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LEVOFLOKSATSIN BILAN Cu(II) KOMPLEKSI: XIRSHFELD SIRTI VA IK SPEKTRI TAHLILI

Annotatsiya: Ushbu maqolada levofloksatsin ishtirokida mis (II) xlorid bilan yangi kompleksining sintezi va tadqiqot natijalari keltirilgan. Sintez qilingan metallokompleksning tarkibi, molekulyar va kristall tuzilishlari rentgen tuzilish tahlili (RTT), IK spektroskopiya natijalari asosida aniqlangan. Kompleksning IK spektri hamda RTT malumotlari asosida Xirshfeld sirt tahlili o‘rganilgan.

Kalit so‘zlar: Levofloksatsin, mis (II) xlorid, xlorid kislota, distillangan suv.

Cu(II) С ЛЕВОФЛОКСАЦИНОМ КОМПЛЕКС: АНАЛИЗ ПОВЕРХНОСТИ И ИК-СПЕКТРА ПО ХИРШФЕЛДУ

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Аннотация: В работе представлены результаты синтеза и исследования нового комплекса с хлоридом меди (II) в присутствии левофлоксатсина. По результатам рентгеноструктурного анализа (РТТ), ИК-спектроскопии определен состав, молекулярная и кристаллическая структура синтезированного металлокомплекса. На основании ИК-спектра и данных РТТ комплекса изучен анализ поверхности Хиршфелда.

Ключевые слова: левофлоксатсин, хлорид меди (II), соляная кислота, дистиллированная вода.

Cu(II) WITH LEVOFLOXACIN COMPLEX: HIRSHFELD SURFACE AND IR SPECTRUM ANALYSIS

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Abstract: This paper presents the synthesis and research results of a new complex with copper (II) chloride in the presence of levofloxacin. The composition, molecular and crystal structures of the synthesized metallocomplex were determined based on the results of X-ray structure analysis (RTT), IR spectroscopy. Based on the IR spectrum and RTT data of the complex, Hirschfeld surface analysis was studied.

Key words: Levofloxacin, copper (II) chloride, hydrochloric acid, distilled water.

Kirish.

So‘ngi yillarda atrof-muhitning turli chiqindilar bilan ifloslanishi oqibatida virus, bakteriya va zamburug‘larning yashashi hamda ko‘payishi uchun qulay sharoitlar yaratilmoqda. Oqibatda kasallik turlari ko‘payib bormoqda. Bu holat kimyo va farmatsevtika sohasidagi olimlarga yangi va samarali dori vositalarini yaratish, ularning konsentratsiya miqdorini kamaytirish hamda tasir doirasini oshirish vazifalarini yuklamoqda. Adabiyotlardan ma’lumki, biologik faol moddalarning antibakteriallik xossalari uning o‘ziga (erkin ligandga) nisbatan biofaol metallar bilan hosil qilgan kompleks birikmalarida faol bo‘lishi o‘rganilgan[1].

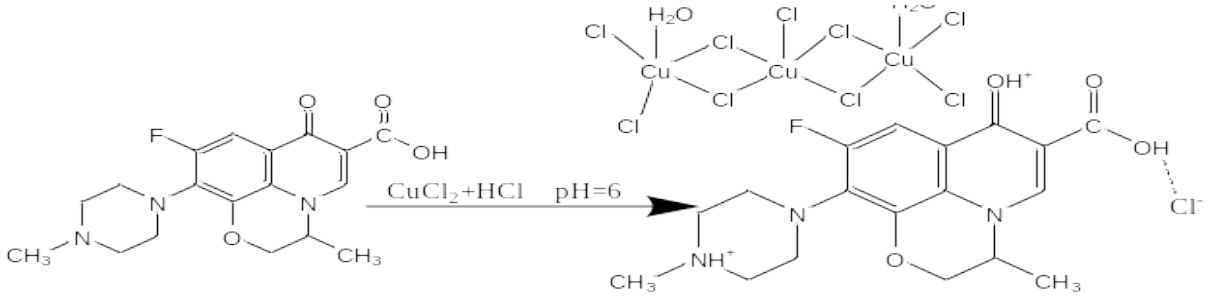
Adabiyotlar tahlili.

