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Investigation of the Effect of Substitutions on the Electronic and Optical Properties of the Sumanene Molecule

Hadis Mohammadpour[1], Pouran Pourhakkak[2, *], Ren Guogang[3], Hamidreeza Shamlouei[1], Mohammadreza Aallaei[4], Nasimeh Mohammadian[5]

[1]Chemistry Department, Lorestan University, Khorram Abad
[2]Department of Chemistry, Payam Noor University, Tehran, Iran
[3]School of Physics, Engineering, and Computer Science, University of Hertfordshire, College Lane, Hatfield AL 109AB, UK
[4]Department of Chemistry, Shahid Bahonar University of Kerman, Kerman, Iran
*[5]Khash School of health, Zahedan University of Medical Sciences*

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ABSTRACT

Sumanene (C21H12) is the smallest bowl-shaped molecule containing a central benzene ring, alternately surrounded by another 3 benzene rings and cyclopentadiene rings. This study investigated the effect of various electron donor and receptor substitutions on its structure, electrical and optical properties. The results showed that the electron-bonding and electron-donor-acceptor groups to sumanene greatly affected the electrical properties. In contrast, the most significant effect occurred when NO and CH2Li substitutions were at the two positions simultaneously. These substitutions also greatly influenced optical properties and significantly increased polarization and polarization values. The most significant effect occurred when BH2 and NCH3Li were replaced in position 1. Finally, the absorption spectrum of the substituted molecules was examined when the BH2-NCH3Li groups were in position 1.
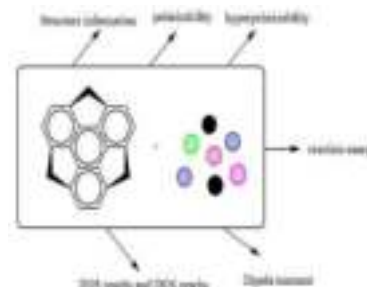
1. Introduction

Current science cannot be envisioned without carbon structures. In natural science, carbon as an element or a particle assumes a fundamental part and can be utilized in all significant disciplines, including materials science, electro-optics, medication, and general science.[1,2] Numerous inorganic analysts have zeroed in on carbon studies beginning around 1950. The disclosure of fullerene and carbon nanotubes was a defining moment in improving established scientific communities.

Fullerenes are bunches of carbon atoms as a generally shut rack and have a few fundamental properties not seen in that frame of mind overall. They structure a fascinating gathering of mixtures that will unquestionably track down applications in innovations later on. Like other significant logical discoveries, fullerenes were found coincidentally. In 1985 Smalley and Kroto got fascinating outcomes on the mass range of carbon tests, which prompted the fullerenes and their security in the gas stage and the quest for different Fullerenes in a circle,

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empty circles, etc.[2] Round drawers that appear as though football is additionally called buckyballs. Research in fullerene science goes on because of the significance of functionalizing these mixtures. For instance, fullerene is insoluble, and adding a fitting gathering can expand its solvency.[3,4]

Polyaromatic hydrocarbons have a π-form bond, collectively of new gems in the π-form carbon frameworks, which have, as of late, been the subject of a few trials or hypothetical examinations.[5,6] Dissimilar to planar fragrant frameworks, these hydrocarbons are not solvent in arrangement and go through stage reversal through a planar progress state. A fundamental contrast between bent hydrocarbons and bent polycarbonate (PAHs) is that the spellbound bent frameworks upgrade the electrostatic connections between these frameworks. In this unique situation, buckybowls, i.e., bowl-formed PAHs, primarily connected with fullerenes, give a desirable option in contrast to stacking communications between raised PAHs. The energy boundary of this reversal is reliant unequivocally on the size and curve of the framework.[7,8] Numerous parts of these designs' theoretical investigations presently cannot be explained, so research in such cases is critical for further development.[9,10]

Like fullerenes, sumanene has benzyl positions for natural responses.[11,12,13,14] The preliminary examination of sumanene started in 2003, while some hypothetical exploration of the saucer-molded atoms had previously been done.[15] The name sumanene is derived from the word Suman, which implies blossom in Hindi and Sanskrit. It alludes to the ring's edges, which look like a blossom and form a petal shape, as shown in Fig. 1.

Early endeavors to orchestrate aromatics in light of planar fragrant mixtures were fruitless. For instance, Tris Bruno methyl tri 1993 gave only one-ring or two-ring items by breaking 1 or 2 external ring bonds under warm decay conditions under streak vacuum (FVP); hence, Suman's ideal tone did not occur 44. One of the reasons for acid reflux is the presence of benzylic corrosive in natural citrus products in three situations with half and half sp^3. After a decade, Sakurai and his partner[16] fostered another manufactured technique to set up a framework in the arrangement stage under gentle circumstances, like Laughton's blend methodology for corannulene.

