Monoxlorsirka kislotasini ftalidometil efirining atomlari zaryad qiymatlari va ayrim energetik parametrlarini Hyperchem dasturida o‘rganish va ChemOffice dasturi bilan taqqoslash

Abrorbek Adhamjon o‘g‘li Nasirdinov
Sherzod Baxodirovich To‘rayev
Hamza Sayidmurodovich Toshov
O‘zbekiston Milliy universiteti

Annotatsiya: Ushbu izlanishda Hyperchem dasturida Monoxlorsirka kislotasini ftalimidometilefirining empirik hosil bo‘lish issiqligi, yarimempirik hosil bo‘lish issiqlik energiyalari, bog‘ uzunliklari, atomlarning zaryad qiymatini, IQ spektrlari, HOMO-LUMO (2D va 3D holati), UB spektrlari o‘rganish natijalari keltirildi. ChemOffice, Hyperchemda olingan nazariy malumotlar, real (amaliy tadqiqotlar) da olingan natijalar bilan taqqoslandi.

Kalit so‘zlar: monoxlorsirka kislotasini ftalimidometilefiri, Hyperchem dasturi, zaryad taqsimoti, hosil bo‘lish issiqligi, IQ, UB

Studying the atomic charge values and some energy parameters of phthalidomethyl ether of monochloroacetic acid in the Hyperchem program and comparing it with the ChemOffice program

Abrorbek Adhamjon oglu Nasirdinov
Sherzod Bakhodirovich Torayev
Hamza Sayidmurodovich Tashov
National University of Uzbekistan

Abstract: In this study, the empirical heat of formation of monochloroacetic acid phthalimidomethylether, semiempirical heat of formation, bond lengths, atomic charge values, IR spectra, HOMO-LUMO (2D and 3D state), UV spectra were studied in the Hyperchem program. the results were presented. The theoretical data obtained in ChemOffice, Hyperchem, were compared with the results obtained in real (practical studies).

Keywords: monochloroacetic acid phthalimidomethylether, Hyperchem program, charge distribution, heat of formation, IR, UV

Kirish: Bugungi kunda dunyo miqyosida alifatik karbon kislota hosilalari oziq-ovqat sanoatida, qishloq xo‘jaligida, farmatsevtika sohasida turli xil preparatlar olishda qo‘llaniladi. Xususan, alifatik karbon kislotalarining alkilimid hosilalaridan o‘smaga, yallig‘lanishga qarshi, og‘riq qoldiruvchi dori vositalari, antioksidantlar, bo‘yoqlar va qishloq xo‘jaligi uchun muhim birikmalar olingan. Bunday birikmalarni yaratish va ularni olish usullarini takomillashtirish kimyo sanoatida muhim ahamiyat kasb etadi.

Jahonda karbon kislotalarning murakkab efirlarini sintez qilish usullarini takomillashtirish, yangi turdagi katalizatorlar - mis sulfamin kislotalar, L-prolin, seziy karbonat, Lyuis kislotalarini qo‘llash orqali mahsulot unumini oshirish ustida ilmiy izlanishlar olib borilmoqda. Bu jarayonda boradigan qo‘shimcha reaksiyalarning oldini olish maqsadida, karbon kislotalarning tuzlaridan foydalanish va bimolekulyar reaksiyalar uchun erituvchi tanlash muhimligi aniqlangan. Bundan tashqari faolligi past bo‘lgan karbon kislotalarning murakkab efirlarini olishda fazalararo kataliz usulida katalizator sifatida kraun efirlarini qo‘llash va mahsulot unumini oshirish alohida ahamiyat kasb etadi. [1-6]

Olingan natijalar tahlili: Monoxlorsirka kislotasini ftalimidometilefiri moddasining ayrim fizik-kimyoviy doimiyliklarini o‘rganish bilan bir qatorda, tuzulishini o‘rganish maqsadida Hyperchem dasturi yordamida turli kvant kimyoviy hisob-kitob ishlarini olib borildi. Monoxlorsirka kislotasini ftalimidometilefirining hosil bo‘lish energiyasi Hyperchem dasturida o‘rganilganda quyidagicha natija olindi: (1-jadval)

1-jadval

Monoxlorsirka kislotasini ftalimidometilefirining ChemOffice va Hyperchem dasturlarida hisoblangan hosil bo‘lish issiqliklari (kkal/mol)

№	Energiya turlari	Chem Office	Hyperchem			
		MM2	MM+	Amber	BioCharm	OPLS
1	Bog'lanish	1.3043	0.678705	0.311805	2.96893	0.178171
2	Valent burchak	23.3919	36.9357	17.5072	21.4194	18.2251
3	Torsion burchak	-4.4108	-3.90637	4.38761	0.239237	0.283065
4	Van-der -Vaals	6.1025	6.59946	2.5525	18.2048	-1.14098
5	Elektrostatik ta’sirlashuv	14.0415	3.32794	0	0	0
6	Umumiy energiya	42.2515	43.71878	24.759149	42.833237	17.545381

Jadvaldan ko‘rinib turibdiki, energiyalar bir-biridan farq qiladi. Chem Office da olingan natijalar monoxlorsirka kislotasining ftalimidometilefirining real (yarim imperik) hosil bo‘lish issiqligidan Amber va OPLS da katta farq qilishi aniqlandi va Hyperchem dasturining OPLS kuch maydoni monoxlorsirka kislotasining ftalimidometilefirining hosil bo‘lish issiqligini hisoblash uchun qulay ekanligi aniqlandi.

2-jadval

Monoxlorsirka kislotasini ftalimidometilefirining Hyperchem(AM1,RM1,PM3) dasturida hisoblangan hosil bo'lish issiqliklari (kkal/mol)

№	Energiya turlari	Hyperchem		
		AM1	RM1	PM3
1	Bog'lanish	-2776.8964	-2188.1320	-2804.0262
2	Atom energiyasi	-75159.2581	-75159.251	-68221.1487
3	Elektron energiyasi	-411606.1757	-413375.0388	-403010.8230
4	Yadrolararo tasir	333670.0211	336027.6486	331985.6480
5	O'zaro ta'sir issiqligi	-100.0644	488.6999	-127.1942
6	Qiyalik	0.0946684	0.0992575	0.1011
7	Umumiy energiya	-77936.1546	-77347.3902	-71025.1749

Yuqoridagi jadvalga asoslanib Hyperchem dasturining AM1 kuch maydonlari monoxlorsirka kislotasining ftalimidometilefirining hosil bo'lish issiqligini hisoblash uchun qulay ekanligi aniqlandi.

3-jadval

Monoxlorsirka kislotasini ftalimidometilefirining Hyperchem(MM+, Amber, BioCharm, OPLS) dasturida hissoblangan bog' uzunliklari , farqlari.

