PIRIDINNING KOBALT (II) XLODID KOMPLEKSI SINTEZI VA TADQIQOTI

Toshtemirov Abdurasul Erkin o’g’li
Termiz davlat universiteti doktoranti
To‘rayev Xayit Xudaynazarovich
Termiz davlat universiteti k.f.d., prof.
Ashurov Jamshid Mengnorovich
O‘zRFA O.S. Sodiqov nomidagi Bioorganik kimyo instituti, k.f.d., prof.
Umbarov Ibrohim Amanovich
Termiz davlat universiteti t.f.d., prof.
DJalilov Abdulaxat Turapovich
O‘zRFA akademigi, Toshkent kimyo-texnologiya ilmiy tadqiqot instituti k.f.d., prof.
E-mail: tosabdurasul20@gmail.com

Annotatsiya: *Ushbu tadqiqot ishida piridin va $CoCl_2$ yordamida yangi, bis(piperidin-1-yl-l3-chloraneyl)cobalt(IV)chloride $CoCl_4(C_5H_6N)_2$ tarkibli kompleks birikma sintez qilindi. Sintez qilingan kompleks birikmaning fizik-kimyoviy tadqiqot usullariga asoslanib tarkibi, kimyoviy formulasi va reaksiya tenglamalari taklif qilindi. IQ spektrlari va 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: *Kobalt (II) xlorid, piridin, xlorid kislota, IQ-spektr, UV yutilish spektri, vodorod bog‘lar geometriyasi.*

СИНТЕЗ И ИССЛЕДОВАНИЕ КОБАЛЬТ(II) ХЛОРИДНОГО КОМПЛЕКСА ПИРИДИНА

[1] Тоштемиров Абдурасул, [2]Тураев Хайит Худайназарович, [3]Ашуров Жамшид Менгнорович, [4]Умбаров Ибрагим Аманович, [5]Джалилов Абдулахат Турапович
[1] Термезский государственный университет докторант
[2]Термезский государственный университет д.х.н., проф.
[3]УзРФА Институт биоорганической химии имени О.С.Содиков д.х.н., проф.
[4]Термезский государственный университет т.х.н., проф.
[5]Академик АН РУз., директор Ташкентского научно-исследовательского института химической технологии д.х.н., проф.
E-mail: tosabdurasul20@gmail.com

Аннотация: В данной работе с использованием пиридина и $CoCl_2$ синтезирован новый бис(пиперидин-1-ил-13-хлоранил) хлоридкобальт (IV) комплекс $CoCl_4(C_5H_6N)_2$. На основе физико-химических методов исследования

предложены состав, химическая формула и уравнения реакций синтезированного комплексного соединения. Молекулярную массу, пространственную форму, расстояние между связями и валентные углы молекулы изучали с использованием, ИК-спектров, рентгеноструктурного анализа (РТТ) и расчетов методом DFT.

Ключевые слова: Хлорид кобальта(II), пиридин, соляная кислота, ИК-спектр, УФ-спектр поглощения, геометрия водородных связей.

STUDYING SYNTHESIS OF THE COBALT (II) CHLORIDE COMPLEX WITH PYRIDINE.

[1]Toshtemirov Abdurasul [2]Hayit Turaev [3]Jamshid Ashurov [4]Umbarov Ibrohim [5]Abdulahat Jalilov

[1]Termez State University doctoral student

[2]Termez State University Doctor of Chemical Sciences, professor

[3]Institute of Bioorganic Chemistry, Academy of Sciences of Uzbekistan Doctor of Chemical Sciences, professor

[4]Termez State University, Doctor of Technical Sciences, Professor

[5]Tashkent Chemical Technology Research Institute, Doctor of chemical sciences, prof., academician of the Academy of Sciences of the Republic of Uzbekistan

E-mail: tosabdurasul20@gmail.com

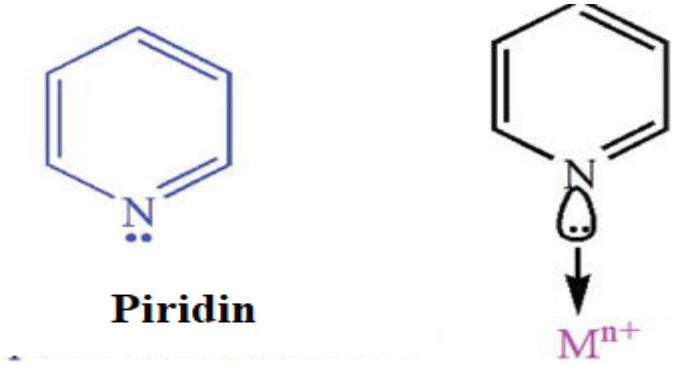
Abstract: *In this paper, a new bis(piperidin-1-yl-l3-chloraneyl)cobalt(IV) chloride $CoCl_4(C_5H_6N)_2$ complex was synthesized using pyridine and $CoCl_2$. Based on the physicochemical research methods, the composition, chemical formula, and reaction equations of the synthesized complex compound were proposed. The molecular mass, spatial shape, distance between bonds, and bond angles of the molecule were studied using, IR spectra, and X-ray structural analysis (RTT) and DFT calculations.*

