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Vibrational Spectroscopy

Elixir Vib. Spec. 159A (2021) 55712-55716

ISSN: 2229-712X

Quantum Chemical and Geometrical Properties of 2, 7-Bis (4-Methoxyphenyl) 9,9-Dipropyl-9h-Flurene

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ARTICLE INFO

Article history:

Received: 11 September 2021;

Received in revised form:

12 October 2021;

Accepted: 24 October 2021;

Keywords

Geometry,

Mulliken Charge,

Chemical Parameters.

ABSTRACT

In this article, we are analysing the arrangements of atoms and charge distribution by using optimized geometry of 2,7-Bis(4-Methoxyphenyl) 9,9-Dipropyl-9H-Flurene (Exalite-389), which has been obtained by DFT study. The solvent effect on the molecular orbitals has been investigated by studying parameters like chemical hardness (η), chemical potential (μ) and global electrophilicity (ω) of the Exalite–389 molecule in vacuum and solvent medium. These outcomes provide a deep understanding of structure of the molecule and electronic properties in different mediums characteristics for optoelectronic applications.

1. Introduction

Laser dyes have several applications such as anticoagulants, fluorescence indicator and possess anthelmintic and optical brightness properties [1]. This Exalite laser dye is a derivative of para-quaterphenylenes and their configurations of molecules were augmented to make best production of the compounds as fluorescent laser grade dyes. To determine the structural properties of the 2,7-Bis(4-Methoxyphenyl) 9,9-Dipropyl-9H-Flurene (Exalite-389) density functional theory approaches, especially those using a hybrid functional, have evolved to a powerful and very reliable tool, being routinely used for the determination of various molecular properties [2]. The present study focuses on determination of ground and excited state mulliken atomic charge distribution and quantum chemical parameter analysis of molecule in different medium using DFT method at the B3LYP/6-311G level of theory.

2. Computational study

Quantum chemical DFT and TD-DFT calculations were executed by using Gaussian 09 [3] to study the optimized structures and charge distribution of Exalite-389 molecule by using the B3LYP/6-311G basis set [4]. From this study, we report, theoretical analysed energy band gap, ionization potential (I), electron affinity (E), chemical hardness (η), chemical potential (μ), chemical softness (s), global electrophilicity (ω) characteristics of the Exalite-389 in vacuum and solvent medium with different polarity (alkanes, alcohols and nitriles) [5-6].

3. Results and Discussion

3.1. Geometrical Properties

The optimized structure of Exalite-389 obtained by density functional theory (DFT/B3LYP/6-311G), Initial geometry obtained from standard parameters which are then reduced to a minimum by the Gaussian program is presented in Figure 1. The bond length (Å), bond angle (º) and dihedral angle (º) [7] of the molecule are tabulated in Table 1.

3.2 Mulliken charge distribution

The Mulliken atomic charge distribution of Exalite-389 have studied in vacuum using DFT (ground state) and TDDFT (excited state) method and tabulated in Table 2. Charge distribution in ground and excited state is represented as shown in Figure 2. Atoms which have the positive charge acts as acceptor and the atoms with negative charge acts as donator, we observed slight changes in charges from ground state to excited state [8].

3.3 Quantum chemical parameters

The quantum chemical parameters are studied by DFT/B3LYP/6-311G in vacuum and various solvent medium [9], the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy levels helps in providing information of chemical parameters, negative of HOMO energy is taken as ionization potential *(I)* and negative of LUMO energy as electron affinity (A) these values helps us to calculate the various parameters of the probe molecule which are reported in Table 3.

The difference between Energy of HOMO and LUMO gives energy band gap (E_g)

$$Eg = E_{HOMO} \sim E_{LUMO} \quad (1)$$

The atom's ability to attract the shared electrons of a covalent bond gives electronegativity (χ)

$$\mathbf{x} = \frac{(I+E)}{2} \quad (2)$$

Half of the energy gap of HOMO and LUMO gives the chemical hardness (η)

$$\boldsymbol{\eta} = \frac{(I-E)}{2} \quad (3)$$

The negative value of electronegativity gives the chemical potential (μ)

$$\mu = -\chi \quad (4)$$

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The electrophilicity index or global electrophilicity (ω) is defined as follows

$$\omega = \frac{\mu^2}{2\eta} \quad (5)$$

4. Conclusion

In this paper, quantum chemical investigation on the geometric and optoelectronic properties obtained by the DFT technique with B3LYP/6-311G basis set in vacuum and solvent medium. The geometric parameters and atomic charge distribution of Exalite-389 are confirmed the stability of structure. HOMO-LUMO gap implies good kinetic stability of the molecule. Finally, the obtained results demonstrate how electronic properties can suggest this compound as a good candidate for optoelectronic applications.