№	Bog'lar	(Chem office)	Hyperchem (A^0)				Farq (A^0)				Eng yuqori mos kelish holati (% da)
			MM+	Amber	Biocharm	OPLS	MM+	Amber	Biocharm	OPLS	
1	C1										Amber metodida bog'lar orasidagi farq eng kam holati kuzatildi va umumiy nazariy va amaliy qiymatlarning mos kelish holati 98.15594% ni tashkil qildi.
2	C2-C1	1.4019	1.351	1.4096	1.3672	1.3434	0.0509	0.0077	0.0347	0.0585	
3	C3-C2	1.4024	1.3479	1.4076	1.3612	1.4639	0.0545	0.0052	0.0412	0.0615	
4	C4-C3	1.3911	1.3343	1.343	1.3561	1.3395	0.0568	0.0481	0.035	0.0516	
5	C6-C1	1.4024	1.3478	1.4075	1.3612	1.464	0.0546	0.0051	0.0412	0.0616	
6	H19-C2	1.1026	1.1039	1.0501	1.0501	1.0498	0.0013	0.0525	0.0525	0.0528	
7	C5-C4	1.3956	1.3484	1.3673	1.4669	1.3603	0.0472	0.0283	0.0713	0.0353	
8	H18-C1	1.1025	1.1039	1.0502	1.0502	1.0498	0.0014	0.0523	0.0523	0.0527	
9	H20-C3	1.1005	1.1032	1.0504	1.0502	1.0499	0.0027	0.0501	0.0503	0.0506	
10	C7-C5	1.4743	1.3554	1.4598	1.46	1.4165	0.1189	0.0145	0.0143	0.0578	
11	C8-C4	1.4757	1.3555	1.4597	1.4605	1.4161	0.1202	0.016	0.0152	0.0596	
12	H21-C6	1.1004	1.1031	1.0503	1.0503	1.0497	0.0027	0.0501	0.0501	0.0507	
13	N9-C8	1.3910	1.3802	1.4124	1.4281	1.392	0.0108	0.0214	0.0371	0.001	
14	C10-N9	1.4704	1.4249	1.4791	1.4611	1.4787	0.0455	0.0087	0.0093	0.0083	
15	O16-C7	1.2208	1.2114	1.2311	1.2305	1.2296	0.0094	0.0103	0.0097	0.0088	
16	O17-C8	1.2206	1.2113	1.231	1.2325	1.2295	0.0093	0.0104	0.0119	0.0089	
17	O11-C10	1.4100	1.4068	1.4178	1.4042	1.4138	0.0032	0.0078	0.0058	0.0038	
18	C12-O11	1.3649	1.3486	1.3334	1.3685	1.3557	0.0163	0.0315	0.0036	0.0092	
19	H22-C10	1.1144	1.1139	1.0902	1.112	1.091	0.0005	0.0242	0.0024	0.0234	
20	H23-C10	1.1145	1.1141	1.0904	1.1121	1.092	0.0004	0.0241	0.0024	0.0225	
21	C14-C12	1.5367	1.5279	1.538	1.5207	1.5281	0.0088	0.0013	0.016	0.0086	
22	O13-C12	1.2159	1.21	1.2304	1.2318	1.2292	0.0059	0.0145	0.0159	0.0133	
23	Cl 15-C14	1.7856	1.8024	1.7711	1.7654	1.7609	0.0168	0.0145	0.0202	0.0247	
24	H24-C14	1.1109	1.1132	1.0903	1.1119	1.0901	0.0023	0.0206	0.001	0.0208	
25	H25-C14	1.1109	1.1132	1.0904	1.1119	1.0901	0.0023	0.0205	0.001	0.0208	
							98.11922%	**98.15594%**	**98.06501%**	**97.5061%**	

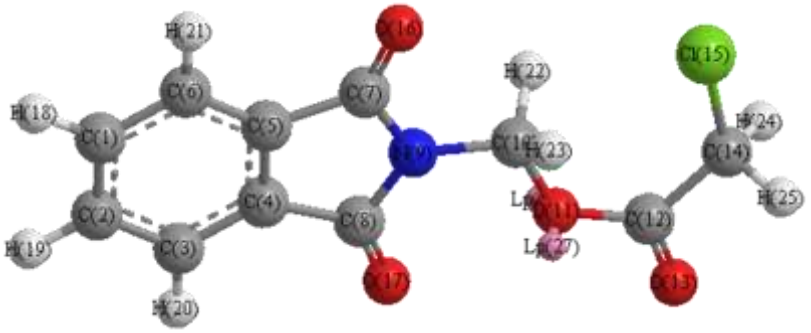
ChemOffice va Hyperchemda (MM+, Amber, BioCharm, OPLS) olingan bog' uzunliklari deyarli farq qilmadi. Amber metodida bog'lar orasidagi farq eng kam holati kuzatildi, umumiy nazariy va amaliy qiymatlarning mos kelish holati 98.15594% ni tashkil qildi.

4-jadval

ChemOffice darturida hisoblangan Monoxlorsirka kislotasini ftalimidometilefirini atom zaryadlari qiymati

№	0	1	2	3	4	5	6	7	8	9
		C -0.029 [C(1)]	C -0.028 [C(2)]	C -0.032 [C(3)]	C 0.013 [C(4)]	C 0.012 [C(5)]	C -0.031 [C(6)]	C 0.408 [C(7)]	C 0.402 [C(8)]	N 404 [N(9)]
1	C 0.202	O	C 0.568	O	C	Cl	O	O	H 0.025	H 0.025

	[C(10)]	-0.095 [O(11)]	[C(12)]	-0.659 [O(13)]	-0.017 [C(14)]	-0.068 [Cl(15)]	-0.643 [O(16)]	-0.649 [O (17)]	[H(18)]	[H(19)]
2	H 0.024 [H(20)]	H 0.024 [H(21)]	H 0.021 [H(22)]	H 0.021 [H(23)]	H 0.051 [H(24)]	H 0.051 [H(25)]				



1-rasm. Monoxlorsirka kislotasini ftalimidometilefirining 3D xolati va raqamlanishi.

Bu zaryad qiymatlaridan ko‘rinib turibdiki, 13-raqamli kislorod eng kichik zaryadga (-0.659) va shu kislorodga birikkan 12-raqamli uglerod atomi esa eng yuqori zaryadga (0.568) ega. Agar moddani reaksiyaga kirishtirilsa shu qisma bilan reaksiyaga kirishadi.

5-jadval

Hyperchem “AM1” dasturida hisoblangan Monoxlorsirka kislotasini ftalimidometilefirining atom zaryadlari qiymati

№	0	1	2	3	4	5	6	7	8	9
		C -0.115 [C(1)]	C -0.115 [C(2)]	C -0.059 [C(3)]	C -0.117 [C(4)]	C -0.117 [C(5)]	C -0.059 [C(6)]	C 0.36 [C(7)]	C 0.366 [C(8)]	N - 0.352 [N(9)]
1	C 0.116 [C(10)]	O -0.286 [O(11)]	C 0.302 [C(12)]	O -0.261 [O(13)]	C 0.176 [C(14)]	Cl -0.043 [Cl(15)]	O -0.280 [O(16)]	O -0.28 [O (17)]	H 0.146 [H(18)]	H 0.146 [H(19)]
2	H 0.161 [H(20)]	H .161 [H(21)]	H 0.117 [H(22)]	H 0.111 [H(23)]	H 0.176 [H(24)]	H 0.136 [H(25)]				

6-jadval

Hyperchem “RM1” dasturida hisoblangan Monoxlorsirka kislotasini ftalimidometilefirining atom zaryadlari qiymati