Sumanene was synthesized in 2003 by Hiro et al.[12] Sumanene with molecular formula $C_{21}H_{12}$, and molecular weight 264.32 gmol^{-1} is a bowl-shaped molecule, π-conjugated, with C_{3v} symmetry, alternate the benzene ring and the cyclopentadiene ring around the central benzene ring.[16] The molecular structure of sumanene was determined by X-ray crystal structure analysis. The structural feature of sumanene is three carbon atoms with sp^3 hybridization at the benzylic positions.

The presence of three carbon atoms in the benzylic position allows the functionalization and, thus, the production of different derivatives with different properties and sometimes increases the possibility of gas adsorption by forming anions, cations, radicals, and carbenes that are not associated with radicals.[18,19] It is different from Corannulene ($C_{20}H_{10}$) and coaderannulene where Sumanene ends are isolated from five and four aromatic rings. This is why sumanene is an attractive molecule for creating newly formed compounds.[20] The structure of sumanene crystals is such that the molecules accumulate in columns, and the axis of concentration of molecules in all columns is directed in one direction. In this makeup, there is a limit between the electron orbitals and the electron movement, which is closely related to the direction of concentration of the crystals that people see. Compared with the structure of fullerenes and carbon nanostructures, the structure of sumanene is more accessible to change. By adjusting the distance between the planes in the structure, the electrical properties of the crystal structure can be controlled. Another interesting dynamic behavior is the bowl-shaped inversion shown in Fig 1.

Due to the presence of three cyclo-pentane rings in this structure, it has a more substantial structure than corynoline, which does not undergo bowl-to-bowl inversion at room temperature. Such excitation properties are studied, especially with fullerene, corannulene, and sumanene structures Tom Reichert et al have got studied the capability of the sumanene molecule to act as a service of the 5FU drug. The inducement to observe sumanene as a capability drug service of 5FU has been located because this molecule Possesses hard and fast consultant physical and chemical properties, established by using numerous studies from Each experimental and theoretical aspect.[21] Artur Kasprzak et al introduced sumanene was found to act as a Cs+ recognition material in its neutral state.[22] It is worth noting that the detection of Cs$^+$ is of the highest environmental importance.[23] Stevan Armakovic et al. investigated the hydrogen storage properties of a compound that serves as a model compound for nanotubes and fullerenes-sumanene[24].

2. Computational Methods

Computational chemistry is a set of techniques to investigate chemical problems using computers

Computational chemistry is divided into two general methods: a) methods in which calculations are made using the laws of classical physics and known as molecular mechanics methods, b): methods in which calculations are made the basis of the mechanics and methods of electronic structure.[17] In this theoretical study, the effect of the number of electron donors and acceptors on the structure, the electron, and the unique properties (NOL) of sumanene were studied. Charge values electrical properties, including orbital values of HOMO and LUMO orbitals, system energy gap (e.g.), and NBO bar, were calculated for all systems using Gaussian09 and GaussSum05 software. The optimized structure was obtained using the B3LYP method and the 6-311G (d, p)basis set. The B3LYP method is a subset of density functional methods that is widely used and has gained tremendous popularity in computational chemistry in recent years. It is prevalent. Frequency calculations were also performed to ensure the stability of the structure due to the lack of imaginary frequency. The energetic values of HOMO and LUMO orbitals were calculated for these structures, which were used to calculate the gap energy value according to the following equation (eq. 1).

E.g., $= E_{LUMO} - E_{HOMO}$ (eq. 1)

For the various structures studied, the values of α (linear optical properties) and β (nonlinear optical properties) were calculated according to the following equations (eq. 2 and 3).

$$\alpha = 1/3 \ (\alpha xx + \alpha yy + \alpha zz) \qquad \text{(eq. 2)}$$

$$\beta 0 = (\beta x2 + \beta y2 + \beta z2) \ ^{1/2} \qquad \text{(eq. 3)}$$

Also, the UV-Vis spectrum of the Sumanene molecule was intact, and the Sumanene molecule had electron donor and receptor substitutions using the TDDFT method.

3. Results and discussion

3.1. Optimized structures

The basic structure of the Sumanene molecule was optimized by the B3LYP computational level, as shown in Fig 1. The structure of this compound includes 21 carbon atoms and 12 hydrogen atoms. The Sumanene nucleus is a benzene ring, and its alternation consists of three benzene rings and three alternating cyclopentadiene rings. This study tried to connect the rings around the nucleus of the electron donor nucleus NHLi, NCH$_3$Li, CH$_2$Li, and the electron acceptor BH$_2$, NO to the π bond. The optimized geometric structures of these compounds are shown in Fig 2. Then, the density values and electrical properties, including HOMO and LUMO orbital energy values, the gap energy of the structures (Eg), and the NBO bar, were calculated for all structures.
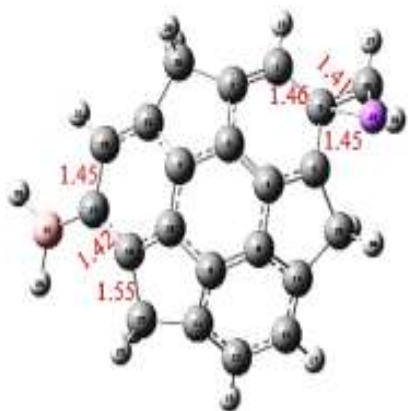
As a result, a shared electron from electron-donating groups increases the length of the π bonds attached to the substitutions.

