			%	%s	%p	%d	H.O	%	%s	%p	%d	H.O
		Н	37.96	99.91	0.09		s	37.62	99.91	0.09		s
$H_{10}-C_6$		С	62.04	29.37	70.55	0.08	$sp^{2.40}$	62.38	28.72	71.20	0.08	sp ^{2.48}
		Н	38.18	99.91	0.09		s	37.82	99.91	0.09		s
H9-C5		С	61.82	29.51	70.41	0.08	sp ^{2.39}	62.18	28.84	71.08	0.08	sp ^{2.46}
		0	65.79	43.45	55.97	0.58	sp ^{1.29}	66.34	44.55	54.93	0.52	sp ^{1.23}
0 0	σ	С	34.21	33.86	65.97	0.17	sp ^{1.95}	33.66	33.61	66.21	0.19	sp ^{1.97}
$O_6 = C_7$	π	0	72.82	0.00	99.49	0.51	°r D	72.27	0.01	99.48	0.51	b
		C	27.18	0.00	99.67	0.33	r D	27.73	0.01	99.64	0.35	r D
		С	47.74	36.39	63.47	0.14	sp ^{1.74}	47.14	36.74	63.13	0.13	sp ^{1.72}
$C_7 - C_6$		С	52.26	30.53	69.36	0.11	sp ^{2.27}	52.86	31.10	68.78	0.11	sp ^{2.21}
		С	31.79	29.63	70.14	0.23	sp ^{2.37}	31.46	29.55	70.20	0.25	sp ^{2.38}
$C_7 - O_5$		0	68.21	34.59	65.02	0.40	sp ^{1.88}	68.54	35.37	64.29	0.34	sp ^{1.82}
		C	50.07	40.16	59.76	0.08	sp ^{1.49}	50.04	40.16	59.76	0.08	sp ^{1.49}
	σ	C	49.93	39.69	60.23	0.08	sp ^{1.52}	49.96	39.71	60.21	0.08	sp ^{1.52}
C_6-C_5		C	49.98	0.00	99.87	0.13	p	49.96	0.00	99.86	0.14	p
	π	C	50.02	0.00	99.87	0.13	r p	50.04	0.01	99.86	0.14	P D
		C	52.39	30.88	69.01	0.11	sp ^{2.24}	52.79	31.45	68.44	0.11	<u>sp^{2.18}</u>
C_5-C_4		C	47.61	35.44	64.42	0.14	sp ^{1.82}	47.21	35.94	63.92	0.14	sp ^{1.78}
		C	32.92	31.14	68.53	0.33	sp ^{2.20}	32.22	30.66	68.98	0.36	sp ^{2.25}
C_4-O_4		0	67.08	38.14	61.73	0.14	sp ^{1.62}	67.78	38.65	61.25	0.09	sp ^{1.58}
		C	33.86	33.37	66.46	0.18	sp ^{1.99}	33.42	33.31	66.49	0.20	sp ²
	σ	0	66.14	42.10	57.39	0.52	sp ^{1.36}	66.58	43.53	55.99	0.48	sp ^{1.29}
$C_4 - O_3$		С	22.45	0.02	99.60	0.38	p	23.91	0.00	99.60	0.40	p
	π	0	77.55	0.03	99.56	0.41	r D	76.09	0.00	99.57	0.43	r D
		0	79.8	30.76	68.89	0.34	sp ^{2.24}	79.70	30.44	69.25	0.31	sp ^{2.27}
$O_5 - H_{11}$		Н	20.11	99.80	0.20		s	20.30	99.79	0.21		s
		С	61.85	30.76	68.89	0.34	sp ^{2.24}	61.57	25.65	74.25	0.10	sp ^{2.90}
C_3-H_7		Н	38.15	99.80	0.20		s	38.43	99.91	0.09		s
		С	34.74	20.92	78.89	0.19	sp ^{3.77}	34.81	21.68	78.13	0.19	sp ^{3.60}
C_3-N_1		N	65.26	26.54	73.28	0.18	sp ^{2.76}	65.19	26.78	73.06	0.16	sp ^{2.73}
		С	52.30	25.80	74.07	0.13	sp ^{2.87}	53.17	26.03	73.84	0.13	sp ^{2.84}
C_2-C_1		С	47.70	36.16	63.71	0.14	sp ^{1.76}	46.83	36.68	63.18	0.14	sp ^{1.72}
		С	61.71	25.54	74.37	0.10	sp ^{2.91}	62.60	24.97	74.94	0.10	sp ³
C_2-H_3		Н	38.29	99.91	0.09		s	37.40	99.91	0.09		s
		С	64.01	27.61	72.31	0.08	sp ^{2.62}	62.80	25.91	73.99	0.10	sp ^{2.86}
$C_2 - H_2$		Н	35.99	99.90	0.10		s	37.20	99.90	0.10		s
		С	35.76	21.16	78.65	0.18	sp ^{3.72}	37.82	23.20	76.64	0.16	sp ^{3.30}
$C_2 - N_1$		Ν	64.24	26.29	73.52	0.19	sp ^{2.80}	62.18	25.99	73.82	0.19	sp ^{2.84}
		Н	18.94	99.85	0.15		s	17.19	99.85	0.15		s
H_5-N_1		Ν	81.06	25.72	74.14	0.14	sp ^{2.88}	82.81	25.30	74.60	0.10	sp ^{2.95}
		С	33.80	34.21	65.62	0.17	sp ^{1.92}	33.27	32.86	66.95	0.19	sp ^{2.04}
0.0	σ	0	66.20	43.57	55.85	0.58	sp ^{1.28}	66.73	43.30	56.15	0.55	sp ^{1.30}
$C_1 - O_2$		С	25.68	0.01	99.60	0.38	p	28.19	1.11	98.53	0.36	p
	π	0	74.32	0.08	99.38	0.54	p	71.81	1.70	97.74	0.56	p
		C	31.29	29.66	70.11	0.23	sp ^{2.36}	30.99	29.29	70.31	0.41	sp ^{2.40}
$C_1 - O_1$		0	68.71	36.35	63.29	0.36	sp ^{1.74}	69.01	36.91	62.99	0.11	sp ^{1.71}
		0	77.09	24.41	75.27	0.33	sp ^{3.08}	76.04	24.44	75.46	0.10	sp ^{3.09}
O_1-H_1		H	22.91	99.83	0.17		S	23.96	99.65	0.35		-r S
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				B3LY	P/6-31++G	(d,p)			B3L	YP/6-31G(c	l,p)	
			%	%s	%р	%d	H.O	%	%s	%р	%d	H.O
$H_{10}-C_{\epsilon}$		Н	37.07	99.95	0.05		S	36.92	99.95	0.05		S
