Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

Synthesis, Crystal Structure and Spectroscopic Studies of a Series of Hexavanadate Hybrids with Multiple Functional Groups

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FT-IR spectra of compounds 2-4

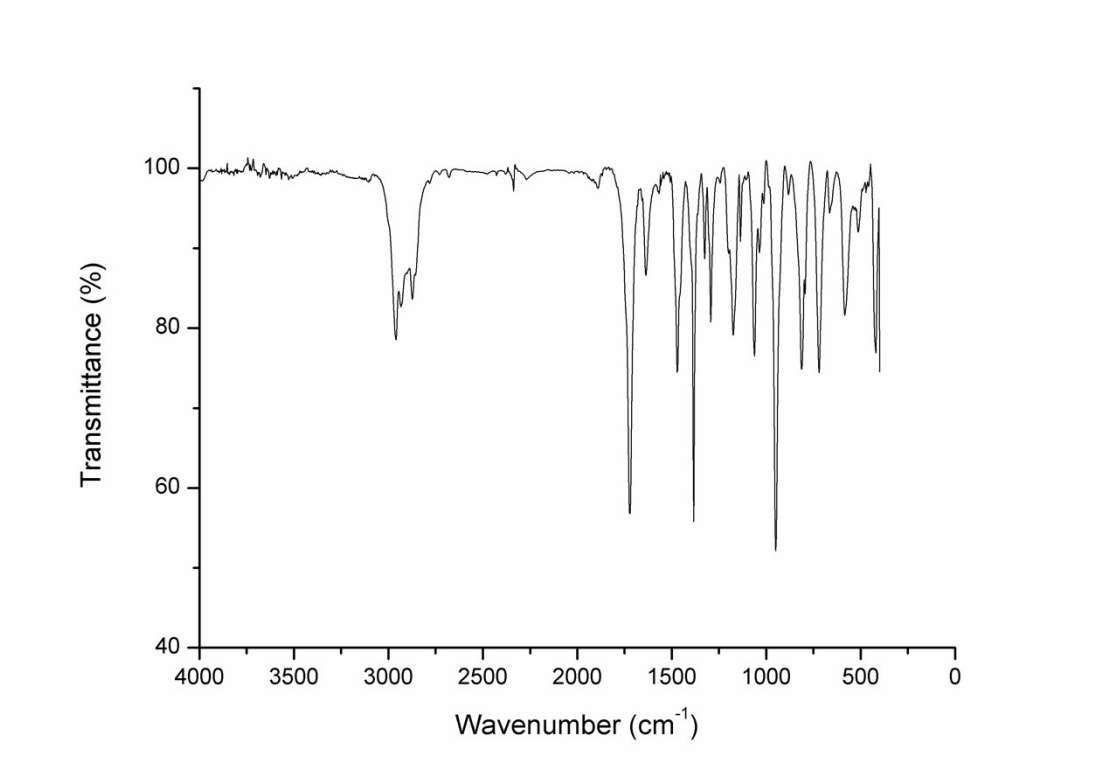

Figure S1. FT-IR spectroscopy studies of compound **2**.

