Supporting information

A new heterogeneous photocatalyst based on Wells -Dawson polyoxometalate and nickel coordination compounds: synthesis, structure and property

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Table S1. Crystal data and structure refinement for complex **NiPW**.

	NiPW
Empirical formula	$C_{90}H_{72}N_{18}Ni_3O_{62}P_2W_{18}$
Formula weight	5945.03
Crystal system	Tetragonal
Space group	$P4_3$
a (Å)	18.6171(5)
b (Å)	18.6171(5)
c (Å)	36.5398(13)
α(°)	90
β (°)	90
γ(°)	90
Volume (Å^3)	12664.6(7)
Z	4
Total reflns/Unique	96109/27107
R(int) /R(sigma)	0.0442/0.0791
GOF	1.139
Final *R* indices [*I*&lt2*σ*(*I*)]	*R*1[a]= 0.0448,
Indices(all data)	*R*1[a]= 0.0484, *wR*2[b]=0.1016

[a] $R_1=\sum||F0|-|Fc||/\sum|F0|$. [b] $wR_2=\{\sum[w(F0^2-Fc^2)^2]/\sum[w(F0^2)^2]\}^{1/2}$

Table S2. Selected bond lengths [Å] and angles [°] for complex NiPW.

W(1)-O(10)	1.746(13)	W(7)-O(1)	1.691(11)	W(13)-O(19)	1.673(11)
W(1)-O(49)	1.883(11)	W(7)-O(32)	1.900(10)	W(13)-O(55)	1.906(13)
W(1)-O(60)	1.898(12)	W(7)-O(41)	1.901(12)	W(13)-O(43)	1.924(11)
W(1)-O(42)	1.938(11)	W(7)-O(28)	1.902(12)	W(13)-O(54)	1.930(11)
W(1)-O(20)	1.975(11)	W(7)-O(29)	1.927(11)	W(13)-O(36)	1.931(11)
W(1)-O(8)	2.390(11)	W(7)-O(62)	2.382(9)	W(13)-O(50)	2.376(12)
W(2)-O(46)	1.686(12)	W(8)-O(12)	1.698(11)	W(14)-O(4)	1.696(12)
W(2)-O(15)	1.873(12)	W(8)-O(37)	1.898(12)	W(14)-O(59)	1.862(11)
W(2)-O(45)	1.904(11)	W(8)-O(32)	1.902(11)	W(14)-O(35)	1.898(12)
W(2)-O(44)	1.910(11)	W(8)-O(45)	1.939(11)	W(14)-O(15)	1.943(12)
W(2)-O(57)	1.936(13)	W(8)-O(49)	1.944(11)	W(14)-O(60)	1.979(11)
W(2)-O(13)	2.353(10)	W(8)-O(13)	2.394(10)	W(14)-O(8)	2.356(10)
W(3)-O(58)	1.711(11)	W(9)-O(30)	1.693(12)	W(15)-O(17)	1.731(11)
W(3)-O(16)	1.889(12)	W(9)-O(23)	1.884(12)	W(15)-O(53)	1.877(11)
W(3)-O(34)	1.892(12)	W(9)-O(18)	1.909(12)	W(15)-O(39)	1.888(11)
W(3)-O(56)	1.902(11)	W(9)-O(52)	1.910(12)	W(15)-O(51)	1.935(11)
W(3)-O(33)	1.955(13)	W(9)-O(48)	1.911(11)	W(15)-O(18)	1.944(12)
W(3)-O(14)	2.329(9)	W(9)-O(38)	2.394(11)	W(15)-O(2)	2.370(11)
W(4)-O(3)	1.693(12)	W(10)-O(31)	1.715(12)	W(16)-O(6)	1.710(12)
W(4)-O(48)	1.885(11)	W(10)-O(26)	1.841(12)	W(16)-O(43)	1.874(12)
W(4)-O(16)	1.899(12)	W(10)-O(28)	1.907(12)	W(16)-O(44)	1.900(11)
W(4)-O(61)	1.924(12)	W(10)-O(23)	1.923(11)	W(16)-O(34)	1.917(12)
W(4)-O(27)	1.927(10)	W(10)-O(22)	1.957(12)	W(16)-O(59)	1.986(11)
W(4)-O(24)	2.398(10)	W(10)-O(38)	2.356(11)	W(16)-O(14)	2.399(10)
W(5)-O(25)	1.716(13)	W(11)-O(11)	1.721(12)	W(17)-O(7)	1.698(12)
W(5)-O(20)	1.873(11)	W(11)-O(57)	1.869(13)	W(17)-O(22)	1.891(12)
W(5)-O(37)	1.892(12)	W(11)-O(55)	1.887(12)	W(17)-O(51)	1.916(12)
W(5)-O(61)	1.913(12)	W(11)-O(41)	1.920(12)	W(17)-O(29)	1.916(11)
W(5)-O(26)	1.949(11)	W(11)-O(40)	1.986(11)	W(17)-O(47)	1.927(13)
W(5)-O(24)	2.351(10)	W(11)-O(62)	2.366(10)	W(17)-O(2)	2.386(10)
W(6)-O(5)	1.713(11)	W(12)-O(9)	1.703(12)	W(18)-O(21)	1.705(12)
W(6)-O(33)	1.844(13)	W(12)-O(40)	1.856(12)	W(18)-O(27)	1.900(11)
W(6)-O(52)	1.884(12)	W(12)-O(36)	1.891(11)	W(18)-O(42)	1.930(12)
W(6)-O(54)	1.932(12)	W(12)-O(47)	1.910(13)	W(18)-O(56)	1.958(11)
W(6)-O(39)	1.945(10)	W(12)-O(53)	1.920(10)	W(18)-O(35)	1.964(12)
W(6)-O(50)	2.324(11)	W(12)-O(2)	2.383(11)	W(18)-O(8)	2.342(10)
Ni(1)-N(3)	2.042(14)	Ni(2)-N(12)	2.041(16)	Ni(3)-N(2)	2.023(17)
Ni(1)-N(1)	2.106(17)	Ni(2)-N(7)	2.051(14)	Ni(3)-N(17)	2.057(14)
Ni(1)-N(9)	2.115(16)	Ni(2)-N(5)	2.063(15)	Ni(3)-N(14)	2.07(2)
Ni(1)-N(15)	2.120(15)	Ni(2)-N(16)	2.068(14)	Ni(3)-N(13)	2.086(16)
Ni(1)-N(6)	2.124(16)	Ni(2)-N(11)	2.089(17)	Ni(3)-N(8)	2.110(18)
Ni(1)-N(4)	2.155(16)	Ni(2)-N(18)	2.099(18)	Ni(3)-N(10)	2.12(2)

