Electronic Supplementary Information

Stabilization of two conformers via intra- or inter-molecular hydrogen bonds in a dinuclear vanadium(V) complex with a pendant Schiff base: A theoretical insight

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(7) ^{1}H NMR spectrum of the complex in DMSO-d_6 medium (**Fig. S3)**.

(8) ^{13}C NMR spectrum of the complex in DMSO-d_6 medium (**Fig. S4)**.

Table S1: Selected bond angles (°) for the complex **$(\mu\text{-}O)_2[V(O)(L)]_2$**.

O(1)-V(1)-O(2)	106.41(11)
O(1)-V(1)-O(11)	97.56(10)
O(1)-V(1)-N(19)	159.43(11)
O(1)-V(1)-N(22)	93.24(10)
O(2)-V(1)-O(11)	103.26(10)
O(2)-V(1)-N(19)	92.85(11)
O(2)-V(1)-N(22)	94.32(11)
O(11)-V(1)-N(19)	84.66(10)
O(11)-V(1)-N(22)	155.76(10)
N(19)-V(1)-N(22)	77.84(10)
O(1)-V(1)-O(1^a)	79.15(9)
O(1^a)-V(1)-O(2)	170.86(10)
O(1^a)-V(1)-O(11)	82.86(8)
O(1^a)-V(1)-N(19)	80.86(9)
O(1^a)-V(1)-N(22)	77.94(9)
O(3^b)-V(2)-N(42)	80.42(9)
O(3)-V(2)-O(4)	107.51(11)
O(3)-V(2)-O(31)	97.73(10)
O(3)-V(2)-N(39)	154.42(10)

O(3)-V(2)-N(42)	93.80(10)
O(3)-V(2)-O(3^b)	78.58(9)
O(4)-V(2)-O(31)	101.68(10)
O(4)-V(2)-N(39)	97.21(11)
O(4)-V(2)-N(42)	92.65(11)
O(3^b)-V(2)-O(4)	171.19(9)
O(31)-V(2)-N(39)	83.29(10)
O(31)-V(2)-N(42)	157.92(10)
O(3^b)-V(2)-O(31)	83.48(8)
N(39)-V(2)-N(42)	78.27(10)
O(3^b)-V(2)-N(39)	76.14(9)

Table S2: Crystal data and refinement details of the complex **(μ-O)$_2$[V(O)(L^1)]$_2$.**

Formula	$C_{24}H_{32}Br_2N_4O_{10}V_2$
Formula Weight	798.22
Temperature(K)	273
Crystal system	Orthorhombic
Space group	*Pbca*
a(Å)	10.0908(9)
b(Å)	13.7330(10)
c(Å)	21.1628(15)
V	2932.7(4)
Z	4

d_{calc}(g cm^{-3})	1.808
μ(mm^{-1})	3.423
F(000)	1600
Total Reflections	22350
Unique Reflections	3030
Observed data [I > 2 σ (I)]	2504
No. of parameters	198
R(int)	0.051
R1, wR2 (all data)	0.0466, 0.0987
R1, wR2 [I > 2 σ (I)]	0.0356, 0.0927

Table S3: Selected bond lengths (Å) for the complex **(μ-O)$_2$[V(O)(L^1)]$_2$**

Bond lengths (Å)	
V(1)-O(1)	1.667(2)
V(1)-O(2)	1.621(2)
V(1)-O(11)	1.909(2)
V(1)-N(19)	2.151(3)
V(1)-N(22)	2.164(3)
V(1)-O(1^c)	2.317(2)

Symmetry transformation; ^{c}= 1-x, 1-y, 1-z.

Table S4: Selected bond angles (°) for the complex **(μ-O)$_2$[V(O)(L^1)]$_2$**.

O(1)-V(1)-O(2)	107.35(11)
O(1)-V(1)-O(11)	99.30(10)
O(1)-V(1)-N(19)	156.24(10)
O(1)-V(1)-N(22)	93.12(10)
O(2)-V(1)-O(11)	102.46(10)
O(2)-V(1)-N(19)	94.67(11)
O(2)-V(1)-N(22)	91.08(11)
O(11)-V(1)-N(19)	84.13(10)
O(11)-V(1)-N(22)	157.86(10)
N(19)-V(1)-N(22)	77.31(10)
O(1)-V(1)-O(1^c)	79.27(9)
O(1^c)-V(1)-O(2)	168.52(10)
O(1^c)-V(1)-O(11)	85.34(8)
O(1^c)-V(1)-N(19)	77.59(9)
O(1^c)-V(1)-N(22)	79.03(9)