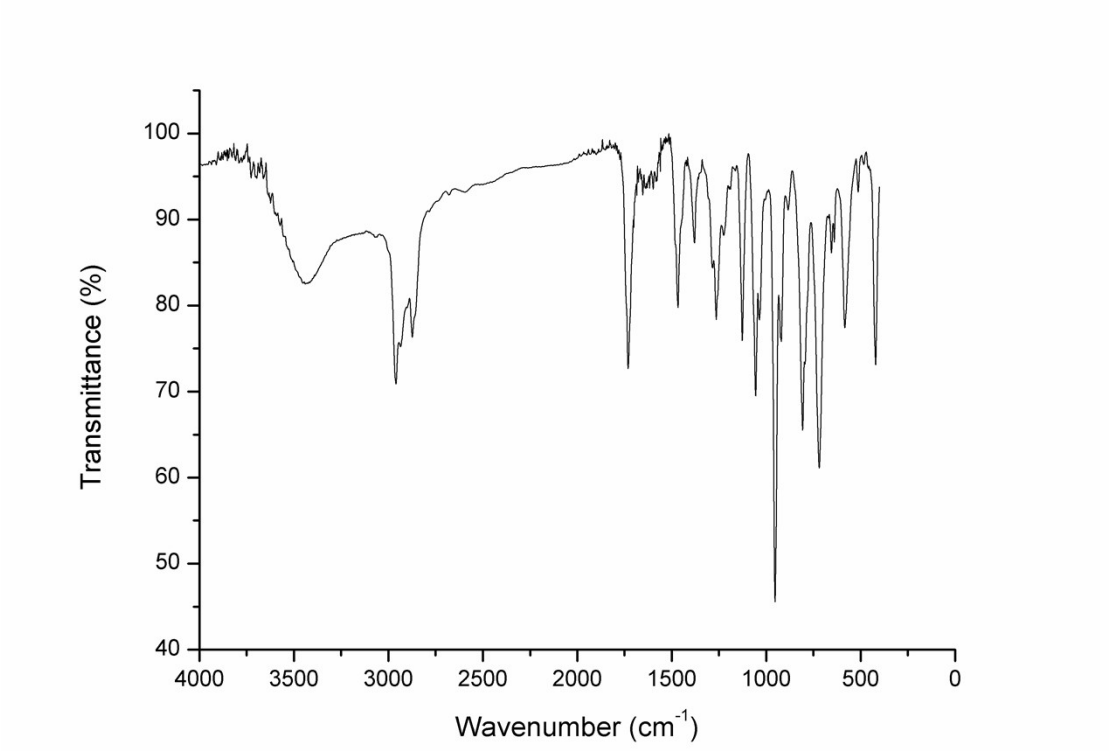

Figure S2 .FT-IR spectroscopy studies of compound **3**.

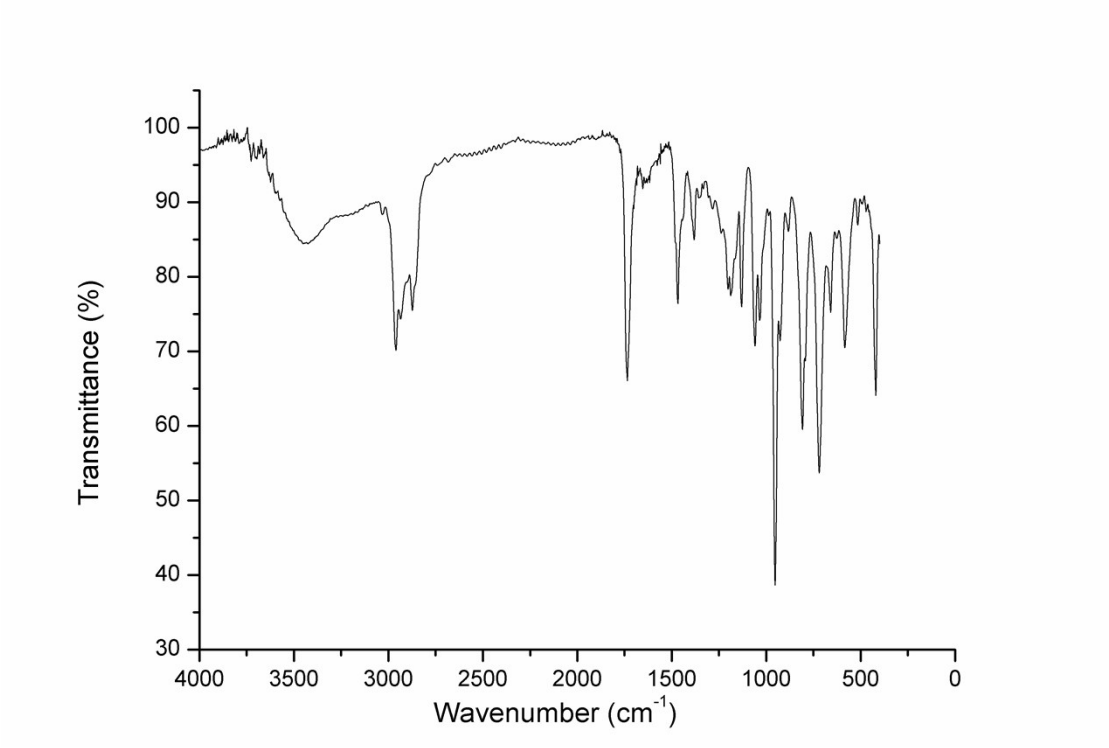

Figure S3. FT-IR spectroscopy studies of compound **4**.

