Electronic Supplementary Material (ESI) for Dalton Transactions.

A pair of new chiral polyoxovanadates with decent NLO property

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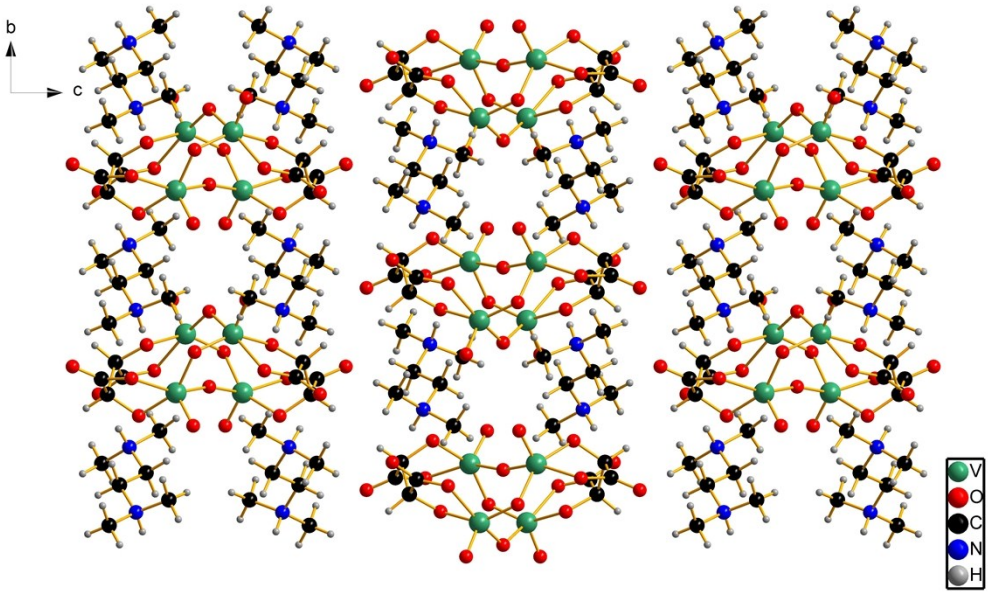

Fig. S1 Representation of the 3D supramolecular structure of 1-L.