№	0	1	2	3	4	5	6	7	8	9
		C -0.084 [C(1)]	C -0.084 [C(2)]	C -0.025 [C(3)]	C -0.130 [C(4)]	C -0.130 [C(5)]	C -0.025 [C(6)]	C 0.441 [C(7)]	C 0.441 [C(8)]	N -0.496 [N(9)]
1	C 0.293 [C(10)]	O -0.307 [O(11)]	C 0.329 [C(12)]	O -0.255 [O(13)]	C 0.009 [C(14)]	Cl -0.187 [Cl(15)]	O -0.294 [O(16)]	O -0.295 [O (17)]	H 0.114 [H(18)]	H 0.114 [H(19)]
2	H 0.130 [H(20)]	H .130 [H(21)]	H 0.083 [H(22)]	H 0.079 [H(23)]	H 0.108 [H(24)]	H 0.111 [H(25)]				

7-jadval

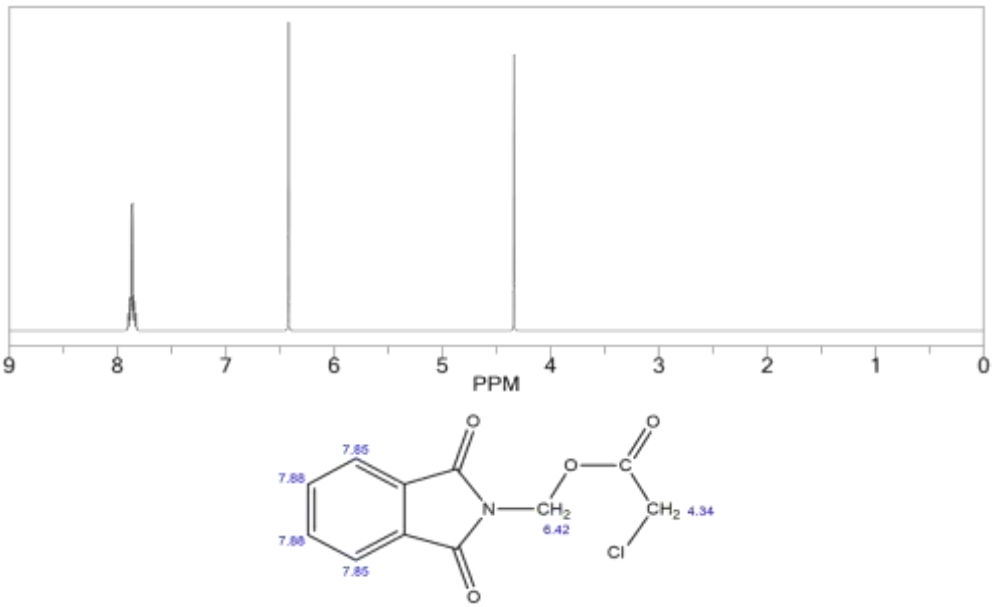
Hyperchem “PM3” darturida hisoblangan Monoxlorsirka kislotasini ftalimidometilefirining atom zaryadlari qiymati.

№	0	1	2	3	4	5	6	7	8	9
		C -0.087	C -0.087	C -0.025	C -0.133	C -0.132	C -0.026	C 0.343	C 0.343 [C(8)]	N -0.125

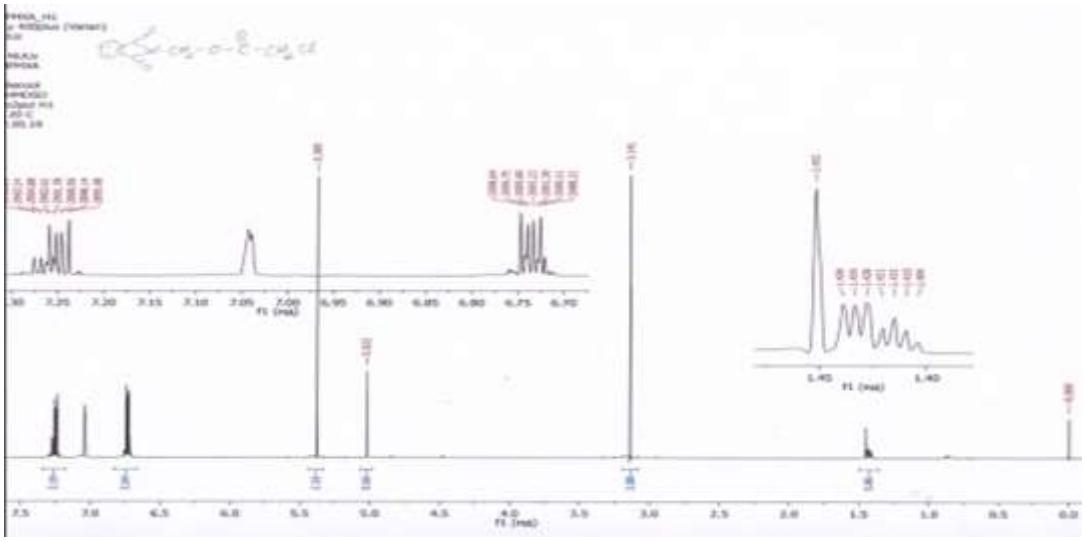
		[C(1)]	[C(2)]	[C(3)]	[C(4)]	[C(5)]	[C(6)]	[C(7)]		[N(9)]
1	C 0.110 [C(10)]	O -0.267 [O(11)]	C 0.350 [C(12)]	O -0.303 [O(13)]	C -0.141 [C(14)]	Cl 0.021 [Cl(15)]	O -0.304 [O(16)]	O -0.307 [O (17)]	H 0.111 [H(18)]	H 0.111 [H(19)]
2	H 0.123 [H(20)]	H .124 [H(21)]	H 0.064 [H(22)]	H 0.062 [H(23)]	H 0.086 [H(24)]	H 0.088 [H(25)]				

Yuqoridagi 5-6 jadvallarda (AM1 va RM1) eng yuqori zaryadga 7 va 8- uglerod atomlariga tegishliligi, eng kichik zaryad esa shu uglerod atomlariga bog‘langan 9-raqamli azot atomiga tegishli ekanligi aniqlandi.

7-jadvalda (PM3) ham eng yuqori zaryad 7 va 8- uglerod atomlari ekanligi, lekin eng kichik zaryad shu uglerod atomlariga bog‘langan kislorod atomlari ekanligi aniqlandi.



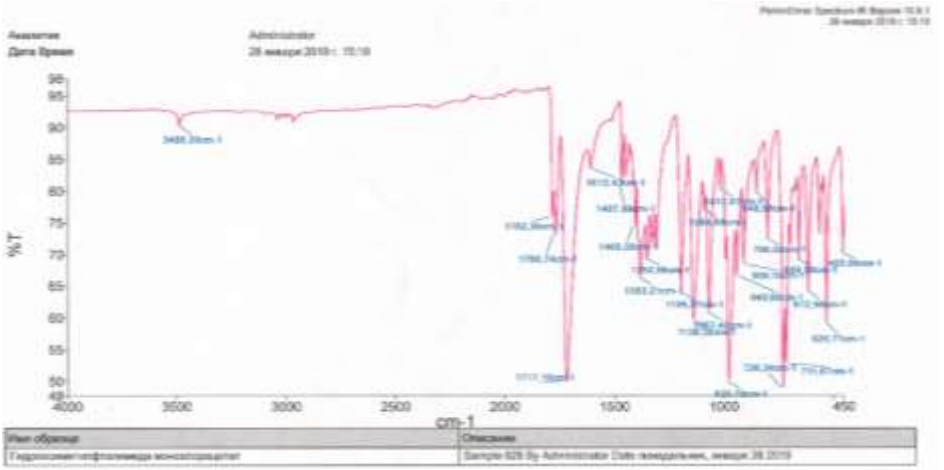
2-rasm. Monoxlorsirka kislotasing ftalimidometilefirining ChemOffice dasturi yordamida nazariy olingan YaMR-1H spektri.



