ORTO-KSILOLNING ATOMLARI ZARYAD QIYMATLARI VA AYRIM ENERGETIK PARAMETRLARINI HYPER CHEM DASTURIDA O‘RGANISH VA CHEM OFFICE DASTURI BILAN TAQQOSLASH

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Annotatsiya: Ushbu izlanishda Hyperchem dasturida orto-ksilolning empirik usulda hosil bo‘lish issiqligi, yarimempirik usulda hosil bo‘lish issiqlik energiyalari, bog‘ uzunliklari, atomlarning zaryad qiymatini, IQ spektrlari, HOMO-LUMO (2D va 3D holati) o‘rganish natijalari keltirildi.

Kalit so‘zlar: Orto-ksilol, Hyperchem dasturi, zaryad taqsimoti, hosil bo‘lish issiqligi, IQ, ChemOffice, yarimempirik, empirik.

Abstract: In this study, the results of the study of the empirical heat of formation of ortho-xylene, semi-empirical heat of formation, bond lengths, atomic charge values, IR spectra, HOMO-LUMO (2D and 3D states) in the Hyperchem program were presented.

Keywords: Ortho-xylene, Hyperchem program, charge distribution, heat of formation, IR, ChemOffice, semi-empirical, empirical.

Аннотация: В данной работе представлены результаты исследования эмпирической и полуэмпирической теплоты образования ортоксилола, длины связей, значений атомных зарядов, ИК-спектров, HOMO-LUMO (2D и 3D состояния) в программе Hyperchem.

Ключевые слова: Орто-ксилол, программа Hyperchem, распределение заряда, теплота образования, ИК, ChemOffice, полуэмпирический, эмпирический.

Kirish

Ksilol–bu kimyo sanoati va tibbiyot texnologiyalarida keng qo‘llaniladigan aromatik uglevodorod bo‘lib, asosan erituvchi sifatida ishlatiladi. U tabiiy ravishda neft, toshko‘mir va yog‘och smolasida uchraydigan, rangsiz va yoqimli hidli suyuqlik yoki gaz holatida bo‘ladi. Kimyoviy formulasi $C_6H_4(CH_3)_2$ bo‘lgan ksilol molekulasi ikki metil guruhi ulangan benzol halqasidan iborat bo‘lib, "dimetilbenzol" deb ham ataladi. Ksilolning uchta izomeri mavjud bo‘lib: orto- (1,2-dimetilbenzol), meta- (1,3-dimetilbenzol) va para-ksilol (1,4-dimetilbenzol).

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U BTEX (benzol, toluol, etilbenzol va ksilollar) guruhi tarkibiga kiruvchi uchuvchi organik birikma sifatida tasniflanadi va bu birikmalarning toksikologik xususiyatlari qat'iy tartibga solingan [1-2]. Orto-ksilol bo'yicha olib borilgan nazariy va eksperimental tadqiqotlar singlet va triplet holatlarining tuzilishini, aniqlashga qaratilgan. Ksilol kauchuk, bo'yoq, charm sanoatida, aviatsiya yonilg'isi va sigaret tutunida keng qo'llaniladi. Shuningdek, orto-ksilol asosidagi sintezlar jarayonida qo'shimcha reaksiyalarda selektivlikni oshirish, atrof-muhitga kam zarar yetkazuvchi texnologiyalarni ishlab chiqish ham alohida e'tiborni talab qiladi. Shu nuqtai nazardan, orto-ksilol va uning hosilalarini chuqur o'rganish va yangi sintez yo'llarini ishlab chiqish kimyo sanoatida muhim nazariy va amaliy ahamiyatga egadir [3-4].