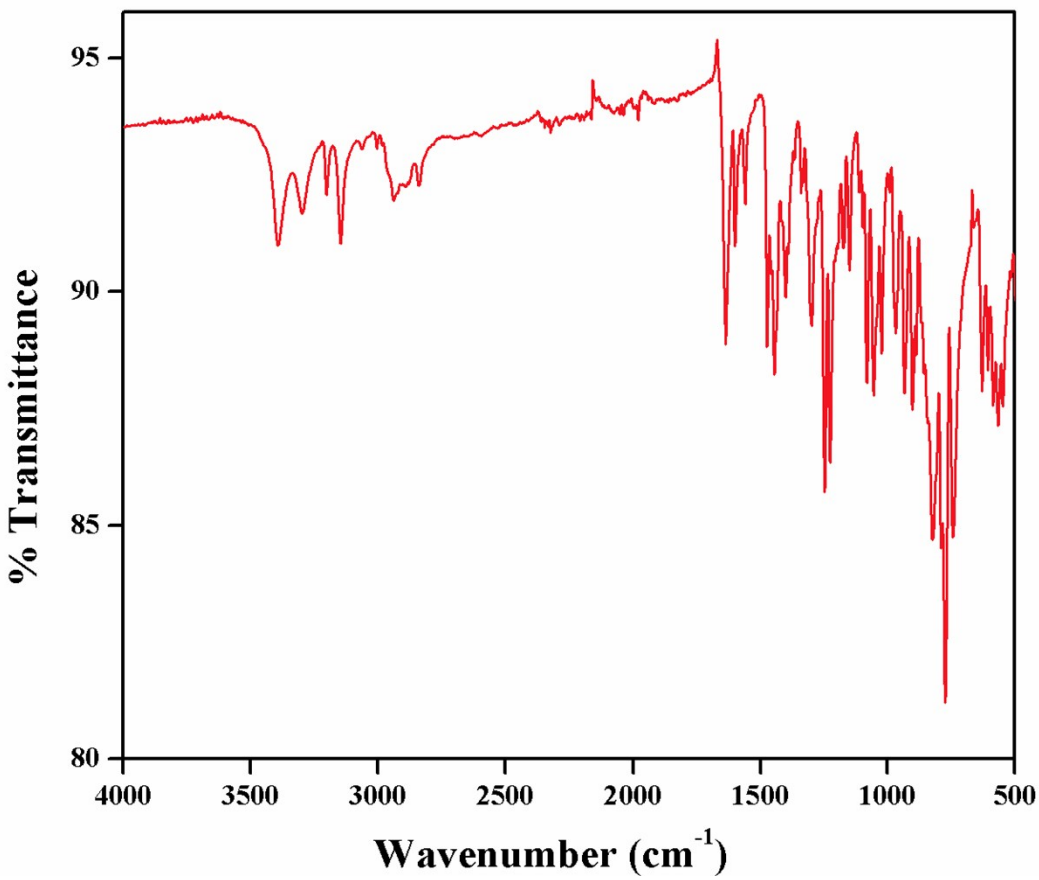

Fig. S1: FT-IR spectrum of the complex.

