The Eurasia Proceedings of Science, Technology, Engineering & Mathematics (EPSTEM)
ISSN: 2602-3199

The Eurasia Proceedings of Science, Technology, Engineering & Mathematics (EPSTEM), 2021

Volume 15, Pages 63-68

ICBAST 2021: International Conference on Basic Science and Technology

Density Functional Theory Studies of Structural Nonlinear Optic and Electronic Properties of Chalcone (E)-3-(Furan-2-Yl)-1-Phenylprop-2-en-1-one Molecule

Guventurk UGURLU
Kafkas University

Abstract: In this study, the geometry optimization of Chalcone (E)-3-(Furan-2-yl)-1-Phenylprop-2-en-1-one molecule was performed at Density Functional Theory (DFT) with Becke-3-Lee-Yang-Parr (B3LYP) the hybrid functional using the 6-311++G(d,p) basis set in the gas phase. The highest occupied molecular orbital (HOMO) energy, the lowest unoccupied molecular orbital (LUMO) energy, the polarizability (α), and hyperpolarizability (β) values of title molecule were calculated DFT/B3LYP/6-311++G(d,p) method in the ground sate. The ^{1}H and ^{13}C NMR spectroscopy values of the molecule were calculated at DFT/B3LYP method using dıfferent basis sets such as 6-31G, 6-31+G, 6-31G(d) and 6-311+(2d,p) and the calculated ^{1}H and ^{13}C NMR values were compared with the experimental values in the literature. The equilibrium state (ground state) dipole moment values of the molecule were calculated as 3.33 Debye by B3LYP/6-311++ G(d,p) method. The electronic energy, dipole moment, polarizability and hyperpolarizability of the title molecule are analyzed and reported. The calculated geometric parameters (bond lengths and bond-dihedral angles) of the molecule were compared with the experimental values in the literature and they were found to be in good agreement The approximate geometry of the molecules in three dimensions was drawn in the GaussView 5.0 molecular imaging program, and all theoretical calculations were used with the Gaussian 09W package program.

Keywords: Chalcone (E)-3-(Furan-2-yl)-1-Phenylprop-2-en-1-one, Dipole moment, HOMO, LUMO, Polarizability

Introduction

Chalcones are found in various types of plants such as vegetables, fruits, tea and soy, and consist of two aromatic rings are linked by a three carbon α, β-unsaturated carbonyl system. Chalcones possess many biological activities such as antidiabetic (Hsieh et al. 2012; Maly et al. 2006), antiviral (de Campos-Buzzi et al. 2006; Kozlowski et al. 2007), antitumor (Kumar et al. 2003), antibacterial (Nielsen et al. 2004;Farooq et al. 2020), anti-inflammatory (Herencia et al. 1998) antifungal (Valla et al. 2006),as well as non-biological applications in solar dyes, chemosensors (Hu et al. 2013), photo-conductors (Girgis et al. 2018), and optoelectronic devices (Xiao et al. 2013).The these compounds are an intermediate for the synthesis of divers heterocyclic compounds like isoxazole (Kaur et al. 2013), pyrazolhine(Reddy et al. 2016), thiazine (Badshah et al. 2016), indazole pyrimidine valuable in pharmaceutical industries. Crystal structure of Chalcone (E)-3-(Furan-2-Yl)-1-Phenylprop-2-en-1-one molecule (1) were determined experimentally using X-ray structure analysis and spectroscopic methods (Vázquez-Vuelvas et al., 2015) but molecular properties such as electronic energy, non-linear optic of title molecule have not been determined.