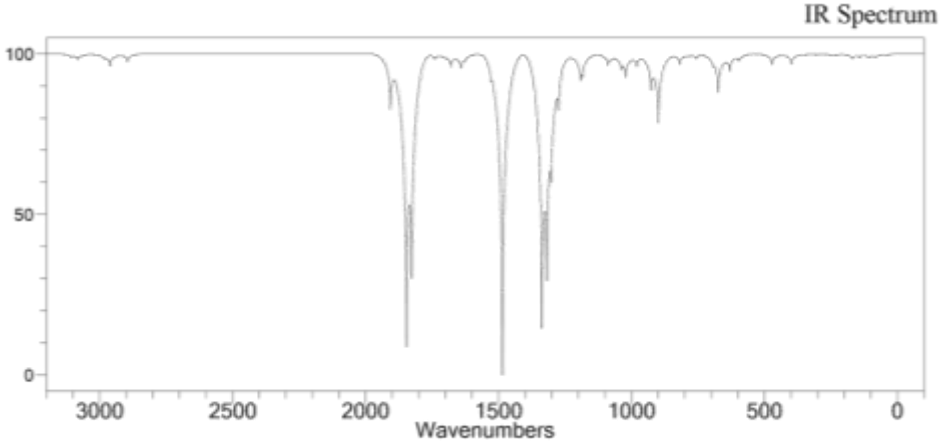
3-rasm Monoxlorsirka kislotasini ftalimidometilefirining amaliy tadqiqotlar natijasida olingan YaMR-1H spektri.

2-rasmdagi (nazariy) spektrlarga ko‘ra 14-uglerod atomiga birikkan ikita vodorod protoni 4.34 m.u da singlet, 10- uglerod atomiga bog‘langan ikkita vodorod protoni 6.42 m.u da singet, benzol halqasidagi 3 va 6 - uglerod atomlariga bog‘langan vodorodlar protoni 7.85 m.u da dublet, 1 va 2-uglerod atomlariga bog‘langan vodorodlar protoni esa 7.88 m.u da triplet signal bergan.

3-rasmda (amaliy) Monoxlor sirkakislotasi ftalimidometilefirining PMR-spektrida metilen guruhlaridagi ikkita vodorod protonining singlet signali δ 3,2 m.u.da (2H, 2CH2), xlorga bog'langan metilen guruhi protonlarining singlet signali δ 5,3 m.u.da (2H, 2CH2), aromatik halqa vodorod protonlarining multiplet signali δ 6,25-7,25 m.u. da (4H, ArH) kuchsiz sohalarda kuzatildi va nazariy olingan spektrga solishtirganda farq qilishi aniqlandi.



4- rasm. Monoxlor sirkakislotasi ftalimidometilefirining amaliy tadqiqotlar natijasida olingan IQ spektri.

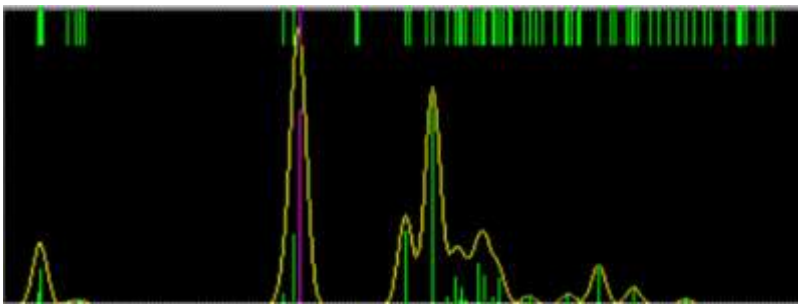


5-rasm. Monoxlor sirkakislotasi ftalimidometilefirining Chem Office dasturi (3-21G) yordamida olingan nazariy IQ spektri.

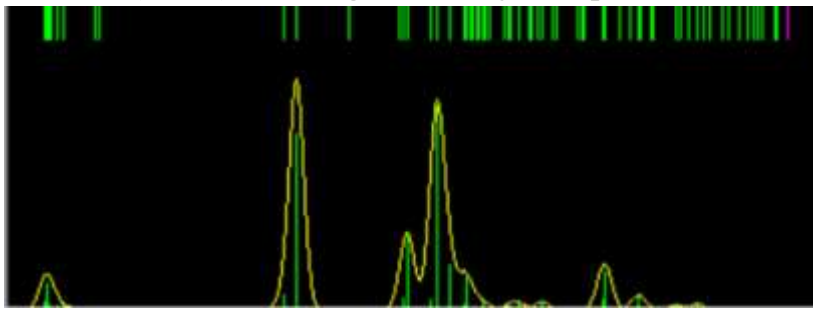
4-rasmda: (amaliy) 1,2-dialmashingan aromatik halqadagi CH bog‘ining deformatsion tebranishlari 721, 798 da; 1496 sm-1 aromatik halqadagi C=C bog‘larning va 3024, 3061 sm-1 C-H bog‘larning valent tebranishlari, 1707, 3454 sm-1 -CO-NH- amid; CH2 guruhining assimmetrik 2962 sm-1 da, simmetrik valent tebranishlari 2939 sm-1 da; azotga bog‘langan CH2 guruhining valent tebranishlari

1396 sm-1 da; 1749, 1707, 1771 sm-1 CH2-COOR murakkab efir bog‘ining valent va 1169 sm-1 -C-O- bog‘ining valent tebranishlari kuzatildi.

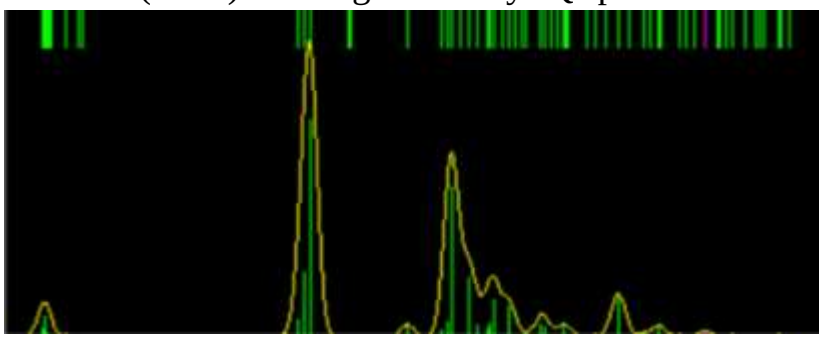
5-rasmda: (Nazariy) Aromatik halqadagi C=C bog‘lar 1490 sm-1 atrofida va 3000- 3100 sm-1 da =C-H bog‘larning valent tebranishlari, -CO-NH- amid 1600-1700 sm-1 orasida, azotga bog‘langan CH2 guruhining valent tebranishlari 1330 sm-1 da; CH2-COOR murakkab efir bog‘ining valent tebranishlari 1600-1700 sm-1 orasida sohalarda tebranishlar kuzatildi. Buni aniqlashda Chem 3D ultra ning STO-2G dan 6-31G gacha bo‘lgan noempirik usullardan foydalanildi va STO-2G, STO-3G, STO-4G, STO-5G, STO-6G dagi natijalar farq qildi. 3-21G dan 6-31G gacha bo‘lgan usullarda natijalar real natijalarga mos keldi va bularni ichida vaqtga nisbadan olganda 3-21G eng qulay usul deb topildi.



