Electronic supplementary materials *Mendeleev Commun.*, 2024, **34**, 382–384

Structure and properties of the metal-containing monomer based on nickel acrylate and 4'-phenyl-2,2':6',2''-terpyridine for self-healing polymers

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I. General

Starting Materials

Acrylic acid, ethanol and benzaldehyde were purified according to standard procedures. 2-Acetylpyridine (C_7H_7NO, ≥99.0 %), nickel chloride hexahydrate ($NiCl_2*6H_2O$, ≥99.0 %), ammonium acetate (NH_4OOCCH_3, ≥98.0 %) and ammonium hydroxide (NH_4OH, ≥99.0 %) were acquired from Aldrich and used without further purification.

Analytical Methods

X-ray diffraction studies of the obtained compound were carried out on single crystals on an Agilent XCalibur CCD diffractometer with EOS detector (Agilent Technologies UK Ltd, Yarnton, Oxfordshire, England). Data acquisition and processing, determination and refinement of unit cell parameters were performed in the CrysAlis PRO program.[S1] Crystals were investigated at a temperature of 273.15 K. Crystallographic data and main parameters of the refinement experiment are presented in Table S1-S5. The structure was solved by dual methods using SHELXT and refined by full-matrix least-squares methods against F^2 by SHELXL using Olex2.[S2-S4] All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were refined isotropic on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Disordered moieties were refined using bond lengths restraints and displacement parameter restraints. Crystallographic data for the structures reported here have been deposited with the Cambridge Crystallographic Data Centre.[S5] CCDC 2338563 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures. This report and the CIF file were generated using FinalCif.[S6]

C, N, H content was studied on a Vario Micro cube elemental analyzer (Elementar GmbH, Hanau, Germany), and the content of nickel was studied on an AAS-3 atomic absorption spectrometer (Zeiss, Jena, Germany).

The ^{1}H NMR mass angel spinning (MAS) NMR spectra were measured with a Bruker AVANCE III 500 MHz spectrometer at Larmor frequency of 500 MHz at room temperature.

IR analysis was performed on a Bruker ALPHA Fourier-IR spectrometer (Bruker Optik GmbH, Germany) equipped with a single reflection diamond prism; the penetration depth for a medium with a sufficiently deep refractive index (2.43) at 1000 cm^{-1} is 1.66 microns. UV spectrometry was carried out on a SPECS-SSP-705-1 spectrometer (JSC Spectroscopic Systems, Moscow, Russia).

Differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) curves were recorded on a METTLER TOLEDO DSC822e differential scanning calorimeter (Mettler Toledo, Switzerland) and a METTLER TGA/SDTA851e thermogravimetric analyzer (Mettler Toledo, Switzerland), the samples were heated in a nitrogen atmosphere.

II. Synthesis

Synthesis of the complex based on nickel(II) acrylate and 4'-phenyl-2,2':6',2''-terpyridine

$(NiOH)_2CO_3$ was obtained according to the described method.[S7]

A solution of 0.92 g $NiCl_2*6H_2O$ (5.5 mmol) in 20 mL water was added to a solution of 0.62 g (5.8 mmol) Na_2CO_3 in 20 mL water under stirring, after which the reaction flask was tightly corked to prevent volatilization of carbon dioxide. The target product was separated by filtration on a Buechner funnel and washed to neutral reaction of the wash water.

Acrylic acid (2 mL, 29 mmol) was added to the obtained $(NiOH)_2CO_3$ in 30 mL of water at 30°C under stirring, the resulting solution was stirred for 1 hour.

4'-Phenyl-2,2':6',2''-terpyridine (PhTpy) was prepared by a procedure similar to that described in previous work.[S8] (^{1}H NMR (500 MHz, Chloroform-d) δ 8.81 – 8.74 (m, 4H), 8.70 (dt, J = 8.0, 1.0 Hz, 2H), 7.97 – 7.86 (m, 4H), 7.57 – 7.51 (m, 2H), 7.51 – 7.44 (m, 1H), 7.37 (ddd, J = 7.5, 4.8, 1.2 Hz, 2H)).[S8]

A solution of nickel(II) acrylate was added to 30 mL of water-alcohol (1:1) suspension of 1.7 g PhTpy (5.5 mmol) under constant stirring at 35°C. The resulting solution was stirred for 4 hours at the same temperature and then evaporated under reduced pressure to remove excess solvent. The residue was recrystallized in diethyl ether. The target product was isolated by filtration under argon atmosphere and dried under vacuum (2.17 g, yield: 65%). The compound was crystallized from the methanol-chloroform solvent system by evaporation at 25°C.

III. Experimental data

Tables

Table S1. Crystallographic data and main refinement parameters of the complex of nickel acrylate and 4'-phenyl-2,2':6',2"-terpyridine ($NiAcr_2PhTpy$).