P(1)-O(24)	1.507(12)	P(1)-O(8)	1.631(11)	P(2)-O(62)	1.527(10)
P(1)-O(13)	1.523(11)	P(2)-O(50)	1.551(12)	P(2)-O(38)	1.531(13)
P(1)-O(14)	1.534(10)	P(2)-O(2)	1.599(11)		

Table S3. Distances [Å] and angles [°]about C–H···O weak interactions in NiPW.

D–H ···A	d(H···A) Å	d(D···A) Å	<DHA °
C60-H60···O25	2.326	3.128	144.28
C79-H79···O4	2.474	3.220	156.73
C79-H79···O59	2.539	3.196	127.98
C61-H61···O19	2.616	3.172	127.584
C8-H8···O42	2.693	3.342	151.771
C20-H20···O58	2.564	3.072	114.721
C41-H41···O25	2.697	3.272	142.836
C71-H71···O5	2.249	2.977	134.63
C86-H86···O7	2.427	3.188	138.98
C17-H17···O9	2.342	3.210	155.09
C39-H39···O9	2.556	3.004	116.63
C73-H73···O11	2.531	3.051	115.64
C29-H29···O11	2.620	2.978	103.49
C81-H81···O17	2.70	3.217	115.34
C59-H59···O18	2.669	3.200	117.01
C37-H37···O21	2.351	2.988	125.53
C7-H7···O3	2.472	3.217	137.20
C68-H68···O41	2.563	3.004	116.63
C85-H85···O45	2.569	2.987	107.73
C44-H44···O49	2.599	3.082	112.85
C62-H62···O54	2.240	3.084	150.56
C66-H66···O58	2.316	3.186	155.53

