

Electronic effect of *para* substituents of 2-hydroxybenzaldehyde co-ligands in a family of hydrazone-oxido vanadium(V) complexes

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Electronic Supporting Information (ESI)

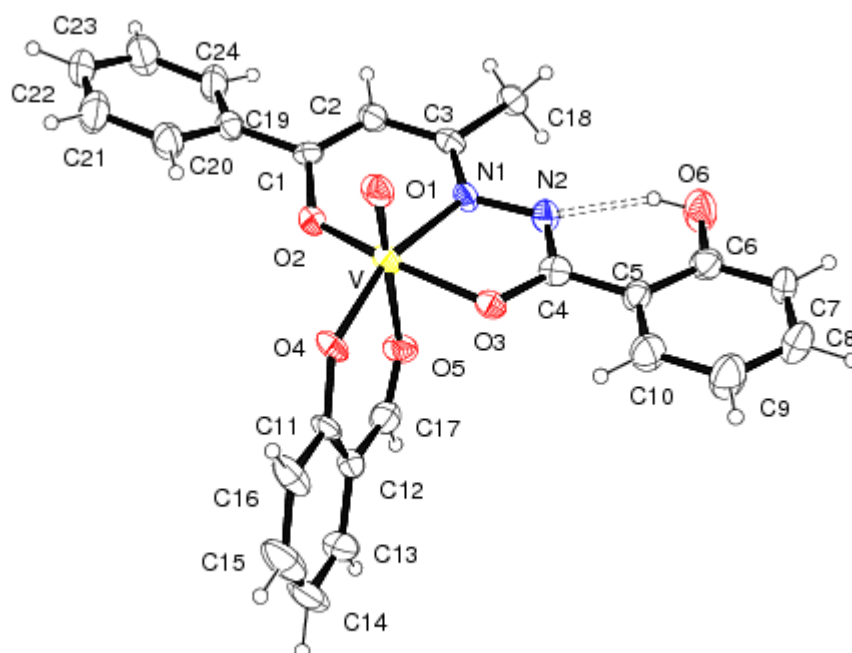


Figure S1: Molecular structure of **5** showing the atom-numbering scheme with ellipsoid at 30% probability. Hydrogen bonds are shown as open bonds.