CCDC number	2338563
Empirical formula	$C_{27.50}H_{22.50}Cl_{1.50}N_3NiO_{4.50}$
Formula weight	578.87
Temperature [K]	273.15
Crystal system	triclinic
Space group (number)	$P\overline{1}$ (2)
a [Å]	8.464(2)
b [Å]	10.921(2)
c [Å]	14.882(3)
α [°]	98.04(3)
β [°]	94.65(3)
γ [°]	105.43(3)
Volume [Å^3]	1302.9(5)
Z	2
ρ_{calc} [gcm^{-3}]	1.476
μ [mm^{-1}]	0.940
F(000)	596
Crystal size [mm^3]	0.35×0.3×0.25
Crystal colour	green
Crystal shape	prizm
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	6.05 to 51.99 (0.81 Å)
Index ranges	$-10 \le h \le 10$ $-13 \le k \le 13$ $0 \le l \le 18$
Reflections collected	5119
Independent reflections	5119 R_{sigma} = 0.0665

Completeness to θ = 25.242°	99.6 %
Data / Restraints / Parameters	5119/15/365
Goodness-of-fit on F^2	1.115
Final R indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0921 wR_2 = 0.2501
Final R indexes [all data]	R_1 = 0.0983 wR_2 = 0.2576
Largest peak/hole [eÅ^{-3}]	1.62/−0.91

Table S2. Atomic coordinates and U_{eq} [Å^2].

Atom	***x***	***y***	***z***	U_{eq}
Ni	0.24218(10)	0.63449(8)	0.31571(6)	0.0196(3)
O1	0.2518(6)	0.4945(5)	0.2046(3)	0.0313(11)
N1	-0.0051(6)	0.5741(5)	0.3397(4)	0.0214(11)
C1	-0.1330(8)	0.5000(7)	0.2795(5)	0.0253(14)
H1	-0.114450	0.474481	0.218507	0.030
O2	0.2739(6)	0.4506(4)	0.3435(3)	0.0249(10)
N2	0.2544(7)	0.7175(5)	0.4442(4)	0.0184(10)
C2	-0.2911(8)	0.4597(6)	0.3033(5)	0.0279(15)
H2	-0.379512	0.407736	0.259224	0.034
O3	0.1953(7)	0.7560(5)	0.2364(4)	0.0318(11)
N3	0.4928(7)	0.7286(5)	0.3473(4)	0.0221(11)
C3	-0.3185(8)	0.4959(7)	0.3918(5)	0.0283(15)
H3	-0.425508	0.467289	0.409898	0.034
O4	0.2165(7)	0.9297(5)	0.3416(4)	0.0388(13)
C4	-0.1877(8)	0.5747(6)	0.4546(5)	0.0222(13)
H4	-0.204134	0.602162	0.515741	0.027
C5	-0.0324(8)	0.6124(6)	0.4257(4)	0.0201(12)
C6	0.1171(7)	0.6972(6)	0.4862(5)	0.0206(13)
C7	0.1222(8)	0.7513(7)	0.5758(5)	0.0237(13)
H7	0.023316	0.738268	0.603775	0.028
C8	0.2724(8)	0.8255(6)	0.6263(5)	0.0229(13)
C9	0.4146(8)	0.8445(6)	0.5795(5)	0.0214(13)
H9	0.519068	0.895111	0.610501	0.026
C10	0.4008(7)	0.7899(6)	0.4896(5)	0.0212(13)
C11	0.5373(8)	0.7995(6)	0.4317(4)	0.0215(13)
C12	0.6982(8)	0.8743(7)	0.4620(5)	0.0263(14)
H12	0.727481	0.923042	0.521941	0.032
C13	0.8159(8)	0.8752(7)	0.4006(5)	0.0283(15)
H13	0.927139	0.925676	0.418530	0.034
C14	0.7698(8)	0.8031(7)	0.3148(5)	0.0288(14)
H14	0.848849	0.802107	0.273117	0.035
C15	0.6073(9)	0.7319(7)	0.2896(5)	0.0267(14)
H15	0.575390	0.683625	0.229533	0.032
C16	0.2861(8)	0.8797(7)	0.7233(5)	0.0258(14)
C17	0.4184(10)	0.9844(8)	0.7642(5)	0.0349(17)
H17	0.499117	1.023022	0.728128	0.042