Tibbiyot amaliyotida dori vositasi sifatida foydalanilib kelayotgan biologik faol birikma hisoblangan keng spektrli ta’sirga ega ftorxinolinlar guruhiga kiruvchi dori vositalaridan levofloksatsin (LEV) eng samarali ftorxinolonlardan biri bo‘lib, klinik amaliyotda ko‘pgina gram-manfiy va ba’zi gram-musbat bakteriyalarga nisbatan antibakterial vosita bo‘lib [2-3], u surunkali prostatit, teri va yumshoq to‘qimalar, o‘pka va peshob yo‘llari infeksiyalari kabi ko‘plab infeksiyalarni klinik davolashda qo‘llaniladi [4-6]. Golovnev N.N. [4], Vasiliev A.D. [2] kabi olimlarning tadqiqotlarida ma’lum biofaol xususiyatga ega bo‘lgan, tarkibida piridin halqasi saqlagan LEV ning metallokomplekslari sintez qilingan va o‘rganilgan [7-8]. Bundan

tashqari Bijay Laxmi Pradhan, Jai Prakash Yadav, Lekhan Lodhi [7] kabi olimlar ham ushbu soha bo‘yicha bir qator tadqiqot ishlarini amalga oshirganlar.

Tadqiqot metodologiyasi.

Tadqiqot jarayonida LEV ning suyultirilgan xlorid kislotadagi eritmasi bilan mis (II) xloridning eritmalaridan foydalanildi. Hosil bo‘lgan eritmalarni mexanik aralashtirgich yordamida 30-35ºC haroratda 20-25 daqiqa davomida qizdirilib aralashtirildi, xona xaroratida og‘zi to‘liq yopiq bo‘lmagan holatda qoldirilib kuzatishga qo‘yildi. Kuzatishlar natijasida 8-12 kundan so‘ng idish tubida yashil rangli kristallar hosil bo‘lgani kuzatildi. RTT usulida tahlil qilinib, kompleksning tuzilishi aniqlandi. Kompleksning hosil bo‘lish reaksiya tenglamasi quyidagicha taklif qilindi (1-rasm).

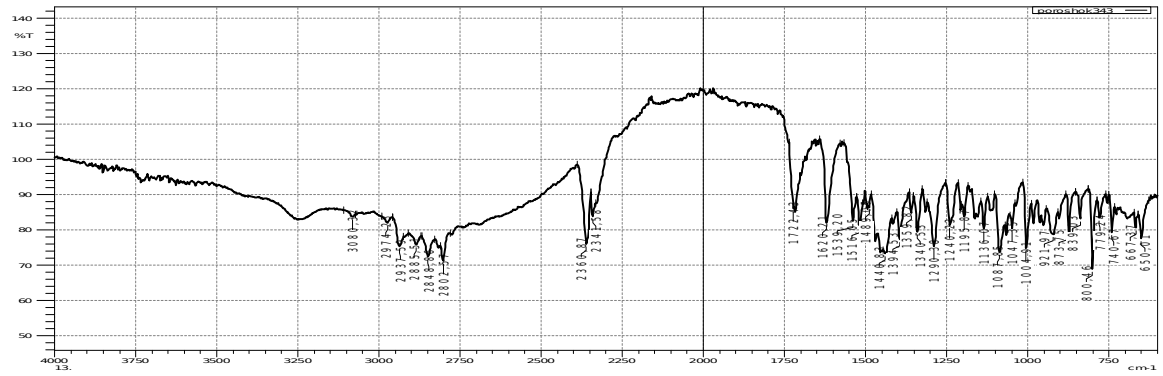


1-rasm. ***[Cu₃Cl₉(H₂O)₂](LEV)Cl tarkibli metallokompleksning sintez reaksiyasi.***

Olingan kompleksning IK spektri hamda RTT ma’lumotlari asosida Xirshfeld sirt tahlili ham o‘rganildi.