In this work, molecular structure, dipole moment, polarizability, first static hyper polarizability, the electronic structure and HOMO-LUMO energies of above-mentioned molecule have been studied. The calculated geometric parameters (bond lengths and bond-dihedral angles) of the molecule were compared with the

experimental values in the literature and they were found to be in good agreement ^{1}H NMR and ^{13}C NMR chemical shifts calculations have been performed. Also, the energy band gap of Chalcone (E)-3-(Furan-2-Yl)-1-Phenylprop-2-en-1-one molecule is calculated by using the highest occupied molecular orbital (HOMO) energy, the lowest unoccupied molecular orbital (LUMO) energy. The molecular structure using numbering scheme of the compound (1) is given in Figure 1

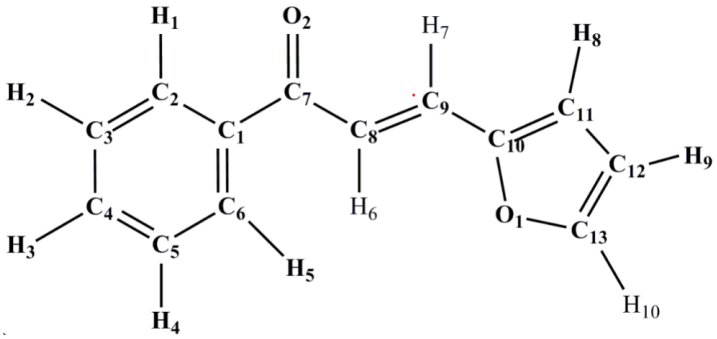

Figure 1. Molecular structure of Chalcone (E)-3-(Furan-2-Yl)-1-Phenylprop-2-en-1-one molecule numbering scheme

Method

The quantum mechanics calculations on the isolated of Chalcone (E)-3-(Furan-2-yl)-1-Phenylprop-2-en-1-one molecule were performed by the aid of Gaussian 09W program package and Gauss view 5.0 molecular visualization programs (Frisch et al., 2010; Dennington et al., 2009) in the gas phase. The geometric parameters of 3-bromo-4-(2-pyridyl) thiophene molecule in the equilibrium state were optimized at DFT with Becke's three parameter hybrid functional (B3) (Becke, 1988) and combined with gradient corrected correlation functional of Lee–Yang–Parr (LYP) (Lee et al., 1988; Becke, 1993) and employing 6-311++G (d,p) basis set (Francl et al., 1982; Rassolov et al., 2001). After optimization, at optimized structures of the title compound obtained B3LYP/6-311++G (d,p) level of theory, dipole moment (μ), polarizability (α), hyperpolarizability (β) based on finite field approach and energy differences of $E_{LUMO} - E_{HOMO}$ were calculated in the same as level of theory. The ^{1}H and ^{13}C NMR chemical shifts were calculated by GIAO approach by using B3LYP level of theory with different basis sets.

Results and Discussion

Firstly, the geometric parameters of the title compound in the ground state were optimized at DFT-B3LYP level of theory using 6-311++G (d, p) as basis set. The optimized geometry of the title molecule performed at B3LYP/6-311G++ (d, p) level with atoms numbering is shown Figure 1. The optimized geometry and Molecular electrostatic potential (MEP) surface values of title molecule obtained B3LYP/6-311++G (d. p) level are presented Figure 2 (a) and (b)

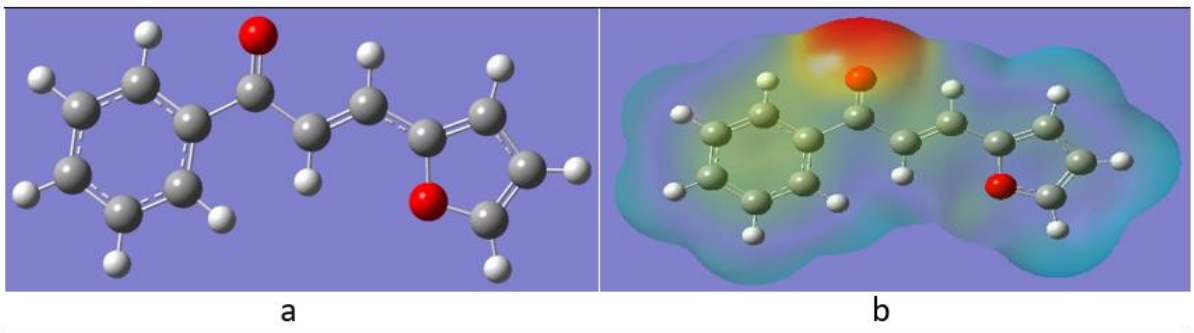

Figure 2. (a)The optimized geometry, (b) Molecular electrostatic (MEP) potential surface (PES) of Chalcone (E)-3-(Furan-2-Yl)-1-Phenylprop-2-en-1-one molecule.