^{1}H NMR spectra of compounds 2-4

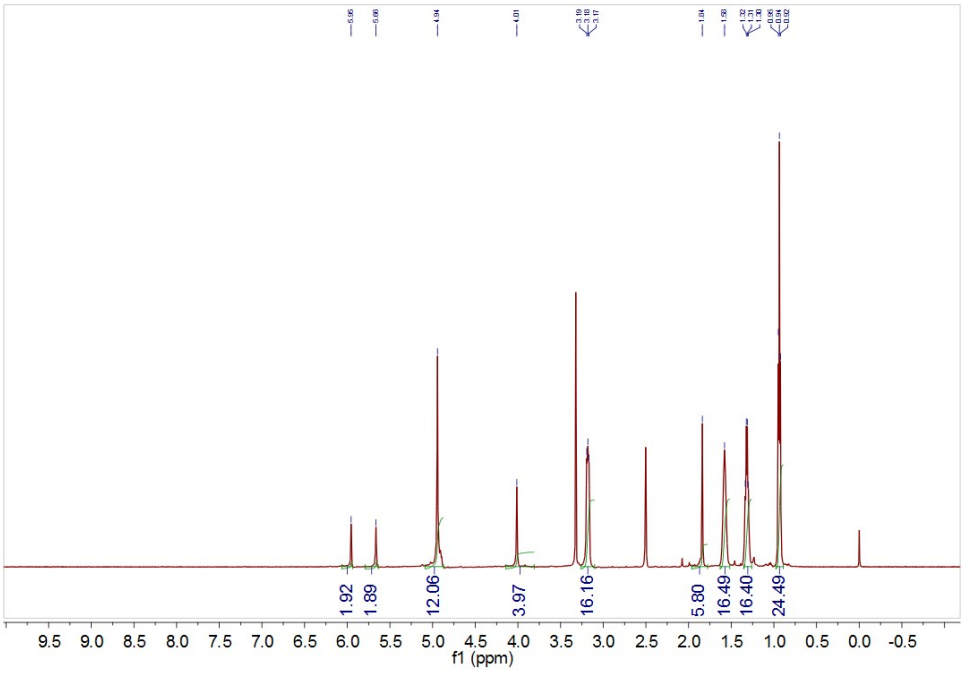

Figure S4. ^{1}H NMR spectra of compound **2** in d_6-DMSO.