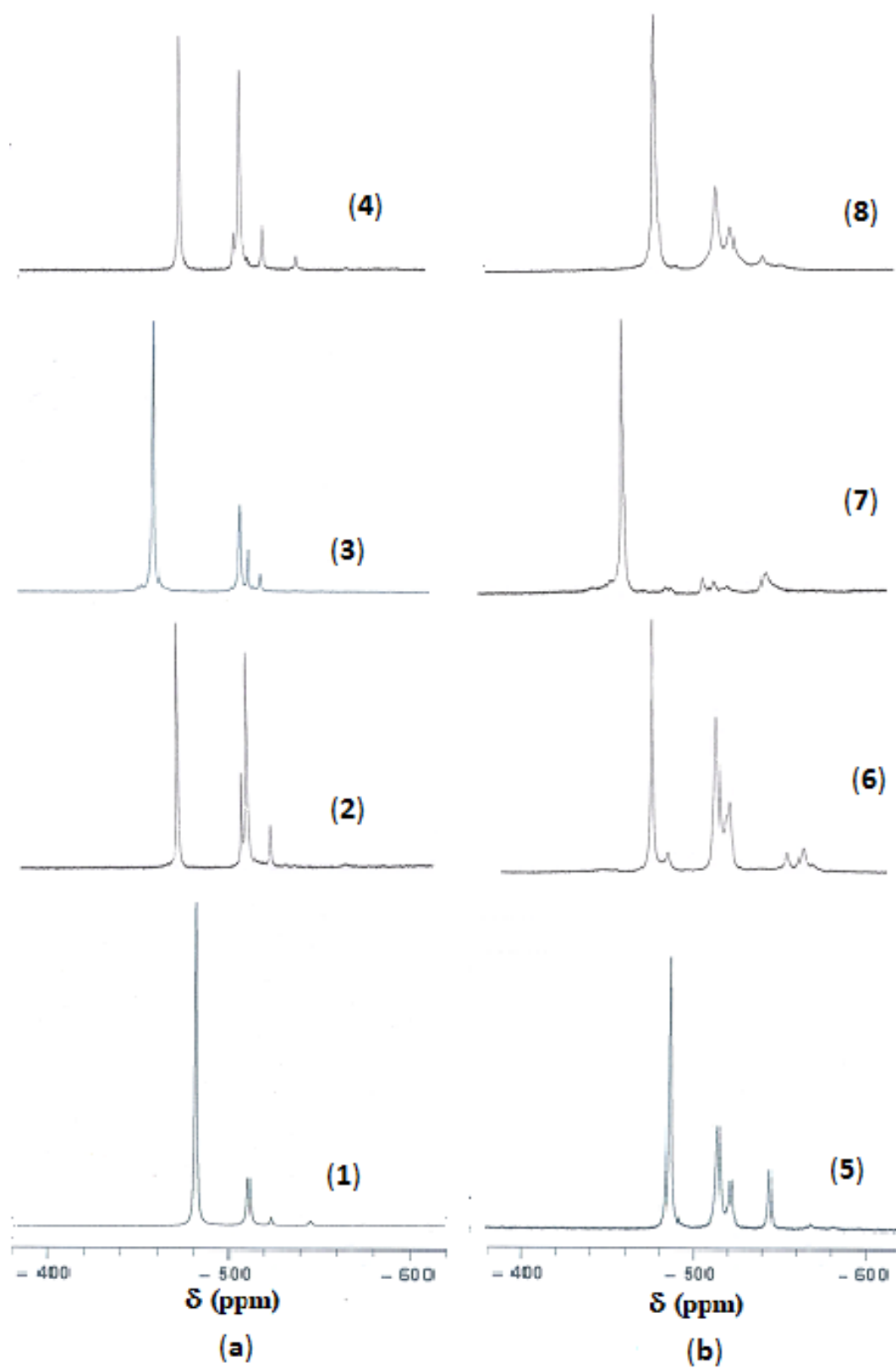


Figure S2: ^{51}V NMR spectra of **1-8** complexes in CDCl_3 solution.