Olingan natijalar tahlili: Orto ksilol 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

Orto-ksilolning ChemOffice va Hyperchem dasturlarida hisoblangan hosil bo'lish issiqliklari (kkal/mol)

№	Energiya turlari	Chem Office	Hyperchem			
		MM2	MM+	Amber	BioCharm	OPLS
1	Bog'lanish	1.6054	0.465605	0.260038	5.16256	0.0815627
2	Valent burchak	0.4261	0.784623	0.656478	1.03641	0.430307
3	Torsion burchak	-7.1200	-7.12	4.45377e-012	0.000184064	0.0003947
4	Van-der - Vaals	4.3963	6.53211	3.04977	26.8979	0.833796
5	Elektrostatik ta'sirlashuv	0.0980	0.109541	0	0	0
6	**Umumiy energiya**	**-0.4533**	**0.774672**	**3.966285**	**33.097074**	**1.346060**

Jadvaldan ko'rinib turibdiki, energiyalar bir-biridan farq qiladi. Chem Office da olingan natijalar Orto ksilolning Hyperchem dasturining Amber va BioCharm metodida olingan hosil bo'lish issiqligidan katta farq qilishi aniqlandi.

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2-jadval

Orto ksilolning Hyperchem (AM1, RM1, PM3) dasturida hisoblangan hosil bo‘lish issiqliklari (kkal/mol)

№	Energiya turlari	Hyperchem		
		AM1	RM1	PM3
1	Bog‘lanish	-1880.3447683	-1533.4277076	-1882.1688
2	Atom energiyasi	-24917.133768	-24917.1337680	-23535.3647700
3	Elektron energiyasi	-125452.54	-125767.0551905	-122971.8863137
4	Yadrolararo tasir	98655.0659	99316.4937149	97554.3527437
5	O‘zaro ta’sir issiqligi	7.7952317	354.7122924	5.9712000
6	Qiyalik	0.0993558	0.0688444	0.0973348
7	**Umumiy energiya**	**-26797.4785363**	**-26450.5614756**	**-25417.5335700**

Yuqoridagi jadvalga asoslanib Hyperchem dasturining AM1 metodi orto ksilolning issiqligini hisoblash uchun qulay ekanligi aniqlandi.

3-jadval

ChemOffice, 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-C2	1,395	1,340	1,4016	1,3655	1,4593	0,055 (95,90)	0,0066 (99,53)	0,0295 (97,84)	0,06 (95,59)	MM+ metodida bog’lar orasidagi farq eng kam holati kuzatildi va umumiy nazariy va amaliy qiymatlarning mos kelish holati **98.5839%** ni tashkil qildi.
2	C1-H9	1,103	1,103	1,0508	1,0517	1,0501	0 (100)	0,0522 (95,03)	0,0513 (95,12)	0,05 (94,96)	
3	C1-C6	1,402	1,347	1,4084	1,3732	1,3424	0,055 (95,92)	0,0064 (99,55)	0,0288 (97,90)	0,06 (95,56)	
4	C2-H10	1,102	1,103	1,0502	1,0497	1,0497	0,001 (99,91)	0,0518 (95,07)	0,0523 (95,02)	0,05 (95,02)	
5	C2-C3	1,393	1,339	1,3996	1,3635	1,3386	0,054 (95,97)	0,0066 (99,53)	0,0295 (97,84)	0,05 (95,94)	
6	C3-H11	1,102	1,103	1,0502	1,0497	1,0497	0,001 (99,91)	0,0518 (95,07)	0,0523 (95,02)	0,05 (95,02)	
7	C3-C4	1,395	1,340	1,4016	1,3655	1,4593	0,055 (95,89)	0,0066 (99,53)	0,0295 (97,84)	0,06 (95,59)	
8	C4-H12	1,103	1,103	1,0508	1,0517	1,0501	0 (100)	0,0522 (95,03)	0,0513 (95,12)	0,05 (94,96)	
9	C4-C5	1,402	1,347	1,4084	1,3732	1,3424	0,055 (95,92)	0,0064 (99,55)	0,0288 (97,90)	0,06 (95,56)	
10	C5-C8	1,513	1,515	1,5235	1,5145	1,5077	0,002 (99,87)	0,0105 (99,31)	0,0015 (99,90)	0,10 (99,65)	
11	C8-H16	1,107	1,109	1,0837	1,1056	1,0853	0,002 (99,82)	0,0233 (97,85)	0,0014 (99,87)	0,10 (98,00)	
12	C8-H17	1,114	1,114	1,0905	1,112	1,0901	0 (100)	0,0235 (97,85)	0,002 (99,82)	0,10 (97,81)	
13	C8-H18	1,114	1,114	1,0905	1,112	1,0901	0 (100)	0,0235 (97,85)	0,002 (99,82)	0,10 (97,81)	
14	C5-C6	1,408	1,352	1,4221	1,3856	1,4778	0,056 (95,86)	0,0141 (99,01)	0,0224 (98,38)	0,10 (95,28)	
15	C6-C7	1,513	1,513	1,5235	1,5145	1,5077	0,004 (99,74)	0,0105 (99,31)	0,0015 (99,90)	0,10 (99,65)	
16	C7-H13	1,107	1,109	1,0837	1,1056	1,0853	0,002 (99,82)	0,0233 (97,85)	0,0014 (99,87)	0,10 (98,00)	
17	C7-H14	1,114	1,114	1,0905	1,112	1,0901	0 (100)	0,0235 (97,85)	0,002 (99,82)	0,10 (97,81)	
18	C7-H15	1,114	1,114	1,0905	1,112	1,0901	0 (100)	0,0235 (97,85)	0,002 (99,82)	0,10 (97,81)	
							98.5839%	**96.667%**	**98.156%**	**96.667%**	