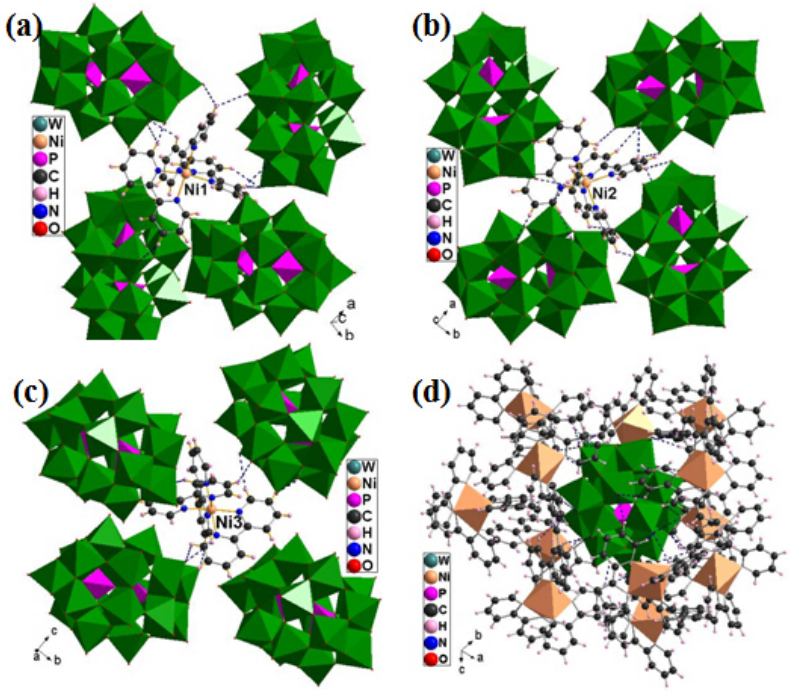

Figure S1. (a) Details of hydrogen bonding of $[Ni1(2,2'\text{-bpy})_3]^{2+}$ in **NiPW**. (b) Details of hydrogen bonding of $[Ni2(2,2'\text{-bpy})_3]^{2+}$ in **NiPW**. (c) Details of hydrogen bonding of $[Ni_3(2,2'\text{-bpy})_3]^{2+}$ in **NiPW**. (d) Details of Wells-Dawson hydrogen bonding in **NiPW**. Green, Purple, and Pink polyhedrons show the $[WO_6]$, $[NiN_6]$, and $[PO_4]$ units, respectively.

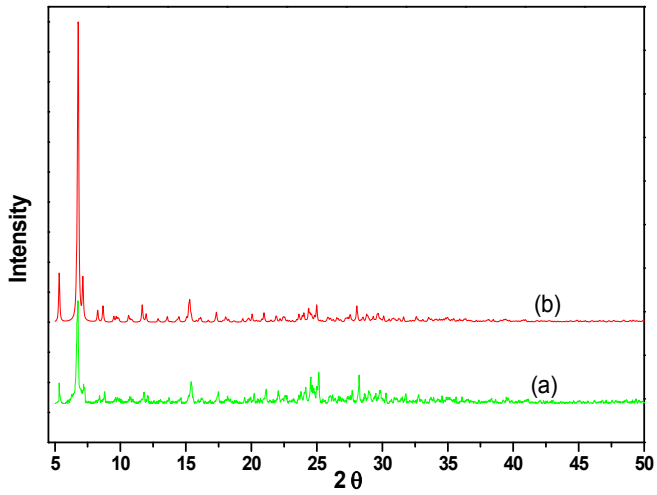

Figure S2. (a) Simulated and (b) Experimental XRPD patterns of complex [Ni(2,2'-bpy)$_3$]$_3$[$P_2W_{18}O_{62}$].