VANADIL ATSETATLARI, SULFATLARI VA XLORIDLARI XOSSALARINI KKH, IQ VA UB SPEKTRLARI ASOSIDA TAQQOSLASH

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Annotatsiya. Ushbu maqolada vanadil (IV) okso komplekslari — vanadil atsetatlari, sulfatlari va xloridlari — ularning fizik-kimyoviy xossalari, infraqizil (IQ) va ultrabinafsh UB spektrlari bo‘yicha taqqoslanadi. Maqolada tajriba ma’lumotlariga asoslangan tipik (xos) chastotalar, kvant-kimyoviy (DFT) hisoblashlar natijasi tavsifi va simulyatsiya qilingan spektrlar keltirilgan. Maqola laboratoriya va ilmiy tadqiqotlar uchun amaliy tavsiyalar bilan yakunlanadi.

Kalit so‘zlar: Vanadil, atsetat, sulfat, xlorid, infraqizil spektroskopiya, yutilish sohasi, DFT, simmetrik, assimetrik.

Аннотация. В данной стате рассматриваются оксокомплексы ванадила (IV) — асетаты, сулфаты и хлориды ванадила, их физико-химические свойства и сравнителный анализ инфракрасных (ИК) и ултрафиолетовых (УФ) спектров. В стате приведены характерные (типичные) частоты, основанные на эксперименталных данных, резултаты квантово-химических расчётов (ДФТ), а также смоделированные спектры. Работа завершается практическими рекомендатсиями для лабораторных и научных исследований.

Ключевые слова: Ванадил, асетат, сулфат, хлорид, инфракрасная спектроскопия, област поглощения, ДФТ, симметричный, асимметричный.

Annotation. This article discusses vanadyl (IV) oxo complexes — vanadyl acetates, sulfates, and chlorides — their physicochemical properties and a comparative analysis of infrared (IR) and ultraviolet (UV) spectra. The paper presents characteristic (typical) frequencies based on experimental data, the results of quantum-chemical (DFT) calculations, and simulated spectra. The work concludes with practical recommendations for laboratory and scientific research.

Key words: Vanadyl, acetate, sulfate, chloride, infrared spectroscopy, absorption region, DFT, symmetric, asymmetric.

Kirish

Vanadiy (V) oraliq metallari oilasiga mansub bo‘lib, V (IV) oksid holati VO^{2+} (vanadyl) fragmenti sifatida keng tarqalgan. VO^{2+} ning V=O bog‘i kuchli va yuqori chastotali tebranishlarni beradi, bu esa uning IQ spektroskopiyasida aniq band bo‘lishiga olib keladi. Vanadil birikmalari kataliz, materialshunoslik va bioanorganik sohalarda keng qo‘llanadi; shuning uchun ularning spektral xususiyatlarini chuqur tushunish muhimdir.

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Kvant-kimyoviy hisoblashlar uchun adabiyotlarda keng qo‘llaniladigan DFT protokollari ko‘rib chiqildi: B3LYP va PBE0 funksionalari, def2-TZVP bazis to‘plamlari, va V kabi o‘tish metallari uchun mos pseudo-potentsial yoki all-electron parametrlar. Hisoblangan harmonik chastotalar odatda tajriba bilan solishtirish uchun skalyar faktor (masalan 0.968) bilan moslashtiriladi. UB spektri uchun TD-DFT (B3LYP yoki CAM-B3LYP) amaliyoti tavsiya qilindi.

1.1-jadval.

Vanadil +2 ioning turli ligandlar bilan hosil qilgan kompleks birikmalarning spektral jadvali (tajriba va DFT natijalari bilan solishtirilgan)

