O-FENILENDIAMINNING NAFTALIN 1,5-DISULFOKISLOTASI BILAN HOSIL QILGAN MOLEKULYAR KOMPLEKSI SINTEZI VA TADQIQOTI

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Annotatsiya: Ushbu tadqiqot ishimizdan asosiy maqsad o-fenilendiaminning kompleks xossalarini va hosil qilingan komplekslarning amaliyotga tadbiqini o'rganishdan iborat. Ilk bor o-fenilendiaminning naftalin 1,5-disulfokislotasi bilan $(C_{10}H_6S_2)^{2-}$,$2(C_6H_9N_2)^+$ tarkibli aralash ligandli kompleks birikmasi sintez qilindi. Sintez qilingan kompleks birikmaning fizik-kimyoviy tadqiqot usullariga asoslanib tarkibi, kimyoviy formulasi va reaksiya tenglamalari taklif qilindi. Rentgen tuzilish tahlili (RTT) va DFT hisoblashlari yordamida molekulaning molekulyar massasi, fazoviy shakli, bog'lar orasidagi masofa va bog' burchaklari o'rganildi.

Kalit so'zlar: o-fenilendiamin, naftalin 1,5-disulfokislota, sokristall, IQ-spektr, vodorod bog'lar geometriyasi.

СИНТЕЗ И ИССЛЕДОВАНИЕ МОЛЕКУЛЯРНОГО КОМПЛЕКСА О-ФЕНИЛЕНДИАМИНА С НАФТАЛИН-1,5-ДИСУЛЬФОКИЛОТОЙ

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Аннотация: Основная цель данной исследовательской работы – изучение комплексных свойств о-фенилендиамина и изучение практического применения образующихся комплексов. Впервые синтезировано сложное сочетание о-фенилендиамина с нафталин-1,5-дисульфокислотой $(C_{10}H_6S_2)^{2-}$,$2(C_6H_9N_2)^{+}$. На основе физико-химических методов исследования предложены состав, химическая формула и уравнения реакций синтезированного комплексного соединения. Рентгеноструктурный анализ (RTT) и расчеты DFT были использованы для изучения молекулярной массы, пространственной формы, расстояния между связями и валентных углов молекулы.

Ключевые слова: о-фенилендиамин, нафталин-1,5-дисульфокислота, сокристалл, ИК-спектр, геометрия водородных связей.

SYNTHESIS AND STUDY OF THE MOLECULAR COMPLEX OF O-PHENYLENEDIAMINE WITH NAPHTHALEN-1,5-DISULPHOCYLOTE

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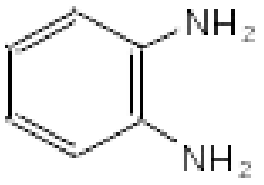
Abstract: The main goal of this research work is to study the complex properties of o-phenylenediamine and to study the practical application of the formed complexes. For the first time, a complex combination of o-phenylenediamine with naphthalene 1,5-disulfoacid (C10H6S2)2-,2(C6H9N2)+ was synthesized. Based on the physico-chemical research methods, the composition, chemical formula and reaction equations of the synthesized complex compound were proposed. X-ray structure analysis (RTT) and DFT calculations were used to study the molecular mass, spatial shape, distance between bonds and bond angles of the molecule.

Key words: o-phenylenediamine, naphthalene 1,5-disulfoacid, cocrystal, IR spectrum, geometry of hydrogen bonds.

Kirish

O-fenilendiaminning boshqa faol ligandlar bilan molekulyar komplekslar va 3d-metall atomlari bilan faol metallokomplekslar hosil qilishi adabiyotlarda keltirilgan[1]. O-fenilendiaminga nisbatan uning sokristallari va xelatlangan komplekslari biologik jihatdan faol ekanligi tajribalarda isbotlangan[2]. O-fenilendiamin asosan tibbiyotda farmatsevtik preparatlar tayyorlashda, qishloq xo'jaligida gerbitsit va fungitsitlar olishda oraliq modda sifatida ishlatiladi. O-fenilendiamin va uning metallokomplekslari bakteriya shtamplariga qarshi antibakterial faolligi yuqori ekanligi isbotlangan[3]. O-fenilendiamin molekulasida $-NH_2$ guruhlari yonma-yon joylashganligi tufayli, elektron zichlik ortadi. Shu sababli uning boshqa izomerlariga nisbatan kompleks hosil qilish qobilyati yuqori hisoblanadi. Azot atomi bunda $-sp^3$ gibridlangan holatda bo'ladi va $-NH_2$ guruhidagi bitta N-H bog'i benzol halqasi bilan bir xil tekislikda yotadi[4-5]. Shuning uchun azot va vodorod atomlarining gomolitik uzilish imkoniyati yuqori bo'ladi va bu fotokimyoviy 3d o'tish jarayonlarida asosiy vodorod manbai bo'lib

xizmat qiladi. Bunda redoks potensiallarining yuqori ritmik ravishda o’zgarishini kuzatishimiz mumkin. Shu sababli o-fenilendiaminning sokristallar hosil qilishi va 3d metallari bilan hosil qilgan kompleks birikmalari muhim ahamiyatga ega hisoblanadi[6-7].



1-rasm. O-fenilendiamin molekulasining tuzilish formulasi.

Fenil halqali birikmalarda asosan polimorfizm hodisasi juda kam uchraydi. Ammo fenil halqali amino birikmalarga aminokislotalarning birikishi natijasida allen tipidagi polimorfizm hodisasining uchrashi o-fenilendiamin hosilalarida ko’p kuzatilgan[8]. O-fenilendiaminning o’zaro sokristallari singoniyasi monoklinik fazoviy shakli C-2 ekanligi tadqiqotlar natijasida aniqlangan[9].

Tadqiqot metadologiyasi

Ushbu tadqiqot ishi xorijiy va mahalliy olimlarning shu sohada olib borgan ilmiy ishlari asosida olib borildi. Hosil qilingan yangi $(C_{10}H_6S_2)^{2-},2(C_6H_9N_2)^+$ tarkibli molekulyar kompleksining tarkibi, tuzilishi va kristall parametrlari zamonaviy fizik-kimyoviy tadqiqot usullari yordamida o’rganildi va xossalari tadqiq qilindi.

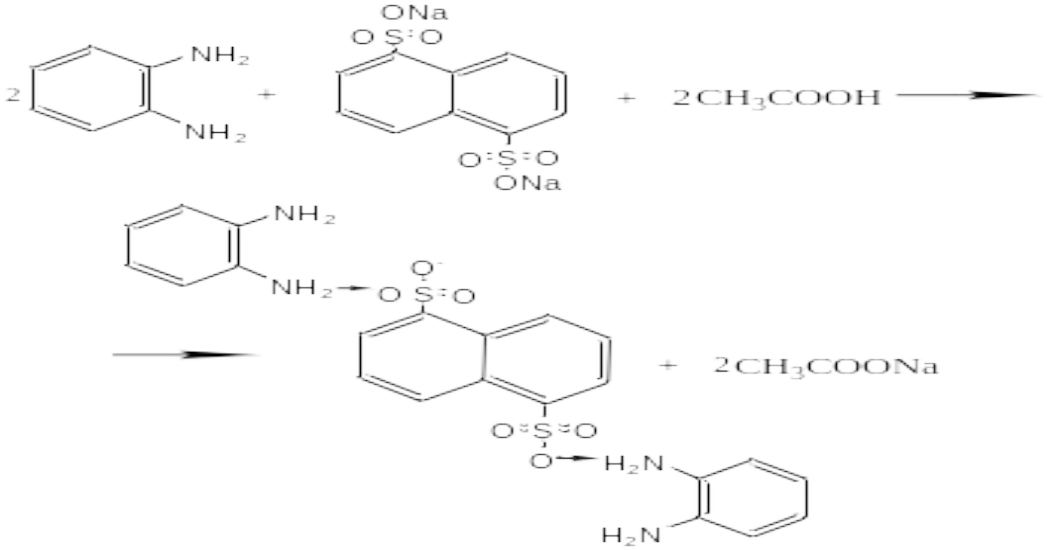
Natijalar va tahlillar

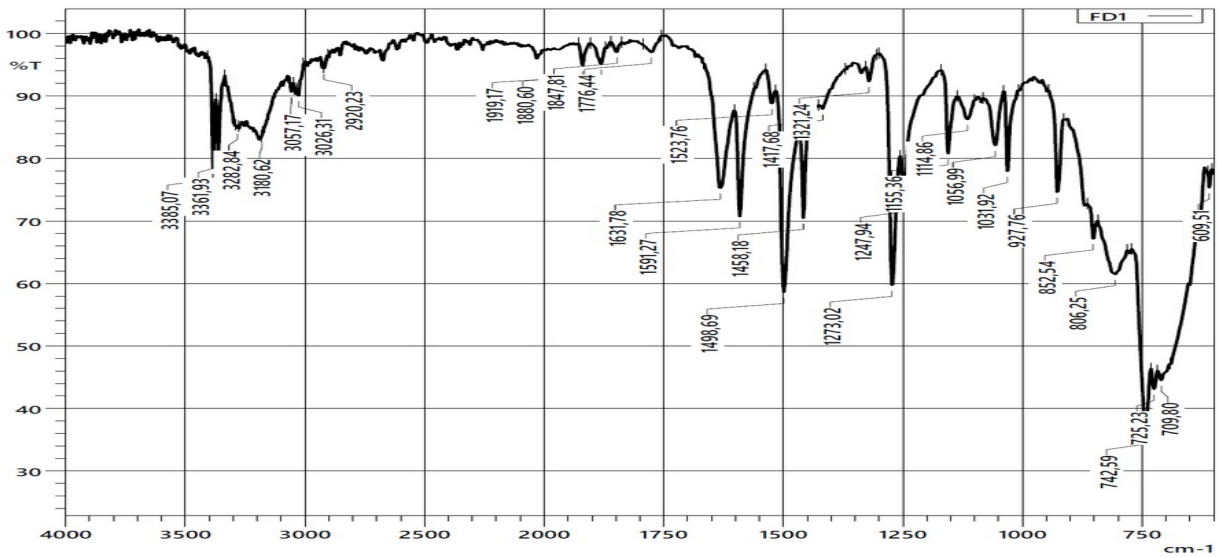
Ushbu tadqiqot ishini bajarishda ishlatiladigan moddalar va reagentlar tijorat manbalaridan (Ilk-Farma) olingan. Olingan ligandlarning tozalik darajasi 99% ni tahkil etadi. Shuningdek reaksiyaga bog’lovchi modda sifatida “muz sirka kislota” ishlatilgan.