1110 00		С	62.93	29.09	70.87	0.04	sp ^{2.44}	63.08	28.37	71.59	0.04	sp ^{2.52}
Ho-Cr		Η	37.11	99.95	0.05		S	36.96	99.95	0.05		S
119 03		С	62.89	29.37	70.59	0.04	sp ^{2.40}	63.04	28.67	71.29	0.04	sp ^{2.49}
	σ	0	64.92	39.96	59.61	0.43	sp ^{1.49}	65.55	41.16	58.47	0.38	sp ^{1.42}
$\Omega_{c} = C_{\pi}$	0	С	35.08	33.77	66.13	0.10	sp ^{1.96}	34.45	33.36	66.53	0.11	sp ^{1.99}
06-07	π	0	68.57	0.01	99.66	0.34	р	67.80	0.02	99.65	0.34	р
	71	С	31.43	0.00	99.83	0.17	р	32.20	0.01	99.81	0.18	р
CC		С	47.98	36.75	63.19	0.07	sp ^{1.72}	47.34	37.28	62.65	0.07	sp ^{1.68}
0/-06		С	52.02	31.17	68.78	0.05	sp ^{2.21}	52.66	31.83	68.12	0.05	sp ^{2.14}
C 0		С	32.69	29.37	70.49	0.15	sp ^{2.40}	32.32	29.20	70.55	0.25	sp ^{2.42}
C7-O5		Ο	67.31	32.51	67.23	0.26	sp ^{2.07}	67.68	33.44	66.49	0.07	sp ^{1.99}
	~	С	49.75	39.82	60.14	0.04	sp ^{1.51}	49.77	39.81	60.15	0.04	sp ^{1.51}
C C	0	С	50.25	39.75	60.21	0.04	$sp^{1.51}$	50.23	39.74	60.22	0.04	sp ^{1.52}
$C_6 - C_5$	~	С	48.43	0.00	99.94	0.05	р	48.43	0.01	99.93	0.06	р
	π	С	51.57	0.00	99.95	0.05	p	51.57	0.01	99.94	0.05	р
C C		С	51.04	30.95	69.00	0.05	sp ^{2.23}	51.56	31.60	68.35	0.05	sp ^{2.16}
$C_5 - C_4$		С	48.96	37.50	62.44	0.06	sp ^{1.66}	48.44	38.04	61.90	0.06	sp ^{1.63}
C 0		С	32.14	28.62	71.12	0.26	sp ^{2.48}	31.56	28.27	71.48	0.25	sp ^{2.53}
$C_4 - O_4$		0	67.86	32.97	66.97	0.06	sp ^{2.03}	68.44	33.57	66.38	0.06	sp ^{1.98}
	_	С	34.92	33.85	66.06	0.09	sp ^{1.95}	34.32	33.63	66.26	0.11	sp ^{1.97}
σ C ₄ -O ₃ π	0	65.08	39.68	59.91	0.42	sp ^{1.51}	65.68	41.06	58.57	0.37	sp ^{1.43}	
		С	29.54	0.01	99.81	0.18	p	30.76	0.00	99.81	0.19	р
	π	0	70.46	0.01	99.67	0.32	p	69.24	0.00	99.67	0.33	р
0.11		0	78.67	28.00	71.74	0.26	sp ^{2.56}	78.32	27.49	72.45	0.06	sp ^{2.64}
$O_5 - H_{11}$		Н	21.33	99.88	0.12		s	21.68	99.75	0.25		s
0.11		0	82.53	30.05	69.91	0.04	sp ^{2.33}	81.87	29.39	70.57	0.04	sp ^{2.40}
O_4-H_4		Н	17.47	99.73	0.27		s	18.13	99.72	0.28		s
C II		С	61.89	25.56	74.38	0.05	sp ^{2.91}	61.68	24.92	75.02	0.06	sp ^{3.01}
C ₃ -H ₇		Н	38.11	99.95	0.05		s	38.32	99.95	0.05		s
C N		С	37.59	22.57	77.29	0.14	sp ^{3.42}	37.92	23.17	76.70	0.13	sp ^{3.31}
$C_3 - N_1$		Ν	62.41	29.68	70.28	0.04	sp ^{2.37}	62.08	29.93	70.03	0.04	sp ^{2.34}
0.0		С	51.17	24.91	75.02	0.06	sp ^{3.01}	52.50	25.53	74.41	0.06	sp ^{2.91}
$C_2 - C_1$		С	48.83	37.84	62.11	0.05	sp ^{1.64}	47.50	38.02	61.92	0.06	sp ^{1.63}
0.11		С	62.45	25.41	74.54	0.05	sp ^{2.93}	62.72	24.80	75.15	0.05	sp ^{3.03}
$C_2 - H_3$		Н	37.55	99.95	0.05		s	37.28	99.95	0.05		s
0.11		С	64.49	26.69	73.27	0.04	sp ^{2.75}	62.55	25.11	74.83	0.05	sp ^{2.98}
$C_2 - H_2$		Н	35.51	99.94	0.06		s	37.45	99.95	0.05		s
		С	39.10	23.08	76.79	0.12	sp ^{3.33}	40.33	24.65	75.24	0.11	sp ^{3.05}
C_2-N_1		Ν	60.90	28.84	71.11	0.05	sp ^{2.47}	59.67	28.66	71.29	0.05	sp ^{2.49}
		Н	27.79	99.89	0.11		s	27.28	99.89	0.11		s
H_5-N_1		Ν	72.21	24.18	75.76	0.05	sp ^{3.13}	72.72	24.46	75.48	0.05	sp ^{3.09}
		C	34.67	33.87	66.03	0.10	sp ^{1.95}	33.99	32.91	66.98	0.11	sp ^{2.03}
a c	σ	0	65.33	40.30	59.27	0.43	sp ^{1.47}	66.01	41.09	58.51	0.40	sp ^{1.42}
$C_1 - O_2$		Č	29.68	0.00	99.80	0.20	D	31.49	0.63	99.18	0.19	-г р
	π	õ	70.32	0.00	99.65	0.35	r n	68.51	0.94	98.70	0.36	r D
		<u> </u>	32.04	28.37	71.39	0.24	sp ^{2.52}	31.53	28.36	71.38	0.26	sp ^{2.52}
C_1-O_1		0	67.96	33.41	66.51	0.08	sp ^{1.99}	68.47	34.41	65.52	0.07	sp ^{1.90}
		0	76.65	22.39	77 53	0.08	sp ^{3.46}	75 40	21.82	78 11	0.07	sp ^{3.58}
O_1-H_1		н	23 35	99.76	0.24	0.00	٩٢ ٩	24 60	99.78	0.22	0.07	٩٢ ٩
			2		N			2 . E. M. M. I.				