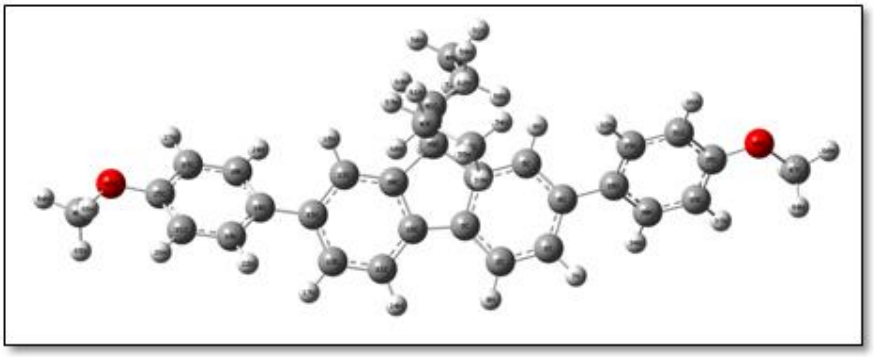

Fig 1. optimized molecular Structure of Exalite-389

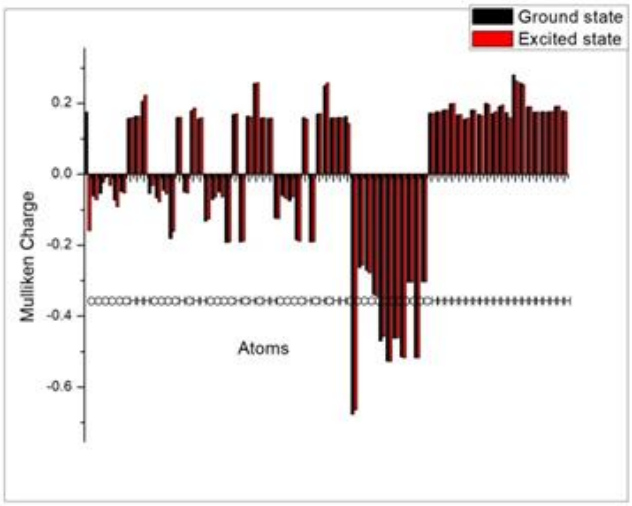

Fig 2. Mulliken atomic charge distribution of Exalite-389 in ground and excited state using DFT and TDDFT

Table 1. bond length (Å), bond angle (º) and dihedral angle (º) of Exalite-389 using DFT/B3LYP/6-311G.

Atoms	Bond length(Å)	Atoms	Bond angle(º)	Atoms	Dihedral angle(º)
2C-1C	1.39557	3C-2C-1C	119.3266	4C-3C-2C-1C	0.373519
3C-2C	1.396234	4C-3C-2C	120.2241	5C-4C-3C-2C	-0.85149
4C-3C	1.414243	5C-4C-3C	119.9775	6C-1C-2C-3C	0.147891
5C-4C	1.38976	6C-1C-2C	121.3873	7H-1C-2C-3C	178.036
6C-1C	1.408905	7H-1C-2C	119.3659	8H-2C-1C-6C	-178.738
7H-1C	1.081812	8H-2C-1C	119.8391	9H-5C-4C-3C	-179.658
8H-2C	1.082699	9H-5C-4C	120.6217	10C-3C-2C-1C	-177.881
9H-5C	1.080848	10C-3C-2C	130.9547	11C-10C-3C-2C	-0.52941
10C-3C	1.466092	11C-10C-3C	131.386	12C-10C-3C-2C	178.5432
11C-10C	1.397035	12C-10C-3C	138.1223	13C-11C-10C-3C	179.3114
12C-10C	2.429833	13C-11C-10C	119.2634	14H-11C-10C-3C	-1.25379
13C-11C	1.395512	14H-11C-10C	120.9009	15C-13C-11C-10C	-0.02031
14H-11C	1.082675	15C-13C-11C	121.5151	16H-12C-10C-3C	-2.19801
15C-13C	1.409802	16H-12C-10C	150.486	17H-13C-11C-10C	178.3261
16H-12C	1.082586	17H-13C-11C	119.3569	18C-15C-13C-11C	-179.878
17H-13C	1.081874	18C-15C-13C	120.8125	19C-18C-15C-13C	39.19033
18C-15C	1.485259	19C-18C-15C	121.3631	20C-18C-15C-13C	-140.805
19C-18C	1.40369	20C-18C-15C	121.1358	21C-19C-18C-15C	-179.942
20C-18C	1.411146	21C-19C-18C	121.7142	22H-19C-18C-15C	1.649933
21C-19C	1.398074	22H-19C-18C	119.4552	23C-20C-18C-15C	179.9804
22H-19C	1.081827	23C-20C-18C	121.395	24H-20C-18C-15C	1.606453
23C-20C	1.388957	24H-20C-18C	119.4498	25C-21C-19C-18C	-0.04172
24H-20C	1.081708	25C-21C-19C	119.5142	26H-21C-19C-18C	-179.393
25C-21C	1.397623	26H-21C-19C	119.3479	27H-23C-20C-18C	-179.315