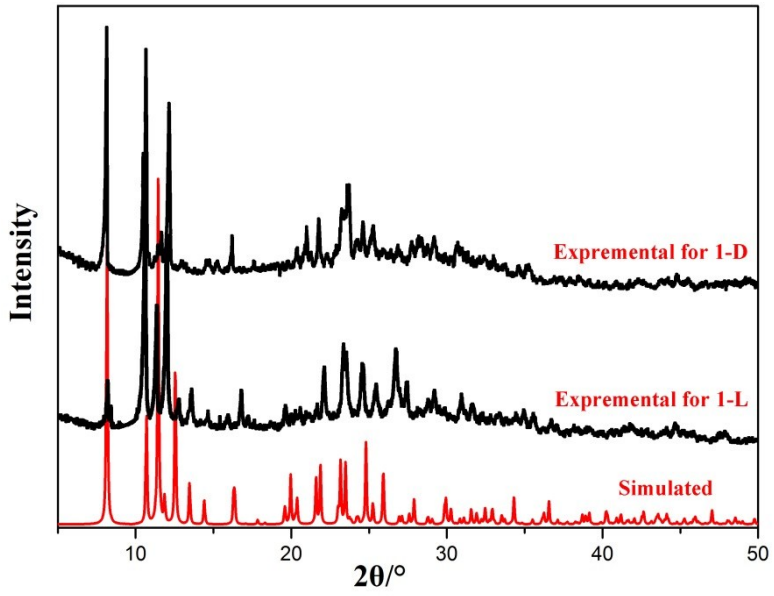

Fig.S2 Experimental and simulated XRD patterns of compound 1-L and 1-D

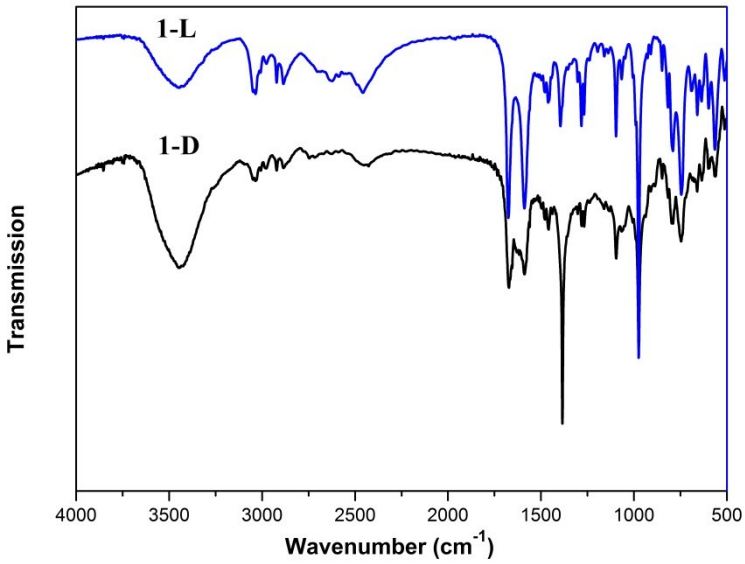

Fig.S3 IR spectrum of compound 1-L and 1-D

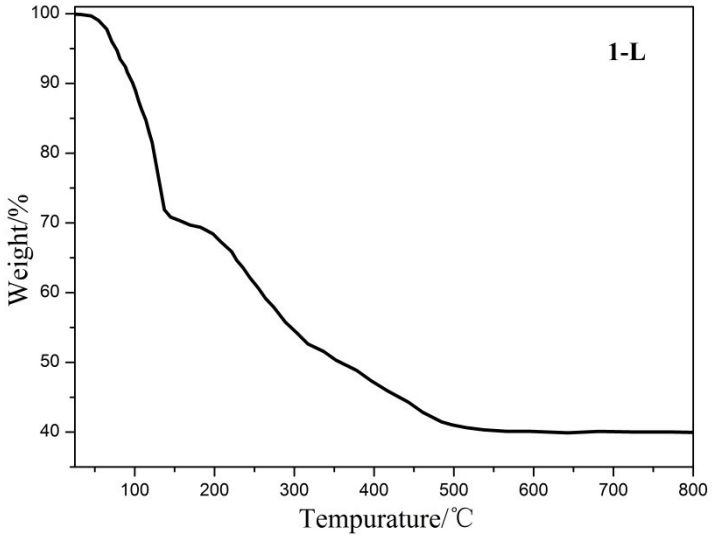

Fig.S4 Thermogravimetric analyses curve of compound 1-L

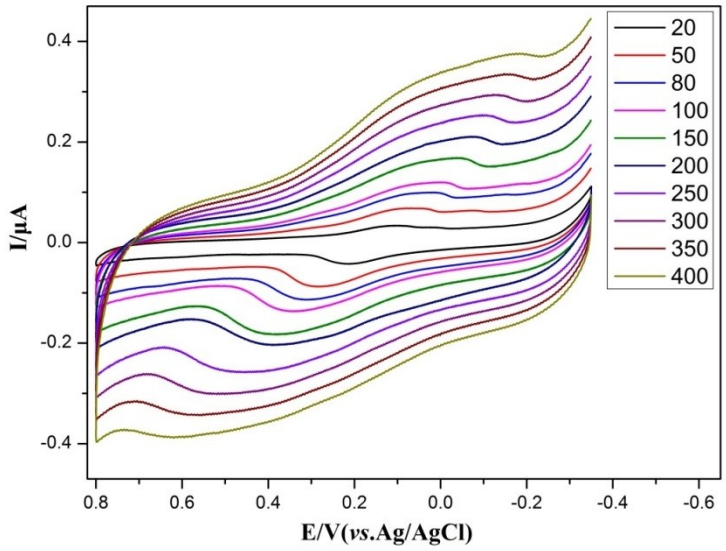

Fig.S5 Cyclic voltammograms of L-CPE in a 1 M Na_2SO_4 solution at different scan rates (from inner to outer: 20, 50, 80, 100, 150, 200, 250, 300, 350 and 400 $mV \cdot s^{-1}$).