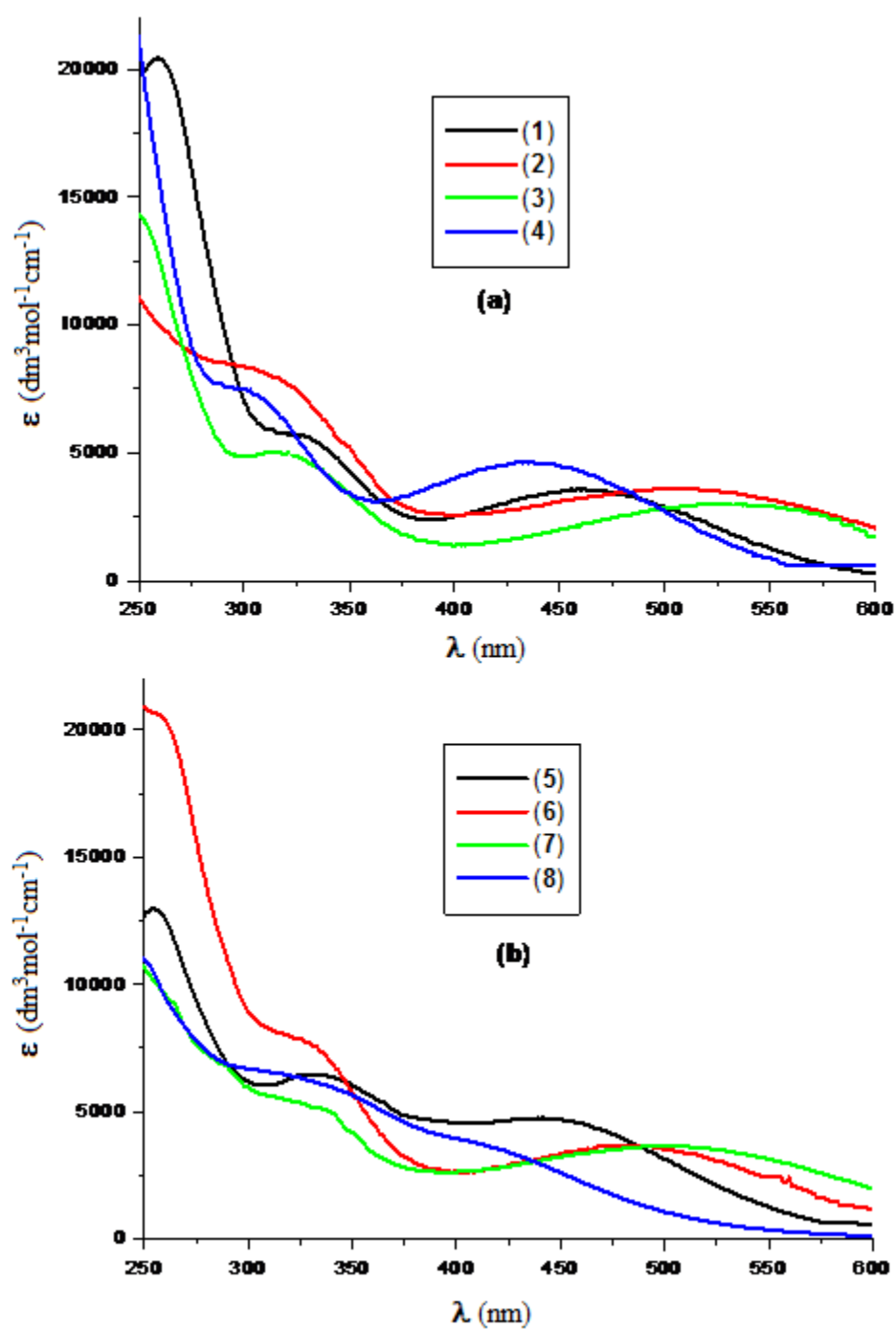


Figure S3: Overlay of the electronic spectra of 1-8 complexes in CH_2Cl_2 solution.