TABLE 4: (a) Second-order perturbation theory analysis of Fock matrix on NBO basis for sarcosine-maleic acid by using the HF and B3LYP methods with 6-31++G(d,p) basis set. (b) Second-order perturbation theory analysis of Fock matrix on NBO basis for sarcosine-maleic acid by using the HF and B3LYP methods with 6-31G(d,p) basis set.

	Occu	ipancies	Acceptor (<i>j</i>)	Occu	pancies	$E(2)^{a}$ ((kcal/mol)	E(j) -	$-E(i)^{b}$ (a.u.)	F(i, j)) ^c (a.u.)
Donor (1)	HF	B3LYP	1 97	HF	B3LYP	HF	B3LYP	HF	B3LYP	HF	B3LYP
σ (H ₁₀ -C ₆)	1.976	1.971	σ^* (H ₉ –C ₅)	0.009	0.011	0.87	0.63	1.48	1.00	0.032	0.023
σ (H ₁₀ -C ₆)	1.976	1.971	σ^{*} (C ₇ -O ₅)	0.067	0.088	5.86	5.13	1.43	0.92	0.083	0.062
$\sigma (H_{10} - C_6)$	1.976	1.971	$\sigma^* (C_6 - C_5)$	0.014	0.017	2.53	1.49	1.68	1.16	0.058	0.037
$\sigma (H_{10}-C_6)$	1.976	1.971	σ^{*} (C ₅ -C ₄)	0.065	0.065	8.54	7.49	1.38	0.93	0.098	0.075
σ (H ₉ -C ₅)	1.977	1.972	$\sigma^{*}(C_{7}-C_{6})$	0.063	0.076	8.69	7.03	1.37	0.92	0.098	0.073
σ (H ₉ -C ₅)	1.977	1.972	σ^{*} (C ₆ -C ₅)	0.014	0.017	2.47	1.66	1.68	1.16	0.058	0.039
$\sigma (O_6 - C_7)$	1.983	1.996	σ^{*} (C ₇ -C ₆)	0.063	0.076	0.85	0.77	2.07	1.45	0.038	0.030
$\sigma (O_6 - C_7)$	1.983	1.996	σ^{*} (O ₅ –H ₁₁)	0.054	0.060	1.43	1.10	2.20	1.51	0.051	0.037
$\pi (O_6 - C_7)$	1.983	1.968	$\pi^* (C_6 - C_5)$	0.027	0.052	6.46	6.67	0.74	0.39	0.062	0.046
σ (C ₇ -C ₆)	1.985	1.986	σ^* (H ₉ –C ₅)	0.009	0.011	2.34	1.81	1.65	1.14	0.056	0.041
σ (C ₇ -C ₆)	1.985	1.986	σ^{*} (C ₆ -C ₅)	0.014	0.017	2.41	1.65	1.84	1.31	0.060	0.041
$\pi (C_6 - C_5)$	1.921	1.876	$\pi^* (O_6 - C_7)$	0.185	0.249	17.06	1.07	0.61	1.38	0.094	0.034
$\pi (C_6 - C_5)$	1.921	1.876	$\pi^* (C_4 - O_3)$	0.257	0.265	18.03	1.60	0.58	1.35	0.096	0.041
σ (C ₄ –O ₃)	1.996	1.996	σ^{*} (C ₆ -C ₅)	0.014	0.017	1.26	1.14	2.34	1.71	0.049	0.040
σ (C ₄ -O ₃)	1.996	1.996	σ^* (C ₅ -C ₄)	0.065	0.065	0.66	1.04	2.04	1.48	0.033	0.035
$\pi (C_4 - O_3)$	1.985	1.975	π^* (C ₆ -C ₅)	0.027	0.052	5.14	5.51	0.75	0.41	0.056	0.043
$\pi (C_4 - O_3)$	1.985	1.975	$\pi^* (C_4 - O_3)$	0.257	0.265	0.71	0.71	0.71	0.38	0.022	0.016
σ (C ₄ –O ₃)	1.985	1.996	σ^{*} (C ₆ -C ₅)	0.014	0.017	52.66	1.14	0.03	1.71	0.098	0.040
σ (C ₅ -C ₄)	1.982	1.982	σ^{*} (H ₁₀ –C ₆)	0.008	0.010	2.34	1.56	1.65	1.17	0.056	0.038
σ (C ₅ -C ₄)	1.982	1.982	σ^{*} (C ₆ -C ₅)	0.014	0.017	2.27	1.82	1.84	1.32	0.058	0.044
σ (O ₅ -H ₁₁)	1.986	1.984	σ^{*} (O ₆ -C ₇)	0.015	0.249	7.88	6.39	2.00	1.37	0.112	0.084
σ (C ₃ -N ₁)	1.993	1.993	$\sigma_{*} (C_{2}-C_{1})$	0.057	0.065	1.20	1.22	1.58	1.08	0.039	0.033
σ (C ₃ -H ₇)	1.992	1.991	σ^{*} (C ₂ –N ₁)	0.011	0.013	3.73	3.18	1.28	0.85	0.062	0.046
σ (C ₃ -H ₈)	1.994	1.992	σ^* (H ₅ –N ₁)	0.017	0.018	2.81	2.25	1.40	0.94	0.056	0.041
σ (C ₂ -C ₁)	1.981	1.979	σ^{*} (C ₁ -O ₂)	0.020	0.024	0.74	0.55	1.84	1.26	0.033	0.024
σ (C ₂ -H ₃)	1.979	1.969	π^* (C ₁ -O ₂)	0.162	0.218	6.89	5.90	0.95	0.52	0.075	0.052
σ (C ₂ -H ₃)	1.979	1.969	σ^{*} (C ₁ –O ₂)	0.020	0.024	1.43	1.56	1.69	1.12	0.044	0.037
σ (C ₂ -H ₂)	1.981	1.971	σ^* (H ₅ –N ₁)	0.017	0.018	2.56	2.00	1.40	0.95	0.053	0.039
σ (C ₂ -N ₁)	1.990	1.989	σ^* (C ₃ –H ₇)	0.003	0.005	1.04	0.91	1.69	1.18	0.043	0.029
σ (C ₂ –N ₁)	1.990	1.989	σ^* (C ₁ –O ₁)	0.069	0.093	2.44	2.23	1.66	1.08	0.058	0.045
σ (H ₅ -N ₁)	1.987	1.986	$\sigma^{*}(C_{2}-C_{1})$	0.057	0.065	0.82	0.73	1.50	1.00	0.032	0.024
σ (H ₅ -N ₁)	1.987	1.986	σ^* (C ₂ –H ₂)	0.008	0.019	1.00	1.54	1.29	1.09	0.032	0.037
σ (H ₅ -N ₁)	1.987	1.986	σ^* (C ₃ –H ₈)	0.004	0.009	2.14	1.71	1.60	1.09	0.052	0.039
π (C ₁ -O ₂)	1.993	1.992	σ^* (C ₂ –H ₂)	0.008	0.019	1.00	0.85	1.29	0.85	0.032	0.024
σ (C ₁ –O ₂)	1.993	1.997	$\sigma^*(C_2-C_1)$	0.057	0.065	0.80	0.83	2.06	1.46	0.059	0.032
σ (C ₁ –O ₂)	1.993	1.997	$\sigma^*(C_2-H_3)$	0.009	0.019	1.29	1.21	1.24	0.81	0.036	0.028
σ (C ₁ -O ₁)	1.996	1.997	σ^* (C ₂ –N ₁)	0.011	0.013	1.13	1.10	1.82	1.28	0.041	0.034
σ (O ₁ -H ₁)	1.987	1.986	σ^* (C ₂ –C ₁)	0.057	0.065	6.59	4.58	1.63	1.12	0.093	0.065
σ (O ₁ -H ₁)	1.987	1.986	σ^* (C ₁ –O ₂)	0.020	0.024	0.77	0.63	1.97	1.35	0.035	0.026
LP1 (O ₂)	1.975	1.976	σ^* (C ₂ –C ₁)	0.057	0.065	3.11	2.58	1.56	1.08	0.063	0.048
LP2 (O ₂)	1.879	1.848	σ^* (C ₂ –C ₁)	0.057	0.065	27.82	19.08	1.06	0.64	0.156	0.101
π^{*} (C ₁ –O ₂)	0.020	0.218	σ^* (C ₂ –H ₃)	0.009	0.019	1.04	0.90	0.48	0.42	0.068	0.051
π^{*} (C ₁ -O ₂)	0.020	0.218	σ^* (C ₂ –H ₂)	0.008	0.018	0.57	0.53	0.53	0.46	0.053	0.041

