Supplementary Material

Synthesis, Crystal Structures and Urease Inhibition of Ni(II) complexes Constructed from Schiff bases with 2,2′-bipyridine as co-ligands

Wen-yang Liu[1†] Hong-lei Li[2†], Jiang-song Jia[1],Wen-ming Zhao[1] and Jun Sun [1,*]

[1]Department of Pharmacy, Henan Provincial People's Hospital; People's Hospital of Zhengzhou University; People's Hospital of Henan University, Zhengzhou, Henan ,450003, China;
[2]Department of Pharmacy, Kangda College of Nanjing Medical University, Lianyungang, 222000, China;
*Correspondence: SJun@zzu.edu.cn; Tel.: (86-371-65580213)
† These authors contributed equally to this work

1. Structure Tables

	C1	C2	C3
CCDC number	2524848	2524939	2524846
Empirical formula	$C_{28}H_{29}Cl_2N_3NiO_6$	$C_{17}H_{21}Cl_2NNiO_7$	$C_{52}H_{44}Cl_4N_6Ni_2O_9$
Formula weight	633.15	480.96	1155.14
Temperature [K]	115.0	116.0	302.00
Crystal system	triclinic	orthorhombic	triclinic
Space group (number)	$P\bar{1}$ (2)	$P2_12_12_1$ (19)	$P\bar{1}$ (2)
***a* [Å]**	9.4508(6)	7.0996(8)	11.081(4)
***b* [Å]**	11.9832(8)	7.9070(9)	15.530(5)
***c* [Å]**	13.2510(7)	35.205(4)	16.391(4)
α [°]	86.307(2)	90	68.900(7)
β [°]	81.250(2)	90	80.093(8)
γ [°]	69.766(2)	90	81.532(10)
Volume [Å³]	1391.58(15)	1976.3(4)	2581.1(14)
Z	2	4	2
ρ_{calc} [gcm⁻³]	1.511	1.616	1.486
μ [mm⁻¹]	0.937	1.292	0.999
***F*(000)**	656	992	1186
Crystal size [mm³]	0.15×0.11×0.1	0.12×0.11×0.09	0.13×0.1×0.08
Crystal colour	clear greenish colourless	clear greenish colourless	clear greenish green
Crystal shape	block	block	block
Radiation	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)
2θ range [°]	4.81 to 55.05 (0.77 Å)	4.63 to 55.00 (0.77 Å)	4.32 to 53.20 (0.79 Å)
Index ranges	−12 ≤ h ≤ 12	−9 ≤ h ≤ 9	−13 ≤ h ≤ 13
	−15 ≤ k ≤ 15	−10 ≤ k ≤ 10	−19 ≤ k ≤ 19
	−17 ≤ l ≤ 14	−45 ≤ l ≤ 45	−17 ≤ l ≤ 20
Reflections collected	27259	25127	39813
Independent reflections	6363	4541	10693
	R_{int} = 0.0785	R_{int} = 0.0887	R_{int} = 0.1654
	R_{sigma} = 0.0642	R_{sigma} = 0.0692	R_{sigma} = 0.1590
Completeness to θ = 25.242°	99.7 %	100.0 %	99.7 %
Data / Restraints / Parameters	6363/0/477	4541/15/246	10693/367/721
Absorption correction	0.5397/0.7456	0.5397/0.7456	0.6624/0.7454
T_{min}/T_{max} (method)	(multi-scan)	(multi-scan)	(multi-scan)
Goodness-of-fit on F^2	1.075	1.210	1.001
Final *R* indexes	R_1 = 0.0434	R_1 = 0.0815	R_1 = 0.0689
[$I \geq 2\sigma(I)$]	wR_2 = 0.0815	wR_2 = 0.1742	wR_2 = 0.1508
Final *R* indexes	R_1 = 0.0600	R_1 = 0.0911	R_1 = 0.1753
[all data]	wR_2 = 0.0996	wR_2 = 0.1806	wR_2 = 0.2063
Largest peak/hole [eÅ⁻³]	0.46/−0.60	1.58/−1.18	0.62/−0.56
Flack X parameter	---	0.12(5)	---
Extinction coefficient	---	---	---

Table 11.-1 Atomic coordinates and U_{eq} [Å²] for C1

Atom	*x*	*y*	*z*	U_{eq}
Ni1	0.47182(4)	0.72784(3)	0.83948(2)	0.01626(10)
Cl1	0.71311(8)	0.74442(7)	0.28820(5)	0.02772(17)
Cl2	0.68531(9)	0.99019(6)	0.62109(5)	0.02716(17)
O1	0.5791(2)	0.81129(16)	0.73324(13)	0.0190(4)

O2	0.6832(2)	0.63135(18)	0.88378(16)	0.0214(4)
O3	0.3641(2)	0.62178(16)	0.92913(13)	0.0189(4)
O4	0.3076(2)	0.45547(16)	0.92512(14)	0.0218(4)
N1	0.5013(2)	0.59992(18)	0.73850(16)	0.0172(4)
N2	0.4126(2)	0.85016(19)	0.95655(16)	0.0176(4)
N3	0.2653(2)	0.85032(19)	0.80211(16)	0.0167(4)
C1	0.6044(3)	0.7929(2)	0.63642(19)	0.0174(5)
C2	0.6569(3)	0.8722(2)	0.5677(2)	0.0196(5)
C3	0.6867(3)	0.8604(3)	0.4637(2)	0.0223(6)
C4	0.6693(3)	0.7642(2)	0.42010(19)	0.0204(6)
C5	0.6207(3)	0.6840(2)	0.4801(2)	0.0189(5)
C6	0.5867(3)	0.6961(2)	0.58701(19)	0.0174(5)
C7	0.5404(3)	0.6036(2)	0.6421(2)	0.0180(5)
C8	0.3724(3)	0.5262(2)	0.88776(19)	0.0176(5)
C12	0.4712(3)	0.4946(2)	0.7841(2)	0.0185(5)
C13	0.6221(3)	0.3950(2)	0.8019(2)	0.0216(6)
C14	0.7254(3)	0.3520(2)	0.7037(2)	0.0187(5)
C15	0.8441(3)	0.3948(3)	0.6702(2)	0.0234(6)
C16	0.9367(3)	0.3587(3)	0.5780(2)	0.0309(7)
C17	0.9103(4)	0.2790(3)	0.5183(2)	0.0303(7)
C18	0.7923(3)	0.2366(3)	0.5497(2)	0.0255(6)
C19	0.7001(3)	0.2727(2)	0.6427(2)	0.0209(6)
C20	0.2027(3)	0.8494(3)	0.7185(2)	0.0220(6)
C21	0.0784(3)	0.9420(3)	0.6914(2)	0.0255(6)
C22	0.0164(3)	1.0400(3)	0.7531(2)	0.0269(6)
C23	0.0791(3)	1.0427(3)	0.8401(2)	0.0245(6)
C24	0.2040(3)	0.9465(2)	0.8628(2)	0.0182(5)
C25	0.2821(3)	0.9430(2)	0.95261(19)	0.0179(5)
C26	0.2249(3)	1.0292(3)	1.0280(2)	0.0232(6)
C27	0.3062(3)	1.0201(3)	1.1090(2)	0.0234(6)
C28	0.4385(3)	0.9251(3)	1.1135(2)	0.0237(6)
C29	0.4878(3)	0.8423(2)	1.0359(2)	0.0202(5)
H2A	0.755(5)	0.664(4)	0.870(3)	0.061(13)
H2B	0.694(4)	0.594(3)	0.941(3)	0.051(12)
H3	0.717(3)	0.913(2)	0.4229(19)	0.006(6)
H5	0.608(3)	0.618(3)	0.452(2)	0.016(7)
H7	0.538(3)	0.537(3)	0.599(2)	0.020(7)
H12	0.419(3)	0.461(2)	0.740(2)	0.015(7)
H13A	0.672(3)	0.424(2)	0.848(2)	0.014(7)
H13B	0.587(3)	0.332(3)	0.834(2)	0.025(8)
H15	0.863(3)	0.446(2)	0.715(2)	0.011(7)
H16	1.017(4)	0.388(3)	0.556(2)	0.027(8)
H17	0.970(4)	0.259(3)	0.456(3)	0.040(10)
H18	0.771(4)	0.181(3)	0.507(3)	0.048(10)
H19	0.620(4)	0.244(3)	0.662(2)	0.032(9)
H20	0.246(3)	0.783(3)	0.679(2)	0.024(8)
H21	0.042(4)	0.935(3)	0.629(3)	0.034(9)
H22	−0.070(4)	1.107(3)	0.737(2)	0.029(8)
H23	0.041(3)	1.108(3)	0.885(2)	0.021(8)
H26	0.132(4)	1.096(3)	1.024(2)	0.033(9)
H27	0.274(3)	1.076(2)	1.159(2)	0.012(7)
H28	0.495(3)	0.916(3)	1.167(2)	0.023(8)
H29	0.577(3)	0.774(3)	1.037(2)	0.020(7)

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

Table 1-12. Anisotropic displacement parameters [Å^2] for C1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2(a^*)^2U_{11} + k^2(b^*)^2U_{22} + \ldots + 2hka^*b^*U_{12}\,]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ni1	0.01802(18)	0.01568(18)	0.01435(17)	0.00008(12)	−0.00183(12)	−0.00503(14)
Cl1	0.0330(4)	0.0344(4)	0.0153(3)	0.0017(3)	0.0001(3)	−0.0127(3)
Cl2	0.0380(4)	0.0248(4)	0.0244(3)	0.0005(3)	−0.0044(3)	−0.0179(3)
O1	0.0251(10)	0.0197(9)	0.0140(9)	0.0008(7)	−0.0012(7)	−0.0106(8)
O2	0.0191(10)	0.0227(10)	0.0216(10)	0.0039(8)	−0.0037(8)	−0.0062(8)
O3	0.0221(10)	0.0181(9)	0.0168(9)	−0.0011(7)	0.0009(7)	−0.0085(8)
O4	0.0263(10)	0.0231(10)	0.0182(9)	0.0015(8)	−0.0004(8)	−0.0127(8)
N1	0.0176(11)	0.0134(11)	0.0176(11)	0.0002(8)	−0.0025(8)	−0.0015(9)
N2	0.0207(11)	0.0162(11)	0.0159(11)	−0.0008(8)	−0.0035(8)	−0.0058(9)
N3	0.0156(11)	0.0167(11)	0.0168(11)	−0.0024(8)	−0.0019(8)	−0.0039(9)
C1	0.0179(13)	0.0165(13)	0.0180(13)	0.0015(10)	−0.0040(10)	−0.0057(10)
C2	0.0224(14)	0.0157(13)	0.0211(13)	0.0018(10)	−0.0037(10)	−0.0073(11)
C3	0.0227(14)	0.0251(15)	0.0185(13)	0.0065(11)	−0.0010(11)	−0.0094(12)
C4	0.0202(14)	0.0254(14)	0.0129(12)	−0.0005(10)	−0.0006(10)	−0.0049(11)
C5	0.0188(13)	0.0169(13)	0.0192(13)	−0.0023(10)	−0.0033(10)	−0.0032(11)
C6	0.0169(13)	0.0190(13)	0.0167(13)	0.0038(10)	−0.0050(10)	−0.0063(11)
C7	0.0174(13)	0.0169(13)	0.0191(13)	−0.0005(10)	−0.0038(10)	−0.0046(11)
C8	0.0180(13)	0.0164(13)	0.0163(12)	0.0012(10)	−0.0023(10)	−0.0033(10)
C12	0.0240(14)	0.0152(13)	0.0171(13)	−0.0018(10)	0.0011(10)	−0.0089(11)
C13	0.0275(15)	0.0157(13)	0.0199(14)	0.0019(11)	−0.0028(11)	−0.0057(12)
C14	0.0181(13)	0.0134(12)	0.0211(13)	0.0010(10)	−0.0046(10)	−0.0004(10)
C15	0.0215(14)	0.0258(15)	0.0240(15)	−0.0004(12)	−0.0052(11)	−0.0085(12)
C16	0.0222(15)	0.0309(17)	0.0380(18)	0.0039(13)	0.0006(13)	−0.0098(13)
C17	0.0308(17)	0.0292(16)	0.0243(16)	−0.0020(13)	0.0030(13)	−0.0043(13)
C18	0.0317(16)	0.0242(15)	0.0202(14)	0.0002(11)	−0.0033(12)	−0.0093(13)
C19	0.0187(14)	0.0167(13)	0.0245(14)	0.0017(11)	−0.0036(11)	−0.0028(11)
C20	0.0213(14)	0.0201(14)	0.0219(14)	−0.0026(11)	−0.0031(11)	−0.0031(11)
C21	0.0246(15)	0.0270(15)	0.0245(15)	−0.0020(12)	−0.0076(12)	−0.0062(12)
C22	0.0253(15)	0.0217(15)	0.0292(16)	0.0010(12)	−0.0107(12)	0.0004(12)
C23	0.0252(15)	0.0205(14)	0.0256(15)	−0.0036(12)	−0.0042(11)	−0.0040(12)
C24	0.0166(13)	0.0187(13)	0.0198(13)	0.0020(10)	−0.0008(10)	−0.0078(11)
C25	0.0209(13)	0.0156(13)	0.0175(13)	0.0008(10)	−0.0010(10)	−0.0073(11)
C26	0.0246(15)	0.0199(14)	0.0229(14)	−0.0024(11)	−0.0025(11)	−0.0046(12)
C27	0.0335(16)	0.0206(14)	0.0168(13)	−0.0042(11)	−0.0007(11)	−0.0104(12)
C28	0.0322(16)	0.0240(15)	0.0163(13)	0.0006(11)	−0.0074(11)	−0.0098(12)
C29	0.0215(14)	0.0181(13)	0.0205(13)	0.0025(10)	−0.0034(10)	−0.0064(11)

