CHEMOFFICE (2006) DASTURIDA 1-(4-BROMFENOKSI)PROPIN-2 NING INFRAQIZIL SPEKTRLARINI NOEMPIRIK USULDA HISOBLASH VA AMALDA OLINGAN NATIJAGA QIYOSIY TAQQOSLASH

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Annotatsiya: Mazkur maqolada 1-(4-bromfenoksi)propin-2 ni ChemOffice (2006) dasturi orqali noempirik usulda HF, MP2 va DFT metodlarida hamda ularga tegishli bazaviy to‘plamlardan foydalangan holda hisoblab olingan IQ-spektr natijalari aniqlangan, shuningdek ushbu birikmaning amalda oligan IQ-spektri bilan dasturda olingan natijalarining qiyosiy tahlil qilindi

Kalit so‘zlar: p-brom arilpropargil efiri, 1-(4-bromfenoksi)propin, noempirik usul, IQ-spektr, HF, MP2, DFT, STO-2G, STO-3G, STO-4G, STO-5G, STO-6G, 3-21G, 6-21G, 4-31G, 5-31G, 6-31G, 6-311G.

Аннотация: В данной статье определены результаты ИК-спектров 1-(4-бромфенокси)пропина-2, рассчитанные с помощью программы ChemOffice (2006) неэмпирическим путем с использованием методов HF, MP2 и DFT и соответствующих им базисных наборов, а также проведен сравнительный анализ результатов, полученных в программе, с реальным ИК-спектром этого соединения и определен оптимальный метод среди них.

Ключевые слова: п-бром арилпропаргиловый эфир, 1-(4-бромфенокси)пропин, неэмпирический метод, ИК спектр, HF, MP2, DFT, STO-2G, STO-3G, STO-4G, STO-5G, STO-6G, 3-21G, 6-21G, 4-31G, 5-31G, 6-31G, 6-311G.

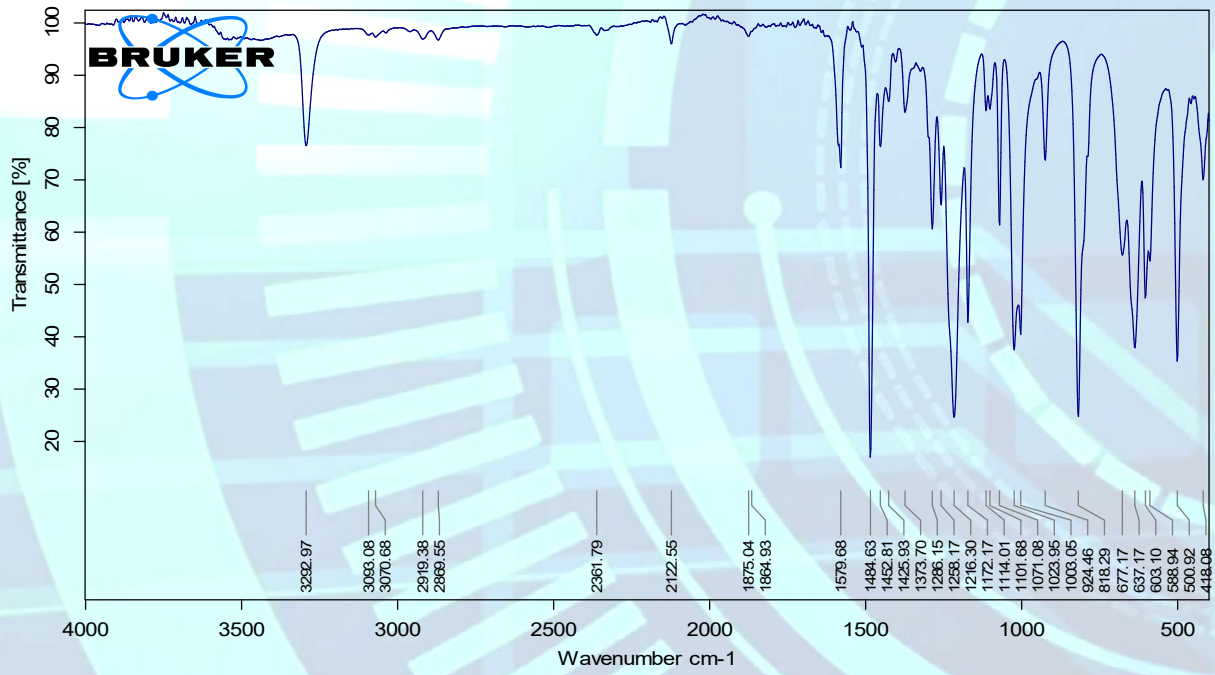
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Abstract: In this article, the IR-spectrum results of 1-(4-bromophenoxy)propyne-2 calculated using the ChemOffice (2006) program in a non-empirical way using the HF, MP2 and DFT methods and their corresponding basis sets were determined, as well as the comparative analysis of the results obtained in the program with the actual IR-spectrum of this compound was performed, and the optimal method was determined among them.