C18	0.4343(11)	1.0330(9)	0.8568(6)	0.045(2)
H18	0.527065	1.102666	0.883786	0.053
C19	0.3171(11)	0.9813(10)	0.9091(6)	0.047(2)
H19	0.327286	1.015838	0.972255	0.057
C20	0.1828(11)	0.8779(10)	0.8700(6)	0.047(2)
H20	0.101491	0.842028	0.906716	0.056
C21	0.1664(9)	0.8264(8)	0.7779(5)	0.0332(16)
H21	0.074565	0.755443	0.751778	0.040
C22	0.2685(7)	0.4194(6)	0.2590(5)	0.0231(14)
C23	0.2863(9)	0.2868(7)	0.2250(6)	0.0361(18)
H23	0.297066	0.232667	0.268507	0.043
C24	0.2876(17)	0.2445(10)	0.1408(8)	0.072(4)
H24A	0.277066	0.296830	0.096029	0.086
H24B	0.299071	0.160634	0.122833	0.086
C25	0.1784(8)	0.8686(7)	0.2641(5)	0.0271(15)
C26	0.1008(10)	0.9250(7)	0.1923(6)	0.0342(17)
H26	0.079303	1.005302	0.210573	0.041
C27	0.0607(13)	0.8724(10)	0.1070(6)	0.050(2)
H27A	0.080310	0.792093	0.086136	0.059
H27B	0.011715	0.914123	0.065295	0.059
C1S	0.7670(9)	0.4773(4)	0.0015(12)	0.049(4)
H1S	0.735474	0.474359	-0.065124	0.058
Cl1S	0.9825(10)	0.5027(7)	0.0217(10)	0.103(4)
Cl2S	0.7097(7)	0.6049(5)	0.0641(4)	0.0426(11)
Cl3S	0.6619(7)	0.3291(4)	0.0318(3)	0.0523(12)
O5	1.3695(16)	0.4306(14)	-0.0597(8)	0.029(3)
H5A	1.274114	0.402418	-0.044059	0.035
H5B	1.416468	0.503373	-0.026072	0.035

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

Table S3. Anisotropic displacement parameters [Å^2].

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}
Ni	0.0142(4)	0.0224(4)	0.0236(4)	0.0029(3)	0.0042(3)	0.0072(3)
O1	0.027(3)	0.038(3)	0.030(3)	0.000(2)	0.007(2)	0.013(2)
N1	0.014(3)	0.023(3)	0.028(3)	0.001(2)	0.005(2)	0.008(2)
C1	0.016(3)	0.029(3)	0.030(4)	0.000(3)	0.003(3)	0.009(3)
O2	0.019(2)	0.020(2)	0.036(3)	0.0044(19)	0.0064(19)	0.0044(18)
N2	0.017(3)	0.020(3)	0.020(3)	0.0037(19)	0.004(2)	0.008(2)
C2	0.015(3)	0.024(3)	0.043(4)	0.002(3)	−0.001(3)	0.004(2)
O3	0.035(3)	0.032(3)	0.033(3)	0.012(2)	0.004(2)	0.014(2)
N3	0.016(3)	0.022(3)	0.030(3)	0.006(2)	0.007(2)	0.007(2)
C3	0.012(3)	0.032(4)	0.039(4)	0.009(3)	0.002(3)	0.002(3)
O4	0.034(3)	0.031(3)	0.049(4)	0.000(2)	0.005(2)	0.010(2)
C4	0.015(3)	0.021(3)	0.032(4)	0.005(2)	0.005(2)	0.007(2)
C5	0.019(3)	0.019(3)	0.023(3)	0.004(2)	0.002(2)	0.008(2)
C6	0.014(3)	0.021(3)	0.031(3)	0.007(2)	0.005(2)	0.011(2)

C7	0.017(3)	0.028(3)	0.028(3)	0.005(3)	0.003(3)	0.011(3)
C8	0.021(3)	0.024(3)	0.029(3)	0.007(2)	0.005(3)	0.014(3)
C9	0.017(3)	0.020(3)	0.029(3)	0.003(2)	0.003(2)	0.009(2)
C10	0.012(3)	0.025(3)	0.030(3)	0.008(2)	0.006(2)	0.007(2)
C11	0.019(3)	0.024(3)	0.027(3)	0.007(2)	0.009(3)	0.012(2)
C12	0.014(3)	0.028(3)	0.036(4)	0.004(3)	0.005(3)	0.005(3)
C13	0.014(3)	0.032(4)	0.042(4)	0.010(3)	0.011(3)	0.008(3)
C14	0.019(3)	0.032(4)	0.040(4)	0.014(3)	0.012(3)	0.007(3)
C15	0.023(3)	0.032(4)	0.028(4)	0.008(3)	0.011(3)	0.008(3)
C16	0.018(3)	0.028(3)	0.036(4)	0.003(3)	0.002(3)	0.015(3)
C17	0.035(4)	0.034(4)	0.035(4)	−0.005(3)	0.001(3)	0.014(3)
C18	0.033(4)	0.056(5)	0.039(5)	−0.012(4)	−0.005(3)	0.017(4)
C19	0.040(5)	0.072(6)	0.030(4)	−0.015(4)	−0.003(3)	0.029(4)
C20	0.039(5)	0.078(7)	0.030(4)	0.002(4)	0.011(3)	0.031(5)
C21	0.026(4)	0.046(4)	0.031(4)	0.004(3)	0.009(3)	0.016(3)
C22	0.006(3)	0.019(3)	0.039(4)	0.000(3)	0.002(2)	−0.002(2)
C23	0.027(4)	0.021(3)	0.057(5)	−0.004(3)	0.013(3)	0.005(3)
C24	0.115(11)	0.031(5)	0.069(7)	0.001(5)	0.042(7)	0.013(6)
C25	0.011(3)	0.031(4)	0.039(4)	0.009(3)	0.007(3)	0.003(3)
C26	0.032(4)	0.027(4)	0.050(5)	0.014(3)	0.016(3)	0.013(3)
C27	0.067(6)	0.066(6)	0.037(5)	0.025(4)	0.019(4)	0.042(5)
C1S	0.053(11)	0.059(12)	0.036(9)	0.005(8)	0.006(8)	0.021(9)
Cl1S	0.036(4)	0.080(4)	0.186(14)	−0.015(6)	0.026(5)	0.018(3)
Cl2S	0.055(3)	0.035(2)	0.035(3)	−0.0028(18)	0.006(2)	0.010(2)
Cl3S	0.088(4)	0.0246(18)	0.038(2)	0.0037(15)	0.018(2)	0.0016(19)
O5	0.033(5)	0.045(5)	0.013(4)	0.003(3)	0.011(4)	0.014(4)