3.2. Electrical properties

The DOS spectrum of the fundamental structure of the sumanene molecule and its corresponding substitute is presented in Figs. 3 and 4.

Figure 1. Sumanene molecule C$_{21}$H$_{12}$

C$_{21}$H$_{12}$ (BH$_2$.CH$_2$Li) (1)

C$_{21}$H$_{12}$ (BH$_2$.CH$_2$Li) (2)

C$_{21}$H$_{12}$ (BH$_2$.CH$_2$Li) (3)

C$_{21}$H$_{12}$ (BH$_2$.NHLi) (1)

C$_{21}$H$_{12}$ (BH$_2$.NHLi) (2)

C$_{21}$H$_{12}$ (BH$_2$.NHLi) (3)

C$_{21}$H$_{12}$ (BH$_2$.NCH$_3$Li) (1)

C$_{21}$H$_{12}$ (BH$_2$.NCH$_3$Li) (2)

C$_{21}$H$_{12}$ (BH$_2$.NCH$_3$Li) (3)

C$_{21}$H$_{12}$ (NO.CH$_2$Li) (1)

C$_{21}$H$_{12}$ (NO.CH$_2$Li) (2)

C$_{21}$H$_{12}$ (NO.CH$_2$Li) (3)

C$_{21}$H$_{12}$ (NO.NHLi) (1)   C$_{21}$H$_{12}$ (NO.NHLi) (2)   C$_{21}$H$_{12}$ (NO.NHLi) (3)
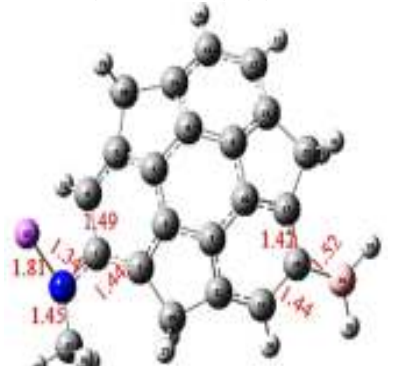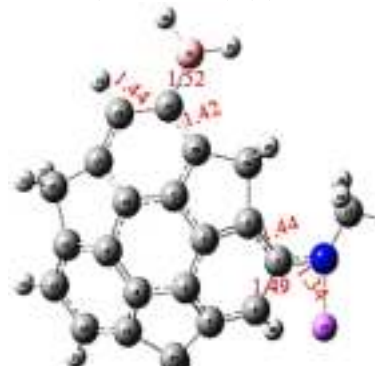
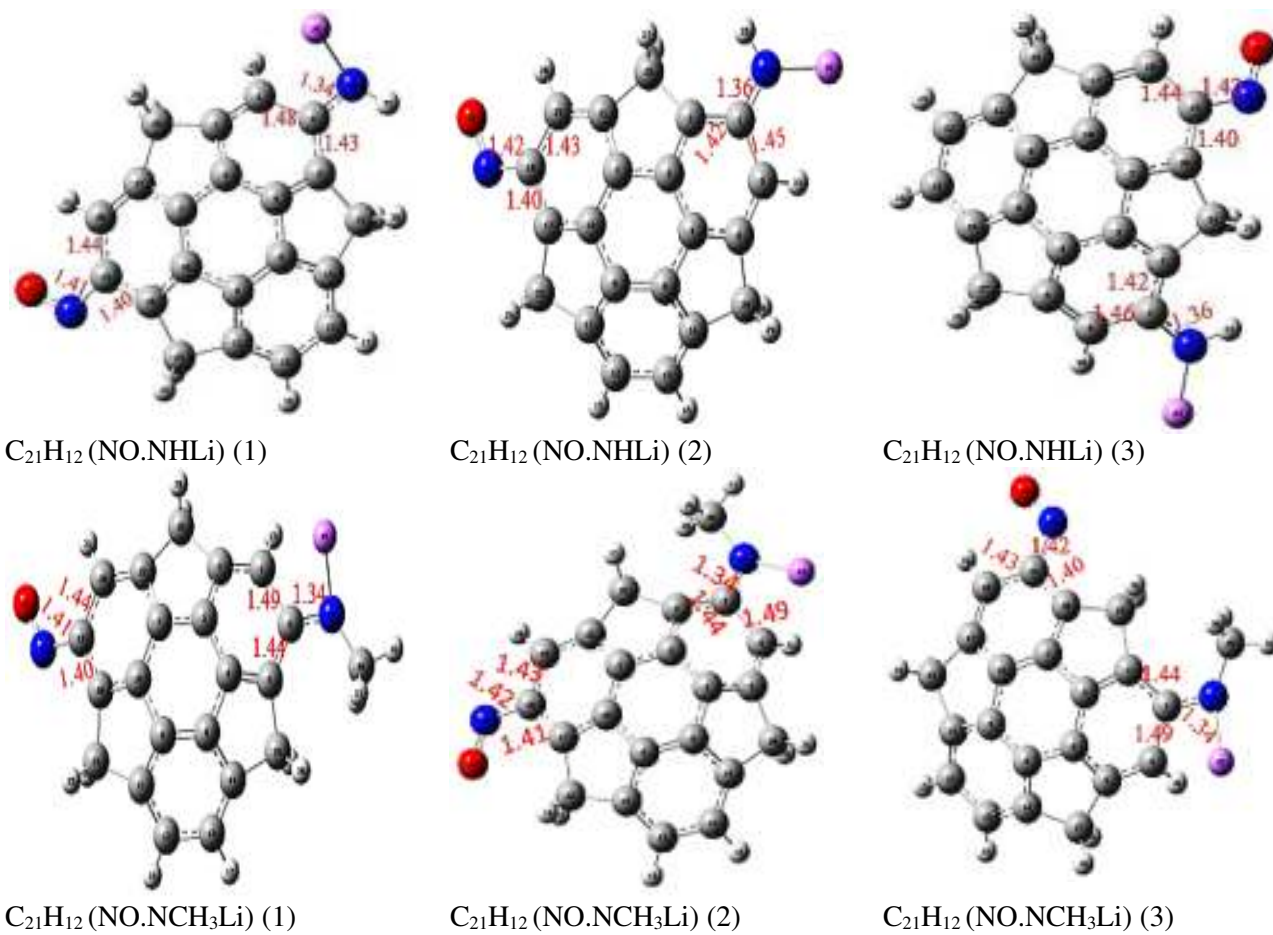C$_{21}$H$_{12}$ (NO.NCH$_3$Li) (1)   C$_{21}$H$_{12}$ (NO.NCH$_3$Li) (2)   C$_{21}$H$_{12}$ (NO.NCH$_3$Li) (3)
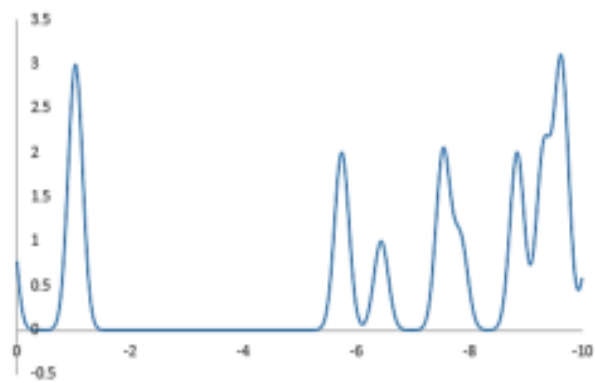
Figure 2. Optimized structures in the substituted state.