Keywords: p-brom arylpropargyl ether, 1-(4-bromophenoxy)propyne, non-empirical method, IR spectrum, HF, MP2, DFT, STO-2G, STO-3G, STO-4G, STO-5G, STO-6G, 3-21G, 6-21G, 4-31G, 5-31G, 6-31G, 6-31G.

Kirish

Brom almashingan arilpropargil efirlar uch bog‘ va efir guruhi tutgan birikmalarning muhim turlaridan biri hisoblanadi. P-brom arilpropargil efirining amalda olingan IQ-spektrida 818 sm^{-1} sohada C-Br, 1484 sm^{-1} sohada -C-O-C- efir, 1875 sm^{-1} sohada sp^2 gibridlangan C=C (aromatik halqa), 2122 sm^{-1} sohada sp gibridlangan C≡C, 2869-2919 sm^{-1} sohada sp^3 gibridlangan C-H, 3070-3093 sm^{-1} sohada esa aromatik halqadagi sp^2 gibridlangan C-H, 3292 sm^{-1} sohada sp gibridlangan C-H bog‘larga tegishli asosiy tebranishlari qayd etildi [1].



1-rasm. 1-(4-bromfenoksi)propin-2 ning amalda olingan IQ-spektri.

OLINGAN NATIJALAR TAHLILI. ChemOffice (2006) dasturida 1-(4-bromfenoksi)propin-2 ning hisoblashning noempirik usullari bo‘lgan HF, MP2 va DFT metodlari va ularga tegishli STO-2G, STO-3G, STO-4G, STO-5G, STO-6G, 3-21G, 6-21G, 4-31G, 5-31G, 6-31G, 6-311G bazaviy to‘plamlaridan foydalanib, IQ-spektri olindi va ushbu birikmaning amalda olingan IQ-spektr natijasi bilan

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qiyosiy taqqoslab tahlil qilindi. Shuningdek, ushbu usullarda olingan natijalarning qay biri amalda olingan natijaga mos kelishi tahlil qilib xulosalar chiqarildi [2].

1-jadval

1-(4-bromfenoksi)propin-2 ning Chem3D Ultra dasturidagi HF metodining noempirik usullarida olingan IQ-spektr qiymatlari

