ESI section

Trinuclear vanadium(IV) and Vanadium(V) complexes derived from 2,4,6-triacetylphloroglucinol and study of their peroxidase mimicking activity

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ES1. Supplementary data of thermogravimetric analysