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A novel Ni-based complex inducing apoptosis through mitochondrial dysfunction in osteosarcoma HOS cells

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S1. Materials and methods

The 4-bpah was synthesized by the methods described previously in the literature.[S1] All other reagents and solvents employed for this synthesis were purchased from commercial sources and used as received without further purification.

S2. Single crystal X-ray diffraction (SCXRD) crystallography

SCXRD data for **Ni complex** was collected with a Bruker SMART APEX II diffractometer with Mo Kα (λ = 0.71073 Å) irradiation source. This system was operated in the ω and θ scan modes. All of the structures were solved by direct methods and refined on F^2 by full-matrix least-squares methods using the SHELXS program provided with the SHELXTL package.[S2] For **Ni complex**, the crystal parameters, obtained data, and refinement data are summarized in Table S1. Selected bond distances and bond angles are listed in Tables S2. Cambridge Crystallographic Data Centre (CCDC) 2351000 for **Ni complex** contains the supplementary crystallographic data supporting the results described in this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

S3. Characterization

The elemental analyses (C, N, and H) were determined with a Perkin-Elmer 240C

elemental analyzer. Powder X-ray diffraction (PXRD) data were collected using a Rigaku diffractometer with Cu Kα radiation. Fourier-transform infrared (FTIR) spectra were recorded with a Varian 640 FTIR spectrometer in the range of 4000–500 cm^{-1} with the use of KBr pellets as sample matrices. Thermogravimetric analyses (TGA) were performed with a METTLER TOLEDO thermal analyzer at a heating rate of 5 °C min^{-1} under a N_2 atmosphere.

Table S1 Crystal and refinement data for **Ni complex**.

Complex	**Ni complex**
Empirical formula	$C_{50}H_{58}N_8NiO_{12}$
F_w	1021.75
Crystal system	Triclinic
space group	*P*–1
a (Å)	10.1444(4)
b (Å)	10.1444(4)
c (Å)	11.9339(4)
α (°)	78.7920(10)
β (°)	74.3180(10)
γ (°)	71.4360(10)
V ($Å^3$), Z, T (K)	1232.62(8), 1, 296(2)
D_c/g cm^{-3}, F(000)	1.376, 538.0
Goodness-of-fit on F^2	1.027
Reflections collected	23976
Uinque data, R_{int}	7624, 0.0297
2*θ* Range (°)	4.346–61.414
R_1 (I > 2σ(I))[a]	0.0405
wR_2[b] (all data)[a]	0.1057

[a]$R_1 = \sum||F_o| - |F_c||/\sum|F_o|$; [b]w$R_2 = \Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]^{1/2}$

Table S2 Selected bond distances (Å) and angles (°) for **Ni complex**.

Ni(1)–O(1)	2.0504(11)	Ni(1)–O(1)#1	2.0504(11)
Ni(1)–O(1W)#1	2.0794(11)	Ni(1)–O(1W)	2.0795(11)
Ni(1)–N(1)	2.1171(12)	Ni(1)–N(1)#1	2.1171(12)
O(1)–Ni(1)–O(1)#1	180	O(1W)#1–Ni(1)–N(1)	90.66(5)
O(1)–Ni(1)–O(1W)#1	88.78(4)	O(1W)–Ni(1)–N(1)	89.34(5)
O(1)#1–Ni(1)–O(1W)#1	91.22(4)	O(1)–Ni(1)–N(1)#1	90.33(5)
O(1)–Ni(1)–O(1W)	91.22(4)	O(1)#1–Ni(1)–N(1)#1	89.67(5)
O(1)#1–Ni(1)–O(1W)	88.78(4)	O(1W)#1–Ni(1)–N(1)#1	89.34(5)
O(1W)#1–Ni(1)–O(1W)	180.00(6)	O(1W)–Ni(1)–N(1)#1	90.66(5)
O(1)–Ni(1)–N(1)	89.67(5)	N(1)–Ni(1)–N(1)#1	180
O(1)#1–Ni(1)–N(1)	90.33(5)		

Symmetry code: #1 $-x + 1, -y + 1, -z + 1$.

Table S3 Hydrogen bonding geometries (Å, °) of the **Ni complex**.

Complex	D–H···A	D–H	H···A	D···A	D–H···A
Ni complex	N4–H4B···O3^{i}	0.86	2.16	2.9879	162
	O1W–H1WB···N2^{ii}	0.85	2.04	2.8445	157
	N3–H3A···O2W^{iii}	0.86	2.24	3.0803	167
	O2W–	0.85	2.43	2.8971	115

Symmetry codes: ^{i} $-x, 2 - y, -z$; ^{ii} $-x, 1 - y, 1 - z$; ^{iii} $1 - x, 1 - y, -z$, ^{iv} $1 - x, 1 - y, 1 - z$.

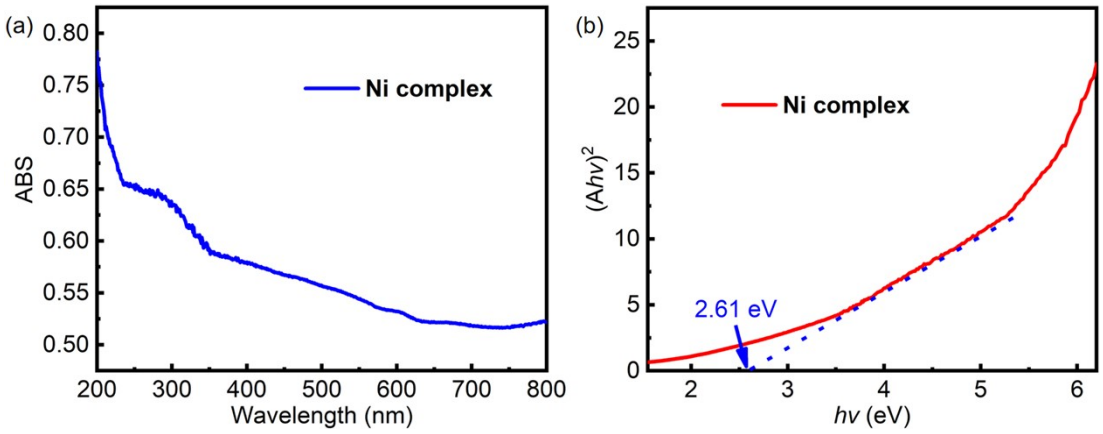

Fig. S1 (a) UV–vis absorption spectrum of **Ni complex**; (b) The bandgap energy of **Ni complex**.

Reference

S1 X. L. Wang, J. Luan, H. Y. Lin, C. Xu, G. C. Liu, J. W. Zhang and A. X. Tian, *CrystEngComm*, 2013, **15**, 9995-10006.

S2 M. S. George, *Acta Cryst.*, 2008, **64**, 112–122.