“JAHON SIVILIZATSIYASIDA BUXORONING O‘RNI: BOY MEROS, BARQAROR RIVOJLANISH, YORQIN KELAJAK”

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@buxdu_uz @buxdu1 @buxdu1 www.buxdu.uz

Tel.: (65) 221-29-14
Faks: (65) 221-27-07

E-mail: buxdu_rektor@buxdu.uz
Manzil: Buxoro shahar, M. Iqbol ko'chasi, 11-uy

STRUCTURE AND PROPERTIES OF N'-[1,1,1-TRIFLUORO-2-HYDROXY-4-(4-METHYLPHENYL)-4-OXOBUTAN-2-YL]BENZOHYDRAZIDE

Savriyeva Nigina Qahramon qizi
PhD Student of the Department of Chemistry and Oil and Gas Technologies
Tursunov Murod Amonovich
Professor of the Department of Chemistry and Oil and Gas Technologies

Annotation. This research focuses on the synthesis, structural characterization, and IR spectroscopic analysis of N'-[1,1,1-trifluoro-2-hydroxy-4-(4-methylphenyl)-4-oxobutan-2-yl]benzohydrazide, a novel hydrazide derivative containing both amide and ketone carbonyl groups. The compound was synthesized via condensation of 4,4,4-trifluoro-1-(4-methylphenyl)butane-1,3-dione with benzohydrazide under reflux conditions in ethanol. Experimental IR spectra (KBr pellet method) were compared with theoretical frequencies calculated using the DFT (B3LYP/6-31G(d)) method with an appropriate scaling factor. The observed shifts in O–H, C=O, and CF_3 vibrational bands, particularly the broadening of the hydroxyl stretching due to hydrogen bonding, were discussed in relation to molecular structure and intramolecular interactions. The results confirm the presence of hydroxyl, carbonyl (amide and ketone), aromatic, and trifluoromethyl functional groups, demonstrating strong agreement between experimental and theoretical data.

Keywords: N'-[1,1,1-trifluoro-2-hydroxy-4-(4-methylphenyl)-4-oxobutan-2-yl]benzohydrazide, hydrazide derivatives, IR spectroscopy, hydroxyl group, carbonyl group, trifluoromethyl group.

Introduction

Hydrazide derivatives hold a special significance in organic and bioorganic chemistry, as the presence of a hydrazine fragment in their molecular structure provides diverse biological activities, coordination abilities, and wide possibilities for synthesis. In recent years, organic compounds containing the trifluoromethyl group have found extensive applications in pharmaceuticals, agrochemicals, and materials science. The trifluoromethyl group imparts high lipophilicity, chemical and thermal stability, as well as unique interaction properties within biological systems[1].

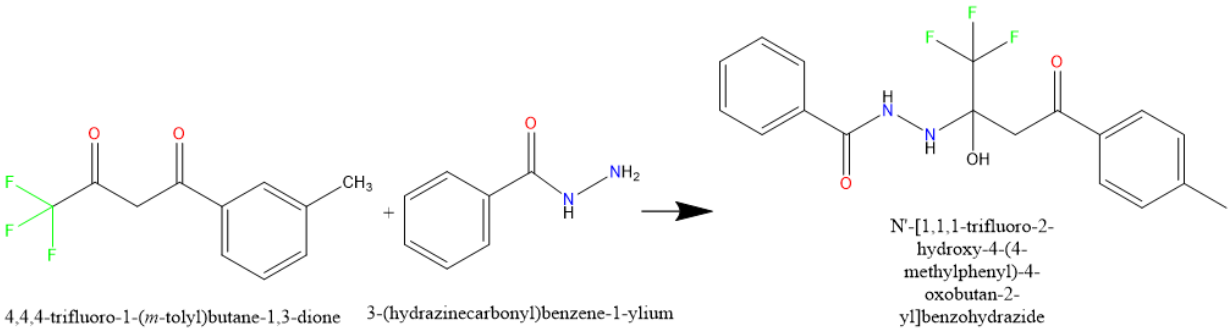
The enrichment of aromatic hydrazides with carbonyl and hydroxyl groups, as well as fluorine atoms, further expands their physicochemical and biological properties. Therefore, the synthesis of hydrazide derivatives bearing a trifluoromethyl group, along with the study of their structure and properties, represents one of the current trends in modern organic chemistry research[2].

In this work, N'-[1,1,1-trifluoro-2-hydroxy-4-(4-methylphenyl)-4-oxobutan-2-yl]benzohydrazide was synthesized for the first time, its structure was characterized using various physicochemical methods, and its main properties were analyzed.

Materials and Methods

All reagents and solvents used for the synthesis — *4,4,4-trifluoro-1-(4-methylphenyl)butane-1,3-dione*, benzohydrazide, and ethanol — were purchased from Sigma-Aldrich and Merck and used without further purification. Distilled water was used in all reactions.