26H-21C	1.079782	27H-23C-20C	121.5542	28C-6C-1C-2C	179.5176
27H-23C	1.080411	28C-6C-1C	120.805	29C-28C-6C-1C	-141.095
28C-6C	1.485606	29C-28C-6C	121.202	30C-28C-6C-1C	38.97916
29C-28C	1.41113	30C-28C-6C	121.31	31C-29C-28C-6C	-179.895
30C-28C	1.403714	31C-29C-28C	121.4026	32H-29C-28C-6C	1.69882
31C-29C	1.389017	32H-29C-28C	119.4622	33C-30C-28C-6C	179.9815
32H-29C	1.081665	33C-30C-28C	121.7227	34H-30C-28C-6C	1.617785
33C-30C	1.398113	34H-30C-28C	119.4559	35C-33C-30C-28C	-0.11413
34H-30C	1.081779	35C-33C-30C	119.5143	36H-31C-29C-28C	-179.364
35C-33C	1.397583	36H-31C-29C	121.5512	37H-33C-30C-28C	-179.421
36H-31C	1.080408	37H-33C-30C	119.3548	38C-12C-10C-3C	0.651697
37H-33C	1.079751	38C-12C-10C	30.0358	39C-38C-12C-10C	178.5763
38C-12C	1.388604	39C-38C-12C	128.6328	40C-39C-38C-12C	-64.9612
39C-38C	1.536594	40C-39C-38C	107.1662	41C-39C-38C-12C	56.12715
40C-39C	1.572706	41C-39C-38C	112.7387	42C-40C-39C-38C	-177.904
41C-39C	1.56022	42C-40C-39C	117.8692	43C-41C-39C-38C	47.62724
42C-40C	1.537943	43C-41C-39C	118.0328	44C-42C-40C-39C	-177.653
43C-41C	1.544953	44C-42C-40C	111.7522	45C-43C-41C-39C	74.36054
44C-42C	1.538171	45C-43C-41C	116.2076	46O-35C-33C-30C	-179.87
45C-43C	1.537132	46O-35C-33C	124.5755	47C-46O-35C-33C	-0.25275
46O-35C	1.393717	47C-46O-35C	119.0066	48O-25C-21C-19C	-179.999
47C-46O	1.451441	48O-25C-21C	124.5771	49C-48O-25C-21C	-0.50064
48O-25C	1.393655	49C-48O-25C	119.0303	50H-44C-42C-40C	60.27942
49C-48O	1.451417	50H-44C-42C	111.2542	51H-44C-42C-40C	-179.619
50H-44C	1.093099	51H-44C-42C	111.1764	52H-44C-42C-40C	-59.6526
51H-44C	1.091913	52H-44C-42C	111.1033	53H-45C-43C-41C	-65.7525
52H-44C	1.092821	53H-45C-43C	112.2296	54H-45C-43C-41C	54.87692
53H-45C	1.08875	54H-45C-43C	111.1545	55H-45C-43C-41C	174.1082
54H-45C	1.093477	55H-45C-43C	110.3037	56H-40C-39C-38C	-54.3983
55H-45C	1.092654	56H-40C-39C	107.6097	57H-40C-39C-38C	59.50025
56H-40C	1.094148	57H-40C-39C	107.0303	58H-42C-40C-39C	61.36318
57H-40C	1.095722	58H-42C-40C	109.849	59H-42C-40C-39C	-56.1944
58H-42C	1.091809	59H-42C-40C	110.3423	60H-43C-41C-39C	-50.2882
59H-42C	1.0935	60H-43C-41C	109.4168	61H-43C-41C-39C	-164.6
60H-43C	1.092845	61H-43C-41C	106.9619	62H-40C-39C-38C	172.1872
61H-43C	1.095512	62H-40C-39C	108.6882	63H-41C-39C-38C	-73.9564
62H-40C	1.094242	63H-41C-39C	106.7434	64H-49C-48O-25C	-179.574
63H-41C	1.095632	64H-49C-48O	105.1216	65H-49C-48O-25C	-60.9513
64H-49C	1.084889	65H-49C-48O	111.3047	66H-49C-48O-25C	61.82861
65H-49C	1.09249	66H-49C-48O	111.315	67H-47C-46O-35C	61.6487
66H-49C	1.092472	67H-47C-46O	111.3008	68H-47C-46O-35C	-179.738
67H-47C	1.092494	68H-47C-46O	105.1235	69H-47C-46O-35C	-61.1164
68H-47C	1.084887	69H-47C-46O	111.3035	-	-
69H-47C	1.092483	-	-	-	-

Table 2. Mulliken atomic charges by DFT/B3LYP/6-311G and TDDFT/ B3LYP/6-311G.

