Supporting Information

Two polyoxovanadates for visible light driven photocatalytic performance

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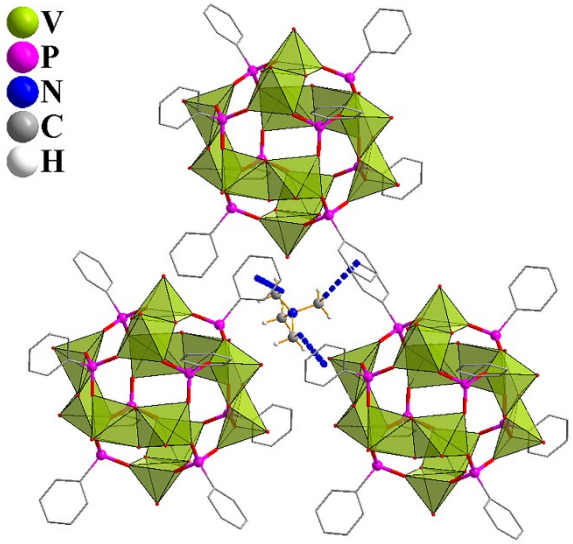

Fig S1. C-H…π interaction in compound **1**.

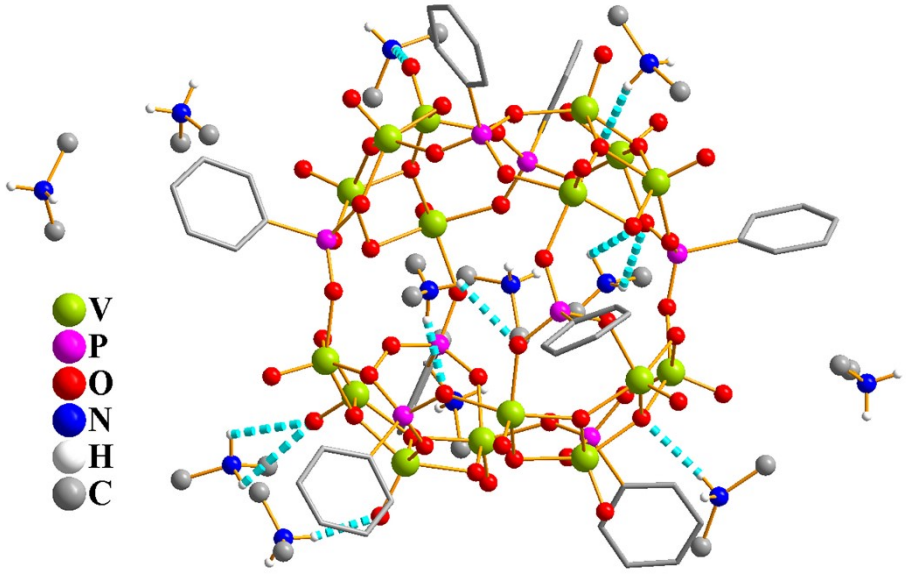

Fig S2. Hydrogen bond interaction in compound **2**.

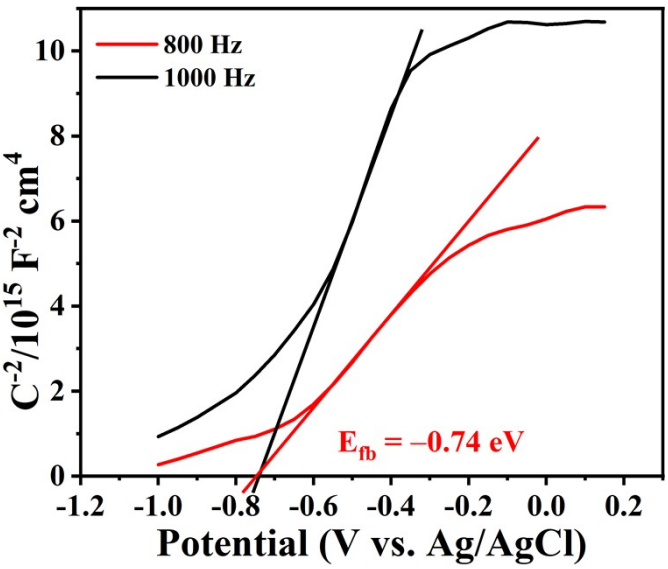

Fig S3. Mott-Schottky plots of **2** at selected frequencies of 800 and 1000 Hz. (The Mott-Schottky test for compound **2** was carried out using a three-electrode system in a 0.2 M Na_2SO_4 solution. Carbon paste electrode as a working electrode, Ag/AgCl as the reference electrode, and a Pt slice as the auxiliary electrode.)