Table1- 13. Bond lengths and angles for 1

Atom–Atom	Length [Å]
Ni1–O1	2.0239(17)
Ni1–O2	2.084(2)
Ni1–O3	2.0966(17)
Ni1–N1	2.018(2)
Ni1–N2	2.081(2)
Ni1–N3	2.105(2)
Cl1–C4	1.746(3)
Cl2–C2	1.738(3)
O1–C1	1.288(3)
O2–H2A	0.89(4)
O2–H2B	0.85(4)
O3–C8	1.274(3)
O4–C8	1.246(3)
N1–C7	1.277(3)
N1–C12	1.461(3)
N2–C25	1.350(3)
N2–C29	1.336(3)
N3–C20	1.335(3)
N3–C24	1.352(3)
C1–C2	1.434(3)
C1–C6	1.437(4)
C2–C3	1.370(4)
C3–C4	1.391(4)

C3–H3	0.90(3)
C4–C5	1.365(4)
C5–C6	1.410(4)
C5–H5	0.95(3)
C6–C7	1.445(3)
C7–H7	1.02(3)
C8–C12	1.528(3)
C12–C13	1.550(4)
C12–H12	1.00(3)
C13–C14	1.505(4)
C13–H13A	0.98(3)
C13–H13B	0.98(3)
C14–C15	1.391(4)
C14–C19	1.389(4)
C15–C16	1.389(4)
C15–H15	0.96(3)
C16–C17	1.387(4)
C16–H16	0.94(3)
C17–C18	1.378(4)
C17–H17	0.92(3)
C18–C19	1.395(4)
C18–H18	0.99(4)
C19–H19	0.93(3)
C20–C21	1.384(4)
C20–H20	0.91(3)
C21–C22	1.376(4)
C21–H21	0.96(3)
C22–C23	1.382(4)
C22–H22	0.97(3)
C23–C24	1.391(4)
C23–H23	0.95(3)
C24–C25	1.484(4)
C25–C26	1.393(4)
C26–C27	1.390(4)
C26–H26	0.96(3)
C27–C28	1.376(4)
C27–H27	0.91(3)
C28–C29	1.387(4)
C28–H28	0.93(3)
C29–H29	0.95(3)

Atom–Atom–Atom	**Angle [°]**
O1–Ni1–O2	88.18(8)
O1–Ni1–O3	170.15(7)
O1–Ni1–N2	98.72(8)
O1–Ni1–N3	87.29(8)
O2–Ni1–O3	92.68(8)
O2–Ni1–N3	170.44(8)
O3–Ni1–N3	93.22(8)
N1–Ni1–O1	90.29(8)
N1–Ni1–O2	89.55(8)
N1–Ni1–O3	79.90(8)
N1–Ni1–N2	170.40(9)
N1–Ni1–N3	98.89(8)
N2–Ni1–O2	94.02(8)
N2–Ni1–O3	91.01(8)
N2–Ni1–N3	78.37(8)
C1–O1–Ni1	125.70(16)
Ni1–O2–H2A	117(3)
Ni1–O2–H2B	124(3)
H2A–O2–H2B	108(4)
C8–O3–Ni1	115.47(16)
C7–N1–Ni1	126.85(18)
C7–N1–C12	119.0(2)
C12–N1–Ni1	114.19(16)
C25–N2–Ni1	115.69(17)
C29–N2–Ni1	126.18(18)
C29–N2–C25	118.1(2)
C20–N3–Ni1	126.30(18)
C20–N3–C24	118.2(2)
C24–N3–Ni1	114.83(17)
O1–C1–C2	120.0(2)
O1–C1–C6	126.0(2)
C2–C1–C6	114.1(2)
C1–C2–Cl2	117.2(2)
C3–C2–Cl2	118.4(2)
C3–C2–C1	124.4(2)
C2–C3–C4	119.1(2)
C2–C3–H3	121.9(16)
C4–C3–H3	119.0(16)
C3–C4–Cl1	119.9(2)
C5–C4–Cl1	119.7(2)
C5–C4–C3	120.3(2)
C4–C5–C6	121.3(2)
C4–C5–H5	121.4(17)
C6–C5–H5	117.2(17)
C1–C6–C7	123.2(2)
C5–C6–C1	120.8(2)
C5–C6–C7	116.0(2)
N1–C7–C6	125.5(2)
N1–C7–H7	118.1(16)
C6–C7–H7	116.3(16)
O3–C8–C12	117.6(2)
O4–C8–O3	125.5(2)
O4–C8–C12	117.0(2)
N1–C12–C8	109.5(2)
N1–C12–C13	110.5(2)
N1–C12–H12	113.0(16)
C8–C12–C13	107.7(2)
C8–C12–H12	108.9(16)
C13–C12–H12	107.0(16)
C12–C13–H13A	109.1(16)
C12–C13–H13B	102.7(18)
C14–C13–C12	112.4(2)
C14–C13–H13A	111.4(16)
C14–C13–H13B	110.1(18)
H13A–C13–H13B	111(2)
C15–C14–C13	120.6(2)

C19–C14–C13	120.6(2)
C19–C14–C15	118.8(2)
C14–C15–H15	117.7(16)
C16–C15–C14	120.9(3)
C16–C15–H15	121.2(16)
C15–C16–H16	120.7(19)
C17–C16–C15	119.5(3)
C17–C16–H16	119.7(19)
C16–C17–H17	118(2)
C18–C17–C16	120.3(3)
C18–C17–H17	122(2)
C17–C18–C19	120.0(3)
C17–C18–H18	121(2)
C19–C18–H18	119(2)
C14–C19–C18	120.5(3)
C14–C19–H19	121(2)
C18–C19–H19	118(2)
N3–C20–C21	123.1(3)
N3–C20–H20	116.1(19)
C21–C20–H20	120.7(19)
C20–C21–H21	118(2)
C22–C21–C20	118.6(3)
C22–C21–H21	124(2)
C21–C22–C23	119.2(3)

C21–C22–H22	122.0(19)
C23–C22–H22	118.8(19)
C22–C23–C24	119.2(3)
C22–C23–H23	122.6(18)
C24–C23–H23	118.3(18)
N3–C24–C23	121.7(3)
N3–C24–C25	115.3(2)
C23–C24–C25	123.0(2)
N2–C25–C24	115.5(2)
N2–C25–C26	122.1(2)
C26–C25–C24	122.4(2)
C25–C26–H26	121(2)
C27–C26–C25	118.8(3)
C27–C26–H26	120.0(19)
C26–C27–H27	121.4(17)
C28–C27–C26	119.1(3)
C28–C27–H27	119.5(17)
C27–C28–C29	118.8(3)
C27–C28–H28	120.9(18)
C29–C28–H28	120.3(18)
N2–C29–C28	123.1(3)
N2–C29–H29	115.3(17)
C28–C29–H29	121.5(17)

Table1- 14. Torsion angles for C1

Atom–Atom–Atom–Atom	Torsion Angle [°]
Ni1–O1–C1–C2	168.86(18)
Ni1–O1–C1–C6	−11.9(4)
Ni1–O3–C8–O4	−174.8(2)
Ni1–O3–C8–C12	5.8(3)
Ni1–N1–C7–C6	6.8(4)
Ni1–N1–C12–C8	20.1(3)
Ni1–N1–C12–C13	−98.4(2)
Ni1–N2–C25–C24	−2.5(3)
Ni1–N2–C25–C26	177.3(2)
Ni1–N2–C29–C28	−177.4(2)
Ni1–N3–C20–C21	−170.2(2)
Ni1–N3–C24–C23	171.4(2)
Ni1–N3–C24–C25	−6.9(3)
Cl1–C4–C5–C6	179.0(2)
Cl2–C2–C3–C4	177.9(2)
O1–C1–C2–Cl2	0.6(3)
O1–C1–C2–C3	−179.9(3)
O1–C1–C6–C5	−178.8(2)
O1–C1–C6–C7	−1.5(4)
O3–C8–C12–N1	−17.0(3)
O3–C8–C12–C13	103.3(3)
O4–C8–C12–N1	163.6(2)
O4–C8–C12–C13	−76.2(3)
N1–C12–C13–C14	−63.5(3)
N2–C25–C26–C27	0.9(4)

N3–C20–C21–C22	0.2(4)
N3–C24–C25–N2	6.3(3)
N3–C24–C25–C26	−173.5(2)
C1–C2–C3–C4	−1.6(4)
C1–C6–C7–N1	4.4(4)
C2–C1–C6–C5	0.4(4)
C2–C1–C6–C7	177.7(2)
C2–C3–C4–Cl1	−177.8(2)
C2–C3–C4–C5	1.1(4)
C3–C4–C5–C6	0.1(4)
C4–C5–C6–C1	−0.9(4)
C4–C5–C6–C7	−178.3(2)
C5–C6–C7–N1	−178.2(2)
C6–C1–C2–Cl2	−178.70(19)
C6–C1–C2–C3	0.8(4)
C7–N1–C12–C8	−159.0(2)
C7–N1–C12–C13	82.5(3)
C8–C12–C13–C14	176.9(2)
C12–N1–C7–C6	−174.3(2)
C12–C13–C14–C15	98.0(3)
C12–C13–C14–C19	−79.3(3)
C13–C14–C15–C16	−177.8(3)
C13–C14–C19–C18	177.4(3)
C14–C15–C16–C17	0.2(5)
C15–C14–C19–C18	0.1(4)
C15–C16–C17–C18	0.5(5)

C16–C17–C18–C19	−0.8(5)
C17–C18–C19–C14	0.6(4)
C19–C14–C15–C16	−0.5(4)
C20–N3–C24–C23	0.1(4)
C20–N3–C24–C25	−178.3(2)
C20–C21–C22–C23	−0.4(4)
C21–C22–C23–C24	0.4(4)
C22–C23–C24–N3	−0.3(4)
C22–C23–C24–C25	177.9(3)
C23–C24–C25–N2	−172.0(2)
C23–C24–C25–C26	8.2(4)
C24–N3–C20–C21	0.0(4)
C24–C25–C26–C27	−179.2(2)
C25–N2–C29–C28	−0.4(4)
C25–C26–C27–C28	−1.5(4)
C26–C27–C28–C29	1.1(4)
C27–C28–C29–N2	−0.1(4)
C29–N2–C25–C24	−179.9(2)
C29–N2–C25–C26	0.0(4)