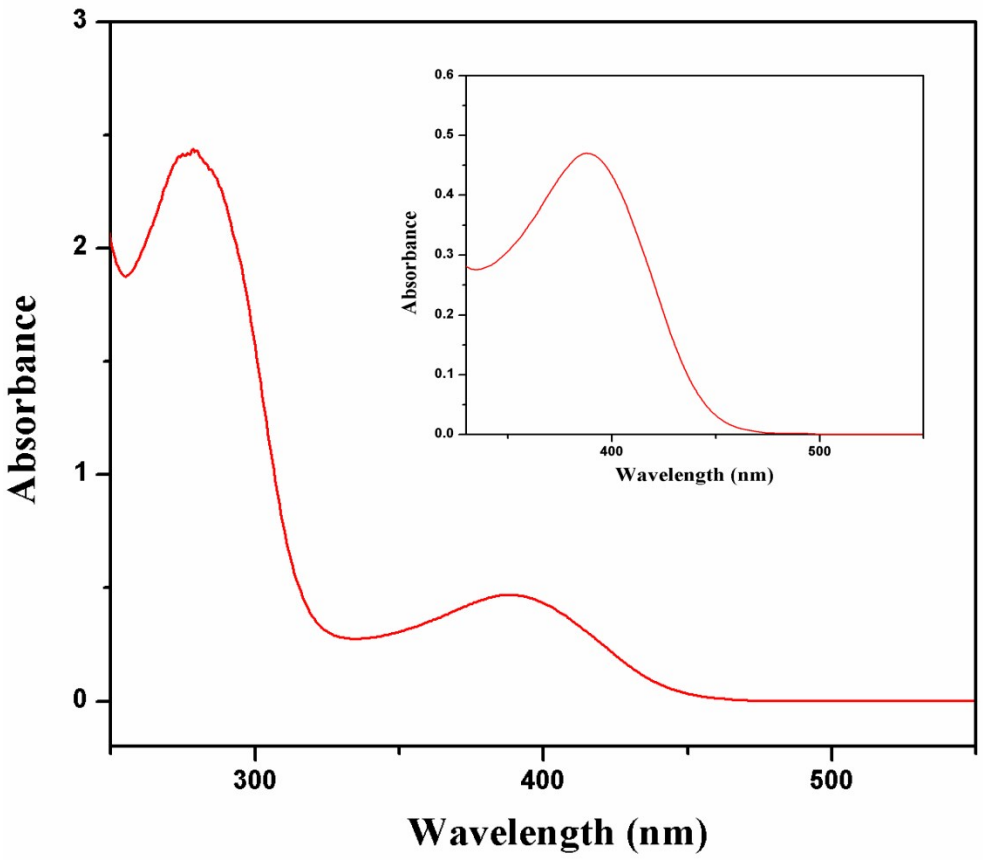

Fig. S2: UV-Vis spectrum of the complex in CH_3CN medium. Inset shows the peak around 390 nm, indicative of LMCT transition.