Figure 3. The DOS spectrum of C$_{21}$H$_{12}$.

C$_{21}$H$_{12}$ (BH$_2$.CH$_2$Li) (1)
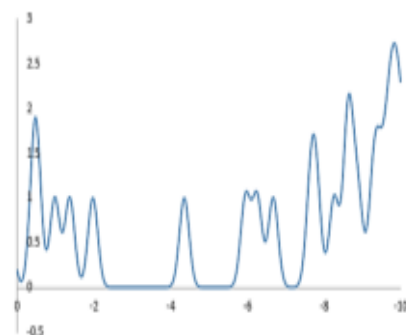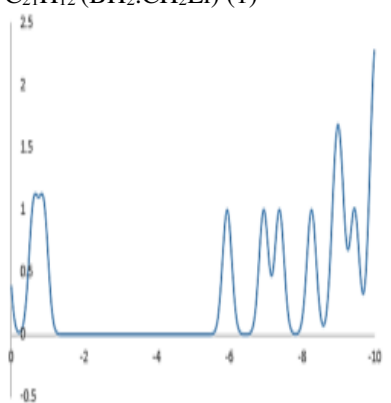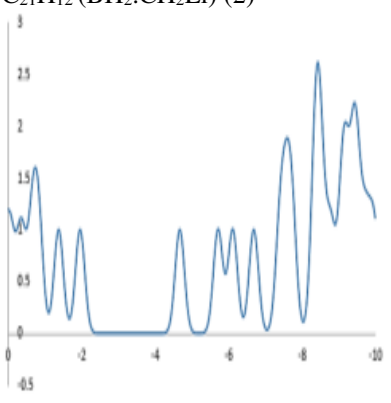
C$_{21}$H$_{12}$ (BH$_2$.CH$_2$Li) (2)

C$_{21}$H$_{12}$ (BH$_2$.CH$_2$Li) (3)