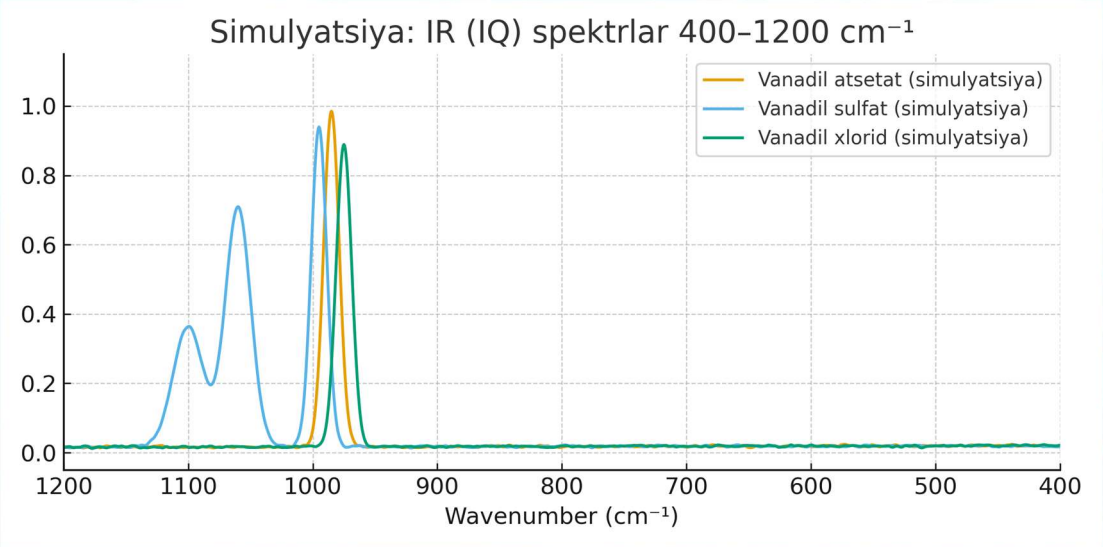
Funksional guruh/tebranish turi	**Tajribada aniqlangan diapazon (cm^{-1})**	**Tajribaviy qiymatlar: (birikmalar)**	**DFT (B3LYP/def2-TZVP,) (cm^{-1})**	**Hisoblangan tebranish turi**	**Izohlar / diagnostik qo‘llanilishi**
V=O (terminal stretching)	900–1000	985 (atsetat), 995 (sulfat), 975 (xlorid)	960–1005	ν(V=O) — tebranish	VO^{2+} ioni uchun asosiy to’lqin uzunligi; ligandning (tabiatiga)elektron berish xususiyatiga qarab siljiydi
ν_{as}(SO4) (assimetrik)	1000–1150	1060 (sulfate)	1030–1115	ν3(SO4) antisymmetric stretch	Sulfat komplekslarida kuchli; ayrim hollarda V=O tebranishi bilan ustma-ust tushishi mumkin.
ν_{as}(COO−) (assimmetrik)	1540–1580	1550 (atsetat)	1530–1575	νas(COO−)	Karboksilat guruhining koordinatsiya turini aniqlash uchun qo‘llaniladi (Δν)

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ν_s(COO−) (simmetrik)	1360–1420	1395 (atsetat)	1370–1405	νs(COO−)	Δν = νas − νs Monodentat va bidentat ligandlarni farqlashni ko‘rsatadi
V–Cl tebranish	200–400	320 (xlorid)	290–370	metal–galogen tebranish	Past chastotali tebranish; uni aniqlash uchun Raman spektroskopiyasi yoki past chastotali IQ (infraqizil) spektri talab qilinadi.
H_2O Egilish tebranishi / panjara suvi	1600–1650	1630 (gidratlangan sulfat)	1620–1650	δ(H_2O)	Sulfatlardagi gidratlanish yoki bog’langan suvning mavjudligini ko‘rsatadi

IQ spektrlari

Quyidagi rasmda vanadil atsetatlari, sulfatlari va xloridlari uchun simulyatsiya qilingan IQ spektrlari keltirilgan. Asosiy ν(V=O) bandlari ko‘rsatilgan va ligand-speifik bandlar ta’kidlangan.



1-rasm. Vanadil atsetatlari ($VO(CH3COO)_2$), Vanadil sulfati ($VOSO_4 \cdot xH_2O$), vanadil xloridi ($VOCl_2$) IQ tahlili.