No.	Atoms	Mulliken Charge		No.	Atoms	Mulliken Charge		No.	Atoms	Mulliken Charge	
		Ground state	Excited state							Ground state	Excited state
1	C	-0.17551	-0.15826	24	H	0.164179	0.161116	47	C	-0.30479	-0.30432
2	C	-0.06195	-0.07167	25	C	0.255823	0.25768	48	O	-0.51734	-0.51792
3	C	-0.05474	-0.02311	26	H	0.158321	0.158277	49	C	-0.30325	-0.30362
4	C	-0.00698	-0.03192	27	H	0.157	0.157275	50	H	0.172826	0.17191
5	C	-0.07371	-0.09166	28	C	-0.1237	-0.12486	51	H	0.175861	0.174994
6	C	-0.0486	-0.05264	29	C	-0.06046	-0.0683	52	H	0.181696	0.180938
7	H	0.157102	0.159049	30	C	-0.0759	-0.06492	53	H	0.198772	0.198259
8	H	0.163327	0.162839	31	C	-0.18555	-0.18863	54	H	0.166923	0.16737
9	H	0.205771	0.222053	32	H	0.160575	0.154511	55	H	0.15458	0.157657
10	C	-0.05463	-0.03199	33	C	-0.19113	-0.19007	56	H	0.180942	0.179571
11	C	-0.06655	-0.07809	34	H	0.169453	0.170124	57	H	0.169134	0.165376
12	C	-0.04605	-0.05588	35	C	0.250154	0.257704	58	H	0.199711	0.195698
13	C	-0.18112	-0.16184	36	H	0.158268	0.158651	59	H	0.171391	0.176467
14	H	0.159916	0.160483	37	H	0.160295	0.159446	60	H	0.191878	0.194899
15	C	-0.05052	-0.05336	38	C	0.163152	0.142653	61	H	0.174216	0.158911
16	H	0.179045	0.186091	39	C	-0.67749	-0.66473	62	H	0.279185	0.262566
17	H	0.15576	0.158122	40	C	-0.26417	-0.25627	63	H	0.256987	0.251718
18	C	-0.13222	-0.12647	41	C	-0.27083	-0.27899	64	H	0.18984	0.19007
19	C	-0.07166	-0.06455	42	C	-0.33951	-0.34328	65	H	0.175593	0.174929
20	C	-0.05034	-0.06479	43	C	-0.46988	-0.4575	66	H	0.175729	0.175519
21	C	-0.19228	-0.19119	44	C	-0.52731	-0.52728	67	H	0.176763	0.176403
22	H	0.168675	0.169414	45	C	-0.46283	-0.46146	68	H	0.190684	0.190872
23	C	-0.19162	-0.18834	46	O	-0.51508	-0.51772	69	H	0.178161	0.176036

Table 3. Quantum chemical parameters of Exalite-389 by DFT/ B3LYP/6-311G basis set.