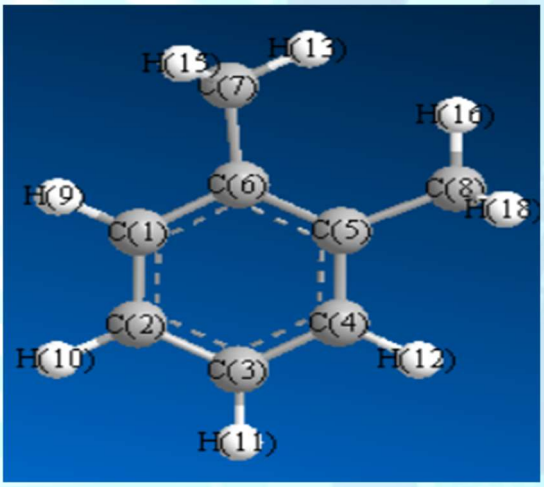
ChemOffice va Hyperchemda (MM+, Amber, BioCharm, OPLS) olingan bog‘ uzunliklari deyarli farq qilmadi. MM+ metodida bog‘lar orasidagi farq eng kam xatolik holati kuzatildi, ikkala dasturda qiymatlarning mos kelish holati **98.5839%** ni tashkil qildi.

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4-jadval

ChemOffice darturida hisoblangan Orto-ksilolning atom zaryadlari qiymati

№	0	1	2	3	4	5	6	7	8	9
		C - 0.056 [C(1)]	C - 0.048 [C(2)]	C - 0.048 [C(3)]	C - 0.056 [C(4)]	C 0.054 [C(5)]	C 0.054 [C(6)]	C - 0.144 [C(7)]	C - 0.144 [C(8)]	H 0.023 [H(9)]
1	H 0.025 [H(10)]	H 0.025 [H(11)]	H 0.023 [H(12)]	H 0.042 [H(13)]	H 0.053 [H(14)]	H 0.053 [H(15)]	H 0.042 [H(16)]	H 0.053 [H(17)]	H 0.053 [H(18)]	



1-rasm. Orto-ksilolning 3D xolati va raqamlanishi

Bu zaryad qiymatlaridan ko‘rinib turibdiki, 7-raqamli uglerod eng kichik zaryadga (-0.144) va shu uglerodga birikkan 15-raqamli uglerod atomi esa eng yuqori zaryadga (0.053) ega.