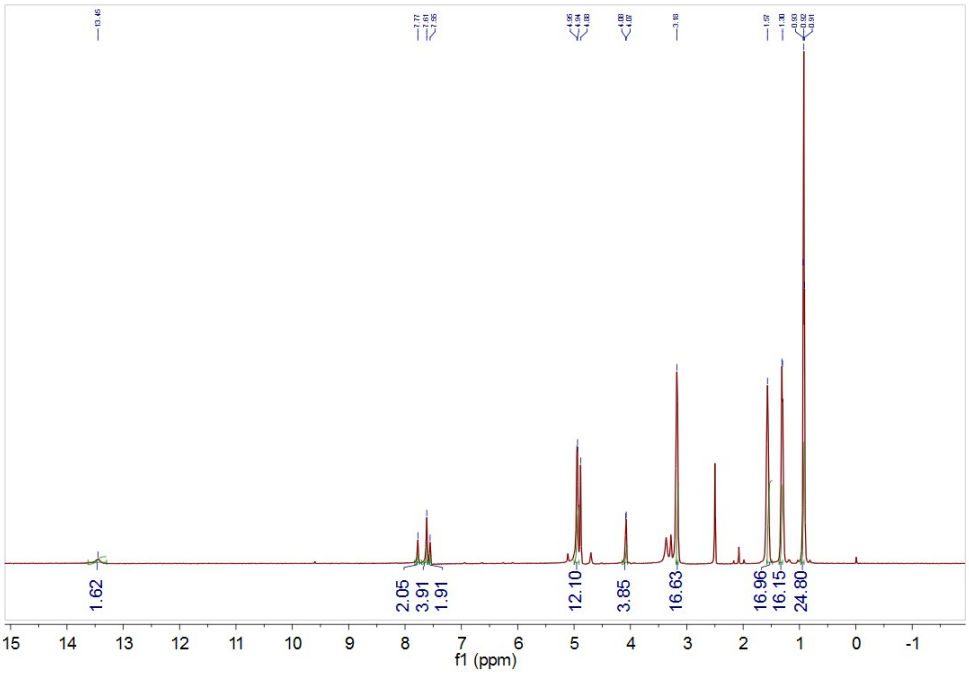

Figure S5. ^{1}H NMR spectra of compound **3** in d_6-DMSO.

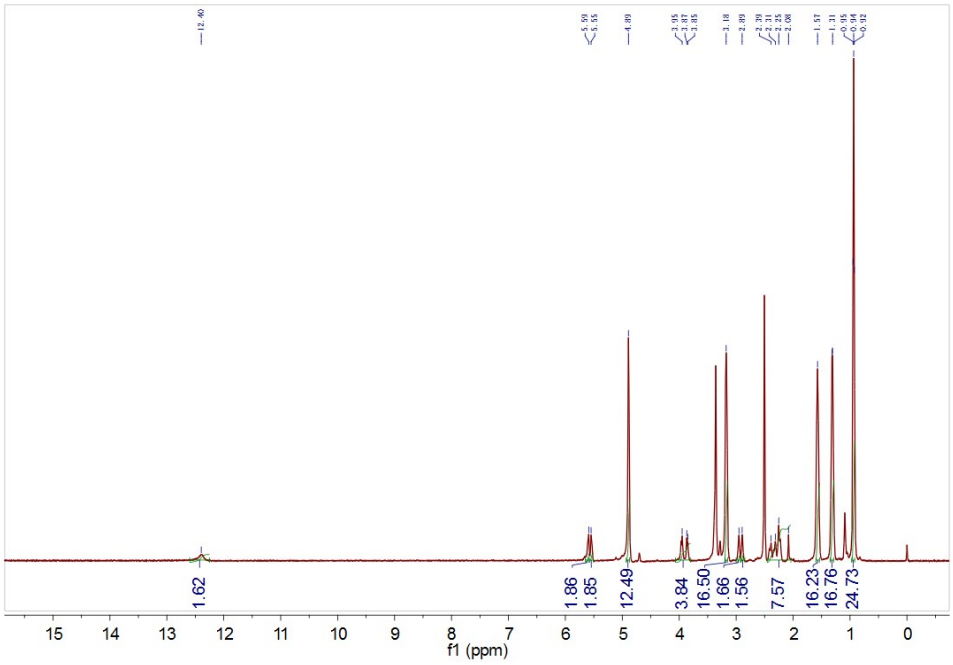

Figure S6. ^{1}H NMR spectra of compound **4** in d_6-DMSO.

* In all the spectra, the solvent d_6-DMSO gives a singlet at 2.5 ppm and the water gives a singlet at 3.3 ppm.