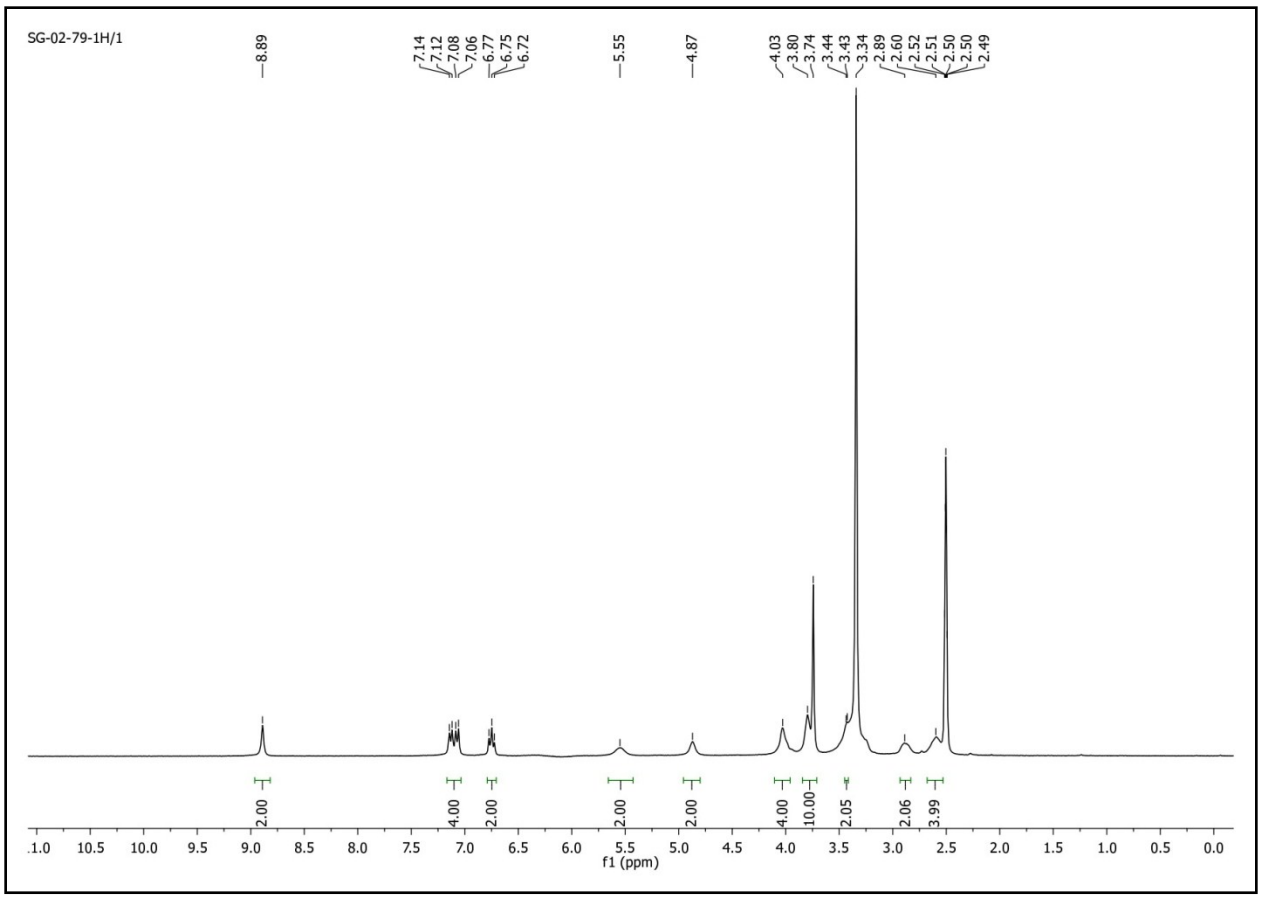

Fig. S3: ^{1}H NMR spectrum of the complex in DMSO-d_6 medium.

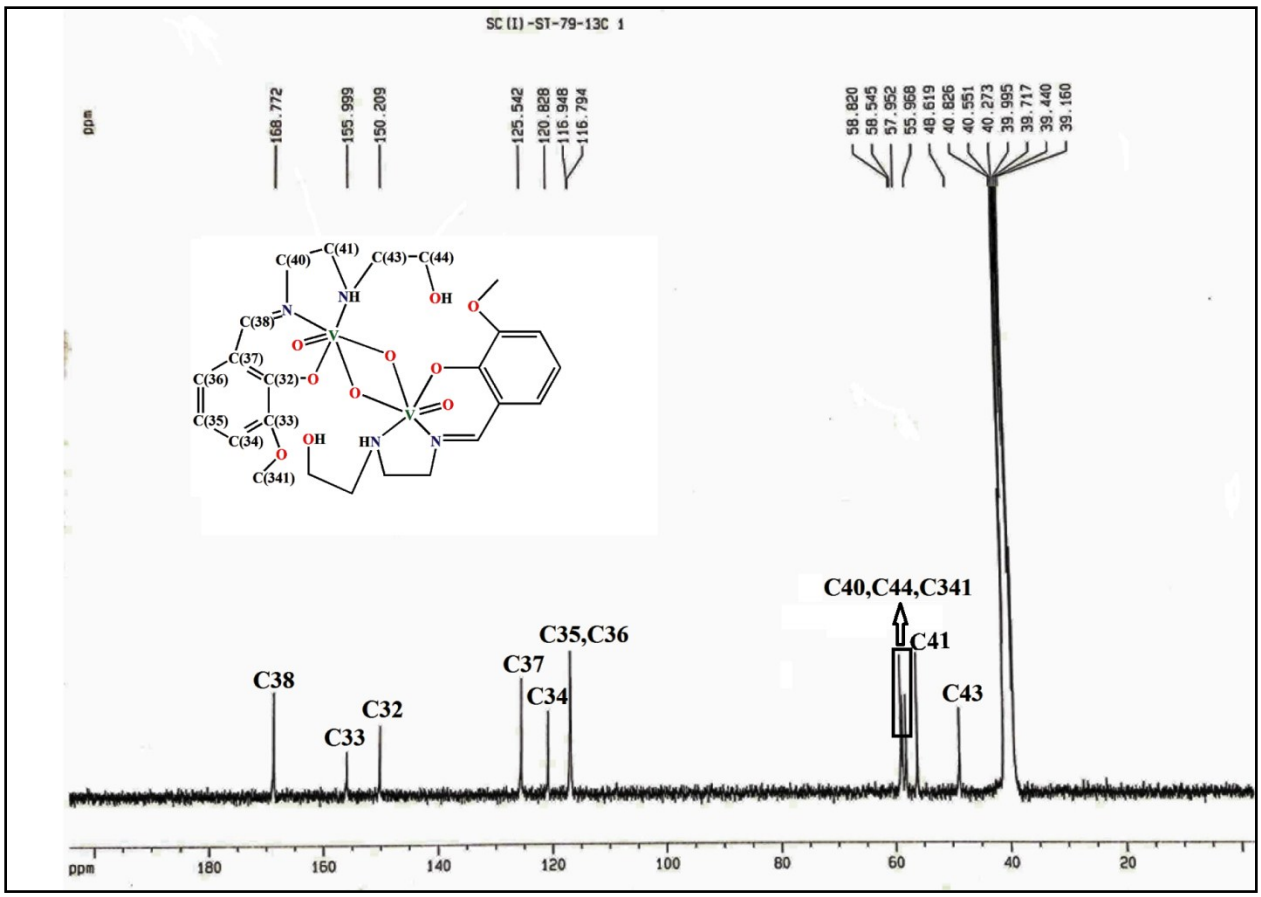

Fig. S4: ^{13}C NMR spectrum of the complex in DMSO-d_6 medium.