(a)

$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Demon(i)	Occu	pancies	Acceptor (j)	Occu	pancies	$E(2)^{a}$	(kcal/mol)	E(j)	$-E(i)^{b}$ (a.u.)	F(i, j)) ^c (a.u.)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Donor (i)	HF	B3LYP		HF	B3LYP	HF	B3LYP	HF	B3LYP	HF	B3LYP
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	σ (H ₁₀ –C ₆)	1.980	1.971	$\sigma^{*} (O_{6}-C_{7})$	0.016	0.019	1.11	0.55	1.40	1.19	0.035	0.023
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	σ (H ₁₀ –C ₆)	1.980	1.971	σ^* (C ₇ –O ₅)	0.026	0.089	8.07	0.61	1.65	1.14	0.103	0.024
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	σ (H ₁₀ –C ₆)	1.980	1.971	σ^* (C ₆ -C ₅)	0.018	0.017	1.09	1.69	1.56	1.17	0.037	0.040
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	σ (H ₁₀ -C ₆)	1.980	1.971	σ^* (C ₅ -C ₄)	0.033	0.065	4.64	7.88	1.54	0.93	0.076	0.077
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	σ (H ₉ -C ₅)	1.980	1.972	σ^* (C ₇ –C ₆)	0.043	0.075	3.72	7.46	1.57	0.92	0.069	0.075
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	σ (H ₉ -C ₅)	1.980	1.972	σ^{*} (C ₆ -C ₅)	0.018	0.017	1.42	1.87	1.56	1.17	0.042	0.042
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	σ (O ₆ –C ₇)	1.991	1.996	σ^* (C ₅ -C ₆)	0.015	0.017	3.63	1.04	1.72	1.78	0.071	0.038
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	σ (O ₆ -C ₇)	1.991	1.996	σ^{*} (O ₅ -H ₁₁)	0.113	0.063	0.69	1.61	1.75	1.60	0.032	0.046
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$\pi (O_6 - C_7)$	1.945	1.967	$\pi^* (C_6 - C_5)$	0.069	0.054	15.39	6.96	0.53	0.39	0.081	0.047
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	σ (C ₇ -C ₆)	1.989	1.988	σ^* (H ₉ –C ₅)	0.010	0.012	3.30	2.28	1.68	1.15	0.066	0.046
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	σ (C ₇ -C ₆)	1.989	1.988	σ^{*} (C ₆ -C ₅)	0.018	0.017	2.05	2.10	1.80	1.31	0.054	0.047
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	π (C ₆ -C ₅)	1.833	1.877	π^* (O ₆ -C ₇)	0.379	0.250	26.74	13.31	0.53	0.31	0.113	0.060
σ (C ₄ -O ₃) 1.988 1.997 σ^* (C ₆ -C ₅) 0.018 0.017 3.33 1.01 1.79 1.72 0.069 0.037	$\pi (C_6 - C_5)$	1.833	1.877	σ^{*} (C ₄ -O ₃)	0.035	0.021	18.46	17.31	0.59	0.29	0.097	0.066
	σ (C ₄ -O ₃)	1.988	1.997	σ^{*} (C ₆ -C ₅)	0.018	0.017	3.33	1.01	1.79	1.72	0.069	0.037
σ (C ₄ -O ₃) 1.988 1.997 σ^* (C ₅ -C ₄) 0.033 0.065 0.80 1.11 2.06 1.49 0.037 0.037	σ (C ₄ -O ₃)	1.988	1.997	σ^{*} (C ₅ -C ₄)	0.033	0.065	0.80	1.11	2.06	1.49	0.037	0.037
π (C ₄ -O ₃) 1.988 1.975 π^* (C ₆ -C ₅) 0.069 0.054 5.52 5.84 0.75 0.41 0.058 0.044	$\pi (C_4 - O_3)$	1.988	1.975	$\pi^* (C_6 - C_5)$	0.069	0.054	5.52	5.84	0.75	0.41	0.058	0.044
π (C ₄ -O ₃) 1.988 1.975 σ^* (C ₄ -O ₃) 0.035 0.021 0.66 0.70 0.72 0.38 0.021 0.016	$\pi (C_4 - O_3)$	1.988	1.975	σ^{*} (C ₄ -O ₃)	0.035	0.021	0.66	0.70	0.72	0.38	0.021	0.016
σ (C ₄ -O ₃) 1.988 1.997 σ^* (C ₆ -C ₅) 0.018 0.017 3.33 1.01 1.79 1.72 0.069 0.037	σ (C ₄ -O ₃)	1.988	1.997	σ^{*} (C ₆ -C ₅)	0.018	0.017	3.33	1.01	1.79	1.72	0.069	0.037
σ (C ₅ -C ₄) 1.989 1.981 σ^* (H ₁₀ -C ₆) 0.001 0.011 2.60 1.74 1.72 1.16 0.060 0.040	σ (C ₅ -C ₄)	1.989	1.981	σ^* (H ₁₀ -C ₆)	0.001	0.011	2.60	1.74	1.72	1.16	0.060	0.040
σ (C ₅ -C ₄) 1.989 1.981 σ^* (C ₆ -C ₅) 0.018 0.017 2.22 2.32 1.83 1.33 0.057 0.050	$\sigma (C_5 - C_4)$	1.989	1.981	$\sigma^* (C_6 - C_5)$	0.018	0.017	2.22	2.32	1.83	1.33	0.057	0.050
σ (O ₅ -H ₁₁) 1.985 1.985 σ^* (O ₆ -C ₇) 0.044 0.250 7.75 6.06 2.00 1.38 0.111 0.082	$\sigma (O_5 - H_{11})$	1.985	1.985	$\sigma^* (O_6 - C_7)$	0.044	0.250	7.75	6.06	2.00	1.38	0.111	0.082
σ (C ₃ -H ₈) 1.991 1.995 σ^* (C ₂ -N ₁) 0.014 0.017 4.77 3.81 1.27 0.84 0.069 0.05	σ (C ₃ -H ₈)	1.991	1.995	σ^{*} (C ₂ -N ₁)	0.014	0.017	4.77	3.81	1.27	0.84	0.069	0.051
σ (C ₃ -H ₆) 1.992 1.992 σ^* (H ₅ -N ₁) 0.010 0.024 3.40 2.73 1.47 0.97 0.063 0.046	σ (C ₃ -H ₆)	1.992	1.992	σ^{*} (H ₅ -N ₁)	0.010	0.024	3.40	2.73	1.47	0.97	0.063	0.046