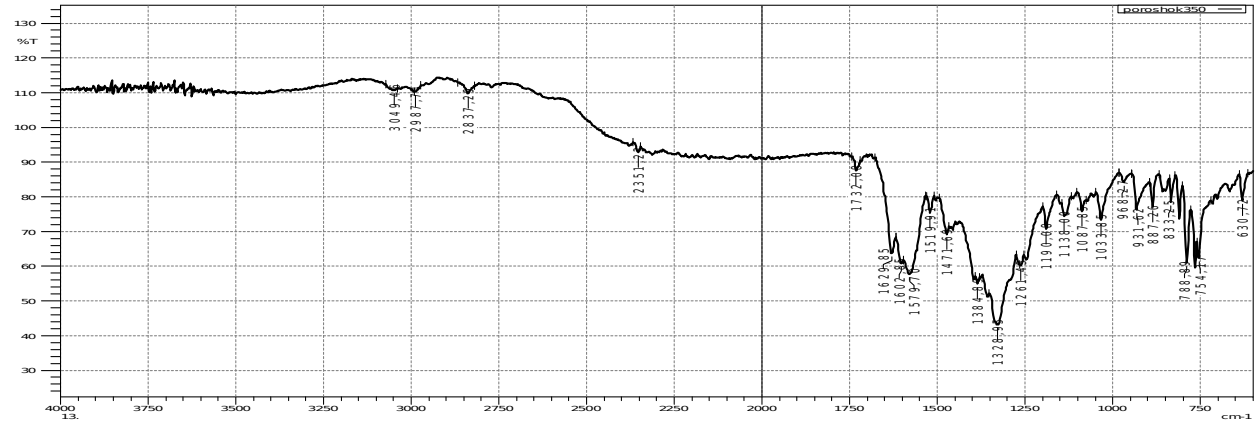
Tahlil va natijalar.

Sintez qilingan metallokompleksning tuzilishini isbotlash maqsadida IK-spektri o‘rganildi. Ushbu ligand hamda yangi sintez qilingan metallokompleks kristallarining IK-spektrlari qiyosiy solishtirib o‘rganildi. Ligand va sintez qilingan kompleks kristalining IK-spektri Yaponiyada ishlab chiqarilgan Shimadzu IK- Furye spektrofotometrida 400-4000 sm-1 sohada olindi.



1-rasm. Ligand LEV ning IK-spektri tahlili

Ligand LEV ning IK-spektri tahlilida quyidagi sohalarda tebranish kuzatildi: Bog‘ hosil qilgan OH-guruhining 3500-3000 sm^{-1} sohasidagi keng va intensiv valent tebranishi 3080.32 sm^{-1} sohasida kuzatildi, >C=O guruhining 1820-1650 sm^{-1} sohasidagi juda intensiv valent tebranishi 1722.43 sm^{-1} sohasida kuzatildi, -CH_3 guruhining 1470-1420 sm^{-1} sohasidagi asimmitrik deformatsion tebranishi 1440.83 sm^{-1} sohasida kuzatildi, >CH_2 guruhining 1350-1150 sm^{-1} sohasidagi urchuqsimon tebranishi 1240.23 sm^{-1} sohasida kuzatildi, C-F bog‘ining 1300-1000 sm^{-1} sohasidagi valent tebranishi 1087.85 sm^{-1} sohasida kuzatildi. -C-O-C- guruhining 1075-1020 sm^{-1} sohasidagi intensiv simmitrik valent tebranishi 1047.35 sm^{-1} sohasida kuzatildi.