Table 1-15. Atomic coordinates and U_{eq} [Å^2] for C2

Atom	*x*	*y*	*z*	U_{eq}
Ni1	0.67779(19)	0.38841(17)	0.69173(4)	0.0117(3)
Cl1	1.1765(4)	0.7084(3)	0.62888(7)	0.0172(5)
Cl2	0.7176(4)	0.8376(4)	0.51092(8)	0.0206(6)
O1	0.8638(10)	0.5148(9)	0.65856(19)	0.0117(15)
O2	0.5408(11)	0.6173(11)	0.7070(2)	0.0198(17)
H2B	0.539777	0.627406	0.731565	0.030
H2A	0.422467	0.611546	0.700635	0.030
O3	0.4698(10)	0.2562(10)	0.7203(2)	0.0136(15)
O4	0.1753(12)	0.1627(9)	0.71427(19)	0.0167(15)
O5	0.8318(12)	0.1638(9)	0.6813(2)	0.0182(16)
H5	0.955(2)	0.165(4)	0.684(3)	0.027
O6	0.8434(10)	0.3991(10)	0.74065(18)	0.0150(15)
H6B	0.802883	0.480356	0.755322	0.022
H6A	0.827133	0.307406	0.754062	0.022
N1	0.4955(11)	0.3673(12)	0.6490(2)	0.0117(17)
C6	0.8250(10)	0.5761(8)	0.62339(15)	0.017(2)
C1	0.9621(8)	0.6802(9)	0.60763(18)	0.017(2)
C2	0.9303(8)	0.7578(8)	0.57279(18)	0.014(2)
H2	1.023953	0.828939	0.562019	0.017
C3	0.7615(9)	0.7312(9)	0.55370(15)	0.015(2)
C4	0.6245(8)	0.6271(9)	0.56945(17)	0.015(2)
H4	0.509076	0.608954	0.556408	0.018
C5	0.6562(9)	0.5495(8)	0.60430(17)	0.016(2)
C7	0.5015(15)	0.4404(12)	0.6170(3)	0.012(2)
H7	0.399042	0.423285	0.600060	0.014
C8	0.3226(16)	0.2737(12)	0.6588(3)	0.0114(18)
H8	0.211874	0.347873	0.653248	0.014
C9	0.3195(16)	0.2284(12)	0.7010(3)	0.0111(18)
C10	0.2990(16)	0.1061(15)	0.6360(3)	0.019(2)
H10A	0.421570	0.046426	0.635449	0.023
H10B	0.208117	0.032716	0.649535	0.023
C11	0.2320(14)	0.1306(14)	0.5959(3)	0.016(2)
C12	0.3386(17)	0.0726(13)	0.5655(3)	0.017(2)
H12	0.458483	0.023293	0.570072	0.020
C13	0.2721(19)	0.0856(16)	0.5281(3)	0.025(3)
H13	0.346737	0.044418	0.507718	0.031
C14	0.0993(17)	0.1575(16)	0.5208(3)	0.023(3)
H14	0.052985	0.166400	0.495555	0.027
C15	−0.0072(17)	0.2180(15)	0.5519(4)	0.023(3)
H15	−0.124912	0.271203	0.547245	0.028
C16	0.0538(16)	0.2021(14)	0.5885(3)	0.017(2)
H16	−0.023482	0.239122	0.608890	0.020
C17	0.7722(19)	−0.0102(17)	0.6837(4)	0.033(3)
H17A	0.734071	−0.049955	0.658530	0.049
H17B	0.665468	−0.019129	0.701274	0.049
H17C	0.876681	−0.079719	0.693093	0.049
O7	1.1436(11)	0.6007(11)	0.7146(2)	0.0230(18)
H7A	1.079206	0.607400	0.693615	0.035
H7B	1.099866	0.511090	0.725895	0.035

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

Table1- 16. Anisotropic displacement parameters [Å^2] for C2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2(a^*)^2U_{11} + k^2(b^*)^2U_{22} + \ldots + 2hka^*b^*U_{12}\,]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ni1	0.0092(6)	0.0113(6)	0.0145(6)	0.0007(5)	0.0005(5)	−0.0009(6)
Cl1	0.0116(11)	0.0134(11)	0.0265(13)	0.0027(10)	−0.0010(11)	−0.0033(11)
Cl2	0.0176(13)	0.0228(14)	0.0215(12)	0.0071(11)	0.0005(10)	−0.0022(11)
O1	0.008(4)	0.018(4)	0.010(3)	0.003(3)	0.003(3)	−0.001(3)
O2	0.022(4)	0.017(4)	0.020(4)	−0.001(4)	0.007(3)	0.005(4)
O3	0.011(4)	0.016(4)	0.013(3)	0.003(3)	0.000(3)	−0.007(3)
O4	0.015(3)	0.017(4)	0.018(3)	0.005(3)	0.001(3)	−0.001(4)
O5	0.015(4)	0.010(3)	0.030(4)	0.000(3)	0.003(3)	−0.002(4)
O6	0.011(3)	0.019(4)	0.015(3)	0.000(3)	0.001(3)	0.002(3)
N1	0.006(4)	0.014(4)	0.015(4)	0.002(4)	0.000(3)	0.001(4)
C6	0.020(5)	0.009(5)	0.021(5)	0.002(4)	0.000(5)	0.004(5)
C1	0.016(5)	0.012(5)	0.024(6)	−0.003(5)	0.004(4)	0.003(4)
C2	0.015(5)	0.009(5)	0.018(5)	0.001(4)	0.006(4)	0.004(4)
C3	0.013(5)	0.017(5)	0.014(5)	0.002(4)	0.003(4)	−0.002(4)
C4	0.013(5)	0.017(6)	0.015(5)	−0.003(4)	0.002(4)	0.009(4)
C5	0.016(5)	0.016(5)	0.015(5)	0.000(4)	0.002(4)	−0.007(4)
C7	0.014(5)	0.009(5)	0.012(5)	−0.002(4)	0.002(4)	0.005(4)
C8	0.012(2)	0.011(2)	0.012(2)	0.0002(13)	0.0003(13)	−0.0006(13)
C9	0.011(4)	0.008(4)	0.014(4)	−0.002(3)	−0.001(4)	0.000(4)
C10	0.019(5)	0.023(5)	0.015(5)	−0.002(5)	−0.001(4)	−0.005(6)
C11	0.016(5)	0.010(5)	0.021(5)	−0.002(4)	0.000(4)	−0.006(4)
C12	0.013(5)	0.015(6)	0.022(5)	0.001(4)	0.003(4)	0.006(5)
C13	0.039(8)	0.022(7)	0.015(5)	−0.002(5)	0.005(5)	−0.003(6)
C14	0.027(6)	0.032(7)	0.008(5)	−0.001(5)	−0.006(4)	0.000(5)
C15	0.014(6)	0.020(6)	0.036(7)	0.007(5)	−0.004(5)	0.008(5)
C16	0.020(6)	0.015(5)	0.015(5)	−0.003(4)	0.000(4)	−0.003(5)
C17	0.033(4)	0.031(4)	0.035(4)	−0.001(2)	−0.001(2)	−0.001(3)
O7	0.019(4)	0.016(4)	0.034(4)	0.000(4)	−0.004(3)	−0.003(4)

Table1- 17. Bond lengths and angles for C2

Atom–Atom	Length [Å]
Ni1–O1	2.026(7)
Ni1–O2	2.123(8)
Ni1–O3	2.070(7)
Ni1–O5	2.118(7)
Ni1–O6	2.087(7)
Ni1–N1	1.990(8)
Cl1–C1	1.711(6)
Cl2–C3	1.753(5)
O1–C6	1.358(8)
O2–H2B	0.8701
O2–H2A	0.8706
O3–C9	1.285(13)
O4–C9	1.240(13)
O5–H5	0.878(13)
O5–C17	1.441(15)
O6–H6B	0.8730
O6–H6A	0.8729
N1–C7	1.269(13)
N1–C8	1.474(13)
C6–C1	1.3900
C6–C5	1.3900
C1–C2	1.3900
C2–H2	0.9500
C2–C3	1.3900
C3–C4	1.3900
C4–H4	0.9500
C4–C5	1.3900
C5–C7	1.466(11)
C7–H7	0.9500
C8–H8	1.0000
C8–C9	1.529(13)
C8–C10	1.557(14)
C10–H10A	0.9900
C10–H10B	0.9900
C10–C11	1.503(14)
C11–C12	1.390(14)
C11–C16	1.410(15)
C12–H12	0.9500
C12–C13	1.401(15)

C13–H13	0.9500
C13–C14	1.377(17)
C14–H14	0.9500
C14–C15	1.416(17)
C15–H15	0.9500
C15–C16	1.363(16)
C16–H16	0.9500
C17–H17A	0.9800
C17–H17B	0.9800
C17–H17C	0.9800
O7–H7A	0.8696
O7–H7B	0.8702

Atom–Atom–Atom	**Angle [°]**
O1–Ni1–O2	91.4(3)
O1–Ni1–O3	173.7(3)
O1–Ni1–O5	88.7(3)
O1–Ni1–O6	95.1(3)
O3–Ni1–O2	88.9(3)
O3–Ni1–O5	91.7(3)
O3–Ni1–O6	91.2(3)
O5–Ni1–O2	174.3(3)
O6–Ni1–O2	90.9(3)
O6–Ni1–O5	83.5(3)
N1–Ni1–O1	91.7(3)
N1–Ni1–O2	88.0(3)
N1–Ni1–O3	82.0(3)
N1–Ni1–O5	97.7(3)
N1–Ni1–O6	173.1(3)
C6–O1–Ni1	124.7(5)
Ni1–O2–H2B	109.5
Ni1–O2–H2A	109.5
H2B–O2–H2A	104.5
C9–O3–Ni1	114.9(6)
Ni1–O5–H5	119(2)
C17–O5–Ni1	129.7(8)
C17–O5–H5	107(2)
Ni1–O6–H6B	109.4
Ni1–O6–H6A	109.8
H6B–O6–H6A	104.3
C7–N1–Ni1	127.7(8)
C7–N1–C8	117.6(9)
C8–N1–Ni1	114.1(6)
O1–C6–C1	115.7(5)
O1–C6–C5	124.2(5)
C1–C6–C5	120.0
C6–C1–Cl1	121.7(4)
C2–C1–Cl1	118.2(4)
C2–C1–C6	120.0
C1–C2–H2	120.0
C1–C2–C3	120.0
C3–C2–H2	120.0
C2–C3–Cl2	119.8(4)
C4–C3–Cl2	120.2(4)
C4–C3–C2	120.0
C3–C4–H4	120.0
C3–C4–C5	120.0
C5–C4–H4	120.0
C6–C5–C7	126.0(6)
C4–C5–C6	120.0
C4–C5–C7	114.0(6)
N1–C7–C5	124.3(9)
N1–C7–H7	117.8
C5–C7–H7	117.8
N1–C8–H8	108.4
N1–C8–C9	110.8(8)
N1–C8–C10	113.4(8)
C9–C8–H8	108.4
C9–C8–C10	107.4(8)
C10–C8–H8	108.4
O3–C9–C8	117.6(9)
O4–C9–O3	123.9(9)
O4–C9–C8	118.5(9)
C8–C10–H10A	108.7
C8–C10–H10B	108.7
H10A–C10–H10B	107.6
C11–C10–C8	114.1(9)
C11–C10–H10A	108.7
C11–C10–H10B	108.7
C12–C11–C10	120.6(10)
C12–C11–C16	118.6(10)
C16–C11–C10	120.6(10)
C11–C12–H12	119.5
C11–C12–C13	121.1(11)
C13–C12–H12	119.5
C12–C13–H13	119.8
C14–C13–C12	120.4(11)
C14–C13–H13	119.8
C13–C14–H14	121.0
C13–C14–C15	118.1(10)
C15–C14–H14	121.0
C14–C15–H15	119.0
C16–C15–C14	122.0(11)
C16–C15–H15	119.0
C11–C16–H16	120.1
C15–C16–C11	119.8(11)
C15–C16–H16	120.1
O5–C17–H17A	109.5
O5–C17–H17B	109.5
O5–C17–H17C	109.5
H17A–C17–H17B	109.5
H17A–C17–H17C	109.5
H17B–C17–H17C	109.5
H7A–O7–H7B	104.5

Table1- 8 Torsion angles for C2

Atom–Atom–Atom–Atom	Torsion Angle [°]
Ni1–O1–C6–C1	170.8(4)
Ni1–O1–C6–C5	−4.9(9)
Ni1–O3–C9–O4	−174.3(8)
Ni1–O3–C9–C8	8.0(11)
Ni1–N1–C7–C5	4.2(15)
Ni1–N1–C8–C9	4.9(10)
Ni1–N1–C8–C10	−116.0(8)
Cl1–C1–C2–C3	176.8(5)
Cl2–C3–C4–C5	−176.9(6)
O1–C6–C1–Cl1	7.4(6)
O1–C6–C1–C2	−175.9(7)
O1–C6–C5–C4	175.6(8)
O1–C6–C5–C7	−6.0(9)
N1–C8–C9–O3	−8.6(12)
N1–C8–C9–O4	173.6(9)
N1–C8–C10–C11	−77.5(11)
C6–C1–C2–C3	0.0
C6–C5–C7–N1	6.7(13)
C1–C6–C5–C4	0.0
C1–C6–C5–C7	178.5(8)
C1–C2–C3–Cl2	176.9(6)
C1–C2–C3–C4	0.0
C2–C3–C4–C5	0.0
C3–C4–C5–C6	0.0
C3–C4–C5–C7	−178.6(7)
C4–C5–C7–N1	−174.8(8)
C5–C6–C1–Cl1	−176.7(6)
C5–C6–C1–C2	0.0
C7–N1–C8–C9	−167.1(9)
C7–N1–C8–C10	72.0(12)
C8–N1–C7–C5	174.9(8)
C8–C10–C11–C12	121.6(11)
C8–C10–C11–C16	−62.9(13)
C9–C8–C10–C11	159.7(9)
C10–C8–C9–O3	115.8(10)
C10–C8–C9–O4	−62.0(12)
C10–C11–C12–C13	176.1(11)
C10–C11–C16–C15	−177.7(11)
C11–C12–C13–C14	0.4(18)
C12–C11–C16–C15	−2.2(16)
C12–C13–C14–C15	0.3(18)
C13–C14–C15–C16	−2.0(19)
C14–C15–C16–C11	3.0(18)
C16–C11–C12–C13	0.5(16)