Table S4. Bond lengths and angles.

Atom–Atom	**Length [Å]**
Ni–O1	2.112(5)
Ni–N1	2.096(5)
Ni–O2	2.186(5)
Ni–N2	1.980(5)
Ni–O3	1.989(5)
Ni–N3	2.079(6)
Ni–C22	2.456(7)
O1–C22	1.257(9)
N1–C1	1.342(9)
N1–C5	1.348(9)
C1–H1	0.9500
C1–C2	1.385(9)
O2–C22	1.249(8)
N2–C6	1.345(8)
N2–C10	1.346(8)
C2–H2	0.9500
C2–C3	1.378(11)
O3–C25	1.290(9)
N3–C11	1.347(9)
N3–C15	1.343(8)
C3–H3	0.9500
C3–C4	1.393(10)
O4–C25	1.222(9)
C4–H4	0.9500
C4–C5	1.392(9)
C5–C6	1.492(9)
C6–C7	1.374(10)
C7–H7	0.9500
C7–C8	1.401(10)
C8–C9	1.422(9)
C8–C16	1.465(10)
C9–H9	0.9500
C9–C10	1.369(9)
C10–C11	1.486(8)
C11–C12	1.390(9)
C12–H12	0.9500
C12–C13	1.404(9)

C13–H13	0.9500
C13–C14	1.371(11)
C14–H14	0.9500
C14–C15	1.379(10)
C15–H15	0.9500
C16–C17	1.395(11)
C16–C21	1.406(10)
C17–H17	0.9500
C17–C18	1.387(11)
C18–H18	0.9500
C18–C19	1.364(14)
C19–H19	0.9500
C19–C20	1.390(14)
C20–H20	0.9500
C20–C21	1.388(11)
C21–H21	0.9500
C22–C23	1.517(9)
C23–H23	0.9500
C23–C24	1.276(14)
C24–H24A	0.9500
C24–H24B	0.9500
C25–C26	1.496(11)
C26–H26	0.9500
C26–C27	1.296(12)
C27–H27A	0.9500
C27–H27B	0.9500
C1S–H1S	1.0000
C1S–Cl1S	1.764(7)
C1S–Cl2S	1.765(7)
C1S–Cl3S	1.765(7)
O5–H5A	0.8481
O5–H5B	0.8540
Atom–Atom–Atom	**Angle [°]**
O1–Ni–O2	61.3(2)
O1–Ni–C22	30.8(2)
N1–Ni–O1	102.4(2)
N1–Ni–O2	89.50(19)
N1–Ni–C22	96.7(2)
O2–Ni–C22	30.5(2)
N2–Ni–O1	158.8(2)
N2–Ni–N1	78.3(2)
N2–Ni–O2	97.6(2)
N2–Ni–O3	107.3(2)
N2–Ni–N3	78.2(2)
N2–Ni–C22	128.1(2)
O3–Ni–O1	94.0(2)
O3–Ni–N1	92.2(2)
O3–Ni–O2	154.9(2)
O3–Ni–N3	95.2(2)