Key words: *Cobalt (II) chloride, pyridine, hydrochloric acid, IR spectrum, UV absorption spectrum, geometry of hydrogen bonds.*

Kirish

So‘nggi yillarda kerakli fizik-kimyoviy va biologik xususiyatlarga ega bo‘lgan yangi koordinatsion birikmalarning sintezi va tavsifiga ilmiy qiziqish ortdi [1]. 3d metalli ionlari turli tirik organizmlarda mikroelement sifatida keng tarqalgan va ko‘plab muhim biokimyoviy jarayonlarda muhim rol o‘ynashi qayd etilgan [2]. Masalan, kobalt ioni B12 vitamini (kobalamin) shaklida bo‘lib, u muhim biokimyoviy birikma hisoblanadi. Biologik tizimdagi makromolekula va bizning hayotimiz uchun zarurdir. Kobaltning muhim hujayrali va biologik yo‘llar bilan bog‘lanishiga ishora qilib, ularning koordinatsion komplekslari bo‘yicha tadqiqotlar bir necha o‘n yillar oldin boshlangan [3].

Ba’zi kobalt (III) komplekslari. antiviral, antikanser, antibakterial, antifungal va antiparazitik xususiyatlar kabi tavsiya etilgan farmakologik xususiyatlar va ular dorivor kimyoda istiqbolli metall asosidagi dorilar nomzodlari sifatida o‘rganilmoqda [4-6]. Piridin va pirazin hosilalari farmatsevtika, parfyumeriya va qishloq xo‘jaligi kimyoviy moddalari uchun muhim komponentlar bo‘lgan eng muhim heterosiklik birikmalardir [7-8]. Piridin (py) keng tarqalgan va nisbatan kuchli s -donor ligand sifatida qaraladi . O‘zining azot atomidagi bog‘ hosil qilishda qatnashmagan juft elektron hisobiga turli xil metallar bilan kompleks hosil qiladi [9]. 1-rasm



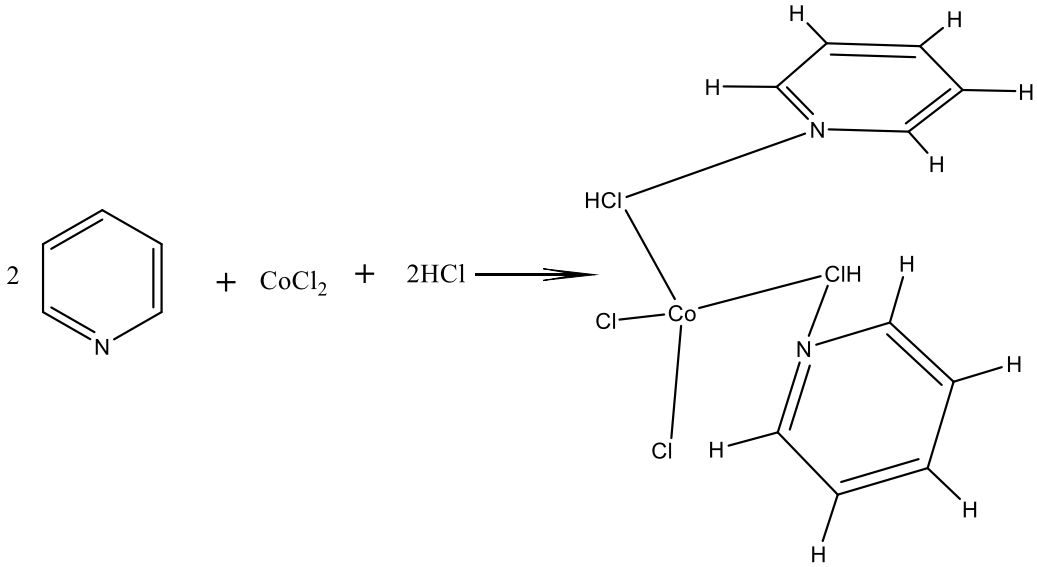
1-rasm. Piridin molekulasining tuzilishi formulasi.