σ (C ₃ -N ₁) 1.991 1.992 σ^* (C ₂ -C ₁) 0.039 0.075 2.93 1.57 1.54 1.06 0.060 0.037	σ (C ₃ -N ₁)	1.991	1.992	$\sigma^{*} (C_{2}-C_{1})$	0.039	0.075	2.93	1.57	1.54	1.06	0.060	0.037
σ (C ₂ -C ₁) 1.989 1.989 σ^* (C ₁ -O ₂) 0.018 0.024 0.86 0.62 1.83 1.26 0.036 0.025	σ (C ₂ -C ₁)	1.989	1.989	$\sigma^* (C_1 - O_2)$	0.018	0.024	0.86	0.62	1.83	1.26	0.036	0.025
σ (C ₂ -H ₃) 1.975 1.977 π^* (C ₁ -O ₂) 0.148 0.207 6.31 3.35 0.88 0.56 0.069 0.04 ¹	σ (C ₂ -H ₃)	1.975	1.977	π^* (C ₁ -O ₂)	0.148	0.207	6.31	3.35	0.88	0.56	0.069	0.041
σ (C ₂ -H ₃) 1.975 1.977 σ^* (C ₁ -O ₂) 0.018 0.024 2.53 2.35 1.69 1.14 0.058 0.046	σ (C ₂ -H ₃)	1.975	1.977	$\sigma^* (C_1 - O_2)$	0.018	0.024	2.53	2.35	1.69	1.14	0.058	0.046
σ (C ₂ -H ₂) 1.982 1.971 σ^* (C ₁ -O ₂) 0.146 0.024 1.85 1.40 1.69 1.14 0.050 0.036	σ (C ₂ -H ₂)	1.982	1.971	$\sigma^* (C_1 - O_2)$	0.146	0.024	1.85	1.40	1.69	1.14	0.050	0.036
σ (C ₂ -N ₁) 1.989 1.988 σ^* (C ₃ -H ₈) 0.006 0.010 1.14 0.99 1.75 1.22 0.040 0.03 ¹	σ (C ₂ -N ₁)	1.989	1.988	$\sigma^* (C_3 - H_8)$	0.006	0.010	1.14	0.99	1.75	1.22	0.040	0.031
σ (C ₂ -N ₁) 1.989 1.988 σ^* (C ₁ -O ₁) 0.050 0.094 2.25 2.32 1.51 1.09 0.052 0.046	σ (C ₂ -N ₁)	1.989	1.988	$\sigma^* (C_1 - O_1)$	0.050	0.094	2.25	2.32	1.51	1.09	0.052	0.046
σ (H ₅ -N ₁) 1.988 1.982 σ^* (C ₂ -C ₁) 0.039 0.075 0.70 0.58 1.46 0.97 0.029 0.02	σ (H ₅ -N ₁)	1.988	1.982	σ^* (C ₂ -C ₁)	0.039	0.075	0.70	0.58	1.46	0.97	0.029	0.022
σ (H ₅ -N ₁) 1.988 1.982 σ^* (C ₂ -H ₃) 0.010 0.018 2.42 2.17 1.58 1.05 0.055 0.043	σ (H ₅ -N ₁)	1.988	1.982	σ^* (C ₂ -H ₃)	0.010	0.018	2.42	2.17	1.58	1.05	0.055	0.043
σ (H ₅ -N ₁) 1.988 1.982 σ^* (C ₃ -H ₆) 0.005 0.009 2.56 2.13 1.60 1.08 0.057 0.043	σ (H ₅ -N ₁)	1.988	1.982	σ^* (C ₃ -H ₆)	0.005	0.009	2.56	2.13	1.60	1.08	0.057	0.043
π (C ₁ -O ₂) 1.992 1.992 σ^* (C ₂ -H ₂) 0.009 0.023 0.84 1.21 1.16 0.81 0.028 0.028	$\pi (C_1 - O_2)$	1.992	1.992	σ^* (C ₂ -H ₂)	0.009	0.023	0.84	1.21	1.16	0.81	0.028	0.028
$\sigma(C_1 - C_2) = 1.993 = 1.996 = \sigma^*(C_2 - C_1) = 0.039 = 0.075 = 0.69 = 0.68 = 2.02 = 1.42 = 0.034 = 0.026$	σ (C ₁ -O ₂)	1 993	1 996	$\sigma^{*}(C_{2}-C_{1})$	0.039	0.075	0.69	0.68	2.02	1 42	0.034	0.028
$\sigma(C_1 - C_2) = 1.993 = 1.996 = \sigma^*(C_2 - H_2) = 0.009 = 0.018 = 1.37 = 1.14 = 1.29 = 0.82 = 0.037 = 0.020$	σ (C ₁ -O ₂)	1 993	1 996	$\sigma^* (C_2 - H_3)$	0.009	0.018	1 37	1 14	1 29	0.82	0.037	0.027
$\sigma(C_1 - C_2) = 1.995 = 1.996 = \sigma^*(C_2 - N_1) = 0.012 = 0.017 = 1.11 = 0.83 = 1.62 = 0.028 = 0.028 = 0.028$	$\sigma (C_1 - O_2)$	1 995	1 996	$\sigma^* (C_2 - N_1)$	0.012	0.017	1 11	0.83	1.62	1.28	0.038	0.029
$\sigma(O_1 - H_1) = 1.987 = 1.985 = \sigma^*(O_2 - O_3) = 0.012 = 0.017 = 1.11 = 0.053 = 1.02 = 1.20 = 0.030 = 0.022$	$\sigma (O_1 - H_1)$	1.995	1.985	$\sigma^* (C_1 - O_2)$	0.012	0.024	5 50	5.84	1.55	1.20	0.082	0.029
LP1 (Ω_2) 1.986 1.977 $\sigma^*(\Omega_2 - \Omega_1)$ 0.039 0.075 2.99 2.69 1.60 1.03 0.062 0.002	LP1 (O_2)	1 986	1.977	$\sigma^* (C_2 - C_1)$	0.039	0.075	2.99	2.69	1.55	1.03	0.062	0.048
$IP2(O_2) = 1929 = 1833 \sigma^*(C_2-C_1) = 0.039 0.075 9.82 20.44 0.98 0.61 0.088 0.107 0.098 0.107 0.098 0.010 0.098 0.010 0.098 0.010 0.098 0.010 0.098 0.010 0.098 0.010 0.098 0.010 0.098 0.010 0.098 0.010 0.098 0.010 0.098 0.010 0.098 0.010 0.098 0.010 0.098 0.010 0.098 0.010 0.098 0.010 0.098 0.010 0.098 0.010 $	$IP2(O_2)$	1 929	1 833	$\sigma^* (C_2 - C_1)$	0.039	0.075	9.87	20.44	0.98	0.61	0.088	0 102
$\pi^*(C_1-C_2) = 0.148 = 0.207 = \sigma^*(C_2-H_2) = 0.009 = 0.018 = 0.78 = 0.63 = 0.61 = 0.000 = 0.012 = 0.0000 = 0.0000 = 0.0000 = 0.0000 = 0.0000 = 0.0000 = 0.0000 = 0.0000 = 0.0000 = 0.0000 = 0.0000 = 0.0000$	$\pi^* (C_1 - O_2)$	0 148	0.207	$\sigma^* (C_2 - H_2)$	0.009	0.018	0.78	0.63	0.50	0.40	0.070	0.102
$\pi^*(C_1-C_2)$ 0.148 0.207 $\sigma^*(C_2-H_2)$ 0.009 0.023 0.70 0.63 0.46 0.40 0.058 0.04	$\pi^* (C_1 - C_2)$	0.148	0.207	$\sigma^* (C_2 - H_2)$	0.009	0.023	0.70	0.63	0.46	0.40	0.058	0.043