The calculated values of the electronic energy, dipole moment, polarizability, hyperpolarizability, using the highest occupied molecular orbital (HOMO) energy, the lowest unoccupied molecular orbital (LUMO) energy and energy gap (ΔEg) at the ground-state equilibrium geometry of studied molecule are listed in Table 1. As seen from Table 1, the equilibrium state (ground state) dipole moment values of the molecule were calculated as 3.33 Debye by B3LYP/6-311++ G(d,p) method. The energy band gap was obtained as 3,83 eV by using HOMO and LUMO energy.

Table 1. The electronic, HOMO, LUMO energy, dipole moment, polarizability, hyperpolarizability, and energy gap (ΔEg) of Chalcone (E)-3-(Furan-2-Yl)-1-Phenylprop-2-en-1-one molecule

DFT/B3LYP/6-311++G (d,p)						
Electronic Energy (a.u)	μ (D)	α (a.u)	β(a.u)	E_{HOMO} (a.u)	E_{LUMO} (a.u)	ΔE_g(eV)
-651.993113415	3.33	183,58	2289,05	-0.232847	-0.092067	3,830

The X-ray crystal structures for studied molecule is available in the literature and (Vázquez-Vuelvas et al., 2015) and the calculated parameter studied molecule of both at the B3LYP/6-311++G (d, p) method in the ground state are tabulated in the Table 2. and findings here. The polarizability, hyperpolarizability of title molecule are calculated as 183,58 a.u and 2289,05 a.u, respectively and studied molecule was found to have a high hyperpolarizability value.

Table 2. Selected structural parameters of Chalcone (E)-3-(Furan-2-Yl)-1-Phenylprop-2-en-1-one molecule

	Bond length (Å)			Bond angle (˚)	
Atoms	DFT	Exp[a].	Atoms	DFT	Exp[a].
O1—C13	1.3568	1.3627(17)	C2-C1-C7	118.77	118.43 (11)
O1—C10	1.3739	1.3628(15)	C6-C1-C7	123.55	122.76 (12)
C1—C2	1.4028	1.3855 (19)	O2-C7-C8	121.14	120.74 (12)
C1—C6	1.4017	1.3857 (18)	O2-C7-C1	119.87	119.78 (12)
C1—C7	1.5032	1.4882 (17)	C8-C7-C1	118.98	119.44 (11)
O2—C7	1.2256	1.2218 (15)	C8-C9-C10	126.31	
C7—C8	1.4801	1.4664 (18)	C8-C9-H9	119.96	116,30
C9—C8	1.3485	1.3308 (17)	C10-C9-H9	117.96	116,30
C9—C10	1.4305	1.4236 (18)	C9-C8-C7	120.16	121.16 (12)
C10—C11	1.3740	1.3468 (18)	C9-C8-H8	119.86	119,40
C11—C12	1.4247	1.407 (2)	C7-C8-H8	119.96	119,40
C6—C5	1.3934	1.3840 (19)	C11-C10-C9	131.60	131.84 (12)
C12—C13	1.3625	1.327 (2)	O1-C10-C9	119.35	118.76 (11)
C2—C3	1.3891	1.377 (2)	C10-C11-C12	106.91	107.32 (12)
C5—C4	1.3931	1.364 (2)	C5-C6-C1	120.53	120.15 (14)
C4—C3	1.3963	1.366 (2			
Dihedral angle (˚)					
C2-C1-C7-O2	10.01	19.4 (2)	C9-C10-C11-C12	-179.94	-176.65 (14)
C6-C1-C7-O2	-169.05	-159.66 (14)	C6-C5-C4-C3	-0.43	-0.1 (2)
C2-C1-C7-C8	-169.00	-158.15 (13)	C5-C4-C3-C2	-0.40	-0.7 (3)
C6-C1-C7-C8	11.00	22.74 (19)	C10-C11-C12-	0.01	-0.29 (17)
C10-C9-C8-	-179.21	-176.31 (13)	C1-C2-C3-C4	0.50	0.7 (3
O2-C7-C8-C9	2.77	-5.4 (2)	C8-C9-C10-O1	0.02	-3.2 (2)
C1-C7-C8-C9	-177.84	172.14 (12)	C11-C12-C13-O1	-0.02	-0.03 (18)
C6-C1-C2-C3	-0.49	0.0 (2)	C13-O1-C10-C11	-0.02	-0.50 (16)
C7-C1-C2-C3	-179.59	-179.11 (14)	C13-O1-C10-C9	179.94	177.07 (12)
C2-C1-C6-C5	0.03	-0.7 (2)	C8-C9-C10-C11	179.96	173.72 (14)
C7-C1-C6-C5	179.07	178.37 (13)	O1-C10-C11-C12	0.01	0.49 (16)
C1-C6-C5-C4	0.43	0.8 (2)	C10-O1-C13-C12	0.02	0.33 (17)