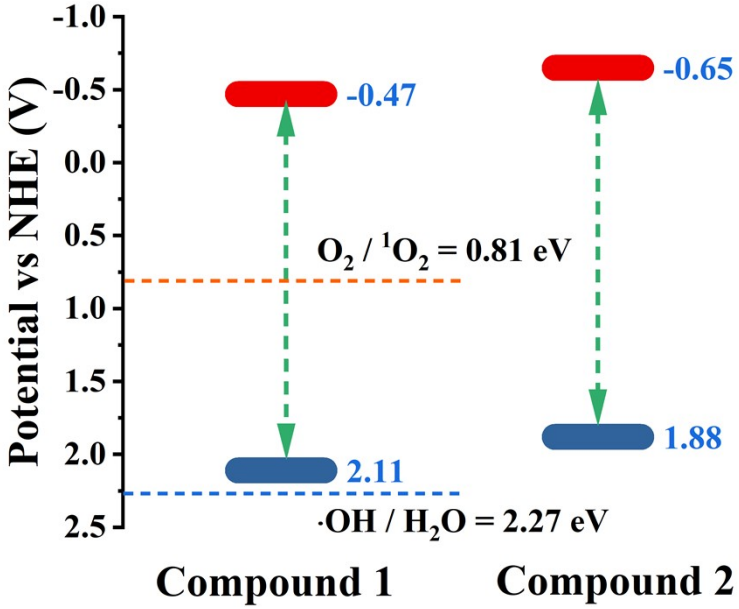

Fig S4. The energy band structure of compound **1** and **2**.

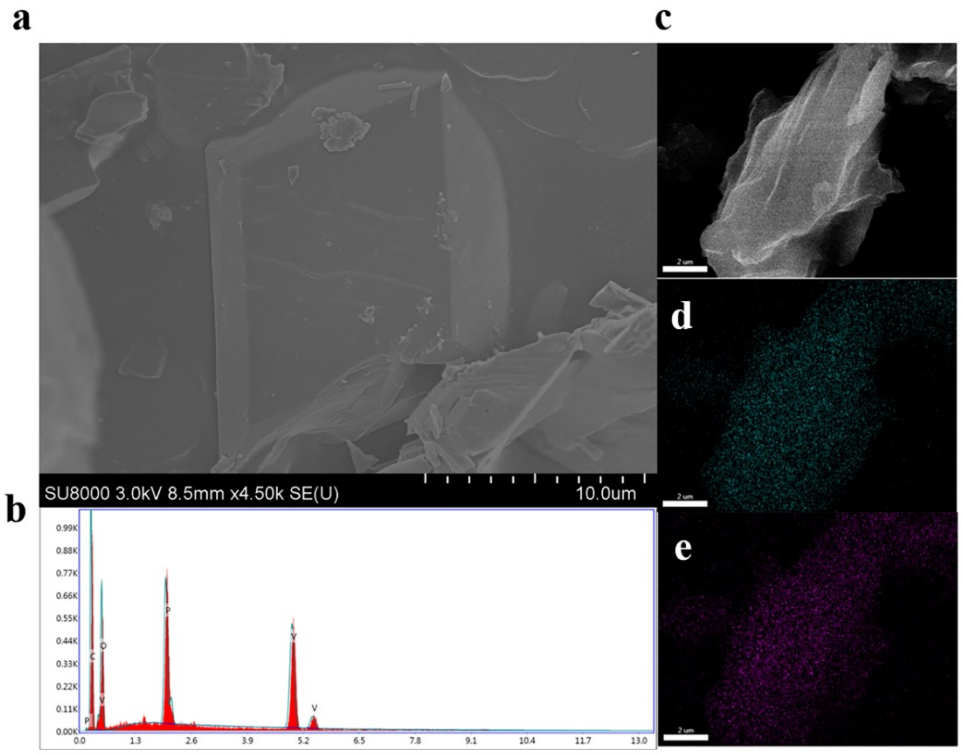

Fig S5. (a) SEM image of compound **1**, (b) EDS pattern of compound **1**, (c) Sample image of compound **1** for EDS test, (d) and (E) Element mapping images of V and P for compound **1**.