5-jadval

Hyperchem (AM1) dasturida hisoblangan orto-ksilolning atom zaryadlari qiymati

№	0	1	2	3	4	5	6	7	8	9
		C - 0.132 [C(1)]	C - 0.131 [C(2)]	C – 0.131 [C(3)]	C - 0.132 [C(4)]	C- 0. 065 [C(5)]	C - 0.065 [C(6)]	C - 0.179 [C(7)]	C – 0.179 [C(8)]	H 0.129 [H(9)]
1	H	H 0.130	H 0.129	H	H	H	H	H 0.083	H	

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	0.130 [H(10)]	[H(11)]	[H(12)]	0.082 [H(13)]	0.083 [H(14)]	0.083 [H(15)]	0.082 [H(16)]	[H(17)]	0.083 [H(18)]	

6-jadval

Hyperchem (RM1) dasturida hisoblangan orto-ksilolning atom zaryadlari qiymati

№	0	1	2	3	4	5	6	7	8	9
		C - 0.097 [C(1)]	C - 0.101 [C(2)]	C – 0.101 [C(3)]	C - 0.097 [C(4)]	C- 0. 067 [C(5)]	C - 0.067 [C(6)]	C - 0.105 [C(7)]	C – 0.105 [C(8)]	H 0.100 [H(9)]
1	H 0.099 [H(10)]	H 0.099 [H(11)]	H 0.100 [H(12)]	H 0.058 [H(13)]	H 0.056 [H(14)]	H 0.056 [H(15)]	H 0.058 [H(16)]	H 0.056 [H(17)]	H 0.056 [H(18)]	

7-jadval

Hyperchem (PM3) darturida hisoblangan orto-ksilolning atom zaryadlari qiymati

№	0	1	2	3	4	5	6	7	8	9
		C - 0.104 [C(1)]	C - 0.104 [C(2)]	C – 0.104 [C(3)]	C - 0.104 [C(4)]	C- 0.070 [C(5)]	C - 0.070 [C(6)]	C - 0.074 [C(7)]	C – 0.074 [C(8)]	H 0.104 [H(9)]
1	H 0.102 [H(10)]	H 0.102 [H(11)]	H 0.104 [H(12)]	H 0.051 [H(13)]	H 0.047 [H(14)]	H 0.047 [H(15)]	H 0.051 [H(16)]	H 0.047 [H(17)]	H 0.047 [H(18)]	

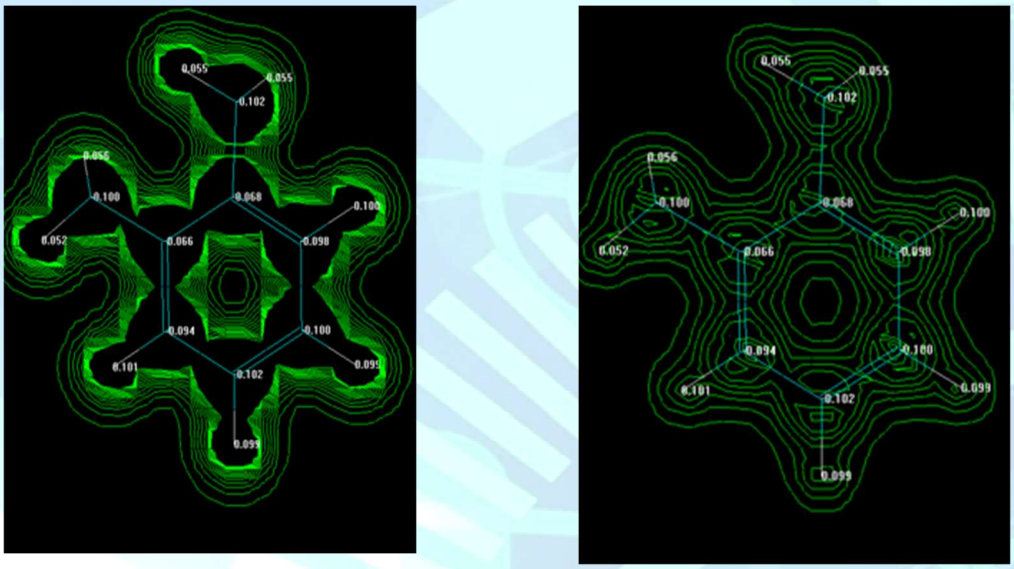
Yuqoridagi **5- jadvalda** (AM1) eng yuqori zaryadga 10 va 11- vodorod atomlariga tegishliligi, eng kichik zaryad esa 7 va 8-uglerod atomlariga tegishli ekanligi aniqlandi.