$(C_{10}H_6S_2)^{2-},2(C_6H_9N_2)^+$ molekulyar kompleksi sintezi. Dastlab analitik tarozida o-fenilendiamindan 0.005 mol (0,54 g) va naftalin-1,5-di-sulfokislotaning dinatriyli tuzidan 0,0025 mol (0,83 g) tortib oldik. O-fenilendiaminning spirtli eritmasi va naftalin-1,5-disulfokislotaning dinatriyli tuzining suvli eritmasidan teng hajmda tayyorlandi. Birinchi va ikkinchi eritmalarni aralashtirib teng hajmda 5 ta flakonga bo’lib soldik va bog’lovchi modda sifatida sirka kislota eritmasidan

foydalandik. Flakonlar 12 kun o’zgarmas 25-28ºC haroratli termostatda qoldirildi. Jarayon oxirida flakonlar tagida qoramtir sariq rangli bis(2-aminoanilin) naftalin-1,5-disulfonat ($(C_{10}H_6S_2)^{2-}$,$2(C_6H_9N_2)^{+}$) kristallar hosil bo’lganligini kuzatdik. Olib borilgan fizik-kimyoviy tadqiqotlar va RTT usuli yordamida sintez qilingan bis(2-aminoanilin) naftalin-1,5-disulfonat ($(C_{10}H_6S_2)^{2-}$,$2(C_6H_9N_2)^{+}$) sokristalining tuzilishi, hosil bo‘lish reaksiya tenglamasi va boshqa kristall parametrlari o‘rganildi.