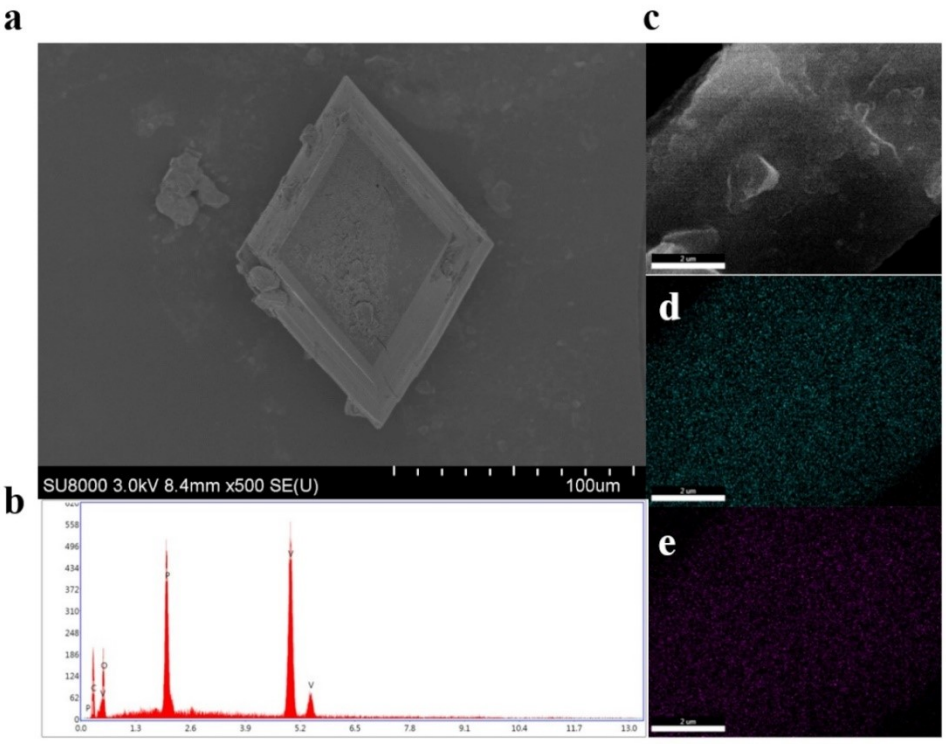

Fig S6. (a) SEM image for compound **2**, (b) EDS pattern of compound **2**, (c) Sample image of compound **2** for EDS test, (d) and (e) Element mapping images of V and P for compound **2**.

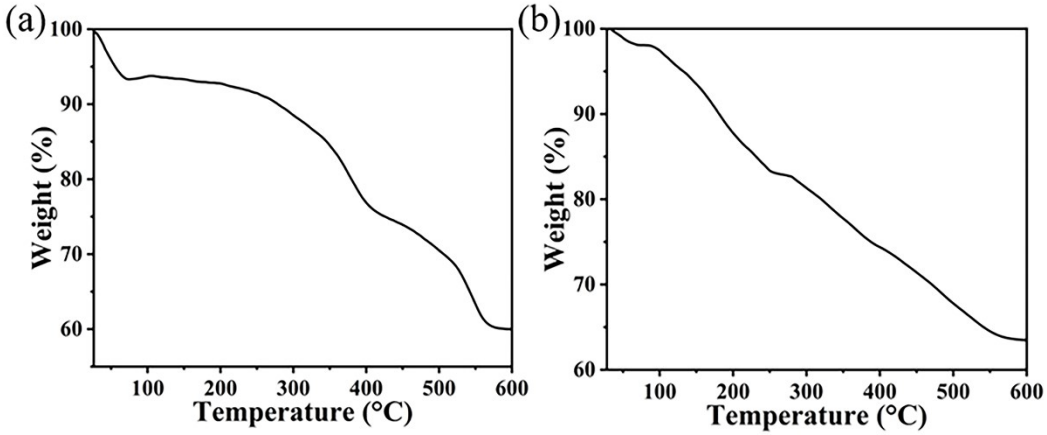

Fig S7. TG curves of compound **1** and compound **2**.