([a]ref Vázquez-Vuelvas et al., 2015)

^{1}H and ^{13}C NMR Chemical Shift

The 1H NMR and 13C NMR chemical shifts of Chalcone (E)-3-(Furan-2-Yl)-1-Phenylprop-2-en-1-one molecule are calculated using the gauge-independent atomic orbital method (GIAO method) and the hybrid three-parameter B3LYP density functional in combination with different basis sets such as 6-31G, 6-31+G and 6-31+G(d) basis sets in gas phase and in solvents (DMSO). The calculated ^{1}H and ^{13}C chemical shielding

values calculated B3LYP/6-31G, B3LYP/6-31+G and B3LYP/6-31+G(d) are given in the Table 3. Also, the value ^{13}C NMR chemical shifts are carried regression analyses and the results were indicated linear correlation. The calculated R^2 (6-31+G(d)) have been 0.9906 (gas phase) and 0.9962 (DMSO) for 13C-NMR chemical shifts values. These results show that there is a good agreement between the experimental values and the theoretical values.

Table 3. The calculated 1H-NMR and 13C-NMR isotropic chemical shifts (ppm) for title molecule.

No	Exp[a].	DFT/B3LYP					
		6-31G		6-31+G		6-31G+(d)	
		GAS	DMSO	GAS	DMSO	GAS	DMSO
C7	189.95	181,48	183,24	183,54	185,92	178,64	181,17
C10	151.69	150,29	149,37	154,40	153,60	149,66	148,94
C13	144.98	140,91	143,81	143,39	146,80	139,50	143,16
C1	138.16	135,05	135,03	138,01	138,21	134,50	134,65
C4	132.82	127,43	129,44	129,08	131,64	126,74	129,32
C9	130.72	125,79	127,58	127,93	130,04	126,00	127,97
C2	128.47	125,67	125,19	127,66	127,40	125,92	125,26
C6	128.47	124,42	125,18	126,24	127,26	123,71	125,23
C3	128.47	123,55	124,91	125,17	127,11	123,21	124,90
C5	128.47	123,27	124,80	125,07	126,99	122,57	124,70
C8	119.30	115,41	118,99	117,70	120,57	113,78	118,01
C11	116.33	115,34	115,02	116,26	117,57	113,27	113,09
C12	112.74	111,08	112,67	111,62	113,67	108,01	109,91
R^2		0.9915	0.9958	0.9885	0.9939	0.9906	0.9962
H1	8.04	8,51	8,36	8,67	8,54	8,45	8,33
H7	8.04	7,89	7,92	8,03	8,10	7,69	7,75
H6	7.61	7,85	7,91	7,82	7,92	7,37	7,48
H10	7.58	7,82	8,06	7,98	8,25	7,96	8,22
H5	7.52	7,57	7,84	7,72	8,02	7,46	7,75
H2	7.52	7,51	7,69	7,54	7,74	7,45	7,62
H3	7.49	7,45	7,72	7,63	7,92	7,51	7,78
H4	7.47	7,44	7,69	7,55	7,82	7,43	7,68
H8	6.72	6,65	7,00	6,82	7,20	6,56	6,92
H9	6.51	6,51	6,79	6,66	6,96	6,41	6,66