Table 1-9 Atomic coordinates and U_{eq} [Å^2] for C3

Atom	*x*	*y*	*z*	U_{eq}
Ni2	0.73381(8)	0.37602(5)	0.14527(5)	0.0347(2)
Ni1	0.25904(8)	0.60240(5)	0.31854(5)	0.0354(2)
Cl4	0.93530(19)	0.18776(13)	−0.03497(11)	0.0567(5)
Cl1	0.1254(2)	0.79122(15)	0.50853(13)	0.0748(7)
Cl2	0.0808(2)	1.09741(14)	0.22385(17)	0.0861(8)
Cl3	0.8354(3)	−0.12481(14)	0.23056(18)	0.1198(13)
O3	0.3162(4)	0.5231(3)	0.2383(3)	0.0392(11)
O7	0.8030(4)	0.2823(3)	0.0850(3)	0.0402(11)
O6	0.6523(4)	0.4542(3)	0.2240(3)	0.0407(11)
O8	0.5729(4)	0.3950(3)	0.0856(3)	0.0463(12)
H8A	0.521902	0.435393	0.099980	0.069
H8B	0.589739	0.418793	0.029898	0.069
O4	0.3910(4)	0.5324(3)	0.1009(3)	0.0482(13)
O2	0.4415(4)	0.5951(3)	0.3427(3)	0.0526(13)
H2A	0.512969	0.566716	0.336862	0.079
H2B	0.453120	0.652436	0.337472	0.079
N1	0.2967(5)	0.7044(3)	0.2036(3)	0.0345(13)
O1	0.2123(4)	0.6968(3)	0.3807(3)	0.0447(12)
N5	0.7991(5)	0.5015(4)	0.0594(3)	0.0379(13)
O5	0.5852(5)	0.4366(3)	0.3637(3)	0.0563(14)
N4	0.6654(4)	0.2738(3)	0.2521(3)	0.0333(12)
N6	0.9026(5)	0.3723(3)	0.1885(3)	0.0365(13)
N2	0.0749(5)	0.5945(4)	0.3087(3)	0.0410(14)
N3	0.2169(6)	0.4842(4)	0.4252(3)	0.0436(15)
C48	0.9004(6)	0.5235(4)	0.0794(4)	0.0382(16)
C49	0.9429(7)	0.6109(5)	0.0383(4)	0.0498(19)
H49	1.014243	0.624417	0.052032	0.060
C47	0.9620(6)	0.4490(4)	0.1497(4)	0.0362(16)
C21	0.0269(6)	0.5171(5)	0.3654(4)	0.0423(17)
C22	0.1061(7)	0.4539(4)	0.4297(4)	0.0445(18)
C9	0.3562(6)	0.5672(5)	0.1603(4)	0.0391(16)
C43	0.9542(6)	0.3019(5)	0.2523(4)	0.0427(17)
H43	0.913288	0.248659	0.279966	0.051
C50	0.8754(8)	0.6776(5)	−0.0240(4)	0.054(2)
H50	0.900968	0.736817	−0.052361	0.065
C34	0.5911(6)	0.3075(4)	0.3200(4)	0.0388(16)
H34	0.613745	0.269265	0.378312	0.047
C42	0.8060(6)	0.1929(4)	0.1199(4)	0.0371(16)
C10	0.2621(6)	0.7909(5)	0.1851(4)	0.0426(17)
H10	0.277021	0.829387	0.126681	0.051
C36	0.6872(6)	0.1866(4)	0.2685(4)	0.0397(17)
H36	0.657707	0.147982	0.324393	0.048
C52	0.7371(6)	0.5685(5)	−0.0018(4)	0.0435(18)
H52	0.666753	0.554395	−0.016497	0.052
C35	0.6124(6)	0.4070(5)	0.3005(5)	0.0427(17)
C17	0.0055(7)	0.6549(5)	0.2491(4)	0.0450(18)
H17	0.038075	0.709006	0.210393	0.054
C33	0.4527(6)	0.3050(5)	0.3184(5)	0.0560(19)
H33A	0.406677	0.334165	0.358968	0.067
H33B	0.433446	0.342849	0.259775	0.067
H33C	0.404954	0.342751	0.350691	0.067
H33D	0.434908	0.331248	0.257877	0.067

C12	0.1652(7)	0.9288(5)	0.2141(5)	0.0500(19)
H12	0.174153	0.958756	0.153268	0.060
C45	1.1240(7)	0.3827(5)	0.2390(5)	0.0509(19)
H45	1.198041	0.387261	0.255965	0.061
C41	0.8646(6)	0.1350(5)	0.0716(4)	0.0409(17)
C19	−0.1596(7)	0.5615(6)	0.2978(6)	0.061(2)
H19	−0.237329	0.549394	0.293136	0.073
C8	0.3645(7)	0.6719(4)	0.1334(4)	0.0482(19)
H8	0.328569	0.704546	0.078500	0.058
C44	1.0653(7)	0.3050(5)	0.2789(5)	0.0501(19)
H44	1.098530	0.254827	0.322908	0.060
C11	0.2010(6)	0.8329(4)	0.2493(4)	0.0395(16)
C23	0.0729(9)	0.3706(5)	0.4917(5)	0.068(3)
H23	−0.004647	0.351914	0.496082	0.081
C51	0.7734(7)	0.6554(5)	−0.0426(5)	0.052(2)
H51	0.727320	0.699540	−0.083561	0.063
C20	−0.0914(7)	0.4992(5)	0.3609(5)	0.058(2)
H20	−0.124152	0.445536	0.400250	0.069
C46	1.0737(7)	0.4549(5)	0.1734(5)	0.0492(19)
H46	1.114809	0.507903	0.144664	0.059
C40	0.8736(7)	0.0400(5)	0.1038(5)	0.053(2)
H40	0.913917	0.006108	0.068855	0.064
C38	0.7638(7)	0.0453(5)	0.2396(5)	0.058(2)
H38	0.730010	0.014082	0.297056	0.069
C24	0.1554(10)	0.3161(5)	0.5463(5)	0.075(3)
H24	0.135427	0.258515	0.586312	0.090
C26	0.2944(8)	0.4297(5)	0.4824(4)	0.058(2)
H26	0.369819	0.450242	0.480751	0.070
C16	0.1848(6)	0.7847(5)	0.3426(4)	0.0400(17)
C37	0.7533(6)	0.1428(4)	0.2079(4)	0.0435(18)
C7	0.5008(7)	0.6871(6)	0.1184(5)	0.069(2)
H7AA	0.548953	0.638547	0.099613	0.082
H7AB	0.526205	0.683435	0.173424	0.082
H7BC	0.533365	0.679737	0.062239	0.082
H7BD	0.538802	0.635346	0.163011	0.082
C30	0.4075(19)	0.2146(12)	0.3404(15)	0.073(3)
C29	0.366(2)	0.1657(14)	0.4277(14)	0.086(3)
H29	0.361316	0.192226	0.470806	0.103
C28	0.330(2)	0.0770(14)	0.4505(14)	0.100(4)
H28	0.301815	0.044181	0.508846	0.120
C27	0.3362(19)	0.0372(12)	0.3860(18)	0.105(4)
H27	0.312384	−0.022102	0.401275	0.126
C32	0.378(2)	0.0862(14)	0.2988(15)	0.096(4)
H32	0.382454	0.059661	0.255664	0.115
C31	0.414(2)	0.1749(14)	0.2760(12)	0.085(4)
H31	0.441956	0.207708	0.217622	0.102
C18	−0.1116(7)	0.6402(6)	0.2431(5)	0.058(2)
H18	−0.157170	0.684128	0.201606	0.070
C13	0.1176(7)	0.9776(5)	0.2684(5)	0.058(2)
C25	0.2659(9)	0.3453(5)	0.5428(5)	0.068(3)
H25	0.321616	0.308753	0.580679	0.082
C14	0.1039(7)	0.9349(5)	0.3589(5)	0.057(2)
H14	0.073182	0.969197	0.395391	0.069
C15	0.1360(7)	0.8414(5)	0.3945(5)	0.051(2)

C39	0.8217(9)	−0.0043(5)	0.1888(5)	0.071(3)
C3	0.5257(7)	0.7815(4)	0.0486(5)	0.066(2)
C2	0.4781(7)	0.8155(5)	−0.0314(5)	0.078(3)
H2	0.423668	0.782312	−0.042851	0.094
C1	0.5119(8)	0.8990(6)	−0.0941(4)	0.103(4)
H1	0.480049	0.921773	−0.147649	0.124
C6	0.5932(8)	0.9486(5)	−0.0770(6)	0.110(3)
H6	0.615811	1.004510	−0.118977	0.132
C5	0.6408(9)	0.9146(6)	0.0030(6)	0.109(3)
H5	0.695193	0.947788	0.014494	0.130
C4	0.6070(8)	0.8311(6)	0.0658(5)	0.091(3)
H4	0.638814	0.808327	0.119294	0.109
C3A	0.553(2)	0.7757(12)	0.1174(18)	0.081(4)
C2A	0.581(3)	0.8362(19)	0.0318(15)	0.093(3)
H2AA	0.576193	0.818150	−0.015785	0.111
C1A	0.614(3)	0.9237(17)	0.0174(14)	0.105(4)
H1A	0.632757	0.964193	−0.039826	0.126
C6A	0.621(2)	0.9507(12)	0.089(2)	0.107(5)
H6A	0.643596	1.009217	0.078998	0.128
C5A	0.594(2)	0.8901(17)	0.1742(16)	0.107(6)
H5A	0.597870	0.908197	0.221863	0.128
C4A	0.560(2)	0.8026(14)	0.1886(13)	0.097(5)
H4A	0.541305	0.762153	0.245906	0.117
C30A	0.4147(12)	0.2076(8)	0.3585(10)	0.071(3)
C29A	0.4137(15)	0.1600(9)	0.4484(10)	0.089(3)
H29A	0.435702	0.188373	0.484203	0.106
C28A	0.3797(16)	0.0699(9)	0.4849(9)	0.104(4)
H28A	0.379027	0.037997	0.545091	0.125
C27A	0.3468(13)	0.0274(7)	0.4315(12)	0.106(4)
H27A	0.324039	−0.032843	0.455876	0.127
C32A	0.3478(13)	0.0751(9)	0.3415(12)	0.099(3)
H32A	0.325727	0.046691	0.305772	0.118
C31A	0.3817(13)	0.1652(9)	0.3051(10)	0.084(3)
H31A	0.382401	0.197067	0.244882	0.100
O9	0.4299(6)	0.6765(4)	0.4644(4)	0.093(2)
H9A	0.416317	0.633883	0.514013	0.140
H9B	0.360967	0.690553	0.444583	0.140

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

Table 1-10 Anisotropic displacement parameters [Å^2] for C3. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2(a^*)^2U_{11} + k^2(b^*)^2U_{22} + \ldots + 2hka^*b^*U_{12}\,]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ni2	0.0372(5)	0.0307(5)	0.0348(5)	−0.0119(4)	−0.0026(4)	0.0008(4)
Ni1	0.0438(5)	0.0307(5)	0.0291(4)	−0.0104(4)	0.0007(4)	−0.0013(4)
Cl4	0.0789(14)	0.0498(11)	0.0382(10)	−0.0172(8)	0.0029(9)	−0.0023(10)
Cl1	0.1096(19)	0.0677(14)	0.0514(12)	−0.0337(11)	0.0123(12)	−0.0139(13)
Cl2	0.108(2)	0.0406(12)	0.1111(19)	−0.0311(12)	−0.0368(15)	0.0293(12)
Cl3	0.199(3)	0.0308(12)	0.0958(19)	−0.0157(12)	0.048(2)	0.0005(15)
O3	0.050(3)	0.033(3)	0.035(2)	−0.013(2)	0.002(2)	−0.008(2)
O7	0.048(3)	0.030(3)	0.039(3)	−0.011(2)	0.000(2)	0.000(2)
O6	0.044(3)	0.034(3)	0.043(3)	−0.016(2)	0.003(2)	0.000(2)
O8	0.050(3)	0.048(3)	0.043(3)	−0.019(2)	−0.012(2)	0.007(2)
O4	0.061(3)	0.053(3)	0.034(2)	−0.025(2)	−0.006(2)	0.010(2)