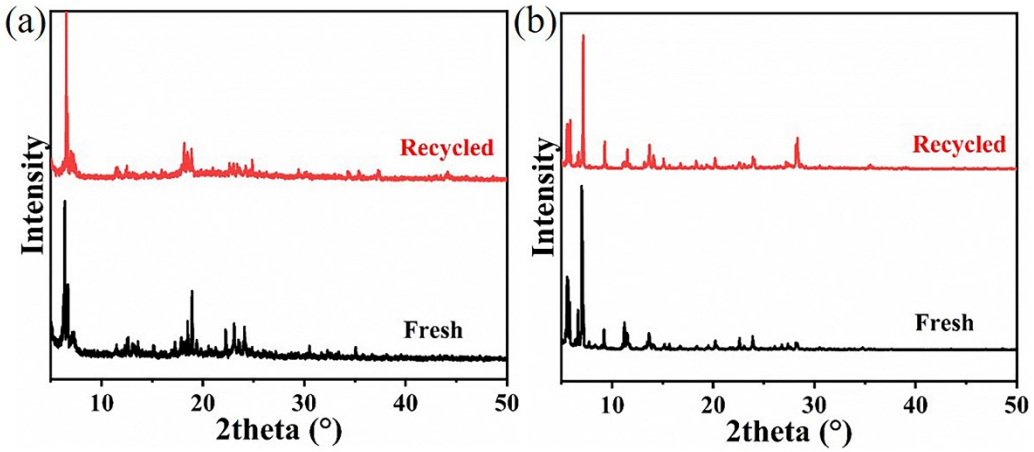

Fig S8. PXRD patterns of compound **1** and compound **2** before and after photocatalytic reaction.

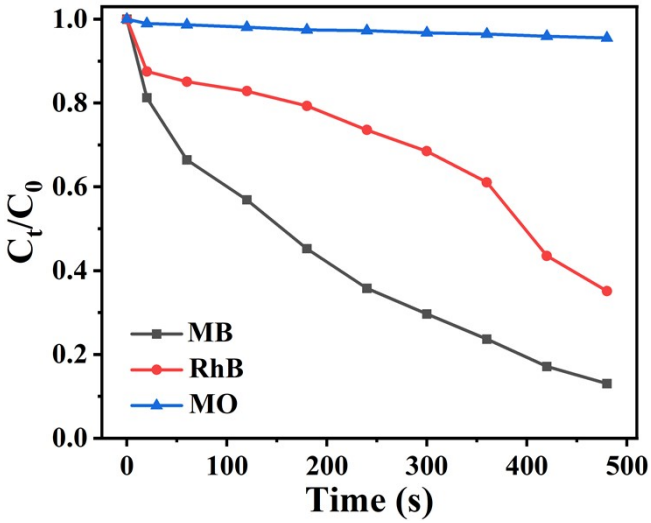

Fig S9. Photodegradation efficiencies of MB, RhB and MO in the presence of compound **1** under visible-light radiation. Reaction conditions: 5 mL dyes solution (15 mg/L), catalyst dosage: 0.5 mg/mL.

Table S1: Crystal data and structure refinement of compound **1** and compound **2**.

Empirical formula	$C_{70}H_{102}N_6O_{50}P_8V_{12}$	$C_{64}H_{104}N_8O_{56}P_8V_{16}$
Formula weight	2686.61	2944.35
Temperature/K	293.15	294.85
Crystal system	triclinic	monoclinic
Space group	P-1	$P2_1/n$
a/Å	15.637(8)	21.110(4)
b/Å	15.719(5)	25.413(4)
c/Å	15.754(6)	26.005(5)
α/°	60.328(11)	90
β/°	65.25(4)	90.082(6)
γ/°	82.83(3)	90
Volume/Å^3	3039(2)	13951(4)
Z	1	4
ρ_{calc}g/cm^3	1.468	1.402
F(000)	1360.0	5920
2Θ range for data collection/°	6.258 to 101.25	4.46 to 50.236
Reflections collected	21198	205792
Independent reflections	6346 [R_{int} = 0.0782, R_{sigma} = 0.0925]	24751 [R_{int} = 0.1223, R_{sigma} = 0.0658]
Data/restraints/parameters	6346/1359/703	24751/2976/1477
Goodness-of-fit on F^2	1.034	1.039
Final R indexes [I>=2σ (I)]	R_1 = 0.0763, wR_2 = 0.1951	R_1 = 0.0804, wR_2 = 0.2105
Final R indexes [all data]	R_1 = 0.1224, wR_2 = 0.2208	R_1 = 0.1338, wR_2 = 0.2472

Table S2: Important bond lengths for compound **1**.