Conclusion

In this work, the lowest unoccupied molecular orbital (LUMO) and the highest occupied molecular orbital (HOMO), bond lengths, electronic parameters, dipole moments and total energy values of Chalcone (E)-3-(Furan-2-Yl)-1-Phenylprop-2-en-1-one molecule were calculated by DFTB3LYP level with the 6-311++G(d,p) basis set. The 1H NMR and 13C NMR chemical shifts of Chalcone (E)-3-(Furan-2-Yl)-1-Phenylprop-2-en-1-one molecule are calculated using the gauge-independent atomic orbital method (GIAO method) and the hybrid three-parameter B3LYP density functional in combination with different basis sets such as 6-31G, 6-31+G and 6-31+G(d) basis sets in gas phase and in solvents (DMSO). As seen from Table 1, the value ^{13}C NMR chemical shifts are carried regression analyses and the results were indicated linear correlation. The calculated R^2 (6-31+G(d)) have been 0.9906 (gas phase) and 0.9962 (DMSO) for ^{13}C-NMR chemical shifts values.

Scientific Ethics Declaration

The authors declare that the scientific ethical and legal responsibility of this article published in EPSTEM journal belongs to the authors.

References

Badshah, S. L., & Naeem, A. (2016). Bioactive thiazine and benzothiazine derivatives: green synthesis methods and their medicinal importance. *Molecules*, *21*(8), 1054.

Becke, A. D. (1988) Density-functional exchange-energy approximation with correct asymptotic behavior. *Physical Review A*, *38*(6), 3098–3100.

Becke, A. D. (1992). Density- functional thermochemistry. I. The effect of the exchange- only gradient correction. *The Journal of chemical physics*, *96*(3), 2155-2160.

de Campos- Buzzi, F., Pereira de Campos, J., Pozza Tonini, P., Corrêa, R., Augusto Yunes, R., Boeck, P., & Cechinel- Filho, V. (2006). Antinociceptive effects of synthetic chalcones obtained from xanthoxyline. *Archiv der Pharmazie: An International Journal Pharmaceutical and Medicinal Chemistry*, *339*(7), 361-365.

Dennington, R., Keith T., Millam, J. (2009). Semichem Inc, In *GaussView* (Version 5). Shawnee Mission.

Farooq, S., Ngaini, Z., & Mortadza, N. A. (2020). Microwave- assisted Synthesis and Molecular Docking Study of Heteroaromatic Chalcone Derivatives as Potential Antibacterial Agents. *Bulletin of the Korean Chemical Society*, *41*(9), 918-924.

Francl, M. M., Pietro, W. J., Hehre, W. J., Binkley, J. S., Gordon, M. S., DeFrees, D. J., & Pople, J. A. (1982). Self- consistent molecular orbital methods. XXIII. A polarization- type basis set for second- row elements. *The Journal of Chemical Physics*, *77*(7), 3654-3665.

Frisch M J, Trucks G W, Schlegel H B, Scuseria G E, Robb M A, Cheeseman J R, Scalmani G, Barone V, Mennucci B, Petersson G A, Nakatsuji H, Caricato M, Li X, Hratchian H P, Izmaylov A F, Bloino J, Zheng G, Sonnenberg J L, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida,M, Nakajima T, Honda Y, Kitao O, Nakai H, Vreven T, Montgomery J A, Vreven T J, Peralta J E, Ogliaro F, Bearpark M, Heyd J. J, Brothers E, Kudin N, Staroverov V N, Kobayashi R, Normand J, Raghavachari K, Rendell A, Burant J C, Iyengar S S, Tomasi J, Cossi M, Rega N, Millam J M, Klene,M, Knox J E, Cross J B, Bakken V, Adamo C, Jaramillo J, Gomperts R, Stratmann R E, Yazyev O, Austin A J, Cammi R, Pomelli C J, Ochterski W, Martin L R, Morokuma K, Zakrzewski V G, Voth G A, Salvador P, Dannenberg J J, Dapprich S, Daniels A D, Farkas O, Foresman J B, Ortiz J V, Cioslowski J, Fox D J, (2009). *Gaussian Inc*. Wallingford.