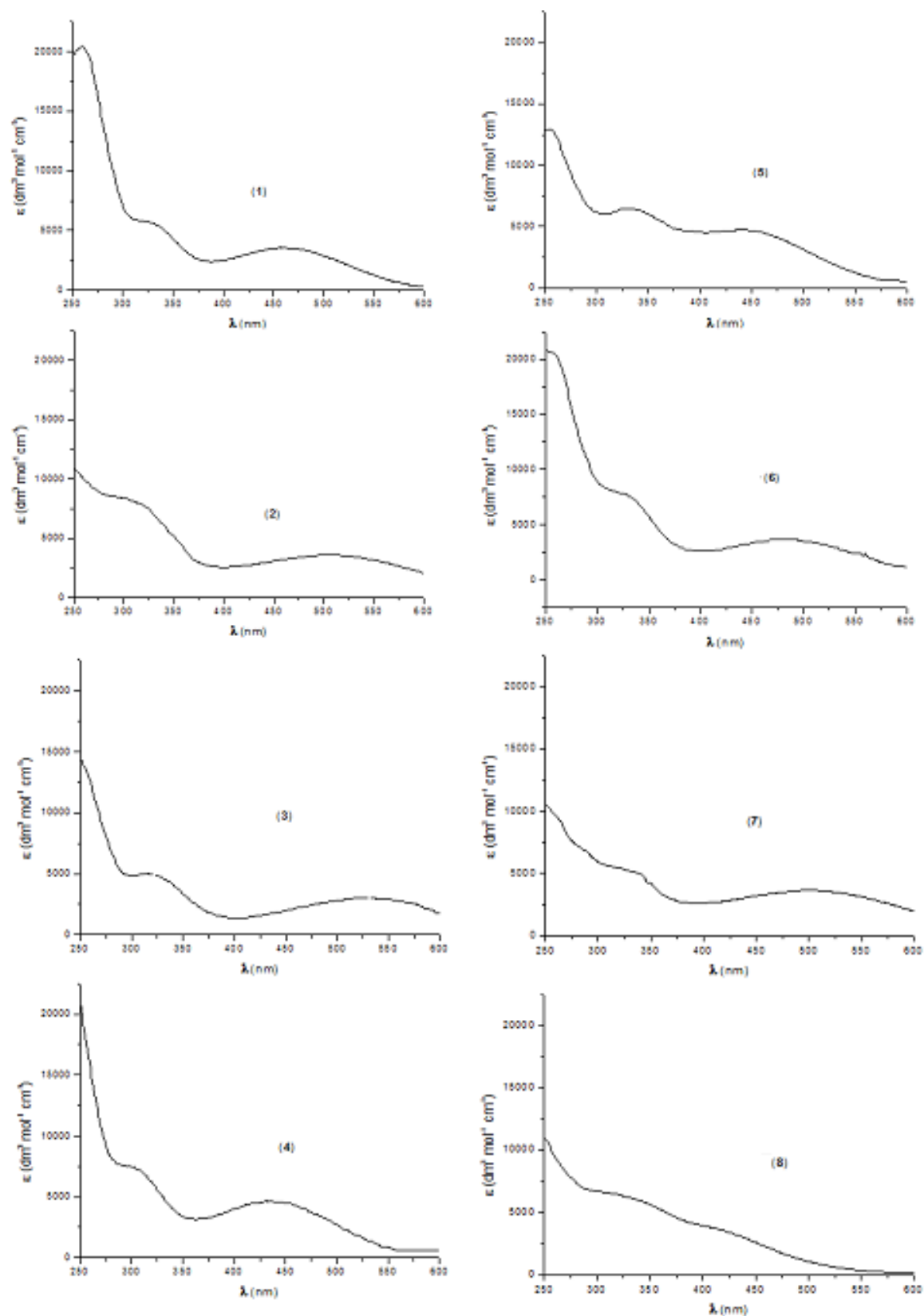


Figure S4: Electronic spectra of 1-8 complexes in CH_2Cl_2 solution.