	Length/Å		**Length/Å**
V1–O6	1.593(8)	V5–O11	1.958(7)
V1–O10	1.990(7)	V5–O13	1.972(8)
V1–O11[1]	1.969(7)	V5–O16[1]	1.983(7)
V1–O16	1.965(7)	V5–O22	1.961(8)
V1–O24	1.960(7)	V6–O1	1.572(8)
V2–O3	1.589(7)	V6–O9	1.969(8)
V2–O4	1.975(8)	V6–O12	1.966(7)
V2–O5	1.956(7)	V6–O15	1.962(7)
V2–O17	1.965(8)	V6–O19	1.972(7)
V2–O18[1]	1.967(7)	P1–O13	1.525(8)
V3–O4	1.973(7)	P1–O14	1.502(8)
V3–O5	1.980(7)	P1–O20	1.520(8)
V3–O8	1.571(7)	P2–O9	1.511(8)
V3–O14	1.972(8)	P2–O18	1.531(8)
V3–O23[1]	1.982(8)	P2–O22	1.518(8)
V4–O2	1.583(8)	P3–O19	1.522(8)
V4–O12	1.958(7)	P3–O23	1.523(8)
V4–O15	1.970(7)	P3–O24	1.520(8)
V4–O20	1.967(8)	P4–O10	1.501(8)
V4–O21	1.964(7)	P4–O17	1.522(8)
V5–O7	1.590(8)	P4–O21	1.517(8)

[1]1-X,1-Y,1-Z

Table S3: Important bond angles for compound **1**.

	Angle/°		Angle/°
O6–V1–O10	106.9(4)	O21–V4–O20	84.4(3)
O6–V1–O11[1]	107.6(4)	O7–V5–O11	108.2(4)
O6–V1–O16	106.4(4)	O7–V5–O13	106.8(4)
O6–V1–O24	106.0(4)	O7–V5–O16[1]	105.7(4)
O11[1]–V1–O10	90.0(3)	O7–V5–O22	103.8(4)
O16–V1–O10	146.4(3)	O11–V5–O13	144.8(3)
O16–V1–O11[1]	76.0(3)	O11–V5–O16[1]	75.9(3)
O24–V1–O10	84.6(3)	O11–V5–O22	90.9(3)
O24–V1–O11[1]	146.0(3)	O13–V5–O16[1]	91.0(3)
O24–V1–O16	90.2(3)	O22–V5–O13	84.7(3)
O3–V2–O4	107.7(4)	O22–V5–O16[1]	150.2(3)
O3–V2–O5	107.4(4)	O1–V6–O9	106.6(4)
O3–V2–O17	105.6(4)	O1–V6–O12	107.5(4)
O3–V2–O18[1]	107.5(4)	O1–V6–O15	107.7(4)
O5–V2–O4	76.2(3)	O1–V6–O19	106.9(4)
O5–V2–O17	90.7(3)	O9–V6–O19	83.4(3)
O5–V2–O18[1]	145.0(3)	O12–V6–O9	145.6(3)
O17–V2–O4	146.5(3)	O12–V6–O19	90.3(3)
O17–V2–O18[1]	82.3(3)	O15–V6–O9	90.1(3)
O18[1]–V2–O4	90.9(3)	O15–V6–O12	76.2(3)
O4–V3–O5	75.7(3)	O15–V6–O19	145.3(3)
O4–V3–O23[1]	91.0(3)	V3–O4–V2	103.4(3)
O5–V3–O23[1]	147.3(3)	V2–O5–V3	103.9(3)
O8–V3–O4	108.9(4)	P2–O9–V6	149.6(5)
O8–V3–O5	106.5(4)	P4–O10–V1	145.9(5)
O8–V3–O14	106.0(4)	V5–O11–V1[1]	104.1(3)
O8–V3–O23[1]	106.1(4)	V4–O12–V6	103.8(3)
O14–V3–O4	144.8(3)	P1–O13–V5	142.8(5)
O14–V3–O5	90.5(3)	P1–O14–V3	146.5(5)
O14–V3–O23[1]	83.4(3)	V6–O15–V4	103.5(3)
O2–V4–O12	107.9(4)	V1–O16–V5[1]	103.4(3)
O2–V4–O15	107.5(4)	P4–O17–V2	143.1(5)
O2–V4–O20	105.0(4)	P2–O18–V2[1]	144.3(5)
O2–V4–O21	107.7(4)	P3–O19–V6	144.4(5)
O12–V4–O15	76.2(3)	P1–O20–V4	144.2(5)
O12–V4–O20	146.8(3)	P4–O21–V4	146.1(5)
O12–V4–O21	89.7(3)	P2–O22–V5	144.5(5)
O20–V4–O15	90.1(3)	P3–O23–V3[1]	143.0(5)
O21–V4–O15	144.6(3)	P3–O24–V1	145.9(5)