C$_{21}$H$_{12}$ (BH$_2$.NHLi) (1)

C$_{21}$H$_{12}$ (BH$_2$.NHLi) (2)

C$_{21}$H$_{12}$ (BH$_2$.NHLi) (3)

C$_{21}$H$_{12}$ (BH$_2$.NCH$_3$Li) (1)

C$_{21}$H$_{12}$ (BH$_2$.NCH$_3$Li) (2)

C$_{21}$H$_{12}$ (BH$_2$.NCH$_3$Li) (3)

C$_{21}$H$_{12}$ (NO.CH$_2$Li) (1)
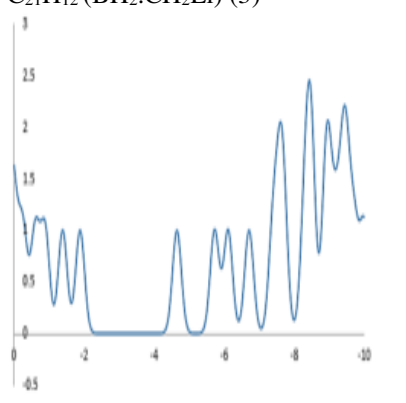
C$_{21}$H$_{12}$ (NO.CH$_2$Li) (2)

C$_{21}$H$_{12}$ (NO.CH$_2$Li) (3)

C$_{21}$H$_{12}$ (NO.NHLi) (1) C$_{21}$H$_{12}$ (NO.NHLi) (2) C$_{21}$H$_{12}$ (NO.NHLi) (3)
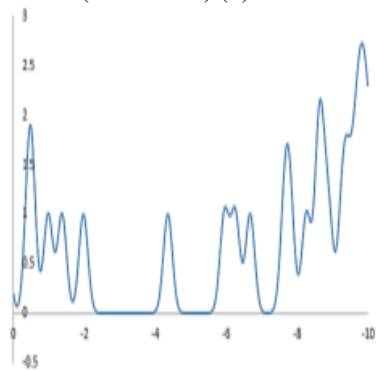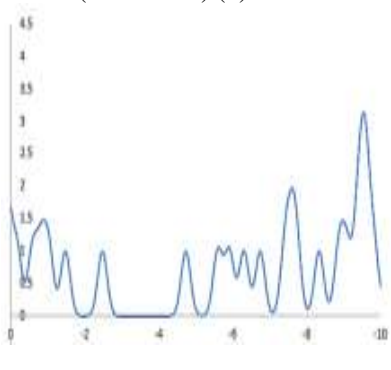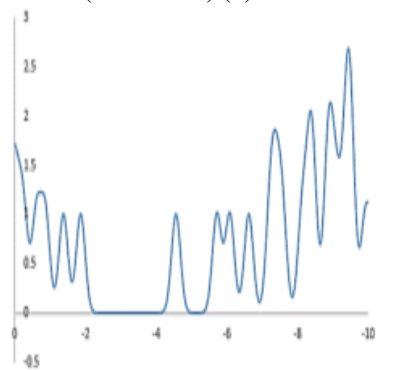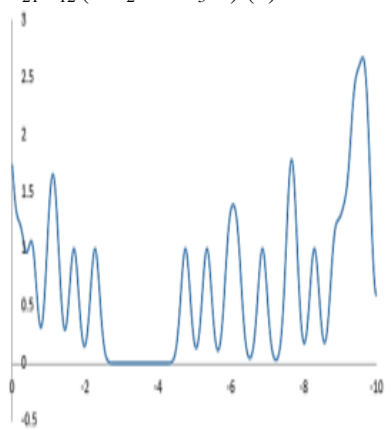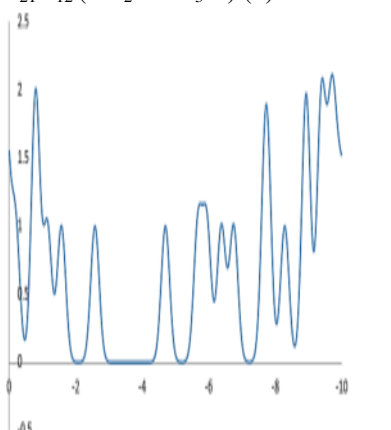
C$_{21}$H$_{12}$ (NO.NCH$_3$Li) (1) C$_{21}$H$_{12}$ (NO.NCH$_3$Li) (2) C$_{21}$H$_{12}$ (NO.NCH$_3$Li) (3)

Figure 4. The DOS spectrum of the Sumanene molecule's initial shape and the substitute state's structure.