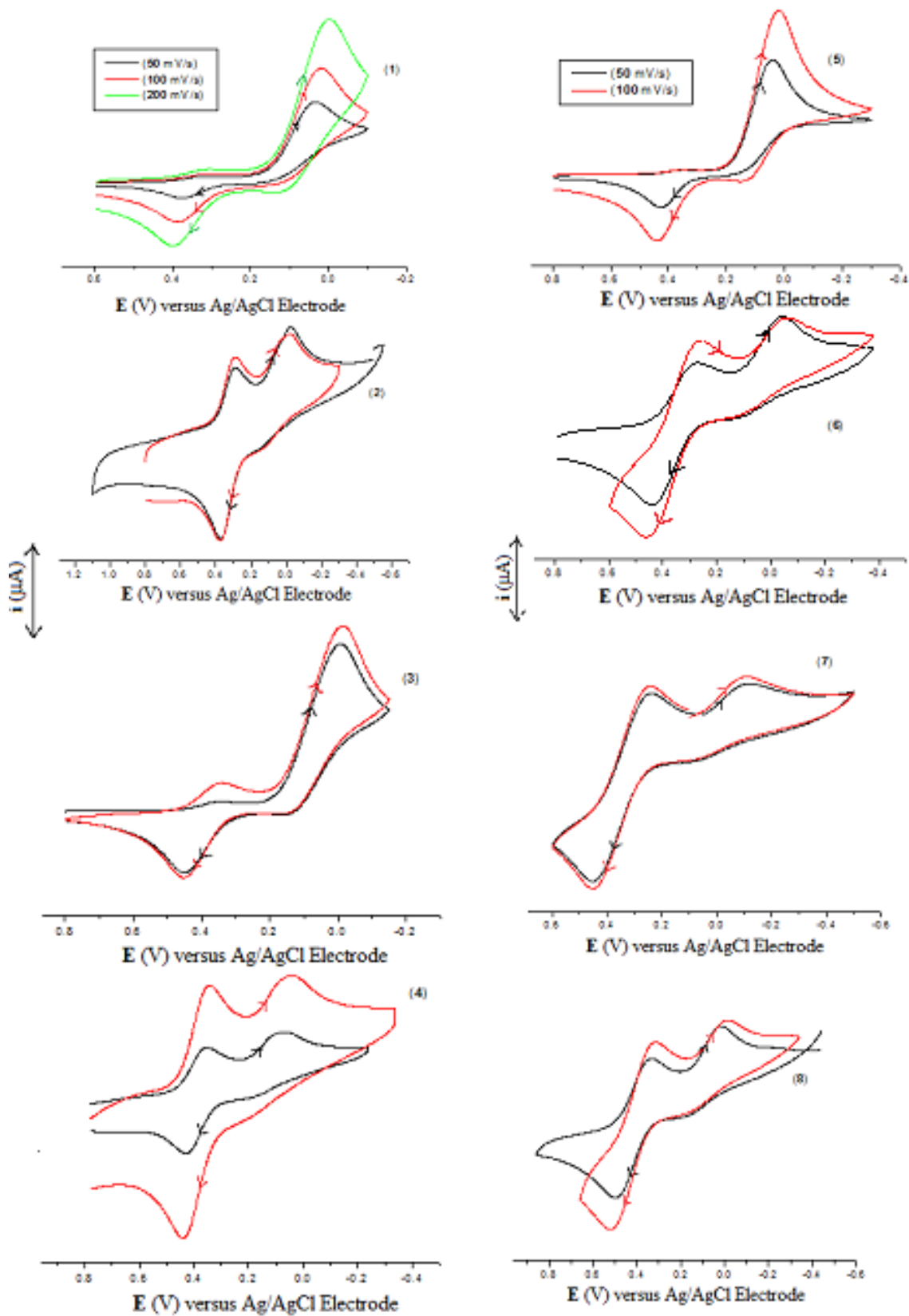


Figure S5: Cyclic voltammogram of 1-8 complexes in CH_2Cl_2 solution at different scan rate. Concentration of the complexes: $\sim 1 \times 10^{-3} \text{ mol dm}^{-3}$; supporting electrolyte: tetrabutylammonium hexafluorophosphate.

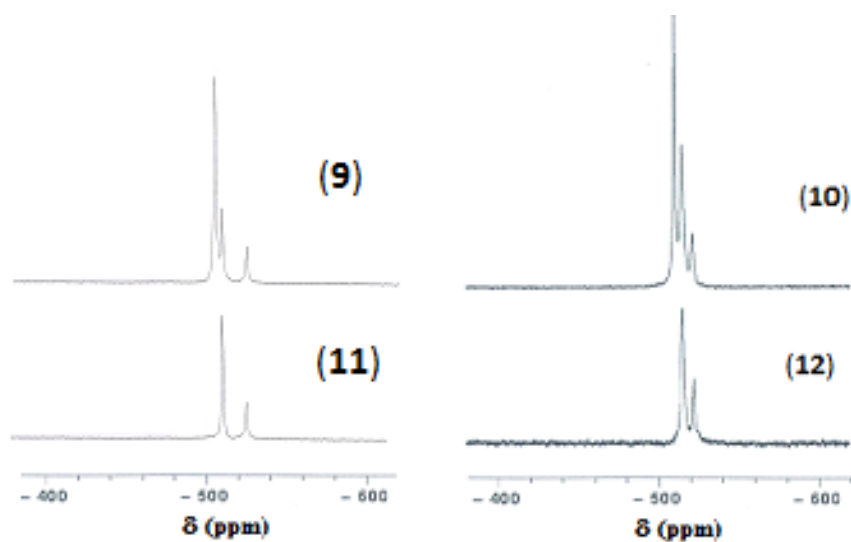


Figure S6: ^{51}V NMR spectra of **9-12** complexes in CDCl_3 solution.