O2	0.049(3)	0.048(3)	0.066(3)	−0.026(3)	−0.015(2)	0.005(2)
N1	0.035(3)	0.033(3)	0.034(3)	−0.014(2)	0.004(2)	−0.001(2)
O1	0.062(3)	0.032(3)	0.038(3)	−0.013(2)	−0.005(2)	0.003(2)
N5	0.036(3)	0.037(3)	0.038(3)	−0.012(3)	0.002(2)	−0.001(3)
O5	0.072(4)	0.059(3)	0.043(3)	−0.030(3)	−0.006(2)	0.007(3)
N4	0.031(3)	0.036(3)	0.034(3)	−0.017(2)	0.001(2)	0.002(2)
N6	0.038(3)	0.030(3)	0.038(3)	−0.012(2)	0.000(2)	0.002(3)
N2	0.047(4)	0.041(3)	0.034(3)	−0.015(3)	0.005(3)	−0.009(3)
N3	0.059(4)	0.033(3)	0.032(3)	−0.010(3)	−0.002(3)	0.008(3)
C48	0.038(4)	0.037(4)	0.040(4)	−0.018(3)	0.005(3)	−0.004(3)
C49	0.061(5)	0.046(4)	0.044(4)	−0.018(4)	0.006(4)	−0.016(4)
C47	0.044(4)	0.036(4)	0.031(3)	−0.018(3)	0.008(3)	−0.006(3)
C21	0.042(4)	0.044(4)	0.044(4)	−0.024(3)	0.009(3)	−0.008(3)
C22	0.066(5)	0.034(4)	0.030(4)	−0.014(3)	0.009(3)	−0.001(4)
C9	0.034(4)	0.043(4)	0.042(4)	−0.020(3)	−0.006(3)	0.003(3)
C43	0.045(5)	0.037(4)	0.043(4)	−0.011(3)	−0.005(3)	−0.001(3)
C50	0.095(7)	0.030(4)	0.033(4)	−0.008(3)	0.002(4)	−0.013(4)
C34	0.044(4)	0.033(4)	0.040(4)	−0.017(3)	−0.002(3)	0.005(3)
C42	0.030(4)	0.040(4)	0.042(4)	−0.017(3)	−0.005(3)	0.004(3)
C10	0.047(4)	0.043(4)	0.031(3)	−0.007(3)	−0.004(3)	0.006(3)
C36	0.042(4)	0.038(4)	0.037(4)	−0.015(3)	0.003(3)	−0.003(3)
C52	0.048(4)	0.043(4)	0.032(4)	−0.006(3)	−0.001(3)	−0.002(3)
C35	0.042(4)	0.044(4)	0.046(4)	−0.023(4)	−0.010(3)	0.008(3)
C17	0.047(5)	0.045(4)	0.039(4)	−0.015(3)	0.000(3)	−0.001(4)
C33	0.049(4)	0.057(4)	0.059(4)	−0.022(4)	0.007(3)	−0.006(3)
C12	0.059(5)	0.034(4)	0.057(5)	−0.018(4)	−0.007(4)	0.002(4)
C45	0.036(4)	0.058(5)	0.066(5)	−0.030(4)	−0.008(4)	−0.003(4)
C41	0.042(4)	0.042(4)	0.037(4)	−0.014(3)	−0.001(3)	−0.001(3)
C19	0.041(5)	0.075(6)	0.081(6)	−0.048(5)	−0.005(4)	−0.005(4)
C8	0.070(5)	0.034(4)	0.031(4)	−0.010(3)	0.008(3)	0.004(4)
C44	0.050(5)	0.052(5)	0.052(5)	−0.023(4)	−0.016(4)	0.006(4)
C11	0.037(4)	0.039(4)	0.041(4)	−0.015(3)	−0.001(3)	0.001(3)
C23	0.101(7)	0.038(5)	0.050(5)	−0.002(4)	0.010(5)	−0.017(5)
C51	0.063(6)	0.043(5)	0.047(4)	−0.013(4)	−0.005(4)	−0.003(4)
C20	0.056(5)	0.048(5)	0.072(6)	−0.031(4)	0.023(4)	−0.019(4)
C46	0.042(5)	0.059(5)	0.054(5)	−0.029(4)	0.000(4)	−0.009(4)
C40	0.076(6)	0.034(4)	0.049(4)	−0.018(3)	0.006(4)	−0.003(4)
C38	0.083(6)	0.030(4)	0.049(4)	−0.009(3)	0.013(4)	−0.008(4)
C24	0.120(9)	0.033(5)	0.049(5)	0.003(4)	0.012(5)	−0.011(5)
C26	0.071(6)	0.056(5)	0.033(4)	−0.009(4)	−0.001(4)	0.018(4)
C16	0.038(4)	0.041(4)	0.043(4)	−0.018(3)	−0.002(3)	−0.002(3)
C37	0.050(4)	0.032(4)	0.041(4)	−0.013(3)	0.006(3)	0.008(3)
C7	0.051(5)	0.074(5)	0.077(5)	−0.028(4)	0.017(4)	−0.019(4)
C30	0.063(5)	0.070(5)	0.076(6)	−0.010(5)	−0.004(5)	−0.021(5)
C29	0.080(6)	0.078(5)	0.086(7)	−0.003(5)	−0.009(5)	−0.030(5)
C28	0.099(6)	0.086(6)	0.097(7)	0.002(6)	−0.015(6)	−0.034(5)
C27	0.106(6)	0.088(6)	0.100(8)	0.005(7)	−0.018(7)	−0.039(6)
C32	0.093(7)	0.087(6)	0.095(8)	−0.005(7)	−0.016(6)	−0.038(6)
C31	0.076(6)	0.079(6)	0.089(7)	−0.005(6)	−0.012(6)	−0.033(5)
C18	0.056(6)	0.065(6)	0.062(5)	−0.033(4)	−0.007(4)	−0.003(4)
C13	0.064(6)	0.038(4)	0.073(6)	−0.020(4)	−0.017(4)	0.003(4)
C25	0.105(8)	0.041(5)	0.041(5)	−0.002(4)	−0.008(5)	0.017(5)
C14	0.053(5)	0.055(5)	0.074(6)	−0.039(4)	−0.005(4)	0.005(4)
C15	0.057(5)	0.044(5)	0.052(4)	−0.023(4)	0.003(4)	0.004(4)

C39	0.110(7)	0.020(4)	0.067(5)	−0.011(4)	0.016(5)	−0.003(4)
C3	0.051(5)	0.069(5)	0.076(5)	−0.026(4)	0.012(4)	−0.018(4)
C2	0.063(5)	0.088(6)	0.074(5)	−0.016(5)	0.007(5)	−0.025(5)
C1	0.085(7)	0.108(7)	0.090(7)	0.002(6)	0.007(6)	−0.040(6)
C6	0.093(6)	0.103(6)	0.114(6)	−0.001(5)	−0.007(5)	−0.046(5)
C5	0.091(6)	0.100(6)	0.119(6)	−0.009(5)	−0.006(5)	−0.041(5)
C4	0.076(5)	0.085(5)	0.106(5)	−0.021(5)	−0.007(5)	−0.024(4)
C3A	0.063(6)	0.080(6)	0.094(6)	−0.022(6)	0.003(6)	−0.022(5)
C2A	0.075(5)	0.089(5)	0.100(5)	−0.014(5)	0.000(5)	−0.028(5)
C1A	0.088(6)	0.097(6)	0.116(6)	−0.012(6)	−0.005(6)	−0.036(6)
C6A	0.088(8)	0.098(8)	0.121(8)	−0.013(7)	−0.007(8)	−0.037(7)
C5A	0.087(9)	0.094(9)	0.124(10)	−0.014(9)	−0.007(9)	−0.027(9)
C4A	0.077(8)	0.087(8)	0.115(8)	−0.016(7)	−0.006(7)	−0.022(7)
C30A	0.060(5)	0.070(5)	0.074(6)	−0.013(5)	−0.002(4)	−0.021(4)
C29A	0.081(6)	0.079(5)	0.087(7)	−0.002(5)	−0.003(5)	−0.027(5)
C28A	0.104(7)	0.091(6)	0.094(7)	0.005(6)	−0.013(6)	−0.028(6)
C27A	0.111(6)	0.086(6)	0.101(8)	0.003(6)	−0.016(6)	−0.034(6)
C32A	0.095(6)	0.086(5)	0.096(7)	0.003(6)	−0.010(5)	−0.044(5)
C31A	0.075(5)	0.075(5)	0.087(7)	−0.004(5)	−0.008(5)	−0.029(5)
O9	0.113(5)	0.106(5)	0.069(4)	−0.043(4)	−0.037(4)	0.030(4)

Table 1-11 Bond lengths and angles for C3

Atom–Atom	Length [Å]
Ni2–O7	2.032(4)
Ni2–O6	2.088(4)
Ni2–O8	2.112(4)
Ni2–N5	2.096(5)
Ni2–N4	2.014(5)
Ni2–N6	2.097(6)
Ni1–O3	2.072(4)
Ni1–O2	2.105(5)
Ni1–N1	2.003(5)
Ni1–O1	2.032(4)
Ni1–N2	2.099(6)
Ni1–N3	2.074(5)
Cl4–C41	1.739(6)
Cl1–C15	1.737(7)
Cl2–C13	1.750(7)
Cl3–C39	1.739(7)
O3–C9	1.252(7)
O7–C42	1.295(7)
O6–C35	1.243(7)
O8–H8A	0.8510
O8–H8B	0.8513
O4–C9	1.256(7)
O2–H2A	0.8560
O2–H2B	0.8898
N1–C10	1.279(7)
N1–C8	1.467(7)
O1–C16	1.294(7)
N5–C48	1.344(8)
N5–C52	1.355(8)
O5–C35	1.253(7)
N4–C34	1.473(7)
N4–C36	1.276(7)
N6–C47	1.342(7)
N6–C43	1.347(8)
N2–C21	1.344(8)
N2–C17	1.347(8)
N3–C22	1.360(9)
N3–C26	1.351(9)
C48–C49	1.391(9)
C48–C47	1.486(9)
C49–H49	0.9300
C49–C50	1.396(10)
C47–C46	1.384(9)
C21–C22	1.471(10)
C21–C20	1.399(10)
C22–C23	1.380(9)
C9–C8	1.537(9)
C43–H43	0.9300
C43–C44	1.387(9)
C50–H50	0.9300
C50–C51	1.342(10)
C34–H34	0.9800
C34–C35	1.507(9)
C34–C33	1.544(9)
C42–C41	1.422(8)
C42–C37	1.436(8)
C10–H10	0.9300
C10–C11	1.453(8)
C36–H36	0.9300
C36–C37	1.440(8)
C52–H52	0.9300
C52–C51	1.359(9)

C17–H17	0.9300
C17–C18	1.376(10)
C33–H33A	0.9700
C33–H33B	0.9700
C33–H33C	0.9700
C33–H33D	0.9700
C33–C30	1.459(16)
C33–C30A	1.507(12)
C12–H12	0.9300
C12–C11	1.412(9)
C12–C13	1.361(10)
C45–H45	0.9300
C45–C44	1.351(9)
C45–C46	1.370(10)
C41–C40	1.371(9)
C19–H19	0.9300
C19–C20	1.381(11)
C19–C18	1.349(10)
C8–H8	0.9800
C8–C7	1.527(10)
C44–H44	0.9300
C11–C16	1.432(8)
C23–H23	0.9300
C23–C24	1.365(12)
C51–H51	0.9300
C20–H20	0.9300
C46–H46	0.9300
C40–H40	0.9300
C40–C39	1.377(9)
C38–H38	0.9300
C38–C37	1.407(9)
C38–C39	1.353(10)
C24–H24	0.9300
C24–C25	1.352(12)
C26–H26	0.9300
C26–C25	1.370(10)
C16–C15	1.425(9)
C7–H7AA	0.9700
C7–H7AB	0.9700
C7–H7BC	0.9700
C7–H7BD	0.9700
C7–C3	1.529(9)
C7–C3A	1.563(15)
C30–C29	1.3900
C30–C31	1.3900
C29–H29	0.9300
C29–C28	1.3900
C28–H28	0.9300
C28–C27	1.3900
C27–H27	0.9300
C27–C32	1.3900
C32–H32	0.9300
C32–C31	1.3900
C31–H31	0.9300

C18–H18	0.9300
C13–C14	1.381(10)
C25–H25	0.9300
C14–H14	0.9300
C14–C15	1.373(9)
C3–C2	1.3900
C3–C4	1.3900
C2–H2	0.9300
C2–C1	1.3900
C1–H1	0.9300
C1–C6	1.3900
C6–H6	0.9300
C6–C5	1.3900
C5–H5	0.9300
C5–C4	1.3900
C4–H4	0.9300
C3A–C2A	1.3900
C3A–C4A	1.3900
C2A–H2AA	0.9300
C2A–C1A	1.3900
C1A–H1A	0.9300
C1A–C6A	1.3900
C6A–H6A	0.9300
C6A–C5A	1.3900
C5A–H5A	0.9300
C5A–C4A	1.3900
C4A–H4A	0.9300
C30A–C29A	1.3900
C30A–C31A	1.3900
C29A–H29A	0.9300
C29A–C28A	1.3900
C28A–H28A	0.9300
C28A–C27A	1.3900
C27A–H27A	0.9300
C27A–C32A	1.3900
C32A–H32A	0.9300
C32A–C31A	1.3900
C31A–H31A	0.9300
O9–H9A	0.8498
O9–H9B	0.8499
Atom–Atom–Atom	**Angle [°]**
O7–Ni2–O6	170.84(17)
O7–Ni2–O8	87.76(18)
O7–Ni2–N5	104.83(18)
O7–Ni2–N6	92.22(19)
O6–Ni2–O8	92.43(18)
O6–Ni2–N5	84.30(18)
O6–Ni2–N6	88.87(18)
N5–Ni2–O8	94.5(2)
N5–Ni2–N6	77.7(2)
N4–Ni2–O7	90.15(18)
N4–Ni2–O6	80.68(18)
N4–Ni2–O8	91.48(19)