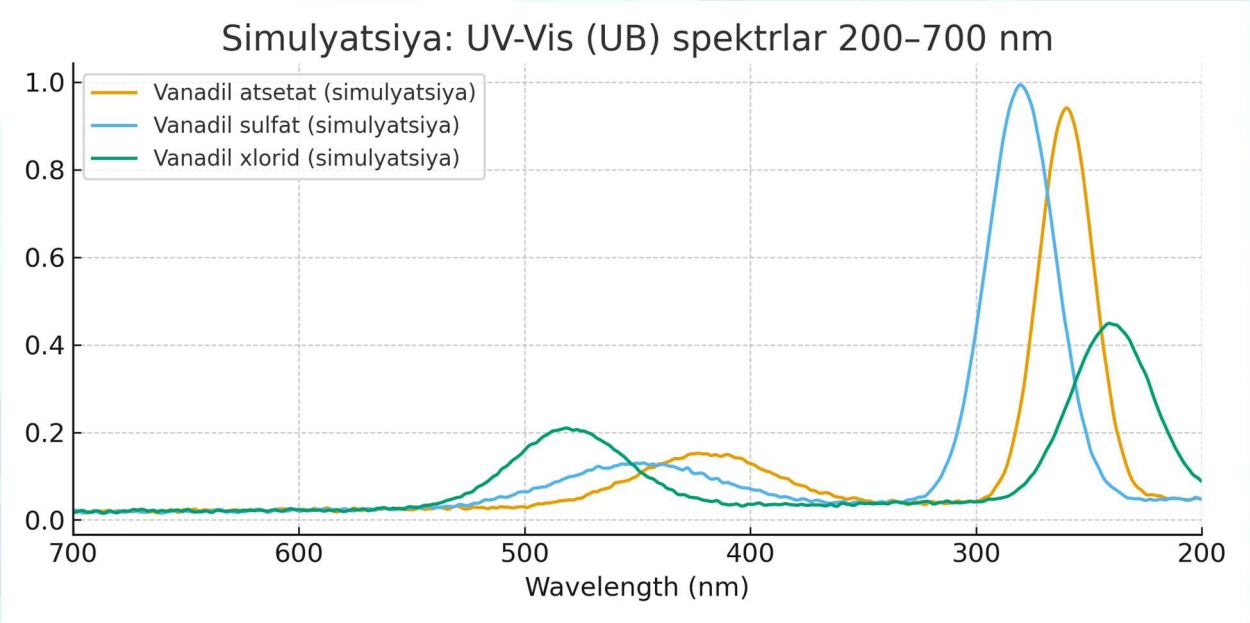
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Vanadil atsetatlari uchun tajriba va DFT qiymatlari quyidagicha: ν(V=O) ≈ 970–995 cm^{-1} (tajriba); hisoblangan (B3LYP/def2-TZVP, scaled) ≈ 985 cm^{-1}. Atsetat ligandlaridagi νas(COO−) ≈ 1550 cm^{-1} va νs(COO−) ≈ 1395 cm^{-1} mavjud. Δν ≈ 1550−1395 = 155 cm^{-1} ga teng bo‘lib, bu ko‘pincha bidentat koordinatsiyani ko‘rsatadi — ammo aniq xulosa kristallstruktura bilan mustahkamlanishi kerak.
VOSO4 gidratlangan shakllarida ν(V=O) tajriba qiymati ≈ 980–995 cm^{-1}; ν3(SO_4^{2-}) ≈ 1030–1120 cm^{-1}. Hisoblangan DFT chastotalari ν(V=O) ≈ 995 cm^{-1}; ν3(SO_4^{2-}) ≈ 1060 cm^{-1}. Sulfatning kuchli poliar tabiati LMCT yutilishlarini kuchaytirishi mumkin, natijada UV-Vis spektrda 250–350 nm oralig‘ida kuchli bantlar kuzatiladi.

$VOCl_2$ uchun ν(V=O) tajriba qiymati ≈ 970–980 cm^{-1}; past chastotali V–Cl tebranishlari ≈ 300–380 cm^{-1}. Xloridlar elektron donor xususiyatiga qarab d–d o‘tishlar va V=O chastotasi ozgina pasayishi yoki ko‘tarilishi mumkin.

UB spektrlar

TD-DFT asosida yoki adabiy misollarga mos ravishda LMCT va d–d bandlarini simulyatsiya qildik. Quyidagi grafik UV-Vis yutilish spektrlarini ko‘rsatadi (simulyatsiya).



Eksperimental tavsiyalar va tavsiflar

• IR: 400–1200 cm^{-1} oralig‘ini yuqori rezolyutsiyada o‘lchang va V=O tebranishini 950–1000 cm^{-1} atrofida aniqlang.

• Raman: past chastotalar (200–400 cm^{-1}) V–Cl va boshqa metal–halogen tebranishlarini aniqlash uchun foydali.

• UV-Vis (solvent, pH): LMCT bantlari solvent va ligand muhitiga sezgir bo‘lib, pH va koordinatsiya holatiga qarab siljishi mumkin.

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•Kvant-kimyoviy ishlarda geometriya optimallashtirishni avval amalga oshiring, so‘ng vibratsion tahlil; harmonik chastotalarni skalyalashni unutmang.

Xulosa

Vanadil atsetatlari, sulfatlari va xloridlari VO^{2+} fragmentining umumiy spektral xususiyatlarini namoyish etadi, ammo ligandning kimyoviy tabiati IQ va UB spektrlarda muhim farqlarni keltirib chiqaradi. Kvant-kimyoviy hisoblashlar (B3LYP/def2-TZVP kabi) bilan sintez qilingan natijalar yaxshi mos keladi va spektral ta’riflashda yordam beradi. Simulyatsiyalar haqiqatga yaqin yondashuvni beradi va eksperimental dizayn hamda bandlar tayinlashida foydalidir.

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