

Supporting Information

Polyoxometalate-Based Ionic Crystal Assembly from Heterometallic Cluster and Polyoxoanion with Visible-Light Catalytic Activity

Zhu-Jun Liu,^a Shuang Yao,^b Zhi-Ming Zhang,^{*a} and En-Bo Wang^{*a}

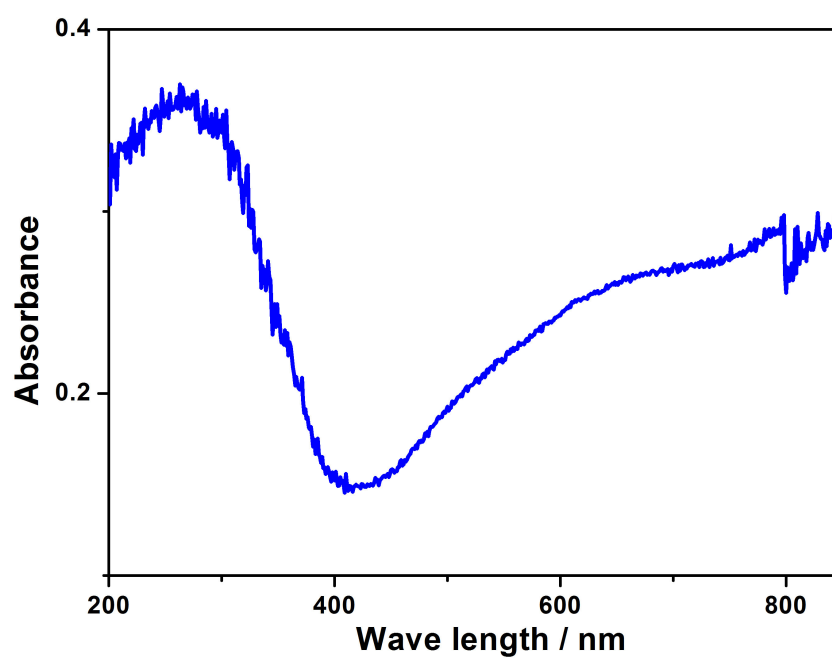


Fig. S1. UV diffuse reflection spectrum of **1**.

Table S1. Crystal Data and Structure Refinement for 1.

	1
Empirical formula	C ₂₅ H ₁₀₄ N ₂₄ Ni ₅ O ₇₃ P ₂ W ₁₉
<i>M</i>	5757.96
<i>A</i> / Å	0.71073
<i>T</i> / K	296(2)
Crystal dimensions / mm	0.21 × 0.20 × 0.18
Crystal system	Cubic
Space group	<i>P</i> 2(1)3
<i>a</i> / Å	21.4954(13)
<i>V</i> /Å ³	9932.0(10)
<i>Z</i>	4
<i>D_c</i> /Mg m ⁻³	3.851
<i>μ</i> /mm ⁻¹	22.967
<i>F</i> (000)	10328
<i>θ</i> Range/°	1.34–25.01
Data/restraints/parameters	5866 / 24 / 446
<i>R</i> ₁ (<i>I</i> > 2σ(<i>I</i>)) ^{<i>a</i>}	0.0377
<i>wR</i> ₂ (all data) ^{<i>b</i>}	0.0955
Goodness-of-fit on <i>F</i> ²	1.022
Flack parameter	0.006(19)
^{<i>a</i>} <i>R</i> ₁ = ∑ <i>F</i> ₀ - <i>F</i> _C /∑ <i>F</i> ₀ ;	
^{<i>b</i>} <i>wR</i> ₂ = ∑[<i>w</i> (<i>F</i> ₀ ² - <i>F</i> _C ²) ²]/∑[<i>w</i> (<i>F</i> ₀ ²) ²] ^{1/2}	

Table S2. Hydrogen Bonds for 1.

D	H	A	[Sym_code for A]	D-H	H...A	D...A	D-H...A
N1	H1C	O2		0.90	2.42	3.30(2)	166
N1	H1D	O16	2-z,-1/2+x,3/2-y	0.90	2.30	3.11(2)	150
N2	H2C	O5	2-x,1/2+y,3/2-z	0.90	2.14	2.98(3)	153
N2	H2D	O1	1/2+y,3/2-z,2-x	0.90	2.06	2.93(2)	163
N3	H3C	O12	1/2+x,1/2-y,2-z	0.90	2.29	3.11(2)	152
N3	H3D	O22	2-x,-1/2+y,3/2-z	0.90	2.58	3.34(2)	143
N4	H4C	O26	z,-1+x,1+y	0.90	2.00	2.87(10)	163
N4	H4D	O11	2-z,-1/2+x,3/2-y	0.90	2.30	3.03(2)	138
N5	H5D	O6	3/2-x,1-y,-1/2+z	0.90	2.56	3.38(2)	152
N7	H7C	OW1		0.90	2.46	3.31(4)	156
N7	H7D	O16	3/2-x,1-y,-1/2+z	0.90	2.27	3.15(3)	165
N8	H8C	O21	2-x,-1/2+y,3/2-z	0.90	2.57	3.46(3)	171
N8	H8C	O26	3/2-y,1-z,-1/2+x	0.90	2.24	2.65(10)	107
N8	H8D	O17	1/2+y,3/2-z,1-x	0.90	2.27	3.07(3)	147