№	Bog‘lar	Nazariy	STO-2G/sm^{-1}	STO-3G/sm^{-1}	STO-4G/sm^{-1}	STO-5G/sm^{-1}	STO-6G/sm^{-1}	3-21G/sm^{-1}	6-21G/sm^{-1}	4-31G/sm^{-1}	5-31G/sm^{-1}	6-31G/sm^{-1}	6-311G/sm^{-1}
1	C-Br	818	771	762	759	759	717	728	Yo‘q	729	729	729	Yo‘q
2	R-O-R’	1484	1711-1639	1683-1597	1684-1591	1688-1591	1684-1611	1383	Yo‘q	1384	1397	1399	Yo‘q
3	C=C (aromatik halqa)	1875	1875	1817	1818	1815	1790	1749	Yo‘q	1771	1785	1789	Yo‘q
4	C≡C	2122	2015	1928	1930	1923	1936	2251	Yo‘q	2268	2279	2281	Yo‘q
5	sp^3 C-H	2919-2869	2519	2448	2430	2420	2423	2958-2917	Yo‘q	2951-2905	2966-2917	2969-2920	Yo‘q
6	sp^2 C-H (aromatik halqa)	3093-3070	3698-3652	3566-3402	3529-3363	3527-3362	3504-3356	3098-3072	Yo‘q	3101-3074	3116-3091	3119-3094	Yo‘q
7	sp C-H	3292	3815	3702	3667	3665	3661	3275	Yo‘q	3298	3318	3322	Yo‘q

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2-jadval

1-(4-bromfenoksi)propin-2 ning Chem3D Ultra dasturidagi MP2 metodining noempirik usullarida olingan IQ-spektr qiymatlari

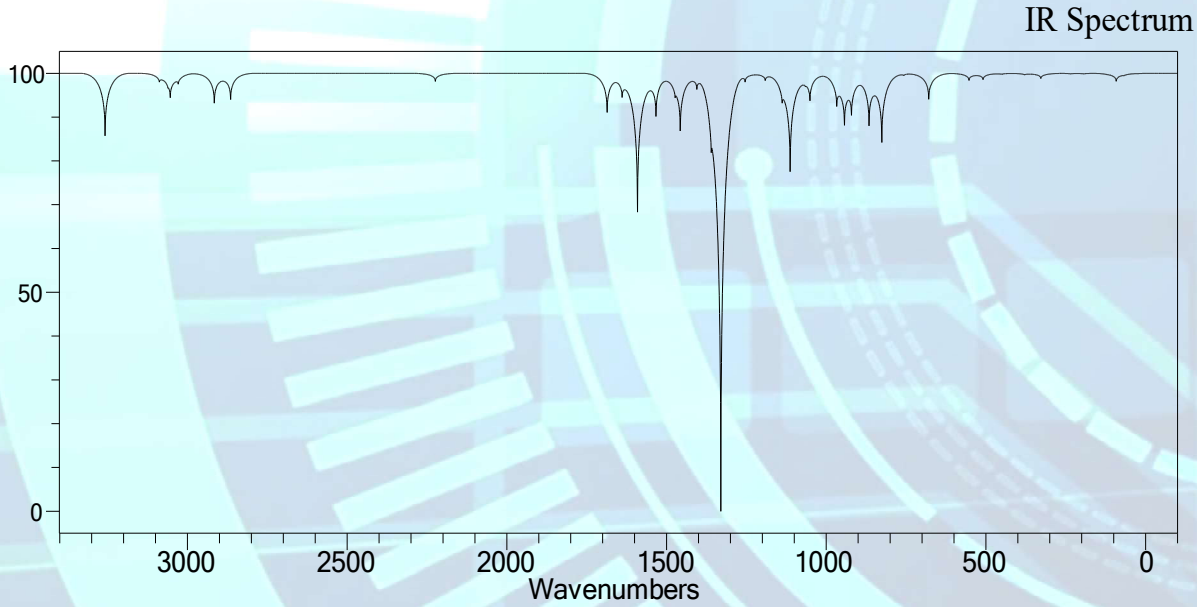
№	Bog'lar	Nazariy	STO-2G/sm^{-1}	STO-3G/sm^{-1}	STO-4G/sm^{-1}	STO-5G/sm^{-1}	STO-6G/sm^{-1}	3-21G/sm^{-1}	6-21G/sm^{-1}	4-31G/sm^{-1}	5-31G/sm^{-1}	6-31G/sm^{-1}	6-311G/sm^{-1}
1	C-Br	818	850	833	842	853	854	816	Yo'q	856	830	823	Yo'q
2	R-O-R'	1484	1580	1524	1520	1520	1542	1357	Yo'q	1349	1360	1362	Yo'q
3	C=C (aromatik halqa)	1875	1783	1712	1711	1708	1683	1659	Yo'q	1576	1592	1592	Yo'q
4	C≡C	2122	1937	1835	1839	1831	2331	2195	Yo'q	2218	2232	2235	Yo'q
5	sp^3 C-H	2919-2869	3476	3345	3307	3305	3296	2950	Yo'q	2949	2967	2971	Yo'q
6	sp^2 C-H (aromatik halqa)	3093-3070	3656-3600	3522-3468	3484-3431	3482-3428	3455-3393	3089-3033	Yo'q	3098-3042	3116-3061	3121-3065	Yo'q
7	sp C-H	3292	3785	3673	3641	3638	3633	3264	Yo'q	3291	3314	3320	Yo'q