Kristal maydon nazariyasida (CFT) ligandlarning spektrokimyoviy seriyasi, hujjat metall d-orbital bo‘linish mavzusiga tegishli ligandlar tartibini tasvirlaydi, piridinni o‘rtacha kuchli ligand tasvirlaydi [10]. Bu bitta piridin elektron juftining metall d-orbitallarga kuchli elektrostatik o‘zaro ta'sirini izohlaydi. Neytral bo‘lishiga qaramay, piridin o‘rta darajada katta d-orbital bo‘linishni hosil qiladi, bu esa metall markazlari bilan kuchli bog'lanish o‘zaro ta'sirini anglatadi [11].

Tajribaviy qism.

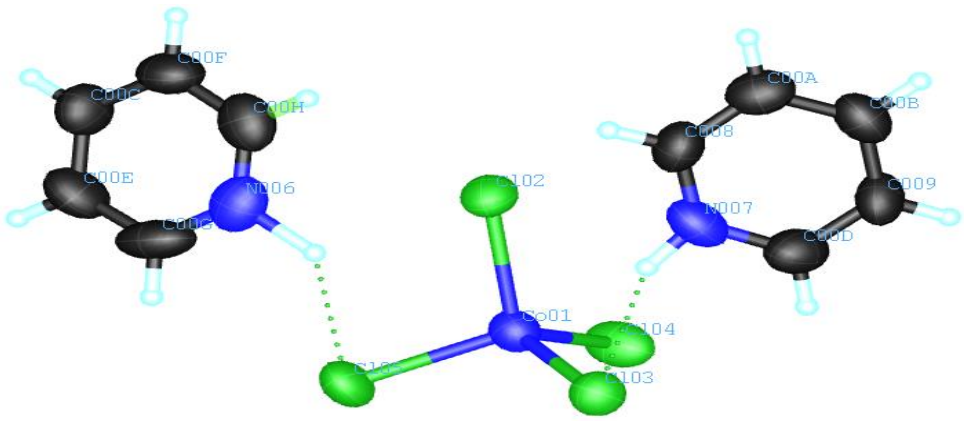
Ushbu tadqiqot ishini bajarishda ishlatiladigan moddalar va reagentlar tijorat manbalaridan («MEDXIMFARMSTROY») olingan.

$CoCl_4(C_5H_5N)_2$ kompleksi sintezi. Dastlab analitik tarozida kobalt (II) xlorid kristallogidratdan 0.002 mol (0,475 g) va piridindan 0,004 mol (0,3163g) tortib oldik. Kobaltning spirtli eritmasi va piridinning ham spirtli eritmasidan teng hajmda tayyorlandi [12]. Eritmalar aralashtirildi, ustidan 0,5 ml 30%li HCl kislota qo‘shildi va 25 ml teflon qoplamali zanglamaydigan po‘latdan yasalgan avtoklavga solinib 10 soat davomida bosim ostida 80 ^{0}C haroratda qizdirildi. Shundan so‘ng, reaktsiya tizimi asta-sekin xona haroratiga sovutildi. Eritma olinib bug‘latish uchun xona harotatida qoldirildi. 20 kundan so‘ng to‘q ko‘k rangli monokristallar bo‘lganini ko‘rdik.



Natijalar tahlili

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. Kompleksining tuzilishi.

Sintez qilingan kompleks birikmada quyi spin-elektron holati yuqori spin-elektron holatiga qaraganda yuqori energetik holatda bo‘ladi. Piridin halqasidagi azot atomida juft elektronlar hisobiga bog‘lanish faqat azot va xlor atomlari orqali amalga oshadi.

Vodorod fraksiyonel atom koordinatalari (Ch104) va ekvivalent izotropik siljish parametrlari (E2Ch103) . Ueq ortogonallashtirilgan Uij izining 1/3 qismi sifatida aniqlanadi.