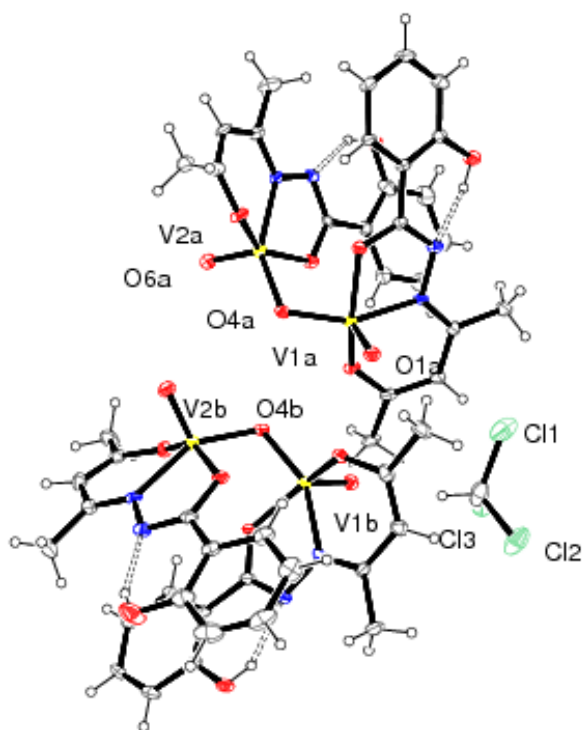
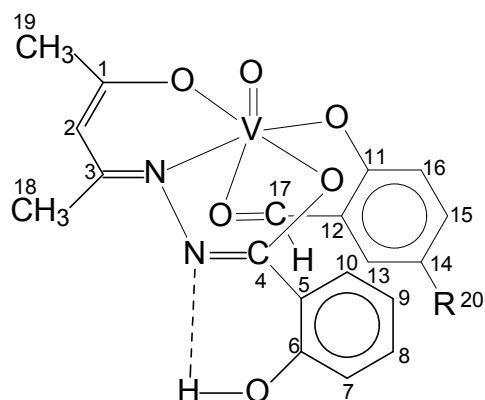
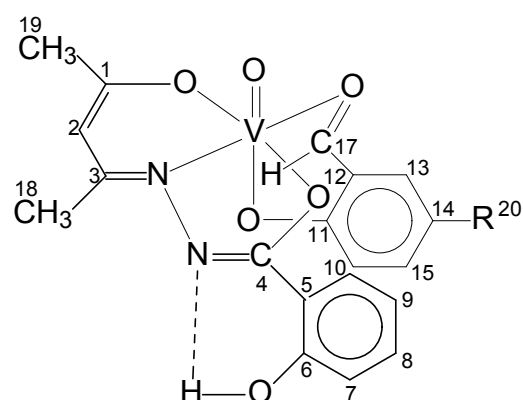


Figure S7: Molecular structure of **11** showing the two molecules in the asymmetric unit with one solvent CHCl_3 molecule. Hydrogen bonds shown as dotted lines