[1]1-X,1-Y,1-Z

Table S4: Important bond lengths for compound **2**.

	Length/Å		Length/Å
V1–O2	1.950(6)	V11–O10	1.969(6)
V1–O8	1.963(6)	V11–O24	1.907(6)
V1–O12	1.986(6)	V11–O40	1.615(5)
V1–O30	1.963(6)	V12–O13	1.948(5)
V1–O41	1.592(6)	V12–O15	1.984(6)
V2–O3	1.945(6)	V12–O22	1.954(6)
V2–O4	1.980(6)	V12–O28	1.979(6)
V2–O9	1.962(6)	V12–O52	1.577(6)
V2–O20	1.967(6)	V13–O3	1.935(6)
V2–O34	1.589(6)	V13–O17	1.931(6)
V3–O7	1.949(6)	V13–O37	1.992(6)
V3–O14	1.965(5)	V13–O44	1.984(6)
V3–O23	1.998(6)	V13–O55	1.595(6)
V3–O27	1.974(6)	V14–O17	1.934(6)
V3–O35	1.586(6)	V14–O29	1.972(6)
V4–O16	1.963(5)	V14–O36	1.985(6)
V4–O19	1.999(6)	V14–O37	1.976(6)
V4–O26	1.940(6)	V14–O53	1.586(6)
V4–O32	1.975(6)	V15–O2	1.932(6)
V4–O38	1.588(6)	V15–O24	1.933(6)
V5–O5	1.936(6)	V15–O43	1.992(6)
V5–O6	1.966(6)	V15–O47	1.978(6)
V5–O7	1.926(6)	V15–O56	1.594(6)
V5–O31	1.972(6)	V16–O24	1.934(6)
V5–O54	1.610(6)	V16–O39	1.976(6)
V6–O13	1.944(5)	V16–O42	1.979(6)
V6–O16	1.986(5)	V16–O43	1.976(6)
V6–O21	1.979(6)	V16–O45	1.595(6)
V6–O26	1.942(6)	P1–O18	1.538(6)
V6–O49	1.598(6)	P1–O19	1.523(6)
V7–O5	1.946(5)	P1–O25	1.513(6)
V7–O7	1.942(6)	P2–O4	1.508(6)
V7–O14	1.981(5)	P2–O32	1.511(6)
V7–O18	1.975(6)	P2–O33	1.532(6)
V7–O46	1.591(6)	P3–O21	1.535(6)
V8–O13	1.933(6)	P3–O23	1.523(6)
V8–O22	1.976(6)	P3–O28	1.510(6)
V8–O26	1.931(6)	P4–O12	1.509(6)
V8–O33	1.968(6)	P4–O27	1.513(6)

V8–O50	1.611(6)	P4–O31	1.526(6)
V9–O1	1.973(6)	P5–O1	1.528(6)
V9–O3	1.923(6)	P5–O15	1.522(6)
V9–O9	1.980(6)	P5–O29	1.516(6)
V9–O17	1.905(6)	P6–O10	1.539(6)
V9–O51	1.614(5)	P6–O11	1.519(6)
V10–O5	1.942(5)	P6–O39	1.506(6)
V10–O6	1.965(6)	P7–O20	1.517(6)
V10–O11	1.988(6)	P7–O42	1.526(6)
V10–O25	1.974(6)	P7–O44	1.525(6)
V10–O48	1.573(6)	P8–O30	1.515(6)
V11–O2	1.913(6)	P8–O36	1.524(6)
V11–O8	1.979(6)	P8–O47	1.534(6)

Table S5: Important bond angles for compound **2**.

