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Supplementary Information

Synthesis, Characterization and Catalytic Activity of Two Novel *cis*-Dioxovanadium(V) Complexes: $[VO_2(L)]$ and $[VO_2(HLox)]$

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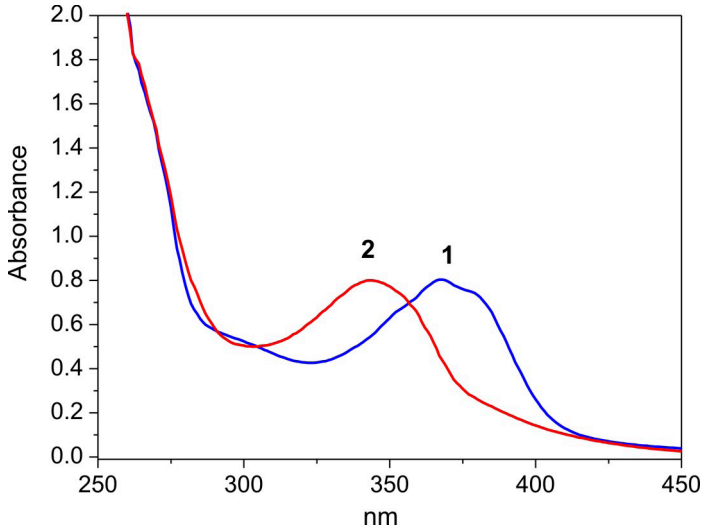

Figure S1. UV-Vis spectra for **1** and **2** recorded in DMSO solutions.

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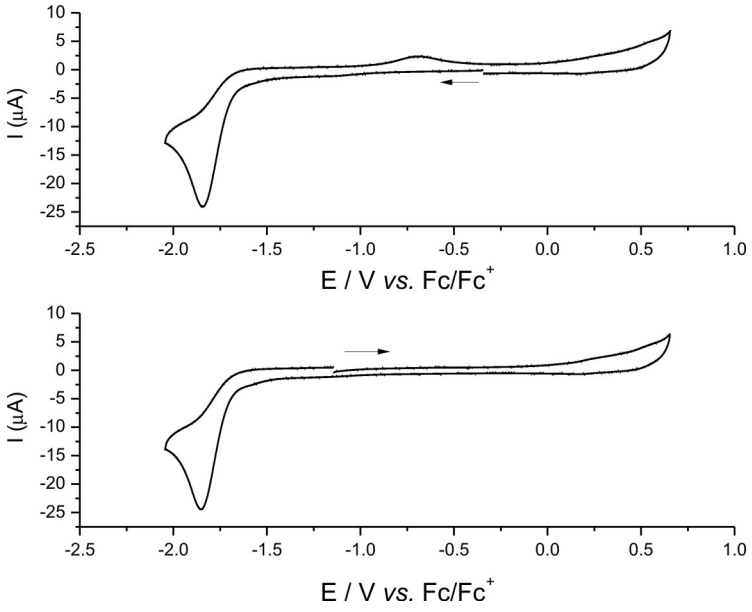

Figure S2. Cyclic voltammograms of complexes **1** in a DMSO/$TBAPF_6$ 0.1 mol L^{-1} solution, scan rate = 0.1 V s^{-1}, working electrode = glassy carbon, reference = Ag/AgCl (DMSO/$TBAPF_6$ 0.1 mol L^{-1}), auxiliary = platinum wire and ferrocene as internal reference. The arrows indicate the scan directions. This figure illustrates the dependence of the process at −0.68 V with the reduction peak at −1.89 V.

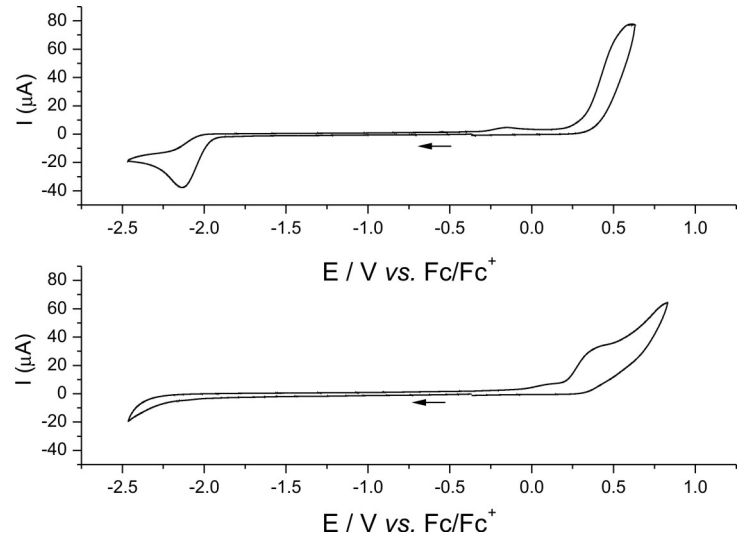

Figure S3. Cyclic voltammograms of the ligands HL (top) and H_2Lox (bottom) in a DMSO/$TBAPF_6$ 0.1 mol L^{-1} solution, scan rate = 0.1 V s^{-1}, working electrode = glassy carbon, reference = Ag/AgCl (DMSO/$TBAPF_6$ 0.1 mol L^{-1}), auxiliary = platinum wire and ferrocene as internal reference. The arrows indicate the scan direction.

Table S1. Summary of the crystal structure data collection and refinement for **1** and **2**

Identification code	$[VO_2(L)]$ (**1**)	$[VO_2(Lox)]$ (**2**)
Empirical formula	$(C_{21}H_{20}N_3O_4V)_2 \cdot H_2O$	$C_{21}H_{21}N_4O_4V$
Formula weight	876.7	444.36
Temperature	293(2) K	293(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	monoclinic	monoclinic
Space group	P 21/c	P21/c
Unit cell dimensions	a = 13.316(3) Å b = 14.293(3) Å c = 22.902(7) Å β = 113.70(2)°	a = 10.126(2) Å b = 15.044(3) Å c = 13.143(3) Å β = 97.61(3)°
Volume	3991.2(17) Å^3	1984.6(7) Å^3
Z	4	4
Density (calculated)	1.459 mg m^{-3}	1.487 mg m^{-3}
Absorption coefficient	0.533 mm^{-1}	0.537 mm^{-1}
F(000)	1816	920
Crystal size	0.26 × 0.25 × 0.13 mm^3	0.47 × 0.22 × 0.14 mm^3
θ range for data collection	5.16 to 25.03°	3.61 to 26.00°
Index ranges	$-15 \le h \le 15$, $-17 \le k \le 17$, $-27 \le l \le 27$	$-12 \le h \le 12$, $-18 \le k \le 17$, $-16 \le l \le 16$
Reflections collected	26034	23865
Independent reflections	6986 [$R_{(int)}$ = 0.0431]	3893 [$R_{(int)}$ = 0.0351]
Completeness to θ = 26.37°	99.1%	99.6%
Absorption correction	empirical	empirical
Max. and min. transmission	0.948 and 0.897	0.931 and 0.785
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	6986 / 2 / 540	3893 / 0 / 271
Goodness-of-fit on F^2	1.169	1.088
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.0578, wR_2 = 0.1291	R_1 = 0.0379, wR_2 = 0.0966
R indices (all data)	R_1 = 0.0872, wR_2 = 0.1386	R_1 = 0.0502, wR_2 = 0.1043
Largest diff. peak and hole	0.487 and –0.364 e.Å^{-3}	0.488 and –0.308 e.Å^{-3}