2-rasm. Sintez qilingan $[Cu_3Cl_9(H_2O)_2](LEV)Cl$ tarkibli metallokompleksning IK-spektri tahlili

2-rasmda sintez qilingan kompleks birikmaning IK-spektri tahlilida quyidagi sohalarda tebranish kuzatildi: Bog‘ hosil qilgan OH-guruhining 3500-3000 sm^{-1} sohasidagi keng va intensiv valent tebranishi 3049.46 sm^{-1} sohasida kuzatildi, NH^+-guruhining 2800-2000 sm^{-1} sohasidagi intensivligi o‘rtacha valent tebranishi 2351.23 sm^{-1} sohasida kuzatildi, >C=O guruhining 1820-1650 sm^{-1} sohasidagi juda intensiv

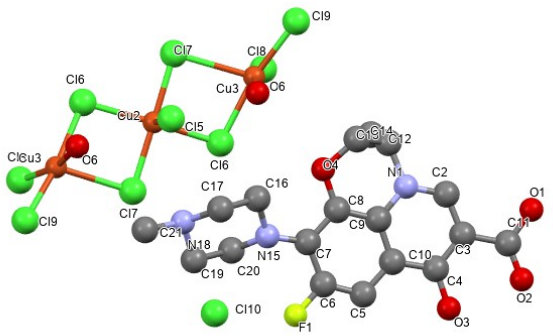
valent tebranishi 1732.08 sm^{-1} sohasida kuzatildi, -CH_3 guruhining 1470-1420 sm^{-1} sohasidagi asimmitrik deformatsion tebranishi 1471.69 sm^{-1} sohasida kuzatildi, >CH_2 guruhining 1350-1150 sm^{-1} sohasidagi urchuqsimon tebranishi 1261.45 sm^{-1} sohasida kuzatildi, C-F bog‘ining 1300-1000 sm^{-1} sohasidagi valent tebranishi 1087.85 sm^{-1} sohasida kuzatildi, -C-O-C- guruhining 1075-1020 sm^{-1} sohasidagi intensiv simmitrik valent tebranishi 1033.85 sm^{-1} sohasida kuzatildi[9]

2-jadval

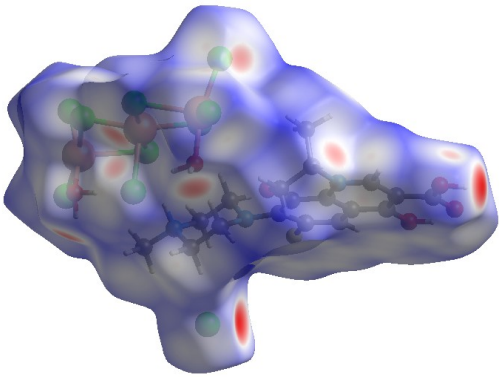
Ligand LEV ва $[Cu_3Cl_9(H_2O)_2](LEV)Cl$ tarkibli kompleksning IK-spektrlari tahlili, sm-1

Tebranish tavsifi	OH	NH^+	>C=O	-CH_3	>CH_2	C-F	-C-O-C-
LEV	3080.32	-	1722.43	1440.83	1240.23	1087.85	1047.35
$[Cu_3Cl_9(H_2O)_2]$ (LEV)Cl	3049.46	2351.23	1732.08	1471.69	1261.45	1087.85	1033.85

$[Cu_3Cl_9(H_2O)_2](LEV)Cl$ tarkibli kompleksning molekulyar tuzilishi rentgen nurlari difraksion tahlili usulida aniqlandi. Molekulalararo o‘zaro ta’sirlar xarakterini tavsiflash uchun Xirshfeld sirtini Crystal Explorer 17.5 [10] dasturi yordamida tahlili amalga oshirildi.