	Angle/°		Angle/°
O2–V1–O8	76.6(2)	O40–V11–O10	111.0(3)
O2–V1–O12	147.9(2)	O40–V11–O24	107.1(3)
O2–V1–O30	89.1(2)	O13–V12–O15	149.4(2)
O8–V1–O12	87.9(2)	O13–V12–O22	77.5(2)
O8–V1–O30	141.7(3)	O13–V12–O28	90.6(2)
O30–V1–O12	86.0(2)	O22–V12–O15	88.5(2)
O41–V1–O2	106.2(3)	O22–V12–O28	143.7(2)
O41–V1–O8	109.3(3)	O28–V12–O15	84.7(2)
O41–V1–O12	105.4(3)	O52–V12–O13	103.8(3)
O41–V1–O30	108.7(3)	O52–V12–O15	106.3(3)
O3–V2–O4	147.9(2)	O52–V12–O22	108.2(3)
O3–V2–O9	76.8(2)	O52–V12–O28	107.9(3)
O3–V2–O20	89.0(2)	O3–V13–O37	145.7(2)
O9–V2–O4	87.6(2)	O3–V13–O44	90.0(2)
O9–V2–O20	141.7(3)	O17–V13–O3	81.7(2)
O20–V2–O4	86.2(2)	O17–V13–O37	77.2(2)
O34–V2–O3	106.0(3)	O17–V13–O44	136.4(3)
O34–V2–O4	105.6(3)	O44–V13–O37	87.1(2)
O34–V2–O9	109.3(3)	O55–V13–O3	106.9(3)
O34–V2–O20	108.8(3)	O55–V13–O17	112.3(3)
O7–V3–O14	77.9(2)	O55–V13–O37	106.0(3)
O7–V3–O23	147.8(2)	O55–V13–O44	111.0(3)
O7–V3–O27	89.6(2)	O17–V14–O29	88.7(2)
O14–V3–O23	87.8(2)	O17–V14–O36	145.5(3)
O14–V3–O27	143.9(2)	O17–V14–O37	77.5(2)
O27–V3–O23	85.3(2)	O29–V14–O36	85.4(3)
O35–V3–O7	105.9(3)	O29–V14–O37	145.0(3)
O35–V3–O14	108.4(3)	O37–V14–O36	88.2(3)
O35–V3–O23	106.0(3)	O53–V14–O17	108.4(3)
O35–V3–O27	107.5(3)	O53–V14–O29	106.6(3)
O16–V4–O19	87.6(2)	O53–V14–O36	105.8(3)
O16–V4–O32	143.8(2)	O53–V14–O37	108.3(3)
O26–V4–O16	78.0(2)	O2–V15–O24	81.5(2)
O26–V4–O19	147.4(2)	O2–V15–O43	145.4(2)
O26–V4–O32	89.6(2)	O2–V15–O47	90.1(2)
O32–V4–O19	85.1(2)	O24–V15–O43	77.0(2)
O38–V4–O16	108.7(3)	O24–V15–O47	136.5(3)
O38–V4–O19	106.4(3)	O47–V15–O43	87.2(2)
O38–V4–O26	105.9(3)	O56–V15–O2	107.0(3)
O38–V4–O32	107.4(3)	O56–V15–O24	112.1(3)