UV-vis spectra of compounds 2-4

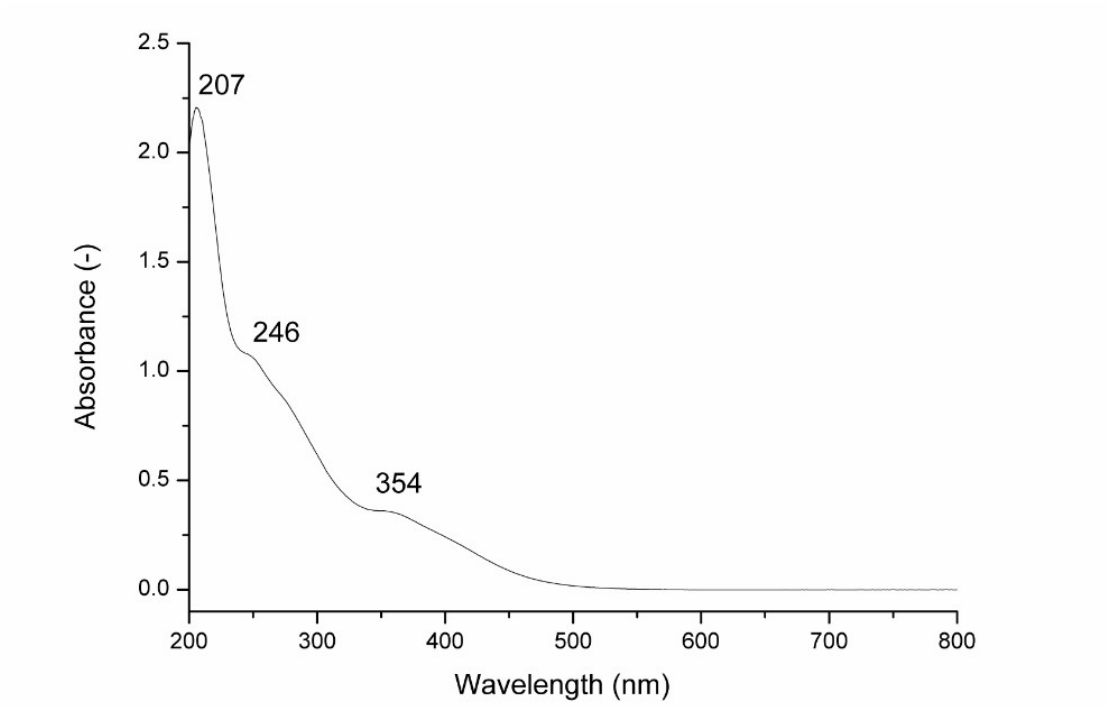

Figure S7. UV-vis spectra of compound **2** in MeCN.