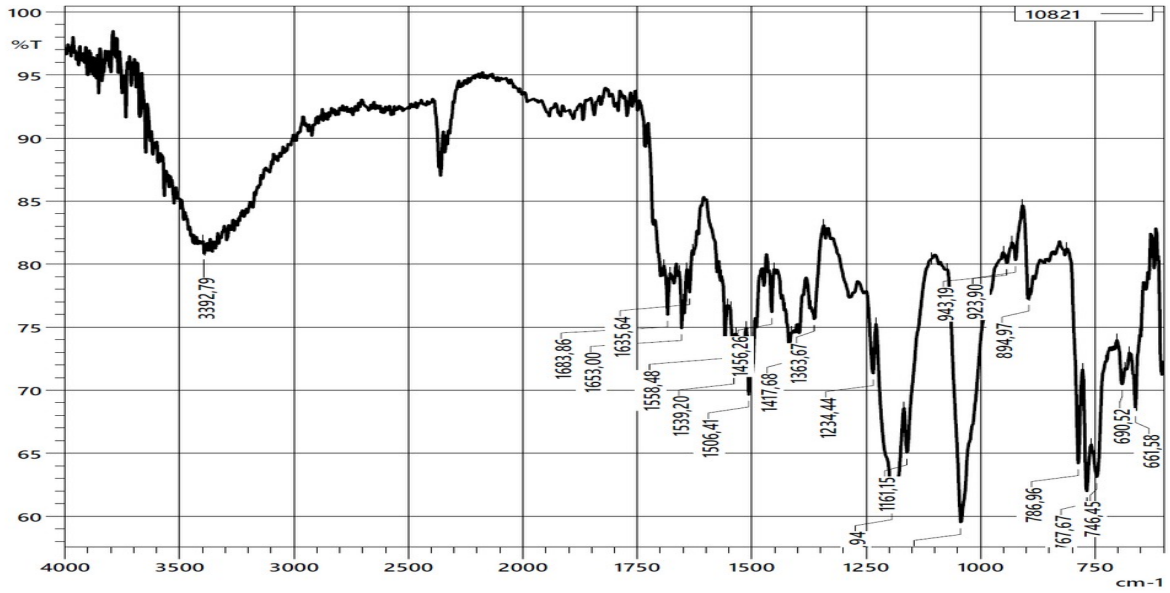
Ushbu tadqiqot ishini bajarishda O‘zRFA O.S. Sodiqov nomidagi Bioorganik kimyo instituti kompleks birikmalar laboratoriyasida mavjud bo’lgan Xcalibur R Oxford Diffraction difraktometri asbobi yordamida RTT usuli orqali molekulaning kristall parametrlari olindi.





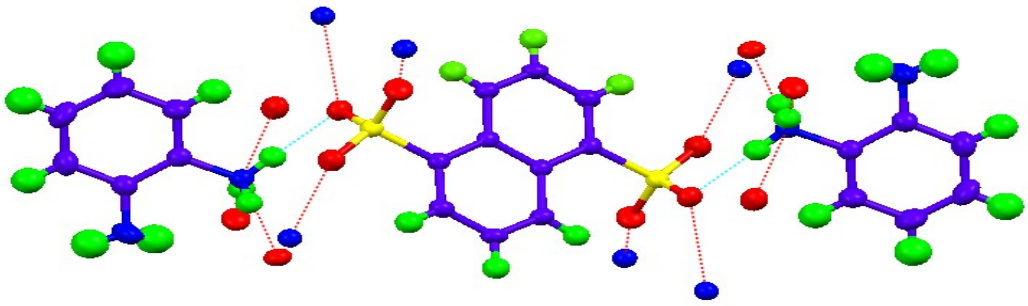
2-rasm. Fenilendiaminning IQ-spektri

2-rasmda 3385,07 sm^{-1} past intensiv sohada ν(Ar)=C-H bog‘ining, 3189.62 sm^{-1} sohada esa aromatik halqadagi C-H bog’ining valent tebranishini va aromatik halqadagi halqa tekisligida bo’layotgan deformatsion tebranishlar natijasida 1631,78 sm^{-1}, 1591.27 sm^{-1} ko’rinadigan yutilish polasalarida NH2 guruhlarining mavjudligini kuzatishimiz mumkin. Spektrdagi 1273.02 sm^{-1} yutilish polasasida C-N guruhining valent tebranishi va 1776.44 sm^{-1} sohada -C=C- bog‘ining valent tebranishlari yuzaga keladi.



3-rasm. Sintez qilingan bis(2-aminoanilin) naftalin-1,5-disulfonat $(C_{10}H_6S_2)^{2-}$,$2(C_6H_9N_2)^+$ tarkibli kompleksning IQ-spektri

3-rasmda tasvirlangan spektrning 3392.79 sm^{-1} yutilish sohasida ν(Ar)=C-H bog‘ining valent tebranishi, 1683.86 sm^{-1} va 1653.00 sm^{-1} yutilish sohalarida esa NH_2 guruhlarining deformatsion tebranishi va 1558.48 sm^{-1} yutilish sohasida esa -C=C- bog‘ining valent tebranishlarini kuzatdik. Aromatik halqa sonining ortishi bilan IQ-spektrning quyi chastotali qismida yutilish polosalari soni ko’payadi. 786.96 sm^{-1} intensiv sohada naftalin halqasining halqa tekisligida deformatsion tebranishi, (Ar(C_6H_6) ning halqa tebranishi 1539,20 sm^{-1} o‘rtacha intensiv soha oralig‘ida va SO_2 bog‘ining assimmetrik valent tebranishi esa 1234,44 sm^{-1} sohalarda kuzatildi.