N4–Ni2–N5	164.1(2)
N4–Ni2–N6	96.6(2)
N6–Ni2–O8	171.93(18)
O3–Ni1–O2	90.18(18)
O3–Ni1–N2	89.95(19)
O3–Ni1–N3	90.41(18)
N1–Ni1–O3	80.99(18)
N1–Ni1–O2	89.2(2)
N1–Ni1–O1	90.23(19)
N1–Ni1–N2	98.0(2)
N1–Ni1–N3	170.7(2)
O1–Ni1–O3	171.13(17)
O1–Ni1–O2	88.36(19)
O1–Ni1–N2	92.6(2)
O1–Ni1–N3	98.43(19)
N2–Ni1–O2	172.72(19)
N3–Ni1–O2	94.4(2)
N3–Ni1–N2	78.3(2)
C9–O3–Ni1	115.3(4)
C42–O7–Ni2	126.9(4)
C35–O6–Ni2	114.1(4)
Ni2–O8–H8A	109.5
Ni2–O8–H8B	109.5
H8A–O8–H8B	104.4
Ni1–O2–H2A	142.6
Ni1–O2–H2B	105.4
H2A–O2–H2B	106.6
C10–N1–Ni1	127.2(4)
C10–N1–C8	118.8(5)
C8–N1–Ni1	113.8(4)
C16–O1–Ni1	125.5(4)
C48–N5–Ni2	115.2(4)
C48–N5–C52	117.5(6)
C52–N5–Ni2	125.9(5)
C34–N4–Ni2	113.4(4)
C36–N4–Ni2	127.5(4)
C36–N4–C34	118.9(5)
C47–N6–Ni2	115.8(4)
C47–N6–C43	117.8(6)
C43–N6–Ni2	126.4(5)
C21–N2–Ni1	114.5(5)
C21–N2–C17	118.4(6)
C17–N2–Ni1	126.9(5)
C22–N3–Ni1	115.4(4)
C26–N3–Ni1	126.0(5)
C26–N3–C22	117.9(6)
N5–C48–C49	122.0(6)
N5–C48–C47	115.4(6)
C49–C48–C47	122.5(7)
C48–C49–H49	120.9
C48–C49–C50	118.3(7)
C50–C49–H49	120.9
N6–C47–C48	114.9(6)
N6–C47–C46	121.0(6)

C46–C47–C48	124.1(6)
N2–C21–C22	116.2(6)
N2–C21–C20	120.4(7)
C20–C21–C22	123.4(7)
N3–C22–C21	114.7(6)
N3–C22–C23	121.1(7)
C23–C22–C21	124.1(8)
O3–C9–O4	125.0(6)
O3–C9–C8	118.6(6)
O4–C9–C8	116.4(6)
N6–C43–H43	118.4
N6–C43–C44	123.3(6)
C44–C43–H43	118.4
C49–C50–H50	120.4
C51–C50–C49	119.2(7)
C51–C50–H50	120.4
N4–C34–H34	109.9
N4–C34–C35	109.4(5)
N4–C34–C33	110.3(5)
C35–C34–H34	109.9
C35–C34–C33	107.3(5)
C33–C34–H34	109.9
O7–C42–C41	121.0(6)
O7–C42–C37	125.2(6)
C41–C42–C37	113.8(6)
N1–C10–H10	117.8
N1–C10–C11	124.4(6)
C11–C10–H10	117.8
N4–C36–H36	117.2
N4–C36–C37	125.7(6)
C37–C36–H36	117.2
N5–C52–H52	118.7
N5–C52–C51	122.7(7)
C51–C52–H52	118.7
O6–C35–O5	124.7(7)
O6–C35–C34	119.0(6)
O5–C35–C34	116.3(6)
N2–C17–H17	118.6
N2–C17–C18	122.8(7)
C18–C17–H17	118.6
C34–C33–H33A	107.9
C34–C33–H33B	107.9
C34–C33–H33C	109.2
C34–C33–H33D	109.2
H33A–C33–H33B	107.2
H33C–C33–H33D	107.9
C30–C33–C34	117.7(10)
C30–C33–H33A	107.9
C30–C33–H33B	107.9
C30A–C33–C34	111.9(8)
C30A–C33–H33C	109.2
C30A–C33–H33D	109.2
C11–C12–H12	119.8
C13–C12–H12	119.8

C13–C12–C11	120.5(7)
C44–C45–H45	120.2
C44–C45–C46	119.5(7)
C46–C45–H45	120.2
C42–C41–Cl4	118.0(5)
C40–C41–Cl4	117.1(5)
C40–C41–C42	124.9(6)
C20–C19–H19	120.5
C18–C19–H19	120.5
C18–C19–C20	119.0(8)
N1–C8–C9	109.2(5)
N1–C8–H8	109.6
N1–C8–C7	111.7(6)
C9–C8–H8	109.6
C7–C8–C9	107.3(6)
C7–C8–H8	109.6
C43–C44–H44	120.9
C45–C44–C43	118.2(7)
C45–C44–H44	120.9
C12–C11–C10	115.1(6)
C12–C11–C16	120.7(6)
C16–C11–C10	124.1(6)
C22–C23–H23	120.4
C24–C23–C22	119.1(9)
C24–C23–H23	120.4
C50–C51–C52	120.2(7)
C50–C51–H51	119.9
C52–C51–H51	119.9
C21–C20–H20	120.0
C19–C20–C21	119.9(7)
C19–C20–H20	120.0
C47–C46–H46	119.9
C45–C46–C47	120.2(7)
C45–C46–H46	119.9
C41–C40–H40	120.6
C41–C40–C39	118.8(6)
C39–C40–H40	120.6
C37–C38–H38	119.1
C39–C38–H38	119.1
C39–C38–C37	121.8(6)
C23–C24–H24	119.8
C25–C24–C23	120.4(8)
C25–C24–H24	119.8
N3–C26–H26	118.8
N3–C26–C25	122.4(8)
C25–C26–H26	118.8
O1–C16–C11	125.1(6)
O1–C16–C15	119.9(6)
C15–C16–C11	115.0(6)
C42–C37–C36	123.8(6)
C38–C37–C42	120.4(6)
C38–C37–C36	115.8(6)
C8–C7–H7AA	109.4
C8–C7–H7AB	109.4

C8–C7–H7BC	106.0
C8–C7–H7BD	106.0
C8–C7–C3	111.2(7)
C8–C7–C3A	125.3(11)
H7AA–C7–H7AB	108.0
H7BC–C7–H7BD	106.3
C3–C7–H7AA	109.4
C3–C7–H7AB	109.4
C3A–C7–H7BC	106.0
C3A–C7–H7BD	106.0
C29–C30–C33	119.4(14)
C29–C30–C31	120.0
C31–C30–C33	120.4(14)
C30–C29–H29	120.0
C28–C29–C30	120.0
C28–C29–H29	120.0
C29–C28–H28	120.0
C29–C28–C27	120.0
C27–C28–H28	120.0
C28–C27–H27	120.0
C32–C27–C28	120.0
C32–C27–H27	120.0
C27–C32–H32	120.0
C27–C32–C31	120.0
C31–C32–H32	120.0
C30–C31–H31	120.0
C32–C31–C30	120.0
C32–C31–H31	120.0
C17–C18–H18	120.3
C19–C18–C17	119.4(8)
C19–C18–H18	120.3
C12–C13–Cl2	119.9(6)
C12–C13–C14	120.9(7)
C14–C13–Cl2	119.1(6)
C24–C25–C26	118.9(8)
C24–C25–H25	120.5
C26–C25–H25	120.5
C13–C14–H14	120.2
C15–C14–C13	119.5(7)
C15–C14–H14	120.2
C16–C15–Cl1	118.4(5)
C14–C15–Cl1	118.2(6)
C14–C15–C16	123.3(7)
C40–C39–Cl3	118.9(6)
C38–C39–Cl3	120.7(6)
C38–C39–C40	120.4(6)
C2–C3–C7	123.4(7)
C2–C3–C4	120.0
C4–C3–C7	116.5(7)
C3–C2–H2	120.0
C1–C2–C3	120.0
C1–C2–H2	120.0
C2–C1–H1	120.0
C2–C1–C6	120.0

C6–C1–H1	120.0
C1–C6–H6	120.0
C5–C6–C1	120.0
C5–C6–H6	120.0
C6–C5–H5	120.0
C6–C5–C4	120.0
C4–C5–H5	120.0
C3–C4–H4	120.0
C5–C4–C3	120.0
C5–C4–H4	120.0
C2A–C3A–C7	111.4(17)
C2A–C3A–C4A	120.0
C4A–C3A–C7	128.1(17)
C3A–C2A–H2AA	120.0
C3A–C2A–C1A	120.0
C1A–C2A–H2AA	120.0
C2A–C1A–H1A	120.0
C6A–C1A–C2A	120.0
C6A–C1A–H1A	120.0
C1A–C6A–H6A	120.0
C5A–C6A–C1A	120.0
C5A–C6A–H6A	120.0
C6A–C5A–H5A	120.0
C6A–C5A–C4A	120.0

C4A–C5A–H5A	120.0
C3A–C4A–H4A	120.0
C5A–C4A–C3A	120.0
C5A–C4A–H4A	120.0
C29A–C30A–C33	120.3(9)
C29A–C30A–C31A	120.0
C31A–C30A–C33	119.7(9)
C30A–C29A–H29A	120.0
C28A–C29A–C30A	120.0
C28A–C29A–H29A	120.0
C29A–C28A–H28A	120.0
C27A–C28A–C29A	120.0
C27A–C28A–H28A	120.0
C28A–C27A–H27A	120.0
C28A–C27A–C32A	120.0
C32A–C27A–H27A	120.0
C27A–C32A–H32A	120.0
C31A–C32A–C27A	120.0
C31A–C32A–H32A	120.0
C30A–C31A–H31A	120.0
C32A–C31A–C30A	120.0
C32A–C31A–H31A	120.0
H9A–O9–H9B	104.5