1A-3A



1B-3B

Complex

1

2

3

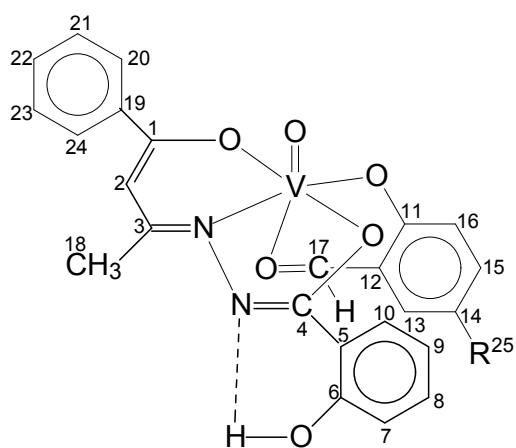
R

H

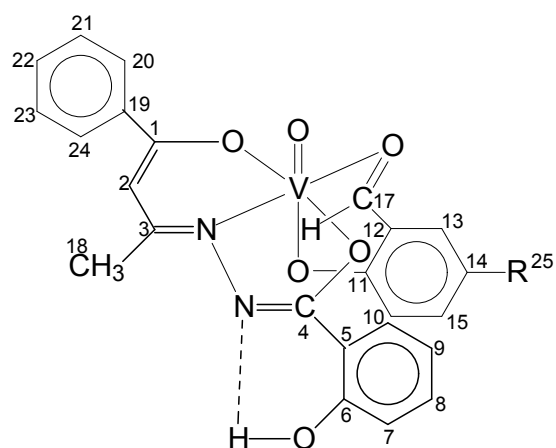
CH₃

OCH₃

Scheme S1: Probable gross structure of the two isomeric forms (**A** and **B**) of complexes **1-3** showing the atom-numbering Scheme for ¹H NMR spectra.