4,4,4-Trifluoro-1-(4-methylphenyl)butane-1,3-dione (0.01 mol) was dissolved in 20 mL of ethanol, and the reaction mixture was stirred on a magnetic stirrer for 5 minutes. Benzohydrazide (0.01 mol) was then added. The mixture was stirred under reflux conditions (80 °C) for 3 hours. Upon completion of the reaction, the mixture was cooled, and the resulting precipitate was collected by filtration. The precipitate was washed with ethanol and dried under vacuum, yielding a white crystalline product. The obtained product was purified by recrystallization. The structure of the compound was confirmed by Infrared (IR) spectroscopy.



Results and Discussion

The synthesized compound, N'-[1,1,1-trifluoro-2-hydroxy-4-(4-methylphenyl)-4-oxobutan-2-yl]benzohydrazide, was analyzed using various physicochemical methods. According to the Infrared (IR) spectrum data (KBr, cm^{-1}) (Figure 1), a broad, intense absorption band observed at around 3153 cm^{-1} corresponds to the stretching vibrations of the hydroxyl (O–H) group. Absorptions at 3001 and 2912 cm^{-1} are assigned to aromatic and aliphatic C–H stretching vibrations, respectively. Strong absorption peaks in the range of 1685–1626 cm^{-1} indicate the presence of a carbonyl (C=O) group[3].

In the 1526–1448 cm^{-1} region, absorptions characteristic of N–H bending vibrations and aromatic C=C stretching were detected. Peaks at 1375–1303 cm^{-1} are attributed to C–N stretching and C–H bending vibrations. Strong absorption bands in the 1247–1138 cm^{-1} range correspond to C–F stretching vibrations of the trifluoromethyl group. Aromatic C–H bending vibrations were recorded between 1024–812 cm^{-1}, while intense peaks at 709 and 696 cm^{-1} are indicative of "out-of-plane" C–H bending vibrations typical of 1,4-disubstituted aromatic rings.

Results confirm the presence of hydroxyl, carbonyl, amino (NH), aromatic ring, and trifluoromethyl functional groups in the synthesized compound. The obtained spectral data are in good agreement with the expected structure based on the proposed synthetic route.

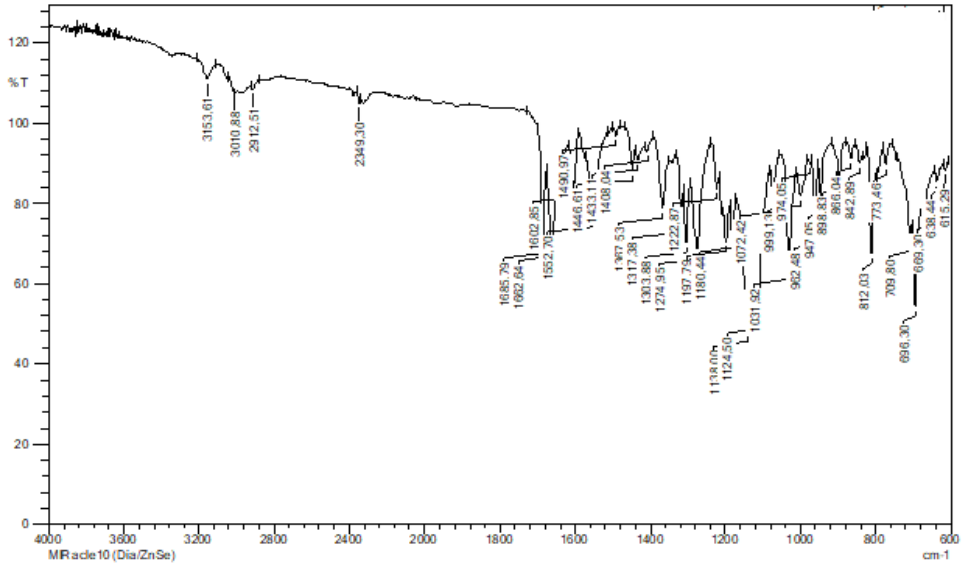


Figure 1. IR spectrum of N'-[1,1,1-trifluoro-2-hydroxy-4-(4-methylphenyl)-4-oxobutan-2-yl]benzohydrazide (KBr, cm^{-1}).

The IR spectrum of the synthesized compound N'-[1,1,1-trifluoro-2-hydroxy-4-(4-methylphenyl)-4-oxobutan-2-yl]benzohydrazide was compared with theoretical calculations (Table 1). The experimental data were obtained using the KBr pellet method, while the theoretical values were calculated at the DFT (B3LYP/6-31G(d)) level and scaled using a scaling factor of ≈ 0.9613.