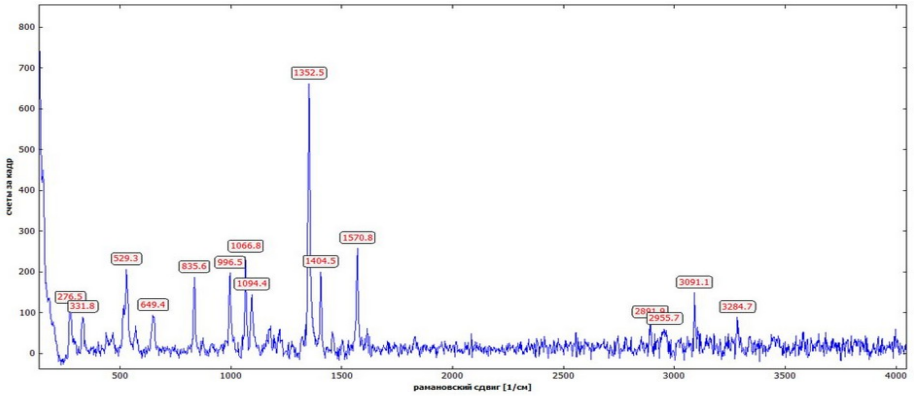
4-rasm. Sintez qilingan bis(2-aminoanilin) naftalin-1,5-disulfonat $(C_{10}H_6S_2)^{2-}$,$2(C_6H_9N_2)^+$ molekulyar kompleksining tuzilishi.

Sintez qilingan kompleks birikmada quyi spin-elektron holati yuqori spin-elektron holatiga qaraganda yuqori energetik holatda bo'ladi. SO_3 va NH_2 funksional guruhlari vodorod bog'lar orqali bog'langan. Naftalin 1,5-disulfonat halqasida mezomer effekt kuzatilganligi sababli bog'lanish faqat SO_3 guruhi orqali amalga oshadi.

$(C_{10}H_6S_2)^{2-}$,$2(C_6H_9N_2)^+$ tarkibli kompleks birikmaning kristall tizimidagi vodorod bog'lar geometriyasi

1-jadval

D-H···A	***D-H,Å***	***H···A,Å***	***D···A,Å***	***DHA, burchak***	***Simmetriya kodlari***
N1 -- H1A -- O3	0.87(3)	2.54(3)	3.240(2)	138(2)	-x,1-y,1-z
N2 -- H2A -- O2	0.89(2)	1.97(2)	2.8578(19)	176(2)	1+x,y,z
N2 -- H2B -- O1	0.90(2)	1.91(2)	2.8100(18)	171.4(16)	-1/2-x,-1/2+y,z
N2 -- H2C -- O2	0.94(2)	1.97(2)	2.8996(19)	171(2)	-1/2-x,-1/2+y,z
C9 -- H9 -- O3	0.9300	2.4300	2.849(2)	107.00	-1/2-x,1/2+y,z
C11 -- H11 -- O1	0.9300	2.5700	3.128(2)	119.00	1/2+x,3/2-y,1-z



5-rasm. Sintez qilingan $(C_{10}H_6S_2)^{2-}$,$2(C_6H_9N_2)^+$ tarkibli kompleks birikmaning Raman-spektri.

5-rasmda sintez qilingan bis(2-aminoanilin) naftalin-1,5-disulfonat raman-spektrining 596,57- 748,28- 1596,65 va 2955,7 sm^{-1} sohalaridagi piklar naftalin disulfokislotaning raman-spektrida tebrangan chiziqlarga yaqin sohalarda mavjud holatda tebrandi. O-fenilendiamin spirtda yaxshi eriganligi sababli, chiziqlar intensivligi juda yuqori bo‘lgan holatda spektri olindi. Molekulyar kompleksda bog‘lar dipol momenti (qutblanishi) ortishi bilan raman-spektrda faol bo‘lmagan holatga o‘tgan. Eritmadagi kompleksning raman-spektri amorf holatdagi raman-spektri bilan qariyb bir xil ekanligi aniqlandi. Bu esa eritmada kompleksning barqaror ekanligini ko‘rsatadi.

Xulosa. Ilk bor o-fenilendiaminning naftalin 1,5-disulfokislota bilan yangi molekulyar kompleksi hosil qilindi va sintez sharoitlari o’rganildi. Hosil qilingan $(C_{10}H_6S_2)^{2-}$,$2(C_6H_9N_2)^+$ molekulyar kompleksning IQ-spektri, Raman-spektri va RTT tahlili yordamida kompleks tuzilish formulalari, reaksiya tenglamalari va boshqa kristall parametrlari o’rganildi.

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