1-jadval

Atom	x	y	z	*Ueq*
H(1)	6470(80)	3260(70)	5480(50)	40(20)
H(6)	9138.89	4207.52	5716.83	76

H(7)	11420.14	2363.02	6359.11	78
H(8)	11005.38	-308.24	6821.77	77
H(9)	8336.15	-1128.48	6558.8	75
H(10)	6115.04	766.42	5898.74	81
H(2)	6890(180)	5820(150)	1560(120)	300(80)
H(1A)	5844.27	7431.36	109.06	95
H(2A)	7450.73	8749.48	-1180.65	86
H(3)	10472.68	8651.94	-1118.23	80
H(4)	11834.92	7320.62	286.95	85
H(5)	10156.12	6000.12	1519.09	84

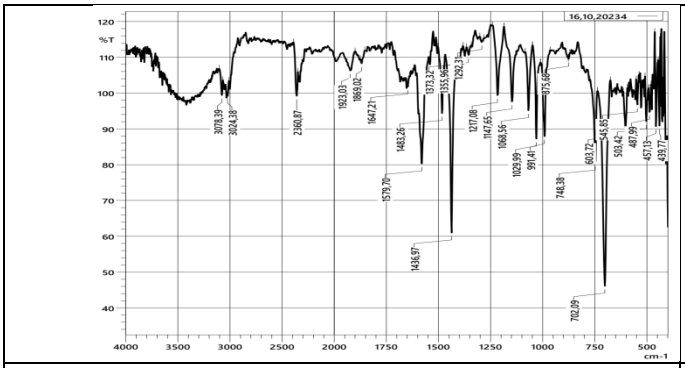
Anizotrop ko'chirish parametrlari (Ch104) . Anizotrop ko'chirish koeffitsienti ko'rsatkichi quyidagi ko'rinishga ega: $-2\pi^2[h^2a^{*2}U_{11}+ \dots +2hka^* Ч b^* Ч U_{12}]$

1-jadval

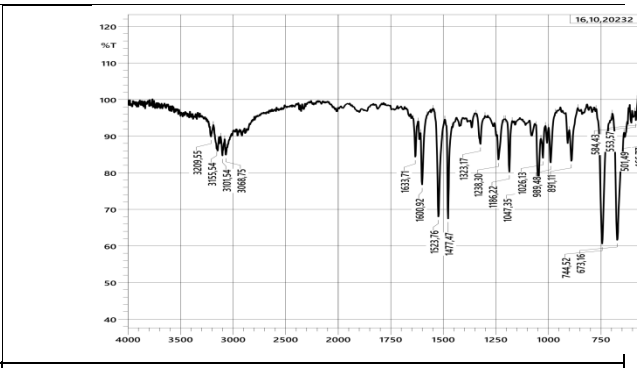
Atom	***U11***	***U22***	***U33***	***U23***	***U13***	***U12***
Co(1)	50.5(9)	45.2(8)	49.5(8)	-0.2(6)	-9.4(7)	-6.2(6)
Cl(1)	59.0(14)	72.6(16)	75.3(17)	24.7(12)	-19.7(13)	-3.8(12)
Cl(2)	56.0(13)	58.5(13)	53.2(13)	3.7(9)	-5.1(11)	-11.0(10)
Cl(3)	59.9(14)	57.5(13)	84.0(17)	-23.6(11)	-16.5(13)	-3.5(11)
Cl(4)	58.1(13)	57.0(13)	63.3(14)	4.6(10)	-17.6(11)	-21.1(10)
N(1)	59(5)	73(6)	59(5)	6(4)	-14(4)	6(4)
C(6)	74(7)	48(6)	68(6)	6(4)	-2(6)	-15(5)
C(7)	62(6)	70(7)	67(7)	-15(5)	-4(5)	-22(5)
C(8)	64(6)	62(6)	58(6)	3(4)	-10(5)	7(5)
C(9)	85(7)	50(5)	57(6)	12(4)	-22(5)	-17(5)
C(10)	62(6)	84(7)	61(6)	9(5)	-11(5)	-21(6)
N(2)	86(7)	48(5)	67(6)	-7(4)	7(5)	-12(5)
C(1)	45(6)	81(8)	112(10)	-24(6)	-3(6)	-16(5)
C(2)	71(7)	82(7)	60(7)	1(5)	-24(6)	1(6)
C(3)	78(7)	72(6)	50(6)	11(5)	-8(5)	-17(5)
C(4)	54(6)	73(7)	92(8)	-4(5)	-16(6)	-18(5)
C(5)	95(8)	48(6)	65(7)	-7(4)	-17(6)	-3(6)

3-rasmda piridinning IQ-spektri 500-800 sm^{-1} C-H gurulari va halqaning deformatsion tebranishi natijasida yuzaga kelgan. C-H guruhlari valent tebranishlari xuddi benzolnikiga o’xshash, 3000-3100 sm^{-1} sohada kuzatiladi. Piridin azot atomi va ushbu tipdagi N atomini tutgan birikmalar bog’lanmagan eletron jufti tufayli tarkibida suv molekulasini tutishi mumkin, buning natijasida 3200-3500 sm^{-1} sohada polosa

kuzatiladi. 4-rasmda Kompleksning IQ-spektri keltirilgan bunda 3209 sm^{-1} yuqori intensiv sohada ν(Ar)=N-H bog‘ining valent tebranishini ko’rishimiz mumkin.