6-rasm. Monoxlor sirkakislotasi ftalimidometilefirining Hyperchem dasturi (AM1) da olingan nazariy IQ spektri.



7-rasm. Monoxlor sirkakislotasi ftalimidometilefirining Hyperchem dasturi (RM1) da olingan nazariy IQ spektri.

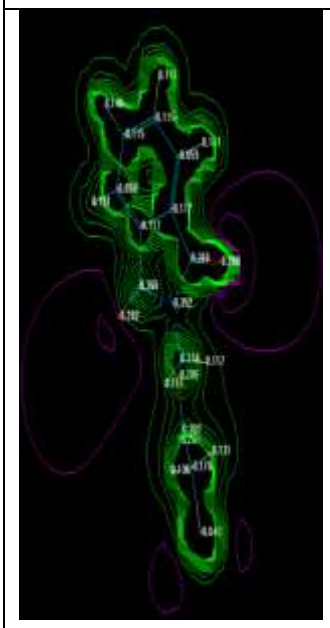
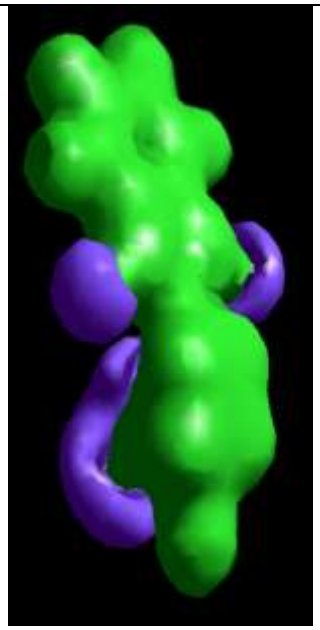
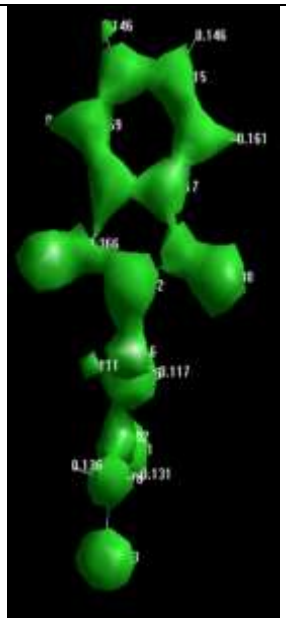


8-rasm. Monoxlor sirkakislotasi ftalimidometilefirining Hyperchem dasturi (PM3) da olingan nazariy IQ spektri.

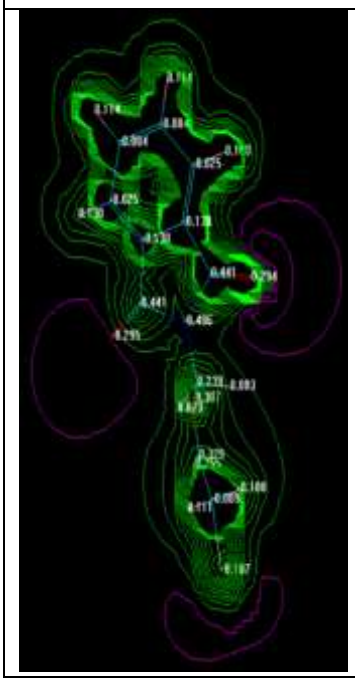
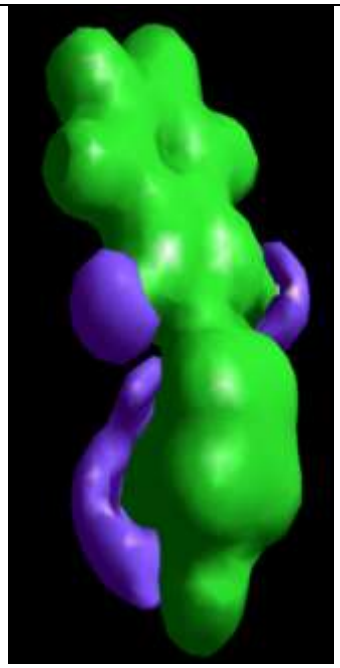
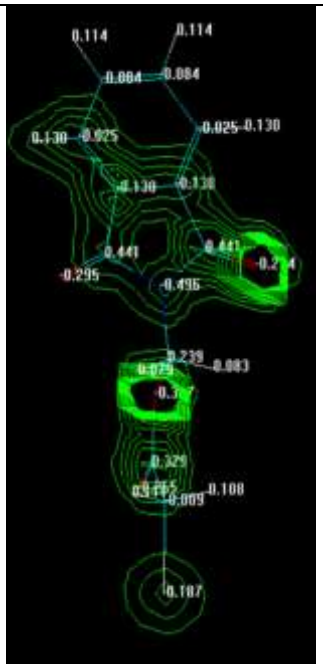
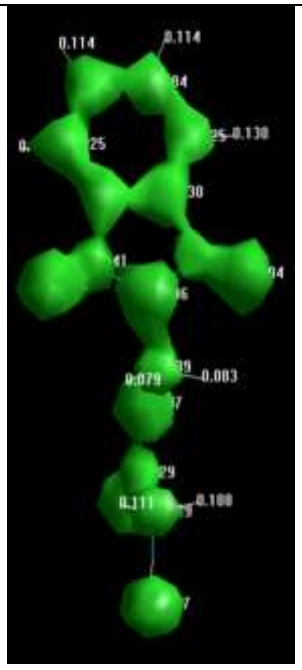
Yuqoridagi 6,7,8-rasmlarda =C-H bog‘larning valent tebranishlari mos ravishda 3170; 3030 ; 3065 sm-1 da, azotga bog‘langan CH2 guruhining valent tebranishlari 1585; 1428; 1400 sm-1 da, -CO-NH- amid 2050; 2059; 2024 sm-1 da signal bergan. -

C-O- bog‘ining valent tebranishlari AM1 va RM1 da 1473; 1549 sm-1 da, C-Cl bog‘i 744;732 sm-1 da tebranish bergan lekin PM3 da bular kuzatilmadi.

