Electronic supplementary material

Vanadium complexes with multidentate amine bisphenols

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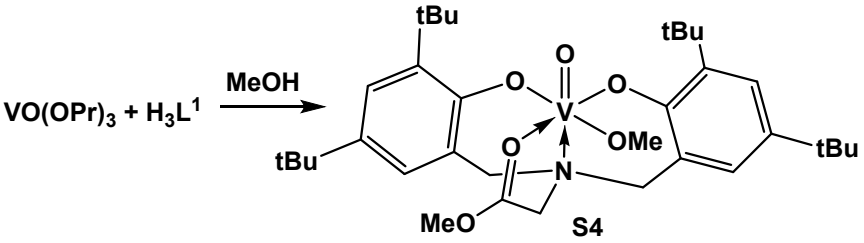
The reaction of glycine bisphenol H_3L^1 with a V(V) precursor [$VO(OPr)_3$] was carried out in various solvents (MeCN, MeOH, EtOH, Et_2O, PhMe). The only characterizable product was mechanically isolated from the mixture, which deposited from the methanol solution.

260 mg (0.51 mmol) of H_3L^1 and 120 µl of [$VO(OPr)_3$] (124 mg, 0.51 mmol) was dissolved in 5 ml of methanol to have a dark solution. The reaction mixture was kept at room temperature for a week while some (ca. 120 mg) crystalline deposition was formed. A selected dark red crystal was analysed by X-ray diffractometry. The oxidation state of the vanadium centre was confirmed by cyclic voltammetry, which show an irreversible one-electron reduction at $E_{1/2}$ = -0.96 V.



S4

Crystal data for S4. $C_{34}H_{52}NO_6V$, M = 621.71, triclinic, a = 9.35040(10), b = 12.4992(2), c = 15.3633(2) Å, α = 106.2400(10), β = 102.8943(25), γ = 91.5820(10)º, V = 1671.58(4) Å^3, space group *P-1* (no. 2), Z = 2, μ(MoKα) = 3.400 mm^{-1}, 26912 reflections measured, 6518 unique (R_{int} = 0.0358), which were used in all calculations. Multi-scan absorption correction made. T_{min} and T_{max} were 0.6662 and 0.7455, respectively. Final R_1 = 0.0378, wR_2 = 0.0918, GOF = 1.077. Minimum and maximum residual electron densities are 0.322 and -0.310 e Å^{-3}, respectively.

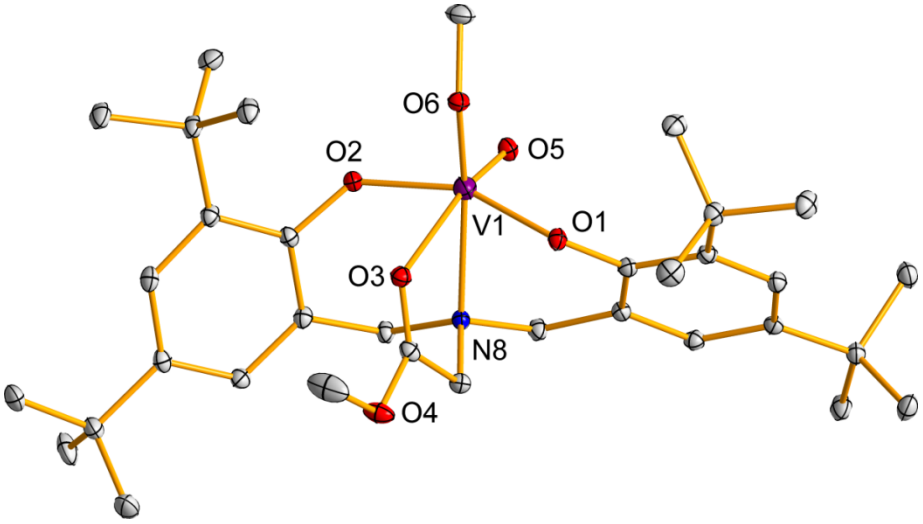


Figure S1. The molecular structure of **S4**. Hydrogen atoms are omitted for clarity.

Table S1. Selected bond lengths [Å] and bond angles [°] in **S4.**

V1-O1	1.5903(12)	O1-V1-O2	100.15(6)
V1-O2	1.8599(11)	O1-V1-O3	97.48(6)
V1-O3	1.8735(11)	O1-V1-O4	165.59(5)
V1-O4	2.3561(12)	O1-V1-O6	104.30(6)
V1-O6	1.7848(11)	O1-V1-N8	92.56(6)
V1-N8	2.2759(14)	O6-V1-N8	162.90(5)
O2-C1	1.354(2)	V1-O2-C1	126.59(10)
O3-C15	1.3475(19)	V1-O3-C15	131.73(10
O4-C17	1.214(2)	V1-O4-C17	113.06(11)
O6-C34	1.417(2)	V1-O6-C34	127.98(12)