O5–V5–O6	77.5(2)	O56–V15–O43	106.1(3)
O5–V5–O31	142.1(2)	O56–V15–O47	111.2(3)
O6–V5–O31	88.1(2)	O24–V16–O39	88.8(2)
O7–V5–O5	82.6(2)	O24–V16–O42	145.5(3)
O7–V5–O6	146.2(2)	O24–V16–O43	77.4(2)
O7–V5–O31	91.3(2)	O39–V16–O42	85.5(3)
O54–V5–O5	108.8(3)	O39–V16–O43	145.0(3)
O54–V5–O6	106.1(3)	O43–V16–O42	88.1(3)
O54–V5–O7	106.1(3)	O45–V16–O24	107.6(3)
O54–V5–O31	108.8(3)	O45–V16–O39	106.9(3)
O13–V6–O16	146.0(2)	O45–V16–O42	106.5(3)
O13–V6–O21	90.5(2)	O45–V16–O43	107.9(3)
O21–V6–O16	87.6(2)	P5–O1–V9	137.2(4)
O26–V6–O13	82.0(2)	V11–O2–V1	104.5(3)
O26–V6–O16	77.3(2)	V11–O2–V15	97.5(3)
O26–V6–O21	138.6(2)	V15–O2–V1	145.2(3)
O49–V6–O13	104.9(3)	V9–O3–V2	104.3(3)
O49–V6–O16	107.6(3)	V9–O3–V13	97.1(3)
O49–V6–O21	110.7(3)	V13–O3–V2	145.4(3)
O49–V6–O26	110.5(3)	P2–O4–V2	140.5(4)
O5–V7–O14	146.2(2)	V5–O5–V7	97.5(2)
O5–V7–O18	90.7(2)	V5–O5–V10	103.3(3)
O7–V7–O5	81.9(2)	V10–O5–V7	143.6(3)
O7–V7–O14	77.6(2)	V10–O6–V5	101.3(3)
O7–V7–O18	139.3(2)	V5–O7–V3	143.5(3)
O18–V7–O14	87.7(2)	V5–O7–V7	98.0(2)
O46–V7–O5	104.9(3)	V7–O7–V3	103.0(3)
O46–V7–O7	110.3(3)	V1–O8–V11	101.6(3)
O46–V7–O14	107.3(3)	V2–O9–V9	101.6(3)
O46–V7–O18	110.3(3)	P6–O10–V11	136.9(4)
O13–V8–O22	77.4(2)	P6–O11–V10	137.4(4)
O13–V8–O33	142.2(3)	P4–O12–V1	140.1(4)
O26–V8–O13	82.5(2)	V6–O13–V12	143.4(3)
O26–V8–O22	145.8(2)	V8–O13–V6	97.6(2)
O26–V8–O33	91.0(2)	V8–O13–V12	103.2(3)
O33–V8–O22	88.4(2)	V3–O14–V7	101.0(3)
O50–V8–O13	108.4(3)	P5–O15–V12	137.5(4)
O50–V8–O22	106.2(3)	V4–O16–V6	100.9(2)
O50–V8–O26	106.3(3)	V9–O17–V13	97.9(3)
O50–V8–O33	109.1(3)	V9–O17–V14	147.9(3)
O1–V9–O9	87.7(2)	V13–O17–V14	104.5(3)
O3–V9–O1	139.3(2)	P1–O18–V7	135.5(4)

O3–V9–O9	76.9(2)	P1–O19–V4	139.8(4)
O17–V9–O1	89.1(2)	P7–O20–V2	137.2(4)
O17–V9–O3	82.7(2)	P3–O21–V6	135.8(4)
O17–V9–O9	144.3(2)	V12–O22–V8	101.5(3)
O51–V9–O1	110.8(3)	P3–O23–V3	139.9(4)
O51–V9–O3	109.7(3)	V11–O24–V15	97.6(3)
O51–V9–O9	106.9(3)	V11–O24–V16	147.7(3)
O51–V9–O17	107.4(3)	V15–O24–V16	104.5(3)
O5–V10–O6	77.4(2)	P1–O25–V10	136.4(4)
O5–V10–O11	149.4(2)	V4–O26–V6	103.4(3)
O5–V10–O25	90.3(2)	V8–O26–V4	143.9(3)
O6–V10–O11	88.6(2)	V8–O26–V6	97.7(2)
O6–V10–O25	143.5(2)	P4–O27–V3	138.4(4)
O25–V10–O11	84.9(2)	P3–O28–V12	136.0(4)
O48–V10–O5	104.3(3)	P5–O29–V14	137.7(4)
O48–V10–O6	108.4(3)	P8–O30–V1	137.5(4)
O48–V10–O11	105.8(3)	P4–O31–V5	136.8(4)
O48–V10–O25	107.9(3)	P2–O32–V4	138.3(4)
O2–V11–O8	77.1(2)	P2–O33–V8	137.0(4)
O2–V11–O10	139.3(2)	P8–O36–V14	140.0(4)
O10–V11–O8	87.5(2)	V14–O37–V13	100.7(3)
O24–V11–O2	82.7(2)	P6–O39–V16	137.7(4)
O24–V11–O8	144.6(2)	P7–O42–V16	140.6(4)
O24–V11–O10	89.3(2)	V16–O43–V15	100.9(3)
O40–V11–O2	109.6(3)	P7–O44–V13	135.8(4)
O40–V11–O8	107.0(3)	P8–O47–V15	136.0(4)