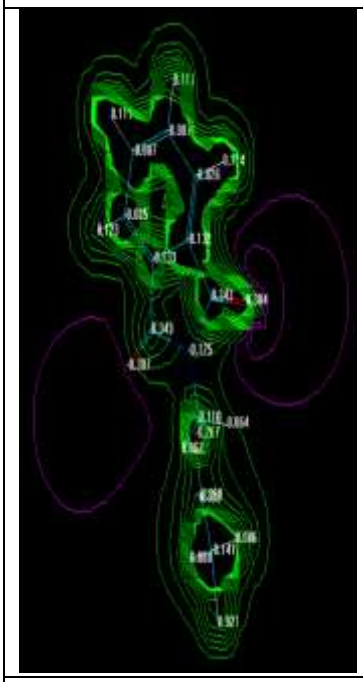
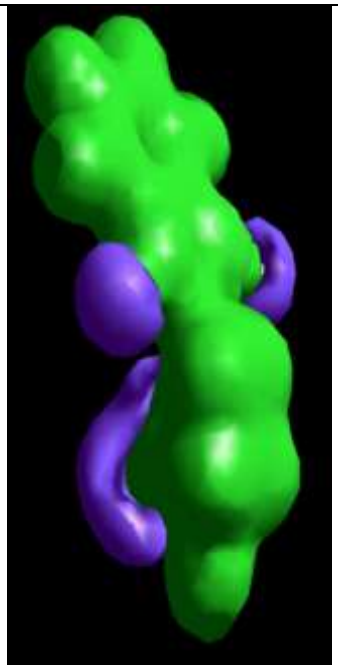
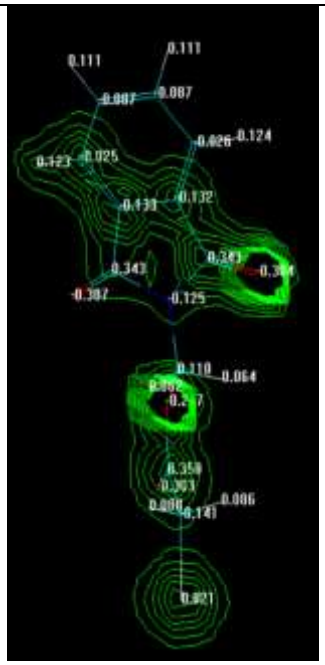
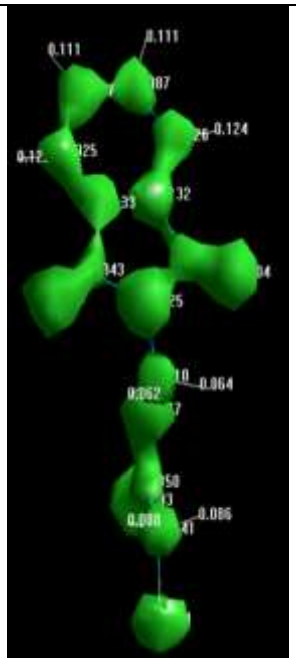
ChemOffice dasturida olingan IQ spektrlari amaliy tadqiqotda olingan spektrdan deyarli farq qilmadi, lekin Hyperchemda olingan IQ spektrlar farq qilishi aniqlandi (=C-H, Azotga bog‘langan CH2, C=C tebranishlari bundan mustasno).

2D	3D	2D	3D
			
Electrostatic Potential		Total charge density	

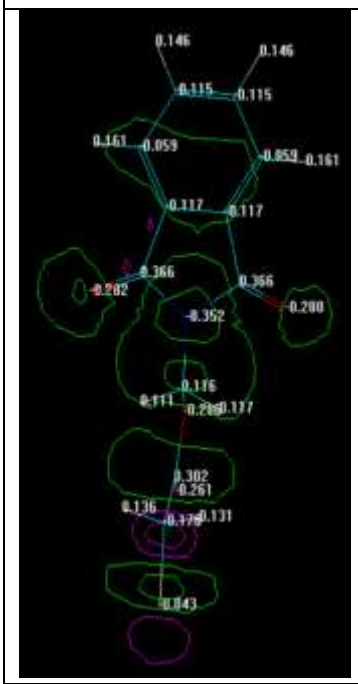
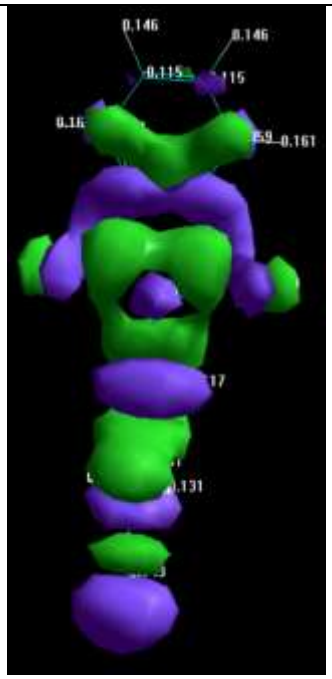
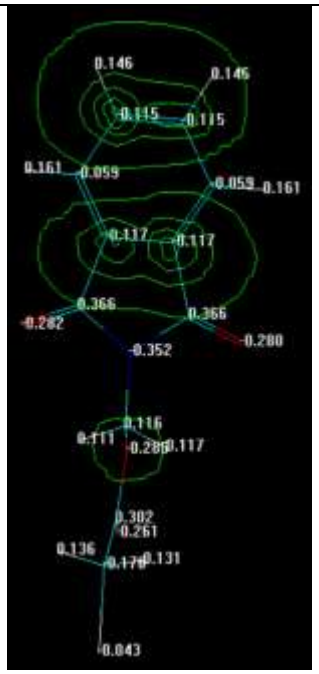
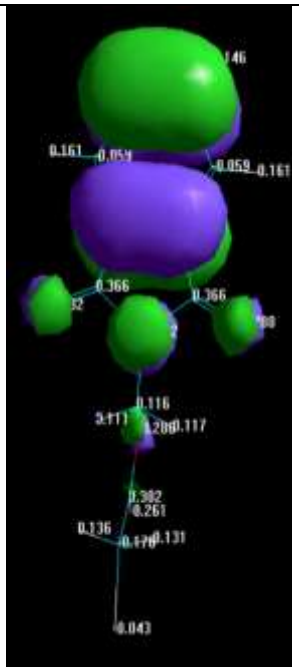
9-rasm. Monoxlor sirkakislotasi ftalimidometilefirining Hyperchem (AM1) da olingan “Electrostatic Potential” va “Total charge density”si