a



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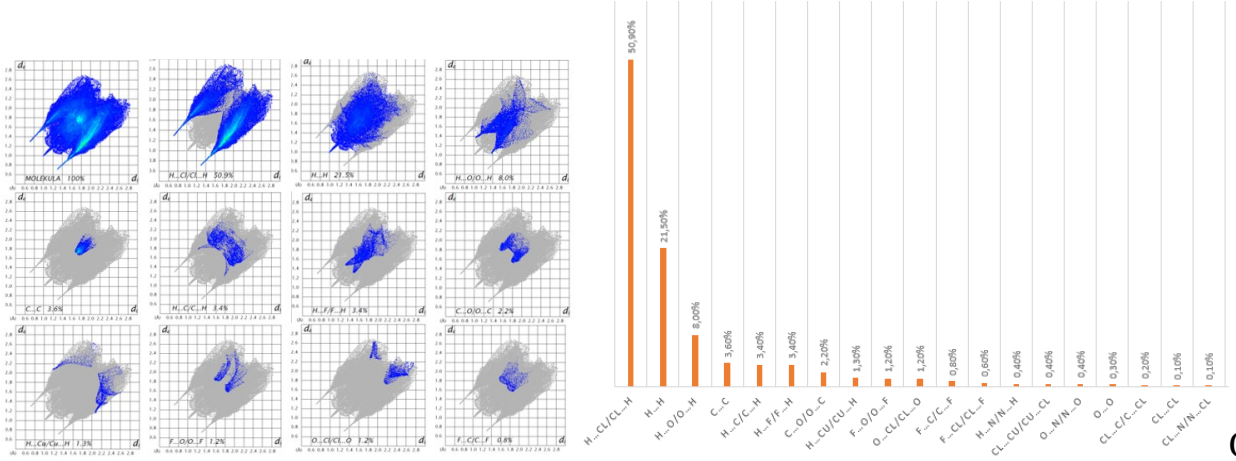
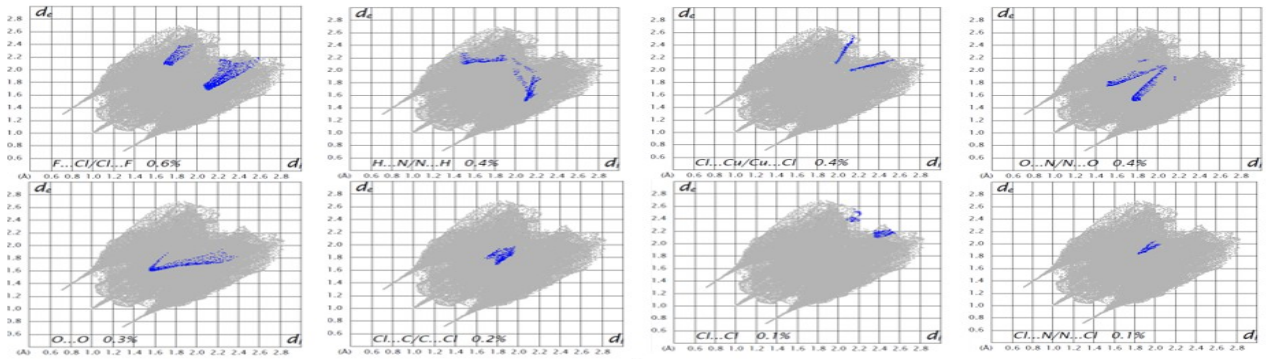