6-jadvalda (RM1) ham eng yuqori zaryad 7 va 8- uglerod atomlari ekanligi, eng kichik zaryad esa 9 va 12 vodorod atomlari ekanligi aniqlandi.

7-jadvalda (PM3) ham eng yuqori zaryad 1va 2,3,4 - uglerod atomlari ekanligi, eng kichik zaryad esa 9 va 12- vodorod atomlari ekanligi aniqlandi.

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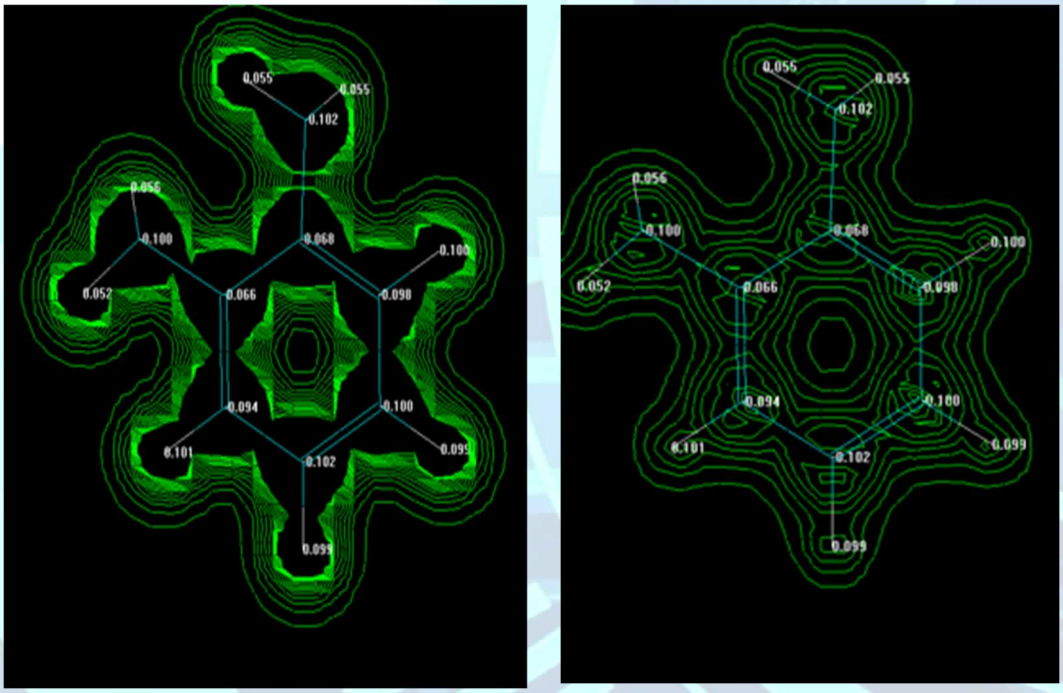
2D 2D



Electrostatic Potential Total charge density

2-rasm. Orto-ksilolning Hyperchem (AM1) da olingan "Electrostatic Potential" va "Total charge density" si