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3-jadval

1-(4-bromfenoksi)propin-2 ning Chem3D Ultra dasturidagi DFT metodining noempirik usullarida olingan IQ-spektr qiymatlari

№	Bog'lar	Nazariy	5-31G/sm^{-1}	6-31G/sm^{-1}	6-311G/sm^{-1}
1	C-Br	818	829	826	Yo'q
2	R-O-R'	1484	1327	1329	Yo'q
3	C=C (aromatik halqa)	1875	1683-1590	1686-1590	Yo'q
4	C≡C	2122	2220	2223	Yo'q
5	sp^3 C-H	2919-2869	2911-2861	2915-2864	Yo'q
6	sp^2 C-H (aromatik halqa)	3093-3070	3083-3024	3087-3028	Yo'q
7	sp C-H	3292	3252	3258	Yo'q



2-rasm. **1-(4-bromfenoksi)propin-2 ning ChemOffice dasturi DFT/B3YLP(6-31G) usulida olingan nazariy IQ-spektri.**

TAJRIBA QISM. 1-(4-Bromfenoksi)propin-2 ning strukturasi Chem Office (2006) dasturining ChemDraw Ultra qismida chizildi va "Structure" bo'limidagi "Clean up Structure" ni tanlab chizilgan birikmaning strukturasi to'g'rilandi. Keyin chizilgan birikmani belgilab, "Edit" bo'limidan "Get 3D Model" ni bosib birikmaning 3D holati olindi va ustidan ikki marta bosish orqali Chem3D Ultra qismiga yo'naltirildi. Ushbu qismda molekulyar mexanika usulida, ya'ni MM2 da

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optimizatsiya qilib olindi. So‘ngra “Calculation” bo‘limining “GAMESS Interface” qismidan “Predict IR/Raman spectrum” bo‘limi orqali kerakli metod va bazaviy to‘plamlar tanlanib, shu usullarga mos IQ-spektr natijalari olindi [3].

XULOSA. ChemOffice (2006) dasturida olingan IQ-spektr natijalari birikmaning amalda olingan IQ-spektridan tegishli metodlar va ularning bazaviy to‘plamlariga qarab farq qildi. Ushbu metodlar bo‘yicha optimallik HF metodidan DFT metodiga qarab ortishi kuzatildi, shuningdek, ushbu metodlarning barchasida STO-2G dan STO-6G gacha bo‘lgan bazaviy to‘plamlardan olingan natijalar amaldagiga nisbatan judayam katta farq bilan xatolik kuzatildi. Lekin bazaviy to‘plamlar 3-21G dan 6-311G gacha o‘tishi bilan birikmaning amalda olingan IQ-spektr natijasiga deyarli mos kelishi kuzatildi [4].

FOYDALANILGAN ADABIYOTLAR

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3. https://en.wikipedia.org/wiki/ChemDraw

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