2D	3D	2D	3D
			
Electrostatic Potential		Total charge density	

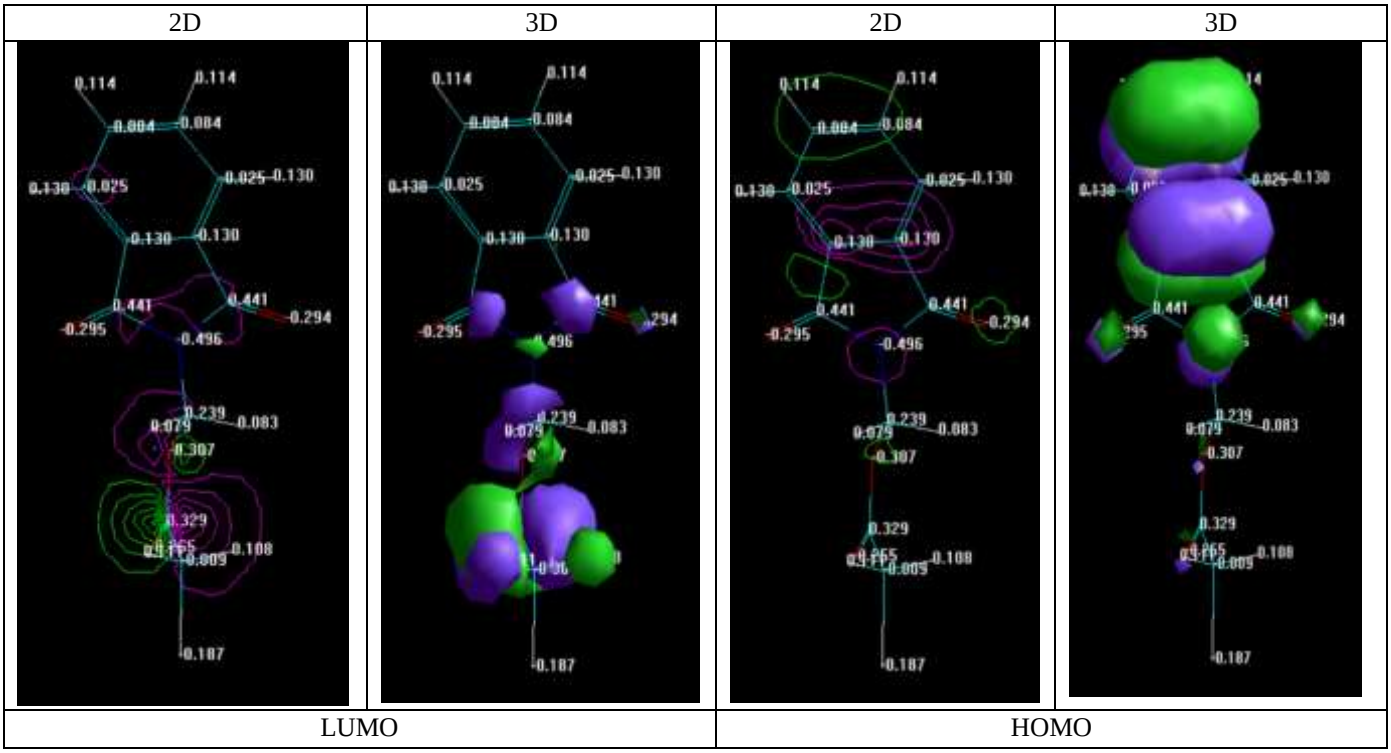
10-rasm. Monoxlor sirkakislotasi ftalimidometilefirining Hyperchem (RM1) da olingan “Electrostatic Potential” va “Total charge density”si

2D	3D	2D	3D
			
Electrostatic Potential		Total charge density	

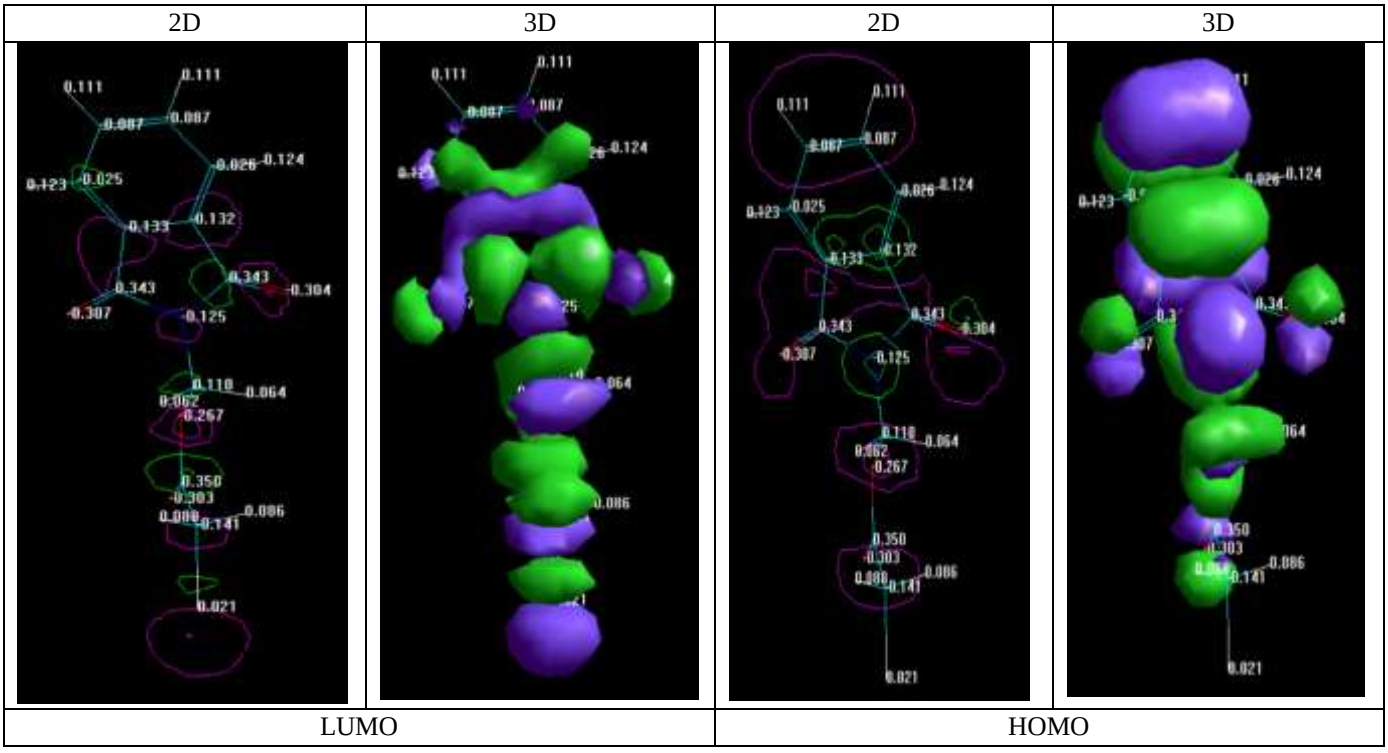
11-rasm. Monoxlor sirkakislotasi ftalimidometilefirining Hyperchem (PM3) da olingan “Electrostatic Potential” va “Total charge density”si

2D	3D	2D	3D
			
LUMO		HOMO	

12-rasm. Monoxlor sirkakislotasi ftalimidometilefirining Hyperchem (AM1) da LUMO va HOMO (2D; 3D) holati



13-rasm. Monoxlor sirkakislotasi ftalimidometilefirining Hyperchem (RM1) da LUMO va HOMO (2D; 3D) holati

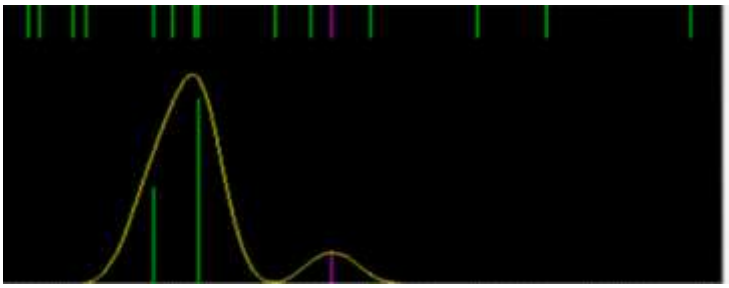


14-rasm. Monoxlor sirkakislotasi ftalimidometilefirining Hyperchem (PM3) da LUMO va HOMO (2D; 3D) holati

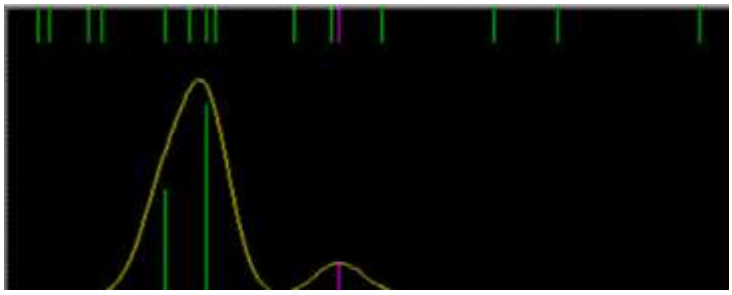
8-jadval

Monoxlor sirkakislotasi ftalimidometilefirining Hyperchem dasturida olingan LUMO va HOMO qiymatlari.