2D 2D

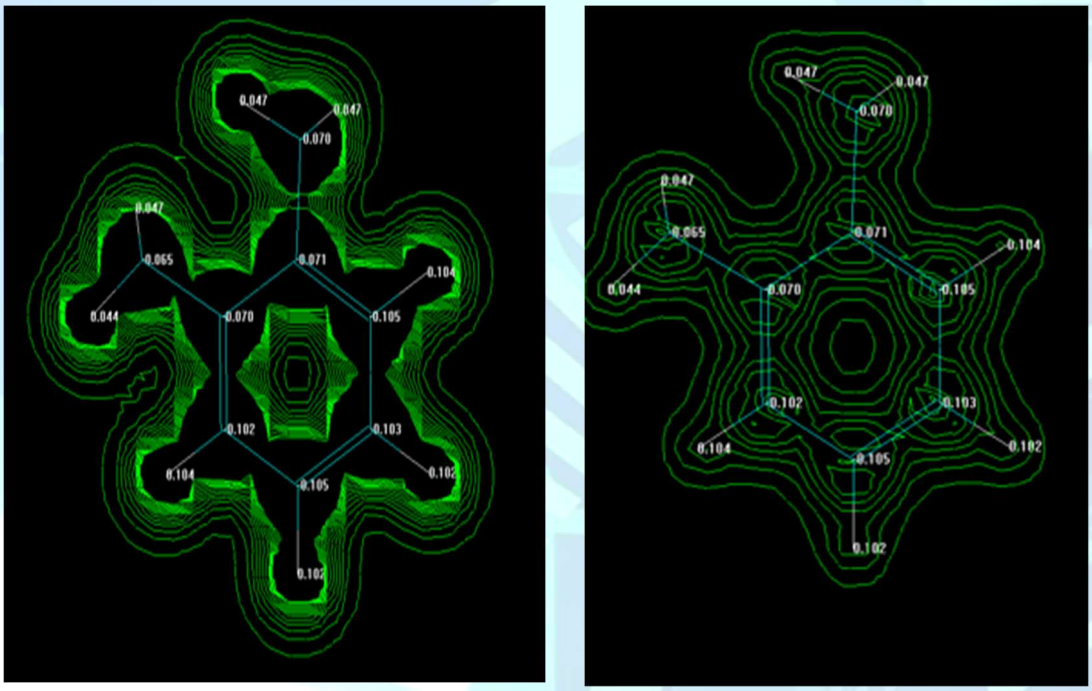


Electrostatic Potential Total charge density

3-rasm. Orto-ksilolning Hyperchem (RM1) da olingan "Electrostatic Potential" va "Total charge density" si.

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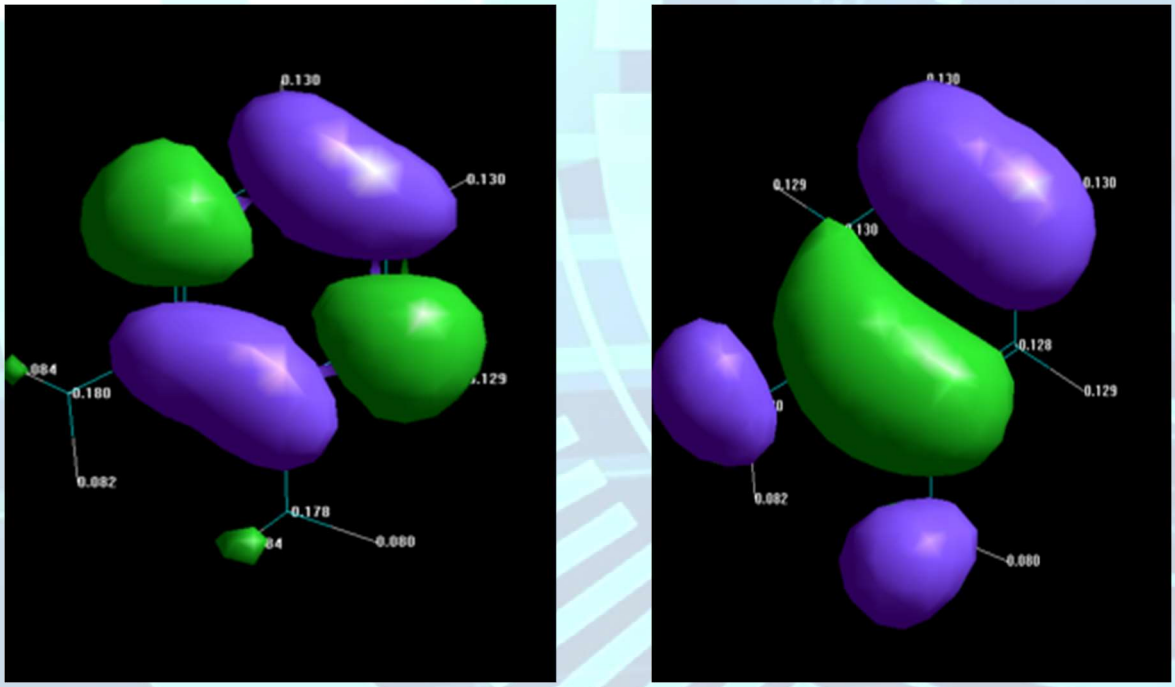
2D 2D