O3–Ni–C22	124.6(2)
N3–Ni–O1	99.4(2)
N3–Ni–N1	156.5(2)
N3–Ni–O2	93.13(19)
N3–Ni–C22	97.4(2)
C22–O1–Ni	89.9(4)
C1–N1–Ni	126.6(5)
C1–N1–C5	118.8(6)
C5–N1–Ni	114.6(4)
N1–C1–H1	118.9
N1–C1–C2	122.3(6)
C2–C1–H1	118.9
C22–O2–Ni	86.8(4)
C6–N2–Ni	119.6(4)
C6–N2–C10	120.7(5)
C10–N2–Ni	119.7(4)
C1–C2–H2	120.5
C3–C2–C1	119.1(6)
C3–C2–H2	120.5
C25–O3–Ni	126.0(5)
C11–N3–Ni	115.0(4)
C15–N3–Ni	125.8(5)
C15–N3–C11	119.0(6)
C2–C3–H3	120.3
C2–C3–C4	119.4(6)
C4–C3–H3	120.3
C3–C4–H4	120.8
C5–C4–C3	118.4(6)
C5–C4–H4	120.8
N1–C5–C4	122.1(6)
N1–C5–C6	114.4(6)
C4–C5–C6	123.5(6)
N2–C6–C5	113.0(6)
N2–C6–C7	121.0(6)
C7–C6–C5	126.0(6)
C6–C7–H7	119.8
C6–C7–C8	120.3(6)
C8–C7–H7	119.8
C7–C8–C9	116.9(6)
C7–C8–C16	122.6(6)
C9–C8–C16	120.5(6)
C8–C9–H9	120.1
C10–C9–C8	119.9(6)
C10–C9–H9	120.1
N2–C10–C9	121.2(6)
N2–C10–C11	112.5(6)
C9–C10–C11	126.3(6)
N3–C11–C10	114.5(6)
N3–C11–C12	122.4(6)
C12–C11–C10	123.1(6)

C11–C12–H12	121.2
C11–C12–C13	117.6(7)
C13–C12–H12	121.2
C12–C13–H13	120.1
C14–C13–C12	119.7(6)
C14–C13–H13	120.1
C13–C14–H14	120.3
C13–C14–C15	119.3(6)
C15–C14–H14	120.3
N3–C15–C14	122.0(7)
N3–C15–H15	119.0
C14–C15–H15	119.0
C17–C16–C8	121.2(7)
C17–C16–C21	118.2(7)
C21–C16–C8	120.6(7)
C16–C17–H17	119.4
C18–C17–C16	121.1(8)
C18–C17–H17	119.4
C17–C18–H18	119.9
C19–C18–C17	120.3(8)
C19–C18–H18	119.9
C18–C19–H19	120.1
C18–C19–C20	119.9(8)
C20–C19–H19	120.1
C19–C20–H20	119.7
C21–C20–C19	120.6(8)
C21–C20–H20	119.7
C16–C21–H21	120.1
C20–C21–C16	119.8(8)
C20–C21–H21	120.1
O1–C22–C23	121.2(7)
O2–C22–O1	122.0(6)
O2–C22–C23	116.8(7)
C22–C23–H23	118.4
C24–C23–C22	123.1(9)
C24–C23–H23	118.4
C23–C24–H24A	120.0
C23–C24–H24B	120.0
H24A–C24–H24B	120.0
O3–C25–C26	114.7(7)
O4–C25–O3	126.4(7)
O4–C25–C26	118.8(7)
C25–C26–H26	117.6
C27–C26–C25	124.8(7)
C27–C26–H26	117.6
C26–C27–H27A	120.0
C26–C27–H27B	120.0
H27A–C27–H27B	120.0
Cl1S–C1S–H1S	108.7
Cl1S–C1S–Cl2S	110.3(6)
Cl1S–C1S–Cl3S	110.3(6)
Cl2S–C1S–H1S	108.7
Cl3S–C1S–H1S	108.7
Cl3S–C1S–Cl2S	110.2(6)
H5A–O5–H5B	108.0

Table S5. Torsion angles.

Atom–Atom–Atom–Atom	Torsion Angle [°]
Ni–O1–C22–O2	−0.6(6)
Ni–O1–C22–C23	−179.5(5)
Ni–N1–C1–C2	176.6(5)
Ni–N1–C5–C4	−176.3(5)
Ni–N1–C5–C6	3.4(7)
Ni–O2–C22–O1	0.6(6)
Ni–O2–C22–C23	179.5(5)
Ni–N2–C6–C5	−1.1(7)
Ni–N2–C6–C7	178.7(5)
Ni–N2–C10–C9	−177.5(5)
Ni–N2–C10–C11	1.7(7)
Ni–O3–C25–O4	14.0(10)
Ni–O3–C25–C26	−164.6(5)
Ni–N3–C11–C10	4.3(7)
Ni–N3–C11–C12	−176.3(5)
Ni–N3–C15–C14	176.1(5)
O1–C22–C23–C24	0.9(12)
N1–C1–C2–C3	−0.4(11)
N1–C5–C6–N2	−1.6(8)
N1–C5–C6–C7	178.6(6)
C1–N1–C5–C4	1.8(9)
C1–N1–C5–C6	−178.4(6)
C1–C2–C3–C4	1.6(11)
O2–C22–C23–C24	−178.0(9)
N2–C6–C7–C8	−2.1(10)
N2–C10–C11–N3	−4.0(8)
N2–C10–C11–C12	176.6(6)
C2–C3–C4–C5	−1.1(10)
O3–C25–C26–C27	−4.0(11)
N3–C11–C12–C13	0.6(10)
C3–C4–C5–N1	−0.6(10)
C3–C4–C5–C6	179.7(6)
O4–C25–C26–C27	177.2(8)
C4–C5–C6–N2	178.1(6)
C4–C5–C6–C7	−1.7(10)
C5–N1–C1–C2	−1.3(10)
C5–C6–C7–C8	177.6(6)
C6–N2–C10–C9	0.1(9)
C6–N2–C10–C11	179.3(5)
C6–C7–C8–C9	2.0(9)
C6–C7–C8–C16	−176.8(6)
C7–C8–C9–C10	−0.8(9)
C7–C8–C16–C17	−158.9(7)
C7–C8–C16–C21	21.7(10)
C8–C9–C10–N2	−0.2(10)
C8–C9–C10–C11	−179.3(6)
C8–C16–C17–C18	−177.8(7)