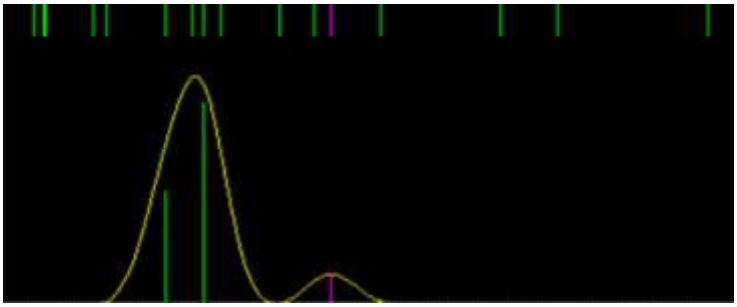
Usul	LUMO	HOMO
AM1	0.5604857	-10.61873
RM1	0.6761852	-10.58845
PM3	0.4635617	-10.462



15-rasm. Monoxlor sirkakislotasi ftalimidometilefirining Hyperchem dasturi (AM1) da olingan UB spektri



16-rasm. Monoxlor sirkakislotasi ftalimidometilefirining Hyperchem dasturi (RM) da olingan UB spektri



17-rasm. Monoxlor sirkakislotasi ftalimidometilefirining Hyperchem dasturi (PM3) da olingan UB spektri

15,16,17- rasmlarda p-p* o‘tishlar mos ravishda 194.74 nm; 192.81 nm; 194.96 nm larda, n-s* o‘tishlar 210.14 nm; 206.26 nm; 210 nm larda, n-p* o‘tishlar 256.86 nm; 251.58 nm; 256.11 nm larda yutilgan.

Tajriba qism: Dastlab Chemdrawda modda chizib oldik va Structure bo‘limidagi “Clean up Structure” ni tanlab chizgan moddamizni strukturasini to‘g‘irlab oldik. Undan so‘ng yana Structure bo‘limiga kirib u yerdan “Predict 1H-NMR Shifts va Predict 13C-NMR Shifts ” bosib moddamizni Spektrlarini oldik uni real tadqiqotlarda olingan YaMR spektri bilan taqqosladik. Moddamizni belgilab, EDIT bo‘limidan

“Get 3D Model” tanlab moddamizni 3D xolatga aylantirdik va ikki marta ustiga bosish orqali Chem3D ultraga o‘tkazdik.

Chem3D ultrada “MM2” bosib moddamizni optimizatsiya qildik. View bo‘limidan “Spectrum viewer” bosib, IQ spektrni ko‘rsatish uchun boshqa oyna ochdik. Unda so‘ng Calculation bo‘limidan “Gamess interface” qismidan “Predict IR/Raman spectrum” bosib STO-2G dan 6-31G gacha bo‘lgan noempirik usullarni ketma-ketlikda tanlab, natijalarni yig‘dik va amalda olingan IQ spektri bilan solishtirib chiqdik va xulosa chiqardik.

Hyperchemda dastlab moddamizni yuklab olib File bo‘limidan “Start log” bosdik va biz bajargan barcha amallarni dastur yozib ola boshladi. Setup bo‘limidan “Molecular mechanics” dan MM+, Amber, Bio-charm, OPLS larni tanlab oldik, optimizatsiya qilib, har biridan zaryadi, hosil bo‘lish issiqlik energiyasi olib jadvalga yozdik song, yana Setup bo‘limidan “Semi-empirical” ni bosib ulardan AM1, RM1, PM3 usullarda IQ spektrini va LUMO-HOMO larini oldik. So‘ngida Compute bo‘limidan “Single point cl” ni bosib UB spektrini oldik.

Xulosa: Chem Office da olingan natijalar monoxlorsirka kislotasining ftalimidometilefirining real (yarim imperik) hosil bo‘lish issiqligidan Amber va OPLS da katta farq qilishi aniqlandi va Hyperchem dasturining OPLS kuch maydoni monoxlorsirka kislotasining ftalimidometilefirining hosil bo‘lish issiqligini hisoblash uchun qulay ekanligi aniqlandi. ChemOffice va Hyperchemda (MM+, Amber, BioCharm, OPLS) olingan bog‘ uzunliklari deyarli farq qilmadi. Amber metodida bog‘lar orasidagi farq eng kam holati kuzatildi, umumiy nazariy va amaliy qiymatlarning mos kelish holati 98.15594% ni tashkil qildi. ChemOffice dasturida olingan IQ spektrlari amaliy tadqiqotda olingan spektrdan deyarli farq qilmadi, lekin Hyperchemda olingan IQ spektrlar farq qilishi aniqlandi (=C-H, Azotga bog‘langan CH2, C=C tebranishlari bundan mustasno).

Foydalanilgan adabiyotlar

1. Turaev Sh.B., Yuldasheva M.R, Synthesis of esters of halogenoacetic acids // Chemistry and chemical engineering. Toshkent, 2020, -№ 3, P. -38-43 (02.00.00, № 3).

2. Turaev Sh.B., Yuldasheva M.R, The synthesis of phthalimidomethylic Ethers of aliphatic carboxylic acids // «Austrian Journal of Technical and Natural Sciences». Austria, 2021, -№ 5-6, P.-13-17 (02.00.00, № 2).

3. Turaev Sh.B., Yuldasheva M.R, N-Gidroksimetil ftalimidning galogensirka kislotalari bilan murakkab efirlari sintezi // “Funksional polimerlar fanining zamonaviy holati va istiqbollari” professor o‘qituvchilar va yosh olimlarning ilmiy-amaliy anjumani materiallari. Toshkent, 2020, 172 b.

4. Turaev Sh.B., Yuldasheva M.R, Galogensirka kislotalarining gidroksimetilftalimid bilan murakkab efirlari sintezi// “Zamonaviy kimyoning dolzarb muammolari” mavzusidagi Respublika ilmiy-amaliy anjumani. Buxoro, 2020, 4-5 dekabr, 326- b.

5. Farhan A. M., Jasim R. A., Ali A. M. Corrosion Protection of Carbon Steel By Voltaren Drug in Acid Media and Theoretical Studies //RESEARCH JOURNAL OF PHARMACEUTICAL BIOLOGICAL AND CHEMICAL SCIENCES. - 2018. - Т. 9. - №. 2. - С. 705-715.

6. Абдураимова З.З., Тошов Ҳ.С., Хаитбаев А.Х. Госсипол ҳосилаларининг металлокомплекслари тадқиқоти. SCIENCE AND EDUCATION SCIENTIFIC JOURNAL. May 2021/ Volume 2 Issue 5. Pp. 24-27