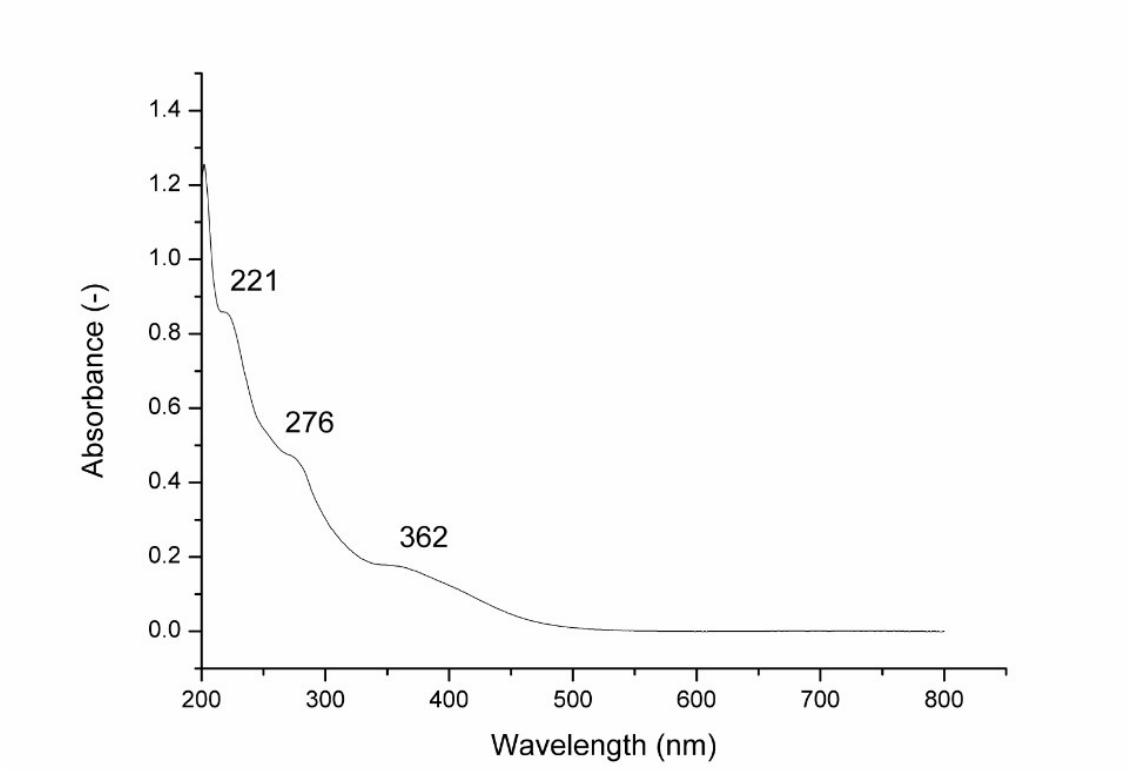

Figure S8. UV-vis spectra of compound **3** in MeCN.

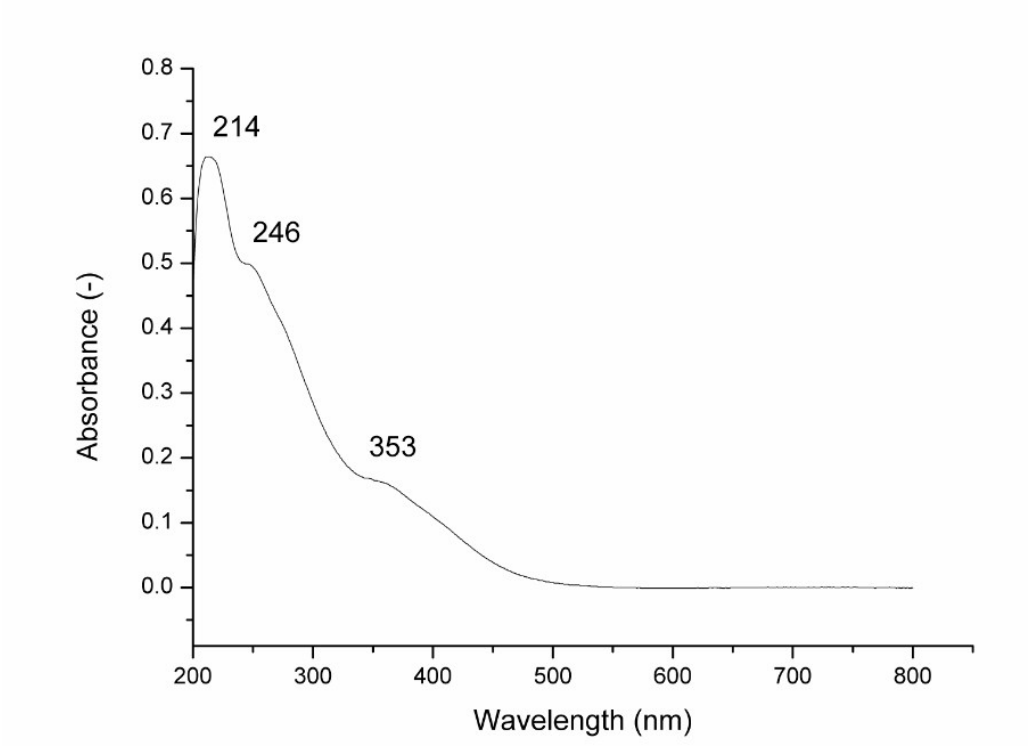

Figure S9. UV-vis spectra of compound **4** in MeCN.