C



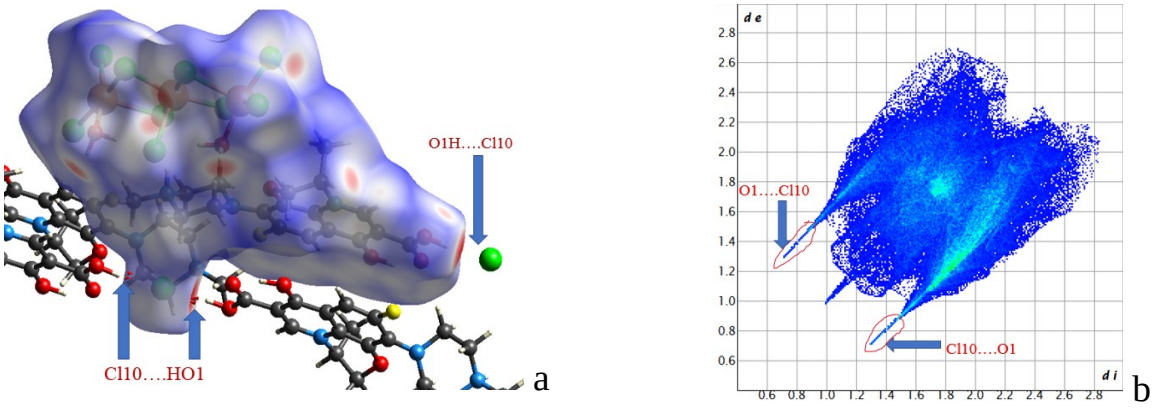
d

3-rasm. Levofloksatsinning mis (II) xlorid bilan hosil qilingan kompleks monokristalining molekulyar tuzilish (a), Xirshfeld sirtlari (b), Xirshfeld barmoq izi diagrammasi (c),

2D Xirshfeld barmoq izi grafigi (d)

LEV ning mis (II) xlorid bilan hosil qilingan kompleksning xirshfeld sirtida qizil rang eng yaqin ta’sirlashuvlarni va ko‘k rang eng uzoq ta’sirlashuvlarni ifodalaydi. Xirshfeld barmoq izi diagrammasi hamda kristall qadoqlashning shakllanishiga individual o‘zaro tasirlarning hissasini ko‘rsatuvchi d_e va d_i funksiyalari yordamida olingan ikki o‘lchamli barmoq izining grafiklari keltirilgan. Shunday qilib Xirshfeld sirtini tahlil qilish natijasida quyidagi tasirlashuvlar aniqlandi: H…Cl/Cl…H (50.9%), H…H (21.5%), H…O/O…H (8.0%), C…C (3.6%), H…C/C…H (3.4%), H…F/F…H (3.4%), O…C/C…O (2.2%), H…Cu/Cu…H (1.3%), F…O/O…F (1.2%), O…Cl/Cl…O (1.2%), F…C/C…F (0.8%), F…Cl/Cl…F (0.6%), H…N/N..H (0.4%), Cl…Cu/Cu…Cl (0.4%), O…N/N…O (0.4%), O…O (0.3%), Cl…C/C…Cl (0.2%), Cl…Cl (0.1%), Cl…N/N…Cl (0.1%) ta’sirlashuvlar kristall qadoqlashning shakllanishiga asosiy hissa qo‘shadi.

Xirshfeld sirt tahlilidan ko‘rinib turibdiki, o‘zaro ta’sirlarning asosiy qismini H…Cl/Cl…H (50.9%), H…H (21.5%) hamda O…H/H…O (8.0%) tashkil qiladi. Molekulalararo vodorod bog‘lanishning asosiy qismi O1H...Cl10 hamda Cl10…HO1 orasidagi bog‘lar hissasiga to‘g‘ri keladi.



4-rasm. Levofloksatsinning mis (II) xlorid bilan hosil qilingan kompleks monokristalining Xirshfeld sirtlarida molekulalararo kuchli vodorod bog‘lanishlar (a), 2D Xirshfeld barmoq izi kuchli vodorod bog‘lanish uchlari grafigi (b)

Xulosa.

Olib borilgan tadqiqotlar natijasida LEV asosida $[Cu_3Cl_9(H_2O)_2](LEV)Cl$ tarkibli yangi metallokompleks sintez qilindi. Sintez qilish uchun optimal sharoitlari o‘rganilib, reaksiya tenglamalari tuzildi. Sintez qilingan yangi metallokompleksning tarkibi, molekulyar va kristall tuzilishlari, rentgen tuzilish tahlili (RTT), IK-spektroskopiya tahlillari yordamida aniqlandi, Xirshfeld sirt tahlili Crystal Explorer 17.5 dasturi yordamida o‘rganildi.

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