^{*a*} ($G_1 G_2$) of H_2 ($G_2 H_2$) of G_2 (G_2 (G_2 (G_2 (G_2 (G_2)) of G_2 ($G_$

Parameters	HF/6-31++G(d,p)	B3LYP/6-31++G(d,p)
Thermal energy, E (kcal/mol)		
Rotational	0.889	0.889
Translational	0.889	0.889
Vibrational	139.016	128.306
Total	140.794	130.083
Heat capacity, C_{ν} (cal/mol K)		
Rotational	2.981	2.981
Translational	2.981	2.981
Vibrational	43.448	46.738
Total	49.409	52.700
Entropy, S (cal/mol K)		
Rotational	32.447	32.665
Translational	41.859	41.859
Vibrational	53.905	59.690
Total	128.210	134.214
Rotational constants (GHz)		
A	1.29083	1.06137
В	0.29960	0.27773
C	0.25715	0.27100
Rotational temperature (Kelvin)		
A	0.06195	0.05094
В	0.01438	0.01333
С	0.01234	0.01301
Thermal properties (Hartree/particle)		
Zero-point correction	0.209706	0.191785
Thermal correction to energy	0.224369	0.207301
Thermal correction to enthalpy	0.225313	0.208245
Thermal correction to gibbs free energy	0.164397	0.144476
Sum of electronic and zero-point energies	-774.972134	-779.355221
Sum of electronic and thermal energies	-774.957471	-779.339706
Sum of electronic and thermal enthalpies	-774.956527	-779.338761
Sum of electronic and thermal free energies	-775.017443	-779.402531
Zero point vibrational energy (kcal/mol)	131.59250	120.34688
E LUMO (eV)	0.418	-2.588
$E_{\rm HOMO}$ (eV)	-10.459	-7.592
$\Delta E_{\rm LUMO} - E_{\rm HOMO}$ (eV)	10.876	5.004
I (eV)	10.459	7.592
A (eV)	-0.418	2.588
<i>χ</i> (eV)	5.021	5.090
η (eV)	5.439	2.502
$S(eV^{-1})$	0.092	0.199

TABLE 5: The calculated thermodynamic and molecular parameters of sarcosine-maleic acid.

1.652 Å for B3LYP/6–31++G(d, p) method and it shows good agreement with the experimental data of 0.940 and 1.530 Å. In the study the N–H···O bond is calculated at 2.588 Å and 2.578 Å with HF and B3LYP method, respectively. But, this bond between sarcosine and maleic acid was not observed

experimentally. According to the results in Table 1, the bond lenghts and angles calculated by HF and B3LYP methods are in good agreement with the experimental values. Moreover, the result suggests that all the calculated bond lengths for this complex are overestimated to some extent.

Property	PNA	HF/6-31++G(d,p)	B3LYP/6-31++G(d,p)
μ_x		-11.66 Debye	-2.38 Debye
μ_{y}		2.88 Debye	3.93 Debye
μ_{z}		-1.62 Debye	-3.22 Debye
μ	2.44 Debye ^a	12.12 Debye	5.61 Debye
α_{xx}		134.96 a.u.	149.33 a.u.
α_{yy}		99.84 a.u.	103.83 a.u.
α_{zz}		77.19 a.u.	105.16 a.u.
$\langle \alpha \rangle$	$22 \times 10^{-24} \mathrm{cm}^{3b}$	$15.41 \times 10^{-24} \mathrm{esu}$	$17.70 \times 10^{-24} \mathrm{esu}$
$\Delta \alpha$		7.47×10^{-24} esu	6.65×10^{-24} esu
β_{xxx}		-189.68 a.u.	-272.95 a.u.
β_{xyy}		17.40 a.u.	-30.49 a.u.
β_{xzz}		10.67 a.u.	36.84 a.u.
β_{yyy}		-18.49 a.u.	10.82 a.u.
β_{xxy}		116.03 a.u.	56.24 a.u.
β_{yzz}		-12.86 a.u.	29.36 a.u.
β_{zzz}		-46.40 a.u.	-3.90 a.u.
β_{xxz}		4.12 a.u.	26.43 a.u.
β_{vzz}		11.38 a.u.	-8.64 a.u.
	20	22	22

 1598.70×10^{-33} esu

TABLE 6: Total static dipol moment (μ), the mean polarizability ($\langle \alpha \rangle$), the anisotropy of the polarizability ($\Delta \alpha$), and the mean first-order hyperpolarizability ($\langle \beta \rangle$) for Sarcosine-maleic acid molecule.

 $\frac{\langle \beta \rangle}{a b c}$ PNA results are taken from references [65-67].