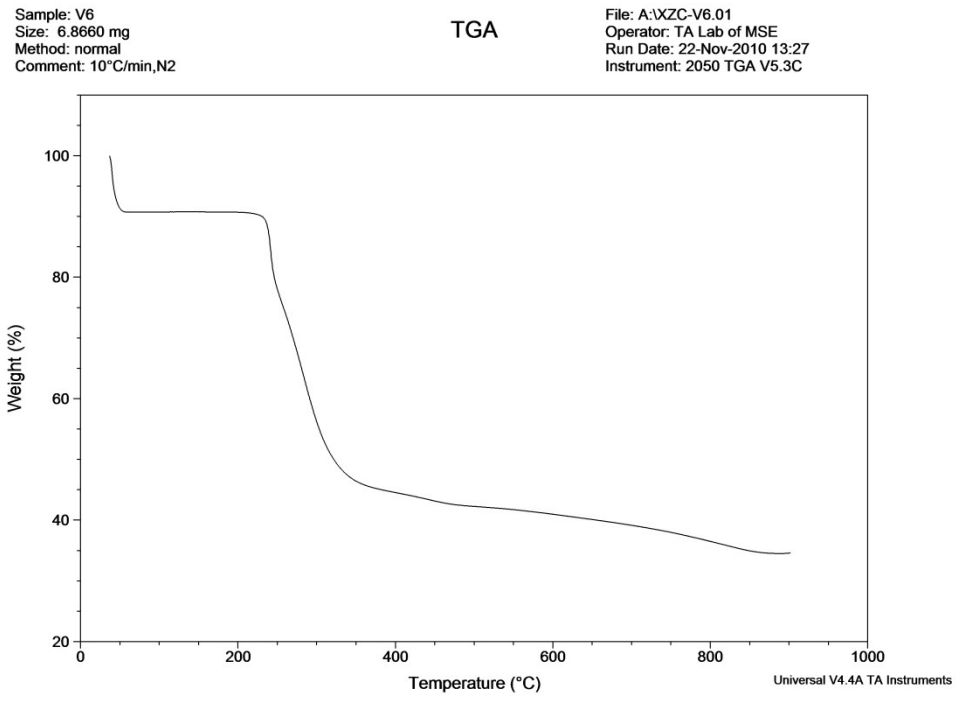

Figure S10. Thermogravimetric curves for compound **1**.

*The loss of solvent molecules in the crytal of compound **1** shows in the temperature range 35 ~ 50 ^{o}C.

Selected Bond Length(Å) and Angle(°)

Table 1: Selected Bond Length(Å) and Angle(°) for Compounds 2-3 and the Two Isomers of Compound 4

Compound 2			
V(1)—O(1)	2.233(9)	V(1)—O(6)	1.833(3)
V(1)—O(2)	2.017(3)	V(1)—O(7)	1.819(3)
V(1)—O(5)	2.017(3)	V(1)—O(8)	1.591(3)
V(2)—O(1)	2.240(9)	V(2)—O(5)	2.008(3)
V(2)—O(3)	2.021(3)	V(2)—O(7)	1.812(3)
V(2)—O(4)	1.815(3)	V(2)—O(9)	1.590(3)
V(3)—O(1)	2.243(10)	V(3)—O(4)	1.831(3)
V(3)—O(2)	2.023(3)	V(3)—O(6)	1.807(3)
V(3)—O(3)	2.018(3)	V(3)—O(10)	1.599(3)
C(2)—O(2)	1.423(5)	C(6)—O(11)	1.273(8)
C(3)—O(3)	1.423(6)	C(6)—O(12)	1.201(9)
C(4)—O(5)	1.425(6)	C(6)—C(7)	1.497(12)
C(5)—O(11)	1.433(6)	C(7)—C(8)	1.342(8)
		C(7)—O(9)	1.463(8)
C(8)—C(7)—C(9)	123.5(12)	C(6)—C(7)—C(8)	121.9(9)
Compound 3			
V(1)—O(2)	1.604(2)	V(1)—O(6)	1.879(2)
V(1)—O(4)	2.244(5)	V(1)—O(8)	1.986(2)
V(1)—O(5)	1.792(2)	V(1)—O(10)	2.028(2)
V(2)—O(1)	1.612(2)	V(2)—O(7)	1.801(2)
V(2)—O(4)	2.234(5)	V(2)—O(9)	2.047(2)
V(2)—O(5)	1.854(2)	V(2)—O(10)	1.996(2)
V(3)—O(3)	1.620(2)	V(3)—O(7)	1.845(2)
V(3)—O(4)	2.251(5)	V(3)—O(8)	2.052(2)
V(3)—O(6)	1.776(2)	V(3)—O(9)	2.007(2)
C(1)—O(8)	1.441(4)	C(7)—C(8)	1.404(5)
C(2)—O(9)	1.433(4)	C(7)—C(12)	1.393(6)
C(3)—O(10)	1.441(4)	C(11)—C(12)	1.394(6)
C(5)—O(11)	1.448(4)	C(12)—C(13)	1.501(5)
C(6)—O(11)	1.311(5)	C(13)—O(13)	1.181(5)
C(6)—O(12)	1.215(5)	C(13)—O(14)	1.340(5)
C(6)—C(7)	1.510(6)		
C(6)—C(7)—C(12)	123.1(4)	C(7)—C(12)—C(13)	119.5(4)
Compound 4			
V(1)—O(2)	1.828(2)	V(1)—O(5)	1.610(2)
V(1)—O(3)	2.250(6)	V(1)—O(8)	2.023(2)
V(1)—O(4)	1.826(2)	V(1)—O(10)	2.020(2)