C8–C16–C21–C20	179.0(7)
C9–C8–C16–C17	22.4(10)
C9–C8–C16–C21	−157.0(7)
C9–C10–C11–N3	175.2(6)
C9–C10–C11–C12	−4.2(11)
C10–N2–C6–C5	−178.7(5)
C10–N2–C6–C7	1.0(9)
C10–C11–C12–C13	180.0(6)
C11–N3–C15–C14	1.6(10)
C11–C12–C13–C14	−0.5(10)
C12–C13–C14–C15	0.9(11)
C13–C14–C15–N3	−1.5(11)
C15–N3–C11–C10	179.4(6)
C15–N3–C11–C12	−1.2(10)
C16–C8–C9–C10	177.9(6)
C16–C17–C18–C19	−1.9(13)
C17–C16–C21–C20	−0.4(11)
C17–C18–C19–C20	1.2(14)
C18–C19–C20–C21	0.0(14)
C19–C20–C21–C16	−0.4(13)
C21–C16–C17–C18	1.5(11)

Table S6. Comparative characterisation of different complexes of metal acrylates and nitrogen-containing chelating ligand.

Complex	Bond length (Å)		Coordination type		Ref.
			Acrylate anion	Nitrogen-containing ligand	
Ni(4'-phenyl-2,2':6',2''-terpy) $(C_3H_3O_2)_2$	Ni–O1	2.112(5)	Mono + bidentate	Tridentate	*This work*
	Ni–O2	2.186(5)			
	Ni–O3	1.989(5)			
	Ni–N1	2.096(5)			
	Ni–N2	1.980(5)			
	Ni–N3	2.079(6)			
Cu(4'-phenyl-2,2':6',2''-terpy) $(C_3H_3O_2)_2$	Cu–O1	2.150(1)	Two monodentate	Tridentate	*S9*
	Cu–O3	1.942(8)			
	Cu–N1	2.034(1)			
	Cu–N2	1.938(1)			
	Cu–N3	2.030(1)			
Ni(2,2′-bipy)$(C_3H_3O_2)_2(H_2O)$	Ni–O1	2.126(3)	Mono + bidentate	Bidentate	*S10*
	Ni–O2	2.147(3)			
	Ni–O3	2.033(3)			
	Ni–N1	2.076(4)			
	Ni–N2	2.065(3)			
Cu(2,2′-bipy)$(C_3H_3O_2)_2(H_2O)$	Cu–O1	1.991(3)	Mono + bidentate	Bidentate	*S10*
	Cu–O2	2.637(3)			
	Cu–O3	1.949(3)			
	Cu–N1	2.021(3)			
	Cu–N2	2.012(3)			
Zn(2,2′-bipy)$(C_3H_3O_2)_2]\cdot H_2O$	Zn–O1	1.994(3)	Two bidentate	Bidentate	*S10*
	Zn–O2	2.490(3)			
	Zn–O3	2.032(3)			
	Zn–O4	2.326(3)			
	Zn–N1	2.100(3)			
	Zn–N2	2.099(2)			
[Cu$(C_3H_3O_2)_2$ (dpa)]$\cdot H_2O$	Cu–O1	2.505(3)	Two bidentate	Bidentate	*S11*
	Cu–O2	1.979(2)			
	Cu–O3	2.566(3)			
	Cu-O4	1.987(3)			
	Cu-N1	1.976(3)			
	Cu-N3	1.967(3)			
Ni$(ctpy)_2\cdot 4H_2O$	Ni-N1	2.109	-	Two tridentate	*S12*
	Ni-N2	1.996			
	Ni-N1	2.109			

Table S7. The results of elemental analysis.

Sample (Estimated formula)	Content of Elements (%) (found/calculated)		
	C	H	N
$NiAcr_2PhTpy$	60,11/63,5	4,34/4,11	7,62/8,2

Table S8. Thermal properties of $NiAcr_2PhTpy$.