Table 1. EHOMO, ELUMO, and Gap energy results (Eg, The initial shape of the Sumanene molecule and the structure are optimized in the substitute state)

	Eg	ε_{LUMO}	ε_{HOMO}
Sumanene	-5.75	-1.04	4.71
BH$_2$-SU-CH$_2$Li(1)	-4.65	-1.78	2.87
BH$_2$-SU-CH$_2$Li(2)	-4.55	-2.03	2.52
BH$_2$-SU-CH$_2$Li(3)	-4.51	-2.11	2.4
BH$_2$-SU-NHLi(1)	-4.79	-1.69	3.1
BH$_2$-SU-NHLi(2)	-4.67	-1.95	2.72
BH$_2$-SU-NHLi(3)	-4.65	-1.89	2.76
BH$_2$-SU- NCH$_3$Li (1)	-4.7	-1.67	3.03
BH$_2$-SU- NCH$_3$Li (2)	-4.58	-1.93	2.65
BH$_2$-SU- NCH$_3$Li (3)	-4.56	-1.86	2.7
NO-SU-CH$_2$Li(1)	-4.76	-2.27	2.49
NO-SU-CH$_2$Li(2)	-4.7	-2.58	2.12
NO-SU-CH$_2$Li(3)	-4.67	-2.54	2.13
NO-SU-NHLi(1)	-4.95	-2.24	2.71
NO-SU-NHLi(2)	-4.53	-2.26	2.27
NO-SU-NHLi(3)	-4.51	-2.24	2.28
NO-SU- NCH$_3$Li (1)	-4.86	-2.22	2.64
NO-SU- NCH$_3$Li (2)	-4.73	-2.47	2.26
NO-SU- NCH$_3$Li (3)	-4.72	-2.42	2.3

Using the DOS range, the HOMO and LUMO energy values and the Gap energy (Eg) of all the structures in the optimized substituted state were calculated. The results are presented in Table 1.

The Eg value for the Sumanene molecule alone is 4.71 eV. The more considerable Eg value for the initial shape of the sumanene indicates that this structure is a semiconductor. According to the results of Table 1, the bonding process of substitution donor and acceptor electrons has led to a decrease in the value of Eg compared to the initial form of the Sumanene molecule. This change indicates that these structures' electrical properties and reactivity have increased. According to the

above values, the highest time effect occurs when NO and CH_2Li substitutions are in position two simultaneously.

3.3. Charge transfer

The structure charge is calculated in the substitute state using NBO calculations, and the results are reported in Table 2. In all substitute structures, the donor electron group BH_2 has a positive charge, which means the charge transfer to the Sumanene molecule, and the NO acceptor electron group, which indicates the charge transfer from molecule Or (In all substitute structures, BH_2 and NO represent a donor and acceptor electron group which results in charge transfer to/from Sumanene molecule, respectively.)

Table 2. NBO results of electron donor and acceptor groups on the Sumanene molecule

Substitute	Charge Q		Substitute	charge Q	
	BH_2	CH_2Li		BH_2	CH_2Li
BH_2-SU-CH_2Li(1)	0.19383	0.48196	**BH_2-SU-NHLi(1)**	0.19338	0.22249
BH_2-SU-CH_2Li(2)	0.21954	0.45346	**BH_2-SU-NHLi(2)**	0.21845	0.20802
BH_2-SU-CH_2Li(3)	0.21989	0.40367	**BH_2-SU-NHLi(3)**	0.2117	0.21126
Substitute	Charge Q		Substitute	charge Q	
	BH_2	NCH_3Li		NO	CH_2Li
BH_2-SU-NCH_3Li (1)	0.19161	0.24094	**NO-SU-CH_2Li(1)**	-0.2959	0.46846
BH_2-SU-NCH_3Li (2)	0.21856	0.22501	**NO-SU-CH_2Li(2)**	-0.25971	0.46583
BH_2-SU-NCH_3Li (3)	0.20939	0.26109	**NO-SU-CH_2Li(3)**	-0.27104	0.47654
Substitute	Charge Q		Substitute	Charge Q	
	NO	NHLi		NO	NCH_3Li
NO-SU-NHLi(1)	-0.29419	0.23135	**NO-SU-NCH_3Li(1)**	-0.29674	0.25192
NO-SU-NHLi(2)	-0.27246	0.11778	**NO-SU-NCH_3Li(2)**	-0.26792	0.23111
NO-SU-NHLi(3)	-0.27951	0.12404	**NO-SU-NCH_3Li(3)**	-0.27255	0.26846

3.4. Optical Properties

The Sumanene molecule's initial linear and nonlinear optical properties and structure were calculated in the

substitute state using the Gaussian09 program. The results are presented in Table 3.