3.2. Assignments of the Vibration Modes. Ilczyszyn et al. have recently investigated the Raman and infrared spectra of the title compound, and have assigned bands vibrations [18]. The experimental vibrational frequencies of sarcosinemaleic acid have been reported [18], and the experimental values are listed in Table 2, accompanied by the calculated data. The agreement between experimental and calculated frequencies for the monomer is excellent. Although different theoretical level gives different frequencies, seeing frequencies do not change the overall picture. The vibrational frequencies calculated by HF method are always higher than those computed by B3LYP method; no matter what basis sets are used. The HF frequencies are in worse agreement with experimental fundamentals than the other method since electron correlation in the HF calculations is neglected. The performance of local- and gradient-corrected DFT in calculating vibrational frequencies has shown that the computing vibrational frequencies provide good agreement with experimental fundamental ones.

 $15.5 \times 10^{-30} \, esu^{c}$

The group of bands in the $3150-3000 \text{ cm}^{-1}$ region in the infrared and Raman spectra of both compounds can be assigned to C-H stretching modes. The C-H bands have been calculated at around 3077-2949 cm⁻¹ using HF and $3084-2980 \text{ cm}^{-1}$ using B3LYP method with 6-31++G(d,p)basis set.

The ionised carboxylic group of semimaleate ion has characteristic antisymmetric stretching vibration at approximately 1574 cm⁻¹ and symmetric stretching vibration at approximately 1433 cm⁻¹ [18]. These bands have been calculated at 1589 cm⁻¹ and 1527 cm⁻¹ for HF level. In the infrared

spectra of Ilczyszyn et al. with the numerous submaxima at 3189, 2764, 2702, 2652, 2573, and 2420 cm⁻¹ was assigned to the ν (O–H) (inter) and ν (N–H) modes. However, we have calculated them at 3369, 3333, and 2292 cm⁻¹ with HF level and at 3361, 3283, and 1899 cm^{-1} with B3LYP level.

 2452.18×10^{-33} esu

The comparative IR and Raman spectra of experimental and calculated HF and DFT are given in Figures 2 and 3, respectively. As can be seen from Table 2 and Figures 2 and 3 there is good agreement with experimental and theoretical ones.

3.3. Natural Bonding Orbital (NBO) Analysis. The NBO analysis provides an efficient method for studying intraand intermolecular bonding and interaction among bonds, and also enables a convenient basis for investigating charge transfer or conjugative interaction in molecular systems.

NBO analysis provides the most accurate "natural Lewis structure" picture of *j*, because all orbital details are mathematically chosen to include the highest possible percentage of the electron density (ED). NBO calculation was performed at the HF/6-31++G(d, p), HF/6-31G(d, p), DFT/B3LYP/6-31++G(d, p), and DFT/B3LYP/6-31G(d, p)levels. According to Goodman and Sauers, NBO results are more susceptible when using a balanced-basis set [47]. The most important interaction between filled (donor) Lewis-type NBOs and empty (acceptor) non-Lewis NBOs is reported in Table 3. The second-order perturbation theory analysis of Fock matrix in the NBO basis of the molecule has also been performed in Table 4.





FIGURE 2: (a) The experimental FT-IR spectrum [18]. (b) The calculated IR spectra of sarcosine-maleic acid.

FIGURE 3: (a) The experimental FT-Raman spectrum [18]. (b) The calculated Raman spectra of sarcosine-maleic acid.

In NBO analysis [6], the hyperconjugative $\sigma \rightarrow \sigma^*$ interactions play a highly important role. These interactions represent the weak departures from a strictly localized natural Lewis structure that constitutes the primary "noncovalent" effects. The results of NBO analysis tabulated in Table 4 indicate that there is a strong hyperconjugative interaction LP2(O2) $\rightarrow \sigma^*$ (C₂-C₁) and σ (O₆-C₇) $\rightarrow \sigma^*$ (O₅-H₁₁) for the title compound is 1.43, 1.10, 27.82, and 19.08 kcal/mol, respectively. The NBO bond polarization and hybridization changes associated with formation of the complex. Herein the percentage changes in the title compound are collected in Table 3. As can be seen in Table 3, the O_5 bond hybrid of the O₅-H₁₁ bond gains 30.76% in s character and 68.89% in p character (with hybrid orbital sp^{2.24}). A more conspicuous discrepancy was seen for the H₂O lone pairs, where the natural hybrids (as well as the numerical maximumoccupancy hybrids) suggest one pure p and one sp^{0.57} lone pair [6]. The π (O₆-C₇) bond (hybrid orbital shows one pure p character) as donor and π^* (C₆-C₅) antibond (hybrid orbital shows one pure p character) as acceptor [π (O₆-C₇) \rightarrow π^* (C₆-C₅)] participates the CT. The CT values are 6.46 and 6.67 kcal/mol (Table 4). The carboxylic group contributes as a better electron-donor. Likewise, the π (C₄-O₃) $\rightarrow \pi^*$ (C_6-C_5) interaction supports the CT.

The second order delocalization energy of σ (H₅–N₁) $\rightarrow \sigma^*$ (C₁–C₂) for the title compound is 0.82 and 0.73 kcal/mol with HF and B3YLP levels. This contributes bond polarization and hybridization changes. The N₁ bond hybrid of the H₅–N₁ bond gains 25.72% in s character and 74.14% in p character (with hybrid orbital sp^{2.88}). The second

order delocalization energies of σ (C₁-O₁) $\rightarrow \sigma^*$ (C₂-N₁) and σ (C₁-O₂) $\rightarrow \sigma^*$ (C₂-C₁) are 1.13, 1.10, 0.80, and 0.83 kcal/mol with HF and B3LYP levels, respectively (in Table 4). The optimized bond lengths C₁-O₁, C₂-N₁, C₁-O₂ and C₂-C₁ are 1.310, 1.474, 1.189, and 1.510 Å(with HF level), the corresponding bonds was observed at 1.307, 1.479, 1.215, and 1.505 Å. The difference between C₁-O₁ and C₁-O₂ bond distances arise from the carboxylic group releasing ability in the title compound. This statement displays delocalization of the title compound.

3.4. Other Molecular Properties. The 3D plots of highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), electrostatic potential (ESP), electron density (ED), and the molecular electrostatic potential map (MEP) figures for the title molecule at the B3LYP method with 6-31++G(d, p) level are shown in Figure 4. The ED plot for molecule shows a uniform distribution. While the negative ESP is localized more over the oxygen atoms, the positive ESP is localized on the rest of the molecule.

MEP has been used primarily for predicting sites and relative reactivities towards electrophilic and nucleophilic attack, and in studies of biological recognition and hydrogen bonding interactions [48–50]. The calculated 3D MEP of the title compound was calculated from optimized molecular structure by using B3LYP/6–31++G(d, p) level and also shown in Figure 4. According to the results, the negative region (red) is mainly over the N and O atomic sites, which were caused by the contribution of lone-pair electrons of



FIGURE 4: Molecular surfaces of the sarcosine-maleic acid (obtained from B3LYP method).