5A-7A



5B-7B

Complex

5

6

7

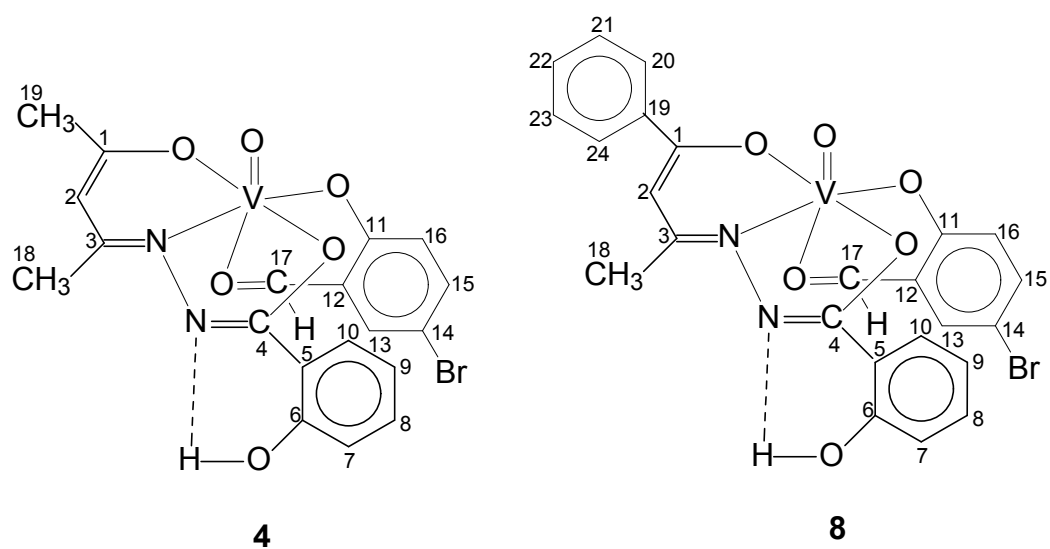
R

H

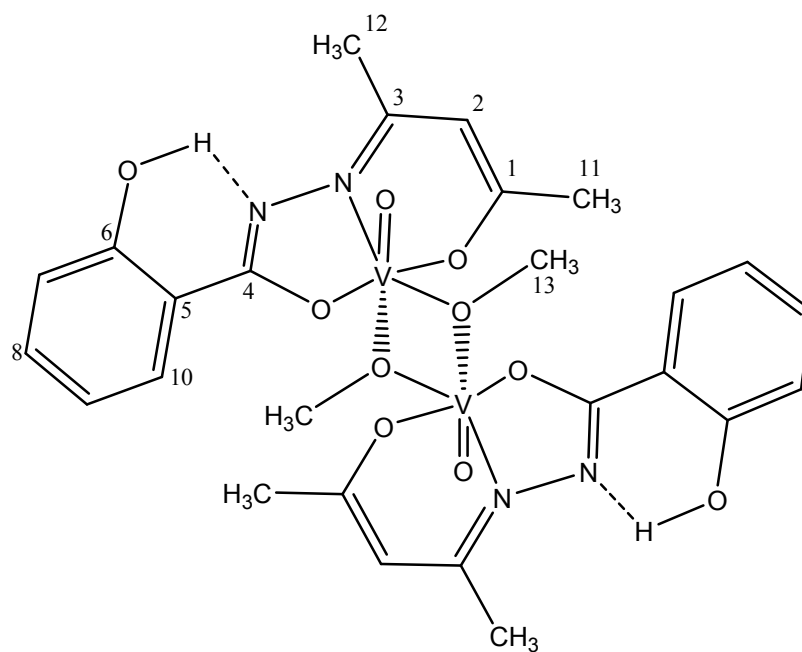
CH₃

OCH₃

Scheme S2: Probable gross structure of the two isomeric forms (**A** and **B**) of complexes **5-7** showing the atom-numbering Scheme for ¹H NMR spectra.



Scheme S3: Probable gross structure of the two isomeric forms (**A** and **B**) of complexes **4** and **8** showing the atom-numbering Scheme for ¹H NMR spectra.



Scheme S4: Probable gross structure of **9** showing the atom-numbering Scheme for ¹H NMR spectra.

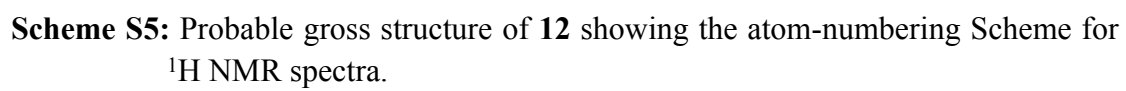


Table S1Crystal data and structure determination summary of **1**, **10** and **11** *

	1	10	11
Empirical formula	C ₁₉ H ₁₇ N ₂ O ₆ V	C ₃₆ H ₃₄ N ₄ O ₁₀ V ₂	C _{24.5} H _{24.5} N ₄ O ₉ Cl _{1.5} V ₂
Formula weight	420.29	784.55	674.04
Crystal colour	black	black	black
Crystal system	monoclinic	orthorhombic	triclinic
Space group	<i>P2₁/c</i>	<i>Pca2₁</i>	<i>P</i> $\bar{1}$
<i>a</i> /Å	11.41(3)	18.5154(18)	11.8887(9)
<i>b</i> /Å	11.09(3)	9.8382(9)	13.9072(11)
<i>c</i> /Å	14.77(4)	19.301(2)	18.0799(14)
α°	(90)	(90)	108.122(7)
β°	92.95(4)	(90)	93.759(6)
γ°	(90)	(90)	90.318(6)
<i>V</i> /Å ³	1866(8)	3515.8(6)	2833.8(4)
<i>Z</i>	4	4	4
$\rho_{\text{calc}}/\text{g cm}^{-3}$	1.496	1.482	1.580
μ/mm^{-1}	0.571	0.596	0.859
F(000)	864	992	1372
Data/restraints/parameters	3518/0/256	5345/1/475	12661/0/751
Goodness-of-fit on <i>F</i> ²	1.032	1.030	0.986
R indices, [<i>I</i> >2σ(<i>I</i>)] R1, wR2	0.0466, 0.1240	0.0286, 0.0655	0.0924, 0.1376
R indices (all data): R1, wR2	0.0736, 0.1469	0.0353, 0.0686	0.1696, 0.1763

*Cell Data for **5**, C₂₄H₁₉N₂O₆V, *M* = 482.35, monoclinic, space group *P2₁/n*, *a* = 13.105(7), *b* = 8.486(4), *c* = 19.710(10) Å, β = 93.973(15)°, *V* = 2186.8(19) Å³, ρ_{calc} = 1.465 gcm⁻³.