V(2)—O(1)	1.811(2)	V(2)—O(7)	1.620(2)
V(2)—O(2)	1.821(2)	V(2)—O(8)	2.027(2)
V(2)—O(3)	2.243(5)	V(2)—O(9)	2.026(2)
V(3)—O(1)	1.843(2)	V(3)—O(6)	1.607(2)
V(3)—O(3)	2.239(5)	V(3)—O(9)	2.007(2)
V(3)—O(4)	1.825(2)	V(3)—O(10)	2.024(2)
C(1)—O(9)	1.433(4)	C(5)—O(11)	1.447(5)
C(2)—O(8)	1.431(4)	C(6)—O(11)	1.278(5)
C(4)—O(10)	1.435(4)	C(6)—O(12)	1.165(6)
C(6)—C(7)	1.519(7)		
C(7)—C(8A)	1.556(9)	C(7)—C(8B)	1.518(12)
C(7)—C(12A)	1.594(8)	C(7)—C(12B)	1.413(12)
C(8A)—C(9A)	1.451(17)	C(8B)—C(9B)	1.810(2)
C(9A)—C(10A)	1.307(17)	C(9B)—C(10B)	1.150(2)
C(10A)—C(11A)	1.464(14)	C(10B)—C(11B)	1.410(2)
C(11A)—C(12A)	1.491(12)	C(11B)—C(12B)	1.478(18)
C(12A)—C(13A)	1.464(11)	C(12B)—C(13B)	1.537(17)
C(13A)—O(13A)	1.265(18)	C(13B)—O(13B)	1.253(17)
C(13A)—O(14A)	1.277(19)	C(13B)—O(14B)	1.249(15)
C(9A)—C(10A)—C(11A)	126.3(10)	C(10A)—C(11A)—C(12A)	111.8(8)
C(9B)—C(10B)—C(11B)	124.8(14)	C(10B)—C(11B)—C(12B)	115.5(10)

Selected Torsion Angle（°）

Table 2: Selected Torsion Angle（°） for Compounds 2-3 and the Two Isomers of Compound 4

Compound 2			
O(12)-C(6)-C(7)-C(8)	175.0(6)	O(12)-C(6)-C(7)-C(9)	1.2(3)
Compound 3			
O(12)-C(6)-C(7)-C(12)	55.2(7)	C(8)-C(7)-C(12)-C(11)	2.1(6)
O(13)-C(13)-C(12)-C(7)	22.7(6)	C(8)-C(9)-C(10)-C(11)	1.8(7)
C(6)-C(7)-C(12)-C(13)	11.0(6)		
Compound 4			
O(12)-C(6)-C(7)-C(12A)	-61.8(10)	C(8A)-C(7)-C(12A)-C(11A)	61.5(9)
O(13A)-C(13A)-C(12A)-C(7)	59.4(14)	C(8A)-C(9A)-C(10A)-C(11A)	3(2)
C(6)-C(7)-C(12A)-C(13A)	66.0(10)		
O(12)-C(6)-C(7)-C(12B)	-109.3(10)	C(8B)-C(7)-C(12B)-C(11B)	-168.8(10)
O(14B)-C(13B)-C(12B)-C(7)	135.0(13)	C(8B)-C(9B)-C(10B)-C(11B)	17(4)
C(6)-C(7)-C(12B)-C(13B)	-67.1(11)		