Table 1

Comparison table of experimental and theoretical IR peaks

Functional group	Experimental (KBr) (cm^{-1})	Theoretical (cm-1)
O–H (Hydroxyl)	3153	~3500–3550
Aromatic C–H	~3001	~3050–3100
Aliphatic C–H	~2912	~2950–3000

C=O (Carbonyl — amide/ketone)	1685–1626	~1730–1670
N–H (amide/–NH– bend)/aromatic C=C	1526–1448	~1550–1500
C–F (CF_3)	1247–1138	~1300–1100

The results indicate that the absorption peaks corresponding to the main functional groups are in good agreement with the theoretical values. In particular, the broad absorption observed at around 3153 cm^{-1} corresponds to the O–H group; its lower position compared to the theoretical value suggests the presence of strong hydrogen bonding in the molecule. The intense peaks in the 1685–1626 cm^{-1} range correspond to the carbonyl (C=O) groups and are slightly shifted relative to the theoretical data due to conjugation effects and intramolecular interactions. Strong absorptions in the 1247–1138 cm^{-1} range are assigned to C–F stretching vibrations of the CF_3 group[4].

Additionally, the peaks observed at 709 and 696 cm^{-1} confirm the out-of-plane C–H bending vibrations typical of 1,4-disubstituted aromatic rings. These results reliably confirm the theoretical structure of the synthesized ligand and the presence of its functional groups through IR spectral analysis.

Reference

1. Mali, S. N., Thorat, B. R., Gupta, D. R., & Pandey, A. (2021). Mini-Review of the Importance of Hydrazides and Their Derivatives—Synthesis and Biological Activity. *Engineering Proceedings*, 11(1), 21.
2. Zhang, D., Li, X., & Hu, J. (2023). Trifluoromethylated hydrazones and acylhydrazones as potent nitrogen-containing fluorinated building blocks. *Beilstein Journal of Organic Chemistry*, 19, 1372–1403. https://doi.org/10.3762/bjoc.19.127
3. **Spectroscopy Tutorial – OrgChemBoulder**. (n.d.). *IR Chart. https://orgchemboulder.com/Spectroscopy/specttutor/irchart.shtml*
4. Chemistry LibreTexts. Infrared Spectroscopy Reference Table. https://chem.libretexts.org/Ancillary_Materials/Reference/Reference_Tables/Spectroscopic_Reference_Tables/Infrared_Spectroscopy_Absorption_Table

BUXORO VILOYATI SHAROITIDA KUZGI BUG‘DOY NAVLARINING SUV TANQISLIGIGA CHIDAMLILIGI.

Sayfiyev Toxir Faxriddinovich
Buxoro davlat universiteti magistranti

Annotatsiya: *Kuzgi bug‘doy navlarining suv tanqisligiga chidamliligi Buxoro viloyati sharoitida juda muhim masaladir. Buxoro viloyati O‘zbekistonning qurg‘oqchil hududlaridan biri bo‘lib, bu erda suv manbalari cheklangan va kuzgi bug‘doy ekinlarini o‘sish va rivojlanishiga ta’sir ko‘rsatuvchi asosiy faktor sifatida suv tanqisligi ahamiyat kasb etadi. Quyidagi maqolada Buxoro viloyatidagi kuzgi bug‘doy navlarining suv tanqisligiga chidamliligi, bu sharoitda eng yaxshi navlar va ularning agrotexnik usullari haqida so‘z yuritiladi.*

Kalit so’zlar: *Kuyzgi bug’doy, suvga chidamlilik. Iqtisodiyotdagi o’rni.*

Kirish: Bug‘doy – O‘zbekistonning asosiy don ekinlaridan biri bo‘lib, uning ishlab chiqarilishi va qishloq xo‘jaligi iqtisodiyotidagi o‘rni katta. Ayniqsa, Buxoro viloyatida bug‘doyning suvga bo‘lgan ehtiyoji va suv tanqisligiga chidamliligi muhim ahamiyatga ega. Buxoroda, suv resurslarining chegaralanganligi tufayli, bug‘doy navlarini tanlashda ularning suvga chidamli bo‘lishi, ya’ni suv taqsimoti va sug‘orish rejimlariga moslashishi katta ahamiyat kasb etadi.

Buxoro viloyatining iqlimi va suv resurslari: Buxoro viloyati O‘zbekistonning qurg‘oqchil hududida joylashgan bo‘lib, bu erdagi iqlimning asosiy xususiyatlari quyidagilardir:

Yuqori harorat: yozda havo harorati +40°C va undan yuqori bo‘lishi mumkin.

Kam yog‘ingarchilik: Yillik yog‘ingarchilik miqdori 100–150 mm atrofida.

Sug‘orishning zaruriyati: Bug‘doy uchun yetarli suv ta’minoti faqat sug‘orish orqali amalga oshiriladi.

Buxoro viloyatidagi sug‘orish tizimlarining samaradorligi va suv resurslarining cheklanganligi kuzgi bug‘doy navlarining o‘sish va rivojlanishiga ta’sir qiladi. Suv tanqisligi sharoitida bug‘doy ekinlarining