Table 3. Results of α (linear optical properties) and β (nonlinear optical properties) initial shape of the sumanene and structure in substitute state

	β_0 (a.u.)	α (a.u.)
Sumanene	210.496	214.601
BH_2-SU-CH_2Li(1)	3402.036	291.717
BH_2-SU-CH_2Li(2)	2155.868	283.100
BH_2-SU-CH_2Li(3)	2808.780	278.930
BH_2-SU-NHLi(1)	4113.883	275.135
BH_2-SU-NHLi(2)	799.623	268.3480
BH_2-SU-NHLi(3)	1254.114	268.766
BH_2-SU- NCH_3Li (1)	5160.392	291.906
BH_2-SU- NCH_3Li (2)	1130.515	283.612
BH_2-SU- NCH_3Li (3)	1104.526	283.896
NO-SU-CH_2Li(1)	3566.108	292.2386
NO-SU-CH_2Li(2)	2020.028	279.8476
NO-SU-CH_2Li(3)	2185.414	279.993

NO-SU-NHLi(1)	3794.0523	272.9106
NO-SU-NHLi(2)	1694.7209	268.6700
NO-SU-NHLi(3)	2035.5586	269.2550
NO-SU- NCH₃Li (1)	4909.7766	289.9323
NO-SU- NCH₃Li (2)	817.2384	278.8813
NO-SU- NCH₃Li (3)	881.4154	281.5716

The Sumanene molecule's initial α and β levels are 214/601 and 210/496, which are increased by the electron donor and acceptor substitution binding to the sumanene. Values of α and β indicate that they had better optical properties than the original form of the Sumanene molecule. The most significant effect occurs when CH_2Li and BH_2 substitutions are in position 1. Table 4 indicates the absorbance values and wavelengths of the UV-Vis spectra of the initial form of the Sumanene molecule and corresponding substituted structures.

Table 4. Adsorbent values and wavelengths of the UV-Vis spectra of the Sumanene molecule with corresponding BH_2 and CH_2Li substituted structures.

State No.	Sumanene		BH₂-SU-CH₂Li(1)		BH₂-SU-CH₂Li(2)		BH₂-SU-CH₂Li(3)	
	(nm)	F	(nm)	f	(nm)	f	(nm)	f
1	324.33	0.0005	531.17	0.1110	603.06	0.0291	649.14	0.0140
2	309.82	0.0000	459.88	0.2774	535.17	0.0652	539.07	0.0554
3	306.02	0.0004	412.49	0.0265	411.18	0.0004	458.96	0.0146
4	306.00	0.0004	395.73	0.0034	384.74	0.0340	384.63	0.0173
5	276.22	0.3247	359.71	0.0476	369.42	0.0117	375.52	0.0184
6	276.22	0.3248	340.80	0.0309	350.15	0.0277	361.15	0.2707
7	256.93	0.0000	333.20	0.0216	343.81	0.0804	334.10	0.1365

The high-intensity adsorption values indicate that the substituted structures have higher adsorption intensity than the Sumanen primary molecule. In Table 4, the maximum adsorption intensity is related to the BH₂-SU-CH₂Li (1) molecule with a value of 0.2774.

Table 5. Adsorbent values and wavelengths of the UV-Vis spectra of the sumanene molecule with structures with BH_2 and NHLi substitutions

State NO	Sumanene		BH₂-SU-NHLi(1)		BH₂-SU-NHLi(2)		BH₂-SU-NHLi(3)	
	(nm)	f	(nm)	f	(nm)	f	(nm)	f
1	324.33	0.0005	471.12	0.0153	553.33	0.0216	558.82	0.0304
2	309.82	0.0000	438.70	0.2896	477.91	0.0048	482.51	0.0113
3	306.02	0.0004	382.15	0.0193	388.63	0.0039	392.79	0.0111
4	306.00	0.0004	373.96	0.0229	379.40	0.0425	373.59	0.0296
5	276.22	0.3247	354.07	0.1040	353.61	0.0816	345.09	0.1330
6	276.22	0.3248	333.44	0.0558	336.60	0.1961	330.04	0.0978
7	256.93	0.0000	327.52	0.0016	331.23	0.1957	322.40	0.1378

The reported adsorption intensity values indicate that the substituted structures have higher adsorption intensity than the Sumanene initial molecule. In Table 5, the highest adsorption intensity is related to the BH₂-SU-NHLi (1) molecule with a value of 0.2896.

Table 6. Adsorbent values and wavelengths of the UV-Vis spectra of the Sumanene molecule with structures with BH_2 and NCH_3Li substitutions

State No	Sumanene		BH₂-SU-(1)	NCH₃Li	BH₂-SU-(2)	NCH₃Li	BH₂-SU-(3)	NCH₃Li
	(nm)	f	(nm)	f	(nm)	f	(nm)	f
1	324.33	0.0005	485.56	0.0146	571.11	0.0217	572.61	0.0338
2	309.82	0.0000	449.77	0.3134	493.61	0.0049	497.57	0.0099
3	306.02	0.0004	390.00	0.0386	394.35	0.0017	400.53	0.0112
4	306.00	0.0004	379.34	0.0203	381.40	0.0346	373.55	0.0185
5	276.22	0.3247	356.16	0.0887	359.07	0.1036	349.8	0.1866
6	276.22	0.3248	333.36	0.0481	339.97	0.0803	334.15	0.0544
7	256.93	0.0000	327.75	0.0009	336.76	0.2965	326.89	0.0855

The reported adsorption intensity values indicate that the substituted structures have higher adsorption intensity than the Sumanen initial molecule. In Table 6, the highest adsorption intensity is related to the BH₂-SU-NHLi (1) molecule with a value of 0.3134.