FIGURE 5: Comparative of Mulliken's plot by HF/6-31++G(d, p) and B3LYP/6-31++G(d, p) of sarcosine-maleic acid.

nitrogen and oxygen atom while the positive (blue) potential sites are around the hydrogen atoms. A portion of a molecule that has a negative electrostatic potential will be susceptible to electrophilic attack—the more negative is the better. It is not as straightforward to use electrostatic potentials to predict nucleophilic attack [28]. Hence, the negative region (red) and positive region (blue) indicate electrophilic and nucleophilic attack symptoms. Also, a negative electrostatic potential region is observed around the O_6 atom.

The charge distribution on the molecule has an important influence on the vibrational spectra. The corresponding Mulliken's plot with different HF/6–31++G(d, p) and B3LYP/6–31++G(d, p) methods are shown in Figure 5. Figure 5 reveals the molecular charge distribution of the title compound. Generally, it is noted that the strong negative and positive partial charges on the skeletal atoms (especially O₅, O₆, O₃, O₄, N₁, O₁, O₂, C₇, C₄, C₂, C₁) for the selected compounds increase with increasing Hammett constant of substituent groups [27, 51]. These distributions of partial charges on the skeletal atoms show that the electrostatic repulsion or attraction between atoms can give a significant contribution to the intra- and intermolecular interaction.

Table 5 indicates the values of some thermodynamical and molecular parameters (such as zero point energy, $E_{\text{HOMO}}, E_{\text{LUMO}}, \Delta E, \eta, \text{ etc.}$) of sarcosine-maleic acid. Thermal energy (E) was calculated as the sum of zero point energy and thermal energy corrections for molecular translation, rotation, and vibration at 298.15 K. Enthalpy at 298.15 K and 1 atm was obtained by adding RT to the electronic energy and thermal energy. These data, as well as the Gibbs free energy, were obtained from the Gaussian output file in hartrees and converted to kJ/mol (1 hartree = 2625.50 kJ/mol). In previously works, the dipole moment and ZPE energies values of some molecules which included 1,2,3/1,2,4-triazole core were obtained to be ~3.0-6.0 D and ~155.0-476.0 kJ mol^{-1} [50, 51]. Besides, the C_v and μ values for the maleic acid were found to be 32.409 cal/mol K and 3.016 Debye [52]. These results are important to test the reliability of our results. As regard as, the results of the energies, dipole moment, entropy, and ZPE can be used to the new synthesis of some molecules which include sarcosine/maleic acid core.

The average HOMO and LUMO energies for the title compound using HF/6-31++G(d, p) and B3LYP/6-31++G(d, p) levels have been obtained to be -10.459 eV, -7.592 eV (HOMO) and 0.418 eV, -2.588 eV (LUMO) (Table 5). These results are consistent with respect to the different molecular structures calculated at semiempirical methods [53, 54]. Obtained average (for η), parameters from these energies using HF and B3LYP levels have been found to be 5.438, 2.502 eV (for η), 0.099 and 0.199 eV (for *S*) for the title compound (Table 5). According to these values, the average variation of η displays influence of the electron donating/withdrawing power of the title compound.

The polarizabilities and hyperpolarizabilities characterize the response of a system in an applied electric field. Electric polarizability is a fundamental characteristic of atomic and molecular systems. The donor and acceptor substituents provide the requisite ground-state charge asymmetry, whereas the π -conjugation system provides a pathway for the redistribution of electric charges under the influence of electric fields. Also, the variation of χ values is supported by the electrostatic potential. Large χ values characterize acids and small χ values are found for bases. For any two molecules, electron will be partially transferred from the one of low χ to that of high χ (electrons flow from high chemical potential to low chemical potential).

p-Nitroaniline (PNA) is one of the prototypical molecules used in the study of the NLO properties of molecular systems. In this study, the typical NLO material, PNA was chosen as a reference molecule; because there were no experimental values about the title compound in the literature. The relatively NLO compounds compared to PNA indicate their promising applications in NLO materials. Therefore it was used frequently as a threshold value for comparative purposes and still continues to be a recognized prototype of organic NLO chromophores. Its hyperpolarizability was studied both experimentally and theoretically in various solvents and at different frequencies [55–58].

The variations of $\langle \alpha \rangle$, $\Delta \alpha$, and $\langle \beta \rangle$ for the title compound are tabulated in Table 6. These variations are caused from the electron donating/withdrawing atom/group and *ab initio* calculations for the title compound. According to *ab initio* calculations, the variation of $\langle \alpha \rangle$ and $\langle \beta \rangle$ values for the title compound is different (Table 6). The results of these variations with HF/6–31++G(d, p) level is larger than ones with the B3LYP/6–31++G(d, p) level. Also, the variation of $\langle \alpha \rangle$ values for the title compound explicitly decreases from the largest molecular structures to the smallest molecular structures. Calculated $\langle \alpha \rangle$ and $\langle \beta \rangle$ values for the title compound are similar to the different theoretical and experimental studies for different molecular structures [25, 28, 29, 31, 59–64].

4. Conclusion

Investigation throughout the work proves that the NLO and NBO analysis of sarcosine-maleic acid can be successfully predicted by *ab-initio* HF and B3LYP methods with

6-31++G(d,p) basis set. To investigate nonlinear optical properties, the compound which have sarcosine and maleic acid substituted by various electron donating/withdrawing atom/group have been used. Also, how NBO analysis change with different two methods and the consistency of these methods have also been investigated. The best fittings between calculated and measured vibrational frequencies were achieved by B3LYP/6-31++G(d, p) level. With this level, the deviations between calculated and experimental values are ignorable for a given type of vibration. These results are accurate enough with the deviations in the same order as anharmonicity corrections and effect from matrix or crystal. Therefore, this study confirms that the theoretical calculation of vibrational frequencies is quite useful for the vibrational assignment and for predicting new vibrational frequencies. The variation of $\langle \alpha \rangle$ and $\langle \beta \rangle$ values with different two methods is different due to the different electron donating/withdrawing atom/group. The η , χ , and S parameters of the compound are directly related to the HOMO and LUMO calculations. The ESP and MEP plots for compound show the distribution of charge of compounds with respect to the difference between positive and negative charge. The small χ values display the $E_{\rm HOMO}$ statement (i.e., Lewis base or nucleophile) and the larger values display E_{LUMO} statement (i.e., Lewis acid or electrophile). To sum up, the negative region (red) is mainly over the N and O atomic sites, which were caused by the contribution of lone-pair electrons of nitrogen and oxygen atom while the positive (blue) potential sites are around the hydrogen atoms. The compound exhibits strong effective intra- and intermolecular charge transfer and shows large second-order nonlinearity. The sarcosine and maleic acid systems can be used as an effective π -bridge in the design of new organic and inorganic acids molecules.

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