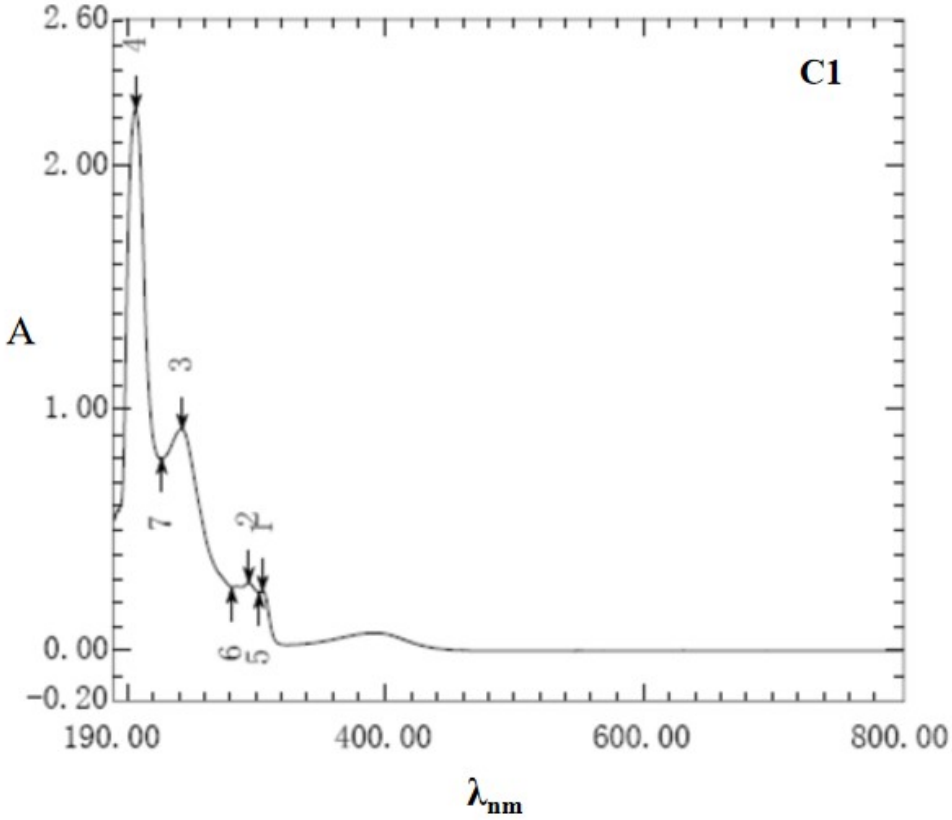
Table 1-12 Torsion angles for C3

Atom–Atom–Atom–Atom	Torsion Angle [°]
Ni2–O7–C42–C41	−175.8(5)
Ni2–O7–C42–C37	4.0(10)
Ni2–O6–C35–O5	163.5(5)
Ni2–O6–C35–C34	−18.1(8)
Ni2–N5–C48–C49	−168.9(5)
Ni2–N5–C48–C47	9.7(7)
Ni2–N5–C52–C51	166.1(5)
Ni2–N4–C34–C35	−13.9(6)
Ni2–N4–C34–C33	103.9(5)
Ni2–N4–C36–C37	−8.7(10)
Ni2–N6–C47–C48	−2.2(6)
Ni2–N6–C47–C46	179.5(5)
Ni2–N6–C43–C44	−178.6(5)
Ni1–O3–C9–O4	−177.4(5)
Ni1–O3–C9–C8	2.8(8)
Ni1–N1–C10–C11	8.5(10)
Ni1–N1–C8–C9	15.8(7)
Ni1–N1–C8–C7	−102.6(6)
Ni1–O1–C16–C11	−10.4(10)
Ni1–O1–C16–C15	170.7(5)
Ni1–N2–C21–C22	4.6(7)
Ni1–N2–C21–C20	−174.5(5)
Ni1–N2–C17–C18	174.5(5)
Ni1–N3–C22–C21	−8.3(7)
Ni1–N3–C22–C23	172.8(5)
Ni1–N3–C26–C25	−169.7(5)
Cl4–C41–C40–C39	178.2(7)
Cl2–C13–C14–C15	−178.1(6)
O3–C9–C8–N1	−12.3(9)
O3–C9–C8–C7	108.9(7)
O7–C42–C41–Cl4	1.4(9)
O7–C42–C41–C40	179.1(7)
O7–C42–C37–C36	1.5(11)
O7–C42–C37–C38	−179.0(7)
O4–C9–C8–N1	167.9(6)
O4–C9–C8–C7	−70.9(8)
N1–C10–C11–C12	−177.0(7)
N1–C10–C11–C16	7.6(11)
N1–C8–C7–C3	−90.7(7)
N1–C8–C7–C3A	−41.5(15)
O1–C16–C15–Cl1	4.5(10)
O1–C16–C15–C14	−179.6(7)
N5–C48–C49–C50	1.5(10)
N5–C48–C47–N6	−5.0(8)
N5–C48–C47–C46	173.2(6)
N5–C52–C51–C50	1.0(11)
N4–C34–C35–O6	21.6(8)
N4–C34–C35–O5	−159.9(6)
N4–C34–C33–C30	64.2(13)
N4–C34–C33–C30A	74.9(9)
N4–C36–C37–C42	1.0(12)
N4–C36–C37–C38	−178.6(7)
N6–C47–C46–C45	−1.8(10)
N6–C43–C44–C45	0.5(10)
N2–C21–C22–N3	2.4(8)
N2–C21–C22–C23	−178.7(6)

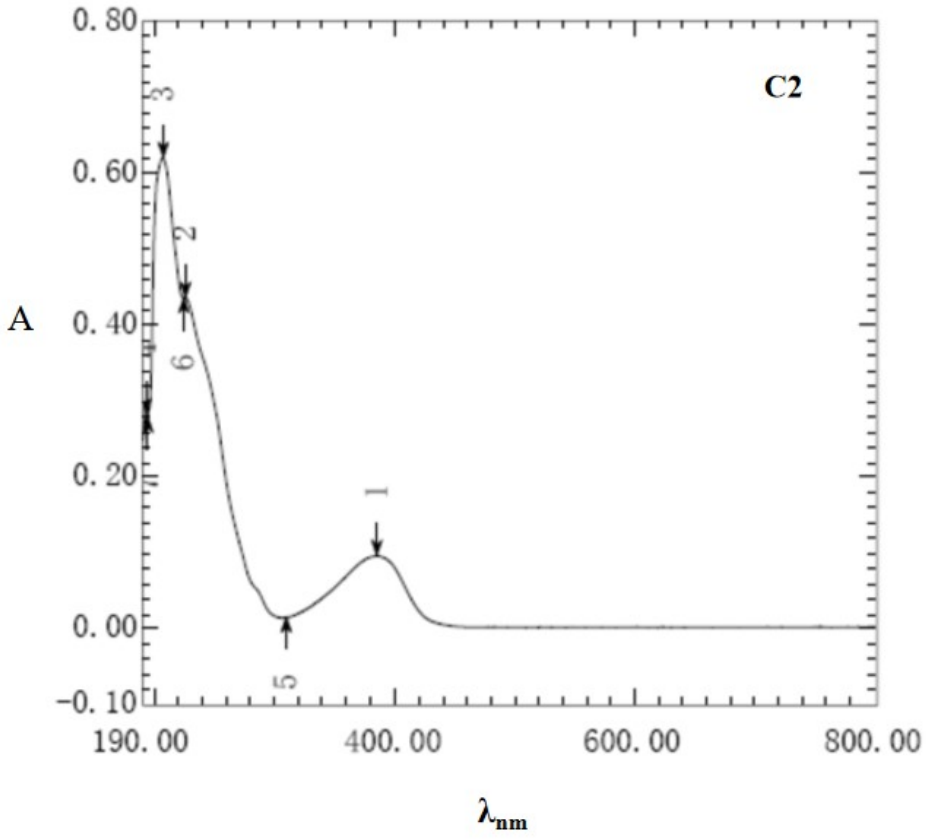
N2–C21–C20–C19	−0.1(10)
N2–C17–C18–C19	−1.0(11)
N3–C22–C23–C24	−3.1(11)
N3–C26–C25–C24	−1.2(12)
C48–N5–C52–C51	0.0(9)
C48–C49–C50–C51	−0.5(10)
C48–C47–C46–C45	−179.9(6)
C49–C48–C47–N6	173.6(6)
C49–C48–C47–C46	−8.1(9)
C49–C50–C51–C52	−0.7(11)
C47–N6–C43–C44	−0.6(9)
C47–C48–C49–C50	−177.0(6)
C21–N2–C17–C18	−1.0(10)
C21–C22–C23–C24	178.0(7)
C22–N3–C26–C25	1.2(10)
C22–C21–C20–C19	−179.1(6)
C22–C23–C24–C25	3.2(13)
C9–C8–C7–C3	149.7(6)
C9–C8–C7–C3A	−161.0(14)
C43–N6–C47–C48	179.5(5)
C43–N6–C47–C46	1.2(9)
C34–N4–C36–C37	177.1(6)
C34–C33–C30–C29	90.0(15)
C34–C33–C30–C31	−85.7(14)
C34–C33–C30A–C29A	68.5(10)
C34–C33–C30A–C31A	−110.8(10)
C42–C41–C40–C39	0.6(12)
C10–N1–C8–C9	−160.2(6)
C10–N1–C8–C7	81.4(8)
C10–C11–C16–O1	−6.3(11)
C10–C11–C16–C15	172.7(7)
C36–N4–C34–C35	161.1(6)
C36–N4–C34–C33	−81.1(7)
C52–N5–C48–C49	−1.2(9)
C52–N5–C48–C47	177.4(5)
C35–C34–C33–C30	−176.6(12)
C35–C34–C33–C30A	−166.0(8)
C17–N2–C21–C22	−179.4(6)
C17–N2–C21–C20	1.5(9)
C33–C34–C35–O6	−98.1(7)
C33–C34–C35–O5	80.4(7)
C33–C30–C29–C28	−175.8(18)
C33–C30–C31–C32	175.7(18)
C33–C30A–C29A–C28A	−179.3(11)
C33–C30A–C31A–C32A	179.3(11)
C12–C11–C16–O1	178.5(7)
C12–C11–C16–C15	−2.5(10)
C12–C13–C14–C15	−1.5(12)
C41–C42–C37–C36	−178.7(7)
C41–C42–C37–C38	0.9(10)
C41–C40–C39–Cl3	−178.8(6)
C41–C40–C39–C38	−0.4(14)
C8–N1–C10–C11	−176.1(6)
C8–C7–C3–C2	−46.0(9)
C8–C7–C3–C4	138.4(6)
C8–C7–C3A–C2A	−97.7(15)
C8–C7–C3A–C4A	74(2)
C44–C45–C46–C47	1.7(10)
C11–C12–C13–Cl2	176.8(6)

C11–C12–C13–C14	0.3(12)
C11–C16–C15–Cl1	−174.5(5)
C11–C16–C15–C14	1.3(11)
C23–C24–C25–C26	−1.1(13)
C20–C21–C22–N3	−178.6(6)
C20–C21–C22–C23	0.3(10)
C20–C19–C18–C17	2.4(11)
C46–C45–C44–C43	−1.0(10)
C26–N3–C22–C21	179.9(5)
C26–N3–C22–C23	0.9(9)
C37–C42–C41–Cl4	−178.4(5)
C37–C42–C41–C40	−0.8(10)
C37–C38–C39–Cl3	178.9(7)
C37–C38–C39–C40	0.6(14)
C7–C3–C2–C1	−175.4(7)
C7–C3–C4–C5	175.7(7)
C7–C3A–C2A–C1A	172.4(19)
C7–C3A–C4A–C5A	−171(2)
C30–C29–C28–C27	0.0
C29–C30–C31–C32	0.0
C29–C28–C27–C32	0.0
C28–C27–C32–C31	0.0
C27–C32–C31–C30	0.0
C31–C30–C29–C28	0.0
C18–C19–C20–C21	−1.9(11)
C13–C12–C11–C10	−173.8(7)
C13–C12–C11–C16	1.8(11)
C13–C14–C15–Cl1	176.5(6)
C13–C14–C15–C16	0.7(12)
C39–C38–C37–C42	−0.8(13)
C39–C38–C37–C36	178.8(8)
C3–C2–C1–C6	0.0
C2–C3–C4–C5	0.0
C2–C1–C6–C5	0.0
C1–C6–C5–C4	0.0
C6–C5–C4–C3	0.0
C4–C3–C2–C1	0.0
C3A–C2A–C1A–C6A	0.0
C2A–C3A–C4A–C5A	0.0
C2A–C1A–C6A–C5A	0.0

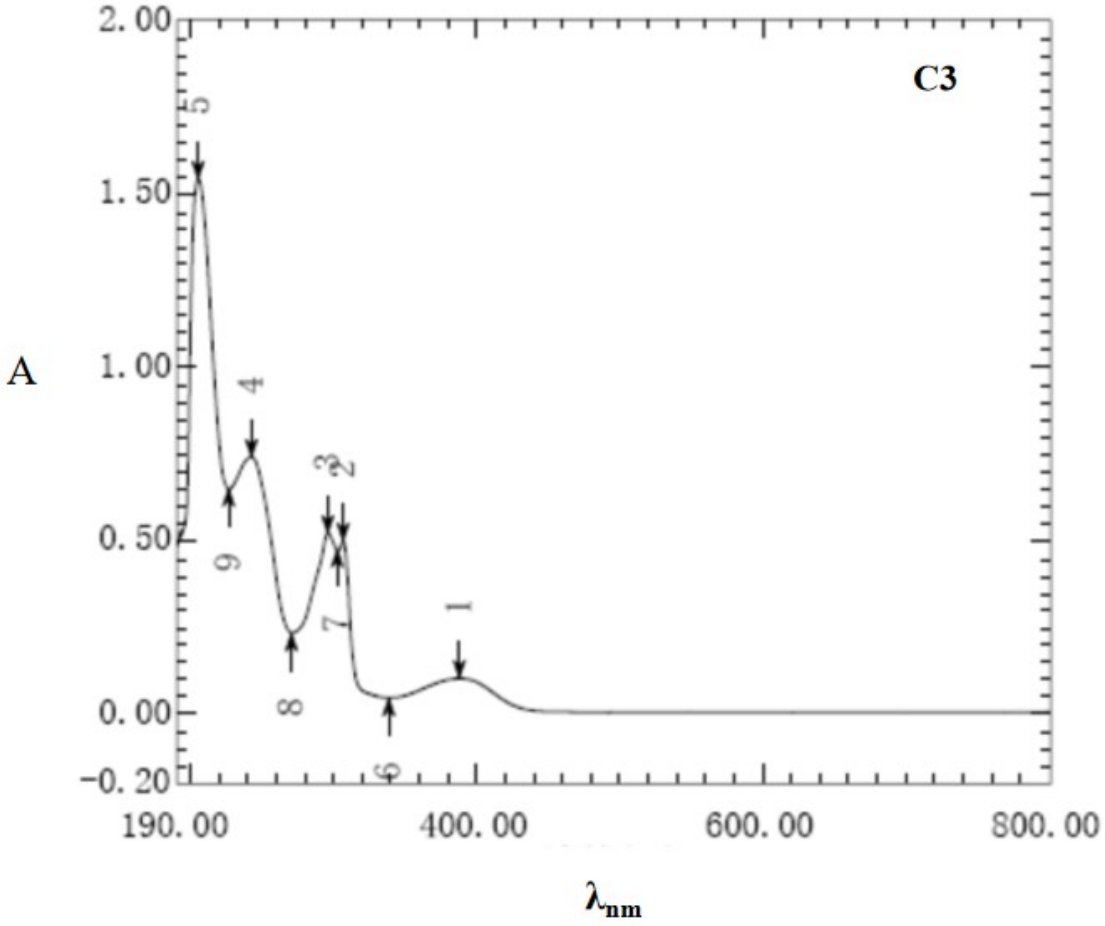
2. UV of C1, C2 and C3



No	P/V	λ_{nm}	A
1	↑	305.2	0.2485
2	↑	294.5	0.2815
3	↑	242.4	0.9151
4	↑	206.9	2.2311
5	↓	302.4	0.2435
6	↓	281.6	0.2644
7	↓	226.6	0.7917