Table.S1 bond valence sum (BVS) calculations of 1-L

BVP	R	s	BVP	R	s
V1-O11	1.785	1.009	V2-O10	1.830	0.877
V1-O2	2.071	0.413	V2-O11	1.875	0.762
V1-O6	1.595	1.827	V2-O3	2.047	0.445
V1-O7	1.817	0.913	V2-O5	1.860	0.799
V1-O9	1.944	0.614	V2-O8	1.587	1.874
calculated value		4.777	calculated value		4.756

Table.S2 hydrogen bond length and Angle of Compound 1-L

D—H···*A*	d(D…A)	d(H…A)	∠(DHA)
N1 -- H1A .. O4	2.712(4)	1.80	176
N2 -- H2B .. O3	2.870(4)	2.04	151
N2 -- H2B .. O11	3.091(4)	2.35	138
C6 -- H6B .. O1	3.376(5)	2.60	138
C7 -- H7B .. O5	3.401(5)	2.53	150
C8 -- H8A .. O7	3.350(4)	2.54	140
C8 -- H8A .. O9	3.385(4)	2.50	152
C8 -- H8B .. O8	3.528(5)	2.58	165
C10 -- H10A .. O3	3.390(5)	2.45	168

Table.S3 Selected bond distances (Å) and angles (º).

V1-O2	2.0713	N2-H2B	0.9100
V1-O6	1.5949	C1-C2	1.535(4)
V1-O7	1.8170	C2-C3	1.541(4)
V1-O9	1.9440	C3-C4	1.505(4)
V1-O11	1.7848	C2-H2A	0.9800
V2-O8	1.587(3)	C3-H3A	0.9800
V2-O10	1.8296(8)	C5-C8	1.499(6)
V2-O11	1.875(3)	C5-H5A	0.9700
V2-O3_a	2.048(2)	C5-H5B	0.9700
V2-O5_a	1.861(2)	C6-H6A	0.9600
O1-C1	1.218(5)	C6-H6B	0.9600
O2-C4	1.270(5)	C6-H6C	0.9600
O3-C1	1.298(5)	C7-H7A	0.9600
O4-C4	1.248(4)	C7-H7B	0.9600
O5-C2	1.406(5)	C7-H7C	0.9600
O9-C3	1.402(3)	C8-H8A	0.9700
N1-C10	1.505(5)	C8-H8B	0.9700
N1-C8	1.504(5)	C9-H9A	0.9600
N1-C9	1.476(5)	C9-H9B	0.9600
N2-C5	1.481(5)	C9-H9C	0.9600
N2-C6	1.487(5)	C10-H10A	0.9600
N2-C7	1.478(5)	C10-H10B	0.9600
N1-H1A	0.9100	C10-H10C	0.9600
O2-V1-O6	93.72	C8-N1-C10	107.9(3)
O2-V1-O7	161.62	C9-N1-C10	110.3(3)
O2-V1-O9	77.44	C5-N2-C7	114.5(3)
O2-V1-O11	87.04	C6-N2-C7	108.7(3)
O6-V1-O7	101.22	C5-N2-C6	110.7(3)
O6-V1-O9	106.28	C8-N1-H1A	108.00
O6-V1-O11	105.95	C10-N1-H1A	108.00
O7-V1-O9	88.04	C9-N1-H1A	108.00
O7-V1-O11	98.92	C6-N2-H2B	108.00
O9-V1-O11	144.93	C7-N2-H2B	108.00
O8-V2-O10	101.24(10)	C5-N2-H2B	108.00
O8-V2-O11	103.28(12)	O1-C1-O3	125.1(3)
O3_a-V2-O8	104.25(11)	O3-C1-C2	111.6(3)
O5_a-V2-O8	101.07(12)	O1-C1-C2	123.0(3)
O10-V2-O11	90.37(10)	O5-C2-C3	107.5(3)
O3_a-V2-O10	154.25(11)	C1-C2-C3	108.3(3)
O5_a-V2-O10	100.57(9)	O5-C2-C1	106.4(3)
O3_a-V2-O11	80.30(10)	C2-C3-C4	108.8(2)
O5_a-V2-O11	150.74(11)	O9-C3-C4	109.6(2)

O3_a-V2-O5_a	78.19(9)	O9-C3-C2	107.3(2)
V1-O2-C4	116.79	O2-C4-O4	124.9(3)
V2_a-O3-C1	113.3(2)	O2-C4-C3	114.8(3)
V2_a-O5-C2	111.7(2)	O4-C4-C3	120.3(3)
V1-O7-V1_a	126.02	O5-C2-H2A	112.00
V1-O9-C3	118.65	C1-C2-H2A	111.00
V2-O10-V2_a	166.05(19)	C3-C2-H2A	111.00
V1-O11-V2	110.85	C2-C3-H3A	110.00
C8-N1-C9	114.9(3)	C4-C3-H3A	110.00