3-rasm. Piridinning IQ-spektri



4-rasm. Kompleksning IQ-spektri

Xulosa. Ilk bor piridin bilan kobalt (II) xlorid kompleksi hosil qilindi va sintez sharoitlari o‘rganildi. Hosil qilingan $(C_5H_5NH)_2CoCl_4$ kompleksning IQ-spektri, RTT tahlili yordamida kompleks tuzilish formulalari, reaksiya tenglamalari va boshqa kristall parametrlari o‘rganildi.

FOYDADANILGAN ADABIYOTLAR:

1. S.A. Abalintsina, M.A. Conde, D.B. Eni, M.O. Agwara, Synthesis, characterization and antimicrobial properties of Cobalt(III), Nickel(III), Copper(II) and Zinc(II) complexes with pyridine and thiocyanate, Scientific African. 18 (2022) e01402. https://doi.org/10.1016/j.sciaf.2022.e01402.

2. X. Zheng, W. Cheng, C. Ji, J. Zhang, M. Yin, Detection of metal ions in biological systems: A review, Reviews in Analytical Chemistry. 39 (2020) 231–246. https://doi.org/10.1515/revac-2020-0118.

3. C.R. Munteanu, K. Suntharalingam, Advances in cobalt complexes as anticancer agents, Dalton Trans. 44 (2015) 13796–13808. https://doi.org/10.1039/C5DT02101D.

4. Pharmaceutics | Free Full-Text | Antibacterial Activity of Co(III) Complexes with Diamine Chelate Ligands against a Broad Spectrum of Bacteria with a DNA Interaction Mechanism, (n.d.). https://www.mdpi.com/1999-4923/13/7/946 (accessed October 17, 2023).

5. A. Mishra, N.K. Kaushik, A.K. Verma, R. Gupta, Synthesis, characterization and antibacterial activity of cobalt(III) complexes with pyridine–amide ligands, European Journal of Medicinal Chemistry. 43 (2008) 2189–2196. https://doi.org/10.1016/j.ejmech.2007.08.015.

6. S. Talebi, A. Abedi, V. Amani, Cobalt(II) complexes with small variations in the heterocycle ligand, crystal structure and DFT calculations, Journal of Molecular Structure. 1230 (2021) 129911. https://doi.org/10.1016/j.molstruc.2021.129911.

7. E.S. Tantawy, A.M. Amer, E.K. Mohamed, M.M. Abd Alla, M.S. Nafie, Synthesis, characterization of some pyrazine derivatives as anti-cancer agents: In vitro and in Silico approaches, Journal of Molecular Structure. 1210 (2020) 128013. https://doi.org/10.1016/j.molstruc.2020.128013.

8. A. Climova, E. Pivovarova, M. Szczesio, A. Olczak, J. Wojciechowski, K. Gobis, D. Ziembicka, A. Korga-Plewko, J. Kubik, M. Iwan, I. Korona-Głowniak, A. Czylkowska, Design of new Zn(II) pyrazine and pyridine derivatives based complexes as potential anticancer agents: from synthesis to structure, Polyhedron. 245 (2023) 116634. https://doi.org/10.1016/j.poly.2023.116634.

9. P. Matczak, Interplay between different metal–ligand binding modes in tin(II) complexes with pyridine, Computational and Theoretical Chemistry. 1226 (2023) 114192. https://doi.org/10.1016/j.comptc.2023.114192.

10. J.E. Huheey, E.A. Keiter, R.L. Keiter, Inorganic chemistry: principles of structure and reactivity, 4th ed, HarperCollins College Publishers, New York, NY, 1993. http://www.gbv.de/dms/bowker/toc/9780060429959.pdf (accessed October 17, 2023).

11. S. Pal, Pyridine: A Useful Ligand in Transition Metal Complexes, in: Pyridine, IntechOpen, 2018. https://doi.org/10.5772/intechopen.76986.

12. Termiz State University, A. Toshtemirov, K.K. Turaev, Termez State University, A.T. Jalilov, Stat Unitary Enterprise Tashkent Scientific Research Institute of Chemical Technology, I.A. Umbarov, Termiz State University, D. Ochilova, Termiz State University, SYNTHESIS AND INVESTIGATION OF LIGANDS BASED ON BENZOTRIAZOLE AND THIOCARBAMIDE., Theoretical & Applied Science. 116 (2022) 687–691. https://doi.org/10.15863/TAS.2022.12.116.57.