Sample	TGA			DSC		Residue at 520°C
$NiAcr_2PhTpy$	1^{st} stage	30-275°C	1.41%	Peak [°C]	Q, [J/g]	
	2^{nd} stage	275-300°C	14.51%			
	3^{rd} stage	300-380°C	29.87%	289.2	133.4	50.41%
	4^{th} stage	380-520°C	3.80%			

Figures

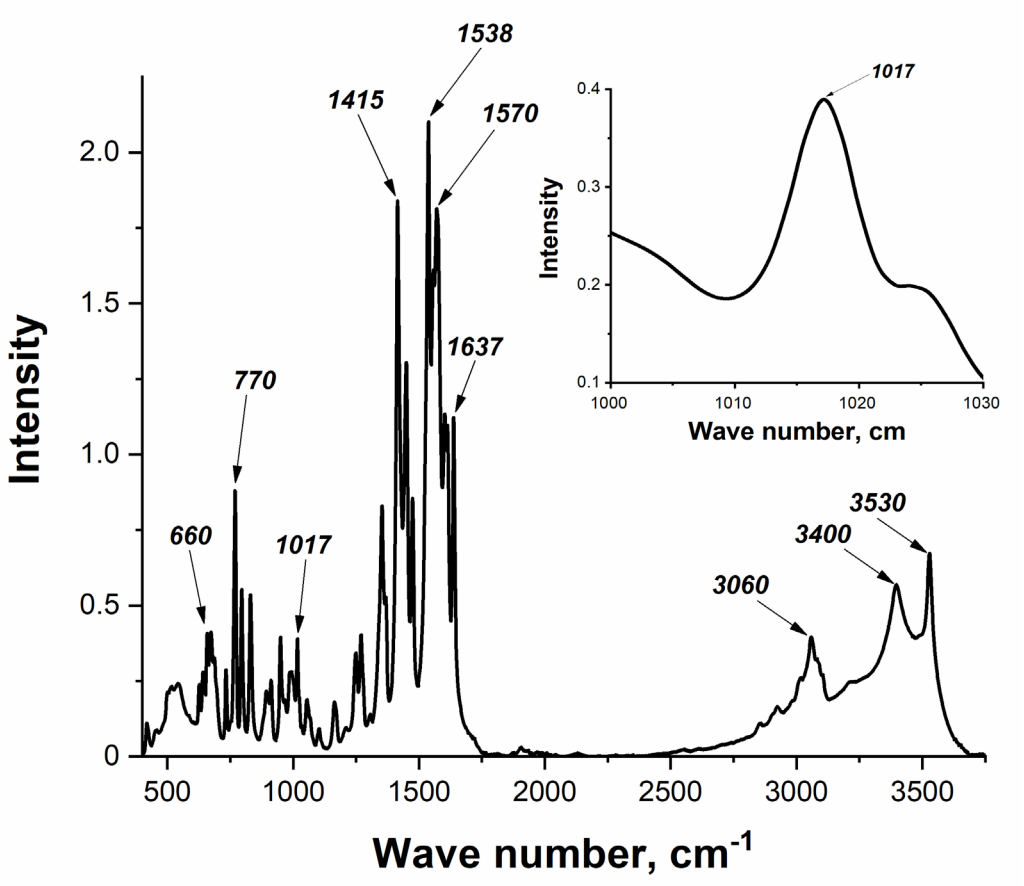

Figure S1. IR-spectrum of $NiAcr_2PhTpy$ (inset - selected region of terpyridine fragment coordination).

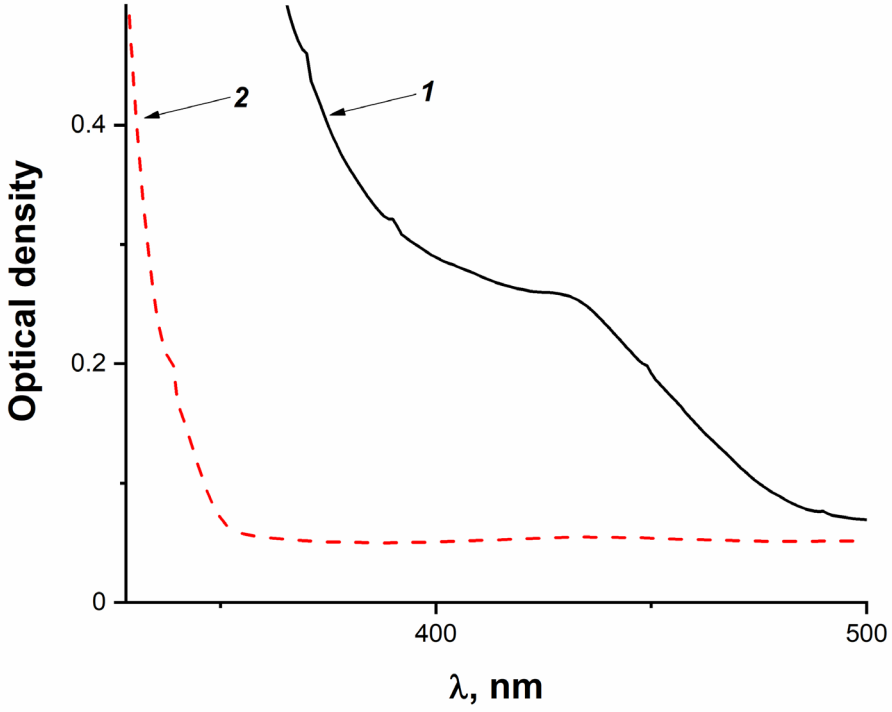

Figure S2. 1 - Absorption spectra of $NiAcr_2PhTpy$ and 2 - 4′-phenyl-2,2′:6′,2″-terpyridine (ethanol solution was used, ethanol absorption spectrum as the base line was subtracted).