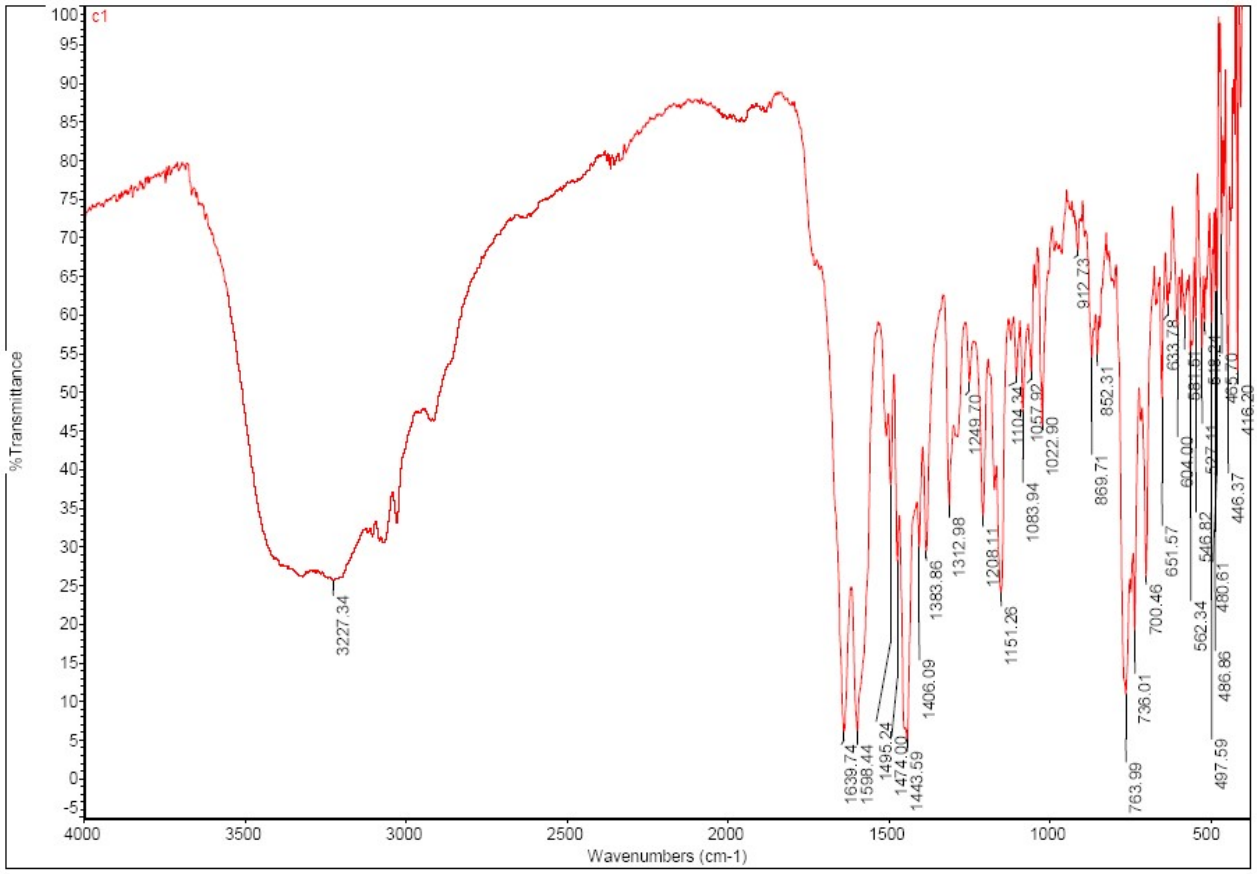


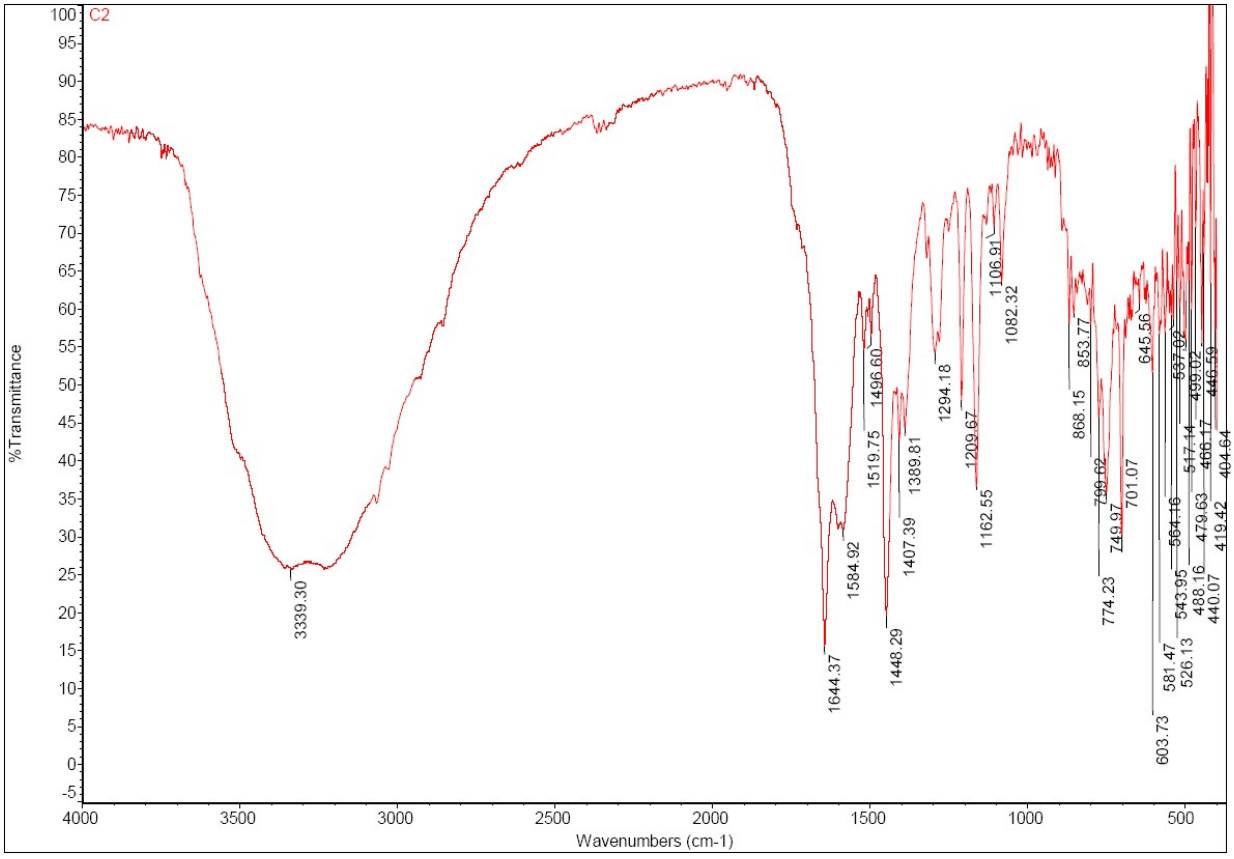
No	P/V	λ_{nm}	A
1	↑	385.0	0.0947
2	↑	225.5	0.4348
3	↑	206.5	0.6195
4	↑	192.7	0.2823
5	↓	310.1	0.0140
6	↓	224.6	0.4346
7	↓	193.6	0.2772

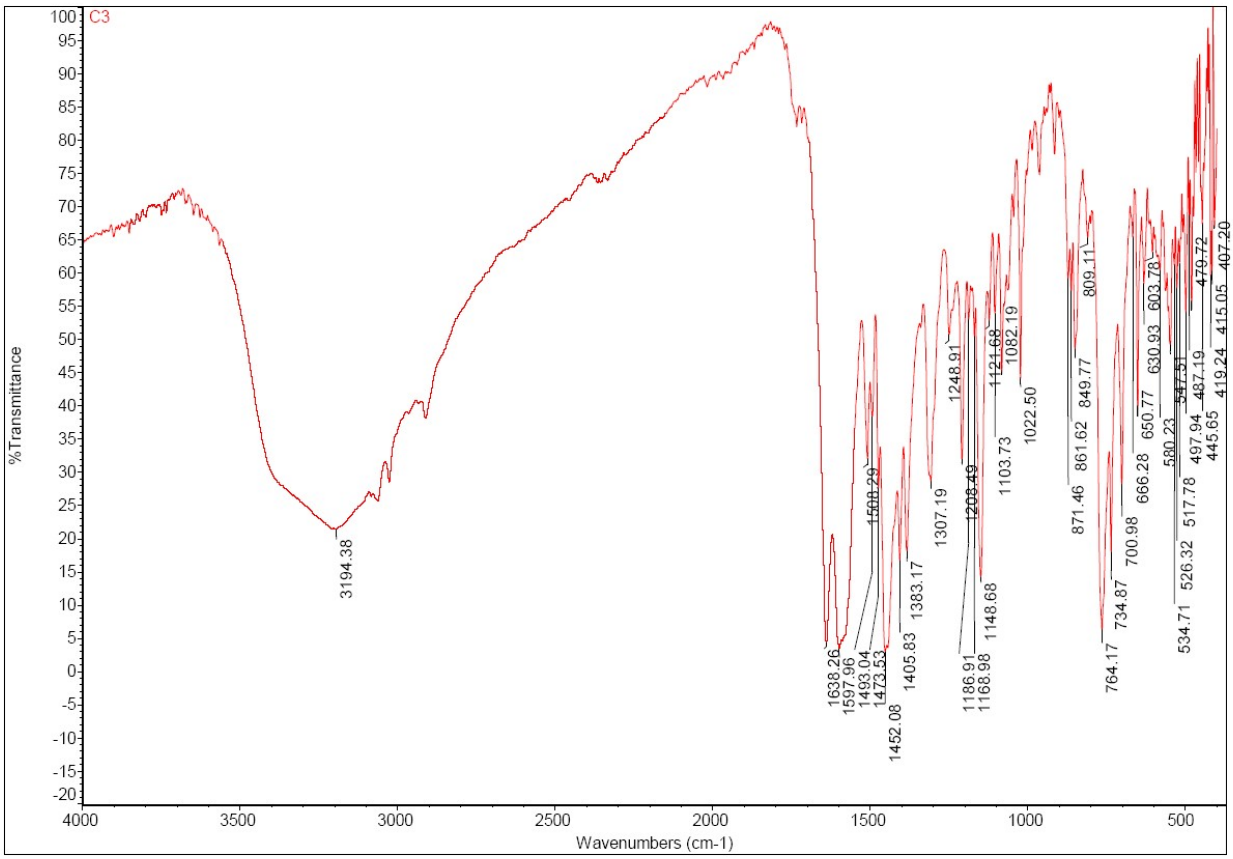


No	P/V	λ_{nm}	A
1	↑	387.3	0.0999
2	↑	306.4	0.4958
3	↑	295.6	0.5206
4	↑	242.1	0.7393
5	↑	204.6	1.5422
6	↓	338.7	0.0438
7	↓	302.7	0.4686
8	↓	270.7	0.2315
9	↓	226.3	0.6464

3. IR of C1, C2 and C3






C3
%Transmittance
Wavenumbers (cm-1)
3194.38
1638.26
1597.96
1493.04
1473.53
1452.08
1405.83
1383.17
1307.19
1248.91
1208.49
1186.91
1168.98
1148.68
1121.68
1103.73
1082.19
1022.50
871.46
861.62
849.77
809.11
764.17
734.87
700.98
666.28
650.77
630.93
603.78
580.23
547.91
534.71
526.32
517.78
497.94
487.19
479.72
445.65
419.24
415.05
407.20