Table 7. Absorbent values and wavelengths of the UV-Vis spectra of the sumanene molecule with structures with NO and CH_2Li substitutions

State NO	Sumanene		NO-SU-CH₂Li(1)		NO-SU-CH₂Li(2)		NO-SU-CH₂Li(3)	
	(nm)	f	(nm)	f	(nm)	f	(nm)	f
1	324.33	0.0005	883.07	0.0002	848.34	0.0002	844.32	0.0002
2	309.82	0.0000	541.59	0.1813	727.92	0.0261	754.39	0.0236
3	306.02	0.0004	519.06	0.1373	526.51	0.0628	521.85	0.0550
4	306.00	0.0004	422.50	0.0155	437.04	0.0191	435.89	0.0060
5	276.22	0.3247	403.87	0.0072	416.54	0.0205	409.98	0.0573
6	276.22	0.3248	385.18	0.1049	378.87	0.0093	367.63	0.1109
7	256.93	0.0000	373.39	0.0011	371.33	0.0751	364.61	0.0464

The reported high adsorption values indicate that the dissociated structures have higher adsorption intensity than the Sumanene initial molecule. In Table 7, the maximum adsorption intensity is related to the NO-SU-CH₂Li (1) molecule with a value of 0.1813.

Table 8. Adsorbent values and wavelengths of the UV-Vis spectra of the sumanene molecule with structures with NO, NHLi substitutions

State NO	Sumanene		NO-SU-NHLi(1)		NO-SU-NHLi(2)		NO-SU-NHLi(3)	
	(nm)	f	(nm)	f	(nm)	f	(nm)	f
1	324.33	0.0005	828.83	0.0002	837.34	0.0003	839.02	0.0002
2	309.82	0.0000	489.02	0.2265	682.94	0.0157	695.45	0.0279
3	306.02	0.0004	461.80	0.0252	662.47	0.0073	659.89	0.0067
4	306.00	0.0004	398.57	0.0293	432.05	0.0386	437.77	0.0170
5	276.22	0.3247	379.66	0.0164	401.32	0.0315	400.46	0.0551
6	276.22	0.3248	369.63	0.1039	391.56	0.0000	397.41	0.0009
7	256.93	0.0000	362.10	0.0010	386.72	0.0005	385.79	0.0022

The reported high adsorption values indicate that the substitute structures have higher adsorption intensity than the Sumanene primary molecule. In Table 8, the maximum adsorption intensity is related to the NO-SU-NHLi (1) molecule with a value of 0.2265.

Table 9. Adsorbent values and wavelengths of the UV-Vis spectra of the sumanene molecule with structures with NO, NCH$_3$Li substitutions

State NO	Sumanene		NO-SU-(1)	NCH$_3$Li	NO-SU- NCH$_3$Li (2)		NO-SU-(3)	NCH$_3$Li
	(nm)	f	(nm)	f	(nm)	f	(nm)	f
1	324.33	0.0005	828.53	0.0002	668.39	0.0142	680.07	0.0311
2	309.82	0.0000	500.34	0.2504	487.02	0.0086	488.19	0.0102
3	306.02	0.0004	475.14	0.0263	419.27	0.0278	416.29	0.0167
4	306.00	0.0004	400.67	0.0092	399.63	0.0164	402.97	0.0226
5	276.22	0.3247	375.73	0.0328	372.16	0.0147	357.67	0.1389
6	276.22	0.3248	375.27	0.1200	361.24	0.1934	353.02	0.0704
7	256.93	0.0000	362.77	0.0007	341.8	0.1538	345.05	0.0153

The reported high adsorption values indicate that the dissociated structures have higher adsorption intensity than the primary Sumanene molecule in Table 9. The maximum adsorption intensity is related to the NO-SU-NCH$_3$Li (1) molecule with a value of 0.2504.

4. Conclusions

The binding of acceptor and electron donor electrons on the Sumanene molecule significantly affects its electrical properties. The most positive change occurs when the NO and CH$_2$Li groups are simultaneously attached to the Sumanene molecule at position 2. Sumanene has the highest polarization and ultra polarization values when BH$_2$ and NCH$_3$Li groups are in position 1. Applying a substitution with the Sumanene molecule reduces the distance between the highest occupied molecular orbital (HOMO) and the lowest orbital molar (LUMO). Decreasing the Eg values of all structures compared to the Sumanene molecule leads to more electrical properties and increases the reactivity of these structures. The NO and CH$_2$Li substitutions have the most significant impact in the second position. The application of the substitutions led to increased adsorption intensity in the UV area, which had the most significant effect when the BH$_2$ and NCH$_3$Li groups were in the first positio

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