Girgis, A. S., Basta, A. H., El-Saied, H., Mohamed, M. A., Bedair, A. H., & Salim, A. S. (2018). Synthesis, quantitative structure–property relationship study of novel fluorescence active 2-pyrazolines and application. *Royal Society Open Science*, *5*(3), 171964.

Herencia, F., Ferrandiz, M. L., Ubeda, A., Domínguez, J., Charris, J. E., Lobo, G. M., & Alcaraz, M. J. (1998). Synthesis and anti-inflammatory activity of chalcone derivatives. *Bioorganic & Medicinal Chemistry Letters*, *8*(10), 1169-1174.

Hsieh, C. T., Hsieh, T. J., El-Shazly, M., Chuang, D. W., Tsai, Y. H., Yen, C. T., ... & Chang, F. R. (2012). Synthesis of chalcone derivatives as potential anti-diabetic agents. *Bioorganic & medicinal chemistry letters*, *22*(12), 3912-3915.

Hu, S., Zhang, S., Hu, Y., Tao, Q., & Wu, A. (2013). A new selective pyrazoline-based fluorescent chemosensor for Cu2+ in aqueous solution. *Dyes and Pigments*, *96*(2), 509-515.

Kaur, N., & Kishore, D. (2013). Application of chalcones in heterocycles synthesis: synthesis of 2-(isoxazolo, pyrazolo and pyrimido) substituted analogues of 1, 4-benzodiazepin-5-carboxamides linked through an oxyphenyl bridge. *Journal of Chemical Sciences*, *125*(3), 555-560.

Kozlowski, D., Trouillas, P., Calliste, C., Marsal, P., Lazzaroni, R., & Duroux, J. L. (2007). Density functional theory study of the conformational, electronic, and antioxidant properties of natural chalcones. *The Journal of Physical Chemistry A*, *111*(6), 1138-1145.

Kumar, S. K., Hager, E., Pettit, C., Gurulingappa, H., Davidson, N. E., & Khan, S. R. (2003). Design, synthesis, and evaluation of novel boronic-chalcone derivatives as antitumor agents. *Journal of Medicinal Chemistry*, *46*(14), 2813-2815.

Lee, C., Yang, W., & Parr, R. G. (1988). Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. *Physical Review B*, *37*(2), 785.

Nielsen, S. F., Boesen, T., Larsen, M., Schønning, K., & Kromann, H. (2004). Antibacterial chalcones—bioisosteric replacement of the 4′-hydroxy group. *Bioorganic & Medicinal Chemistry*, *12*(11), 3047-3054.

Rassolov, V. A., Ratner, M. A., Pople, J. A., Redfern, P. C., & Curtiss, L. A. (2001). 6- 31G* basis set for third- row atoms. *Journal of Computational Chemistry*, *22*(9), 976-984.

Xiao, D., Xi, L., Yang, W., Fu, H., Shuai, Z., Fang, Y., & Yao, J. (2003). Size-tunable emission from 1, 3-diphenyl-5-(2-anthryl)-2-pyrazoline nanoparticles. *Journal of the American Chemical Society*, *125*(22), 6740-6745.

Vázquez-Vuelvas, O. F., Enríquez-Figueroa, R. A., García-Ortega, H., Flores-Alamo, M., & Pineda-Contreras, A. (2015). Crystal structure of the chalcone (E)-3-(furan-2-yl)-1-phenylprop-2-en-1-one. *Acta Crystallographica Section E: Crystallographic Communications*, *71*(2), 161-164.

Author Information

Guventurk UGURLU
Kafkas University
Department of Physics, Kars 36100 Turkey
gugurlu@kafkas.edu.tr

To cite this article:

Ugurlu, G. (2021). Density functional theory studies of structural nonlinear optic and electronic properties of chalcone (E)-3-(Furan-2-Yl)-1-Phenylprop-2-en-1-one molecule. *The Eurasia Proceedings of Science, Technology, Engineering & Mathematics (EPSTEM), 15*, 63-68.