Solvents	HOMO (Harties)	LUMO (Harties)	HOMO (eV)	LUMO (eV)	Energy band gap (E_g)	Ionization potential (I)	Electron affinity (A)	Electronegativity (χ)	Chemical hardness (η)	Chemical potential (μ)
Vacuum	-0.1987	-0.04674	-5.4068257	1.27184214	4.13498356	5.4068257	1.27184214	3.33933392	2.06749178	-3.33933392
Chloroform	-0.15537	-0.0632	-4.22777307	-1.7197352	2.50803787	4.22777307	1.7197352	2.973754135	1.254018935	-2.973754135
DMSO	-0.16893	0.0073	-4.59675423	0.1986403	4.79539453	4.59675423	-0.1986403	2.199056965	2.397697265	-2.199056965
THF	-0.16614	0.00948	-4.52083554	0.25796028	4.77879582	4.52083554	-0.25796028	2.13143763	2.38939791	-2.13143763
ALKANES										
Acetone	-0.16825	0.00911	-4.57825075	0.24789221	4.82614296	4.57825075	-0.24789221	2.16517927	2.41307148	-2.16517927
Aniline	-0.16589	0.00952	-4.51403279	0.25904872	4.77308151	4.51403279	-0.25904872	2.127492035	2.386540755	-2.127492035
Pentane-01	-0.15065	-0.06237	-4.09933715	-1.69715007	2.40218708	4.09933715	1.69715007	2.89824361	1.20109354	-2.89824361
Benzene	-0.15959	0.01068	-4.34260349	0.29061348	4.63321697	4.34260349	-0.29061348	2.025995005	2.316608485	-2.025995005
Cyclohexane	-0.15851	0.01089	-4.31321561	0.29632779	4.6095434	4.31321561	-0.29632779	2.00844391	2.3047717	-2.00844391
Dichloroethane	-0.16699	0.00933	-4.54396489	0.25387863	4.79784352	4.54396489	-0.25387863	2.14504313	2.39892176	-2.14504313
Dichloromethane	-0.16667	0.00938	-4.53525737	0.25523918	4.79049655	4.53525737	-0.25523918	2.140009095	2.395248275	-2.140009095
Toluene	-0.15995	0.01061	-4.35239945	0.28870871	4.64110816	4.35239945	-0.28870871	2.03184537	2.32055408	-2.03184537
Heptane	-0.15034	-0.06233	-4.09090174	-1.69606163	2.39484011	4.09090174	1.69606163	2.893481685	1.197420055	-2.893481685
ALCOHOL										
methanol	-0.16869	0.00904	-4.59022359	0.24598744	4.83621103	4.59022359	-0.24598744	2.172118075	2.418105515	-2.172118075
Ethanol	-0.16847	0.00908	-4.58423717	0.24707588	4.83131305	4.58423717	-0.24707588	2.168580645	2.415656525	-2.168580645
Butanal	-0.16801	0.00915	-4.57172011	0.24898065	4.82070076	4.57172011	-0.24898065	2.16136973	2.41035038	-2.16136973
1-Propanol	-0.16823	0.00911	-4.57770653	0.24789221	4.82559874	4.57770653	-0.24789221	2.16490716	2.41279937	-2.16490716
1-Pentanol	-0.16782	0.00919	-4.56655002	0.25006909	4.81661911	4.56655002	-0.25006909	2.158240465	2.408309555	-2.158240465
1-Hexanol	-0.16745	0.00925	-4.55648195	0.25170175	4.8081837	4.55648195	-0.25170175	2.1523901	2.40409185	-2.1523901
1-Heptanol	-0.16725	0.00928	-4.55103975	0.25251808	4.80355783	4.55103975	-0.25251808	2.149260835	2.401778915	-2.149260835
1-Nonanol	-0.16657	0.0094	-4.53253627	0.2557834	4.78831967	4.53253627	-0.2557834	2.138376435	2.394159835	-2.138376435
1-Decanol	-0.16618	0.00947	-4.52192398	0.25768817	4.77961215	4.52192398	-0.25768817	2.132117905	2.389806075	-2.132117905
NITRILES										
Acetonitrile	-0.15958	-0.06402	-4.34233138	-1.74204822	2.60028316	4.34233138	1.74204822	3.0421898	1.30014158	-3.0421898
Nitromethane	-0.16878	0.00902	-4.59267258	0.24544322	4.8381158	4.59267258	-0.24544322	2.17361468	2.4190579	-2.17361468
Nitroethane	-0.15877	-0.06397	-4.32029047	-1.74068767	2.5796028	4.32029047	1.74068767	3.03048907	1.2898014	-3.03048907
2-Nitropropane	-0.16848	0.00907	-4.58450928	0.24680377	4.83131305	4.58450928	-0.24680377	2.168852755	2.415656525	-2.168852755
Propanonitrile	-0.15879	-0.06398	-4.32083469	-1.74095978	2.57987491	4.32083469	1.74095978	3.030897235	1.289937455	-3.030897235
Butanonitrile	-0.16843	0.00908	-4.58314873	0.24707588	4.83022461	4.58314873	-0.24707588	2.168036425	2.415112305	-2.168036425
Benzonitrile	-0.15869	-0.06395	-4.31811359	-1.74014345	2.57797014	4.31811359	1.74014345	3.02912852	1.28898507	-3.02912852
O-Nitrotoluene	-0.16848	0.00907	-4.58450928	0.24680377	4.83131305	4.58450928	-0.24680377	2.168852755	2.415656525	-2.168852755
Nitobenzene	-0.1687	0.00903	-4.5904957	0.24571533	4.83621103	4.5904957	-0.24571533	2.172390185	2.418105515	-2.172390185

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