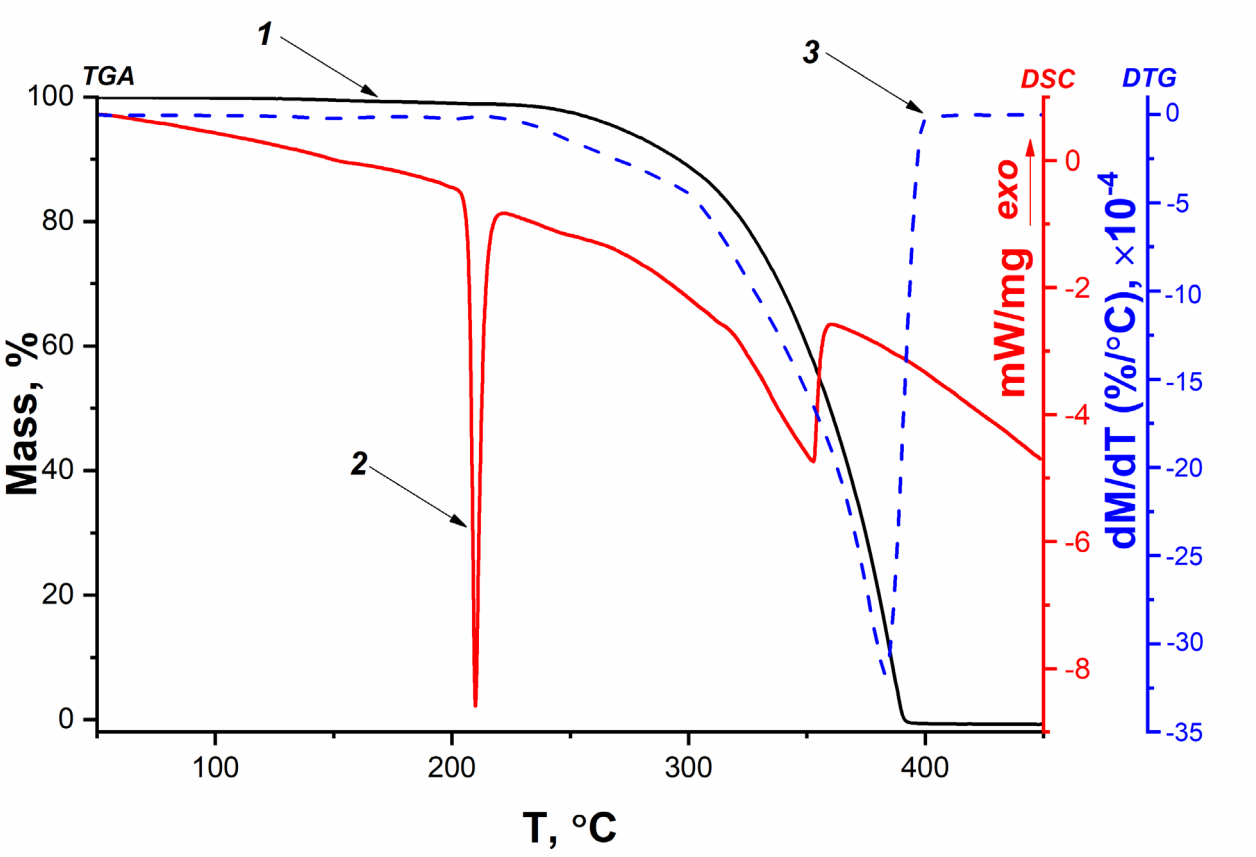

Figure S3. 1 - TGA, 2 - DSC and 3 - DTG curves of 4′-phenyl-2,2′:6′,2″-terpyridine (heating rate - 10°C/min).

IV. Calculation of activation energy

DSC spectra were taken at different heating temperatures to estimate the effective activation energy of solid-phase polymerisation. According to ASTM E698, since the transformation rate is proportional to the heating rate β, the formula can be written as follows:

$$\beta = Af(\alpha) \cdot \exp\left(-\frac{E_a}{RT}\right), \quad (S1)$$

whence, having logarithmized, to obtain:

$$ln\beta = lnAf(\alpha) - \frac{E_a}{R} \cdot \frac{1}{T}, \quad (S2)$$

where A is the pre-exponential multiplier; R is the gas constant (J mol^{-1}·K^{-1}); E_a is the activation energy (J mol^{-1}); f(α) is a function of the transformation degree, depending on the reaction type.[S13] Then, the activation energy can be found from the slope of the straight line in coordinates lnβ - 1/T.

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