Electrostatic Potential Total charge density

4-rasm. Orto-ksilolning Hyperchem (PM3) da olingan "Electrostatic Potential" va "Total charge density" si.

3D 3D

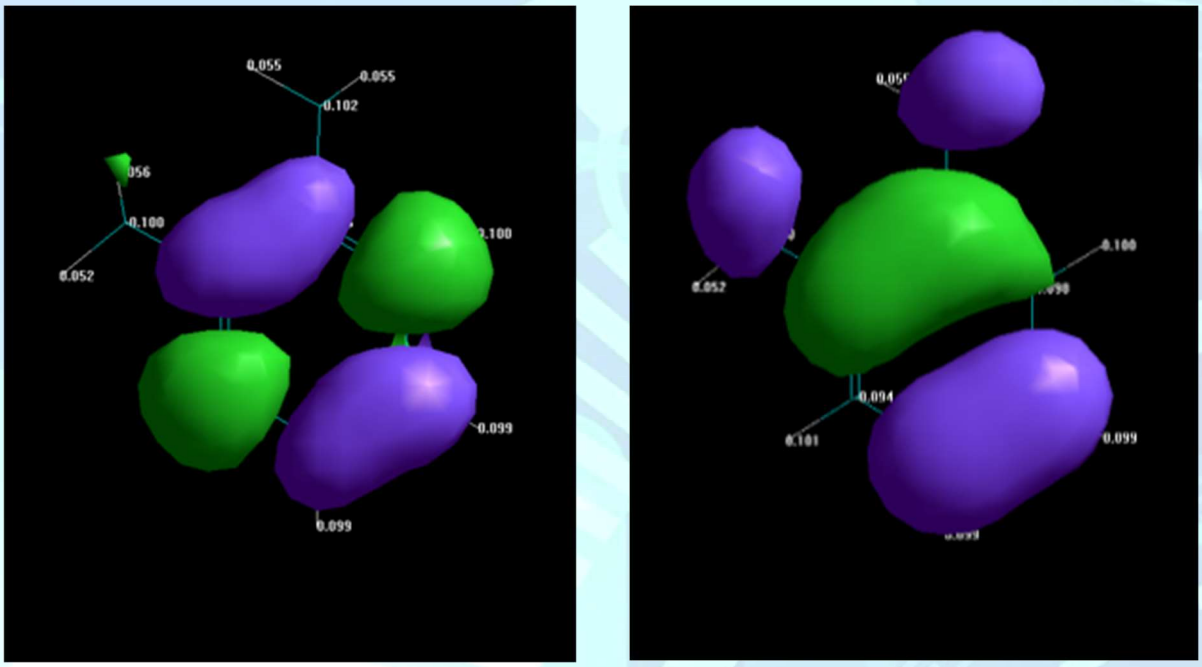


LUMO HOMO

5-rasm. Orto-ksilolning Hyperchem (AM1) da LUMO va HOMO (3D) holati

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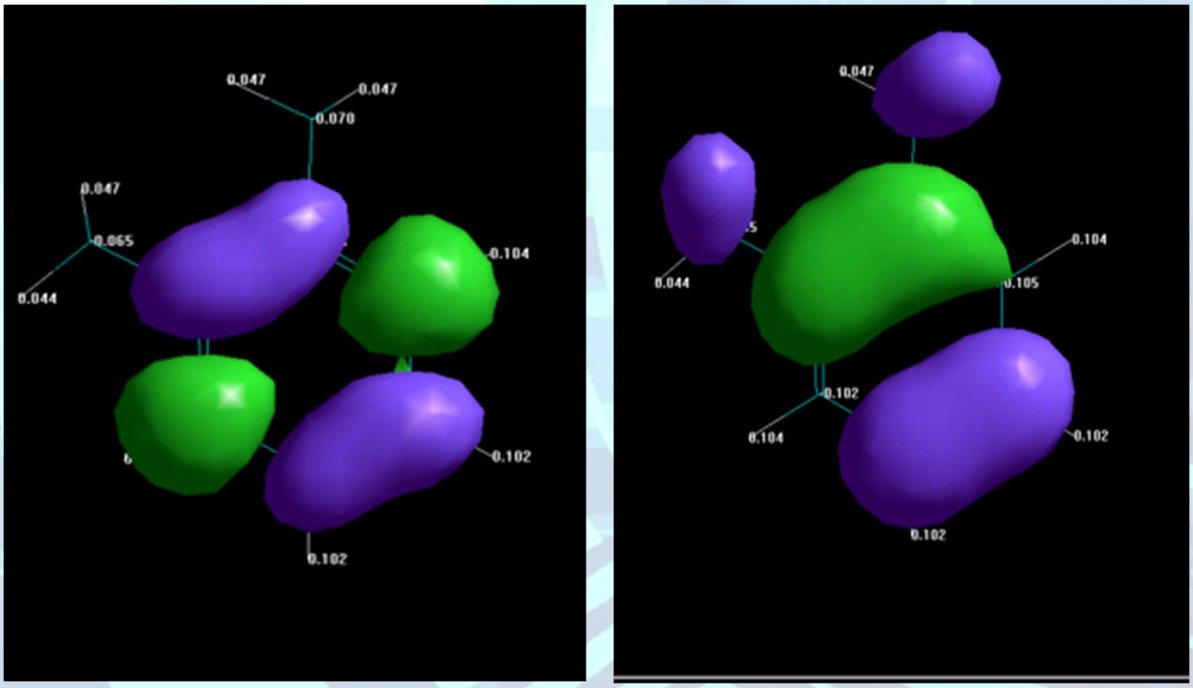
3D 3D



LUMO HOMO

6-rasm. Orto-ksilolning Hyperchem (RM1) da LUMO va HOMO (3D) holati

3D 3D



LUMO HOMO

7-rasm. Orto-ksilolning Hyperchem (PM3) da LUMO va HOMO (3D) holati.

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8-jadval

Hyperchem dasturida olingan LUMO va HOMO qiymatlari

Usul	LUMO	HOMO
AM1	0,6115233	-9,168556
RM1	0,6295907	-9,156899
PM3	0,4571528	-9,28669

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” tanlab moddamizni spektrlarini oldik. 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” metodida optimizatsiya qildik.

Hyperchemda dastlab moddamizni yuklab olib File bo‘limidan “Start log” bosdik va biz bajargan barcha amallarni dastur yozib ola boshladi. Setup bo‘limida “Molecular mechanics” dan MM+, Amber, Bio-charm, OPLS larni tanlab oldik hamda optimizatsiya qilib, hosil bo‘lish issiqlik energiyasi olib jadvalga yozdik, Setup bo‘limidan “Semi-empirical”ni tanlab AM1, RM1, PM3 usullarda IQ spektrini va LUMO-HOMO qiymatlarini oldik [5].

Xulosa: Chem Office da olingan natijalar orto ksilolning hosil bo‘lish issiqligidan Amber va BioCharm da katta farq qilishi aniqlandi va Hyperchem dasturining OPLS kuch maydoni 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, qiymatlarning mos kelish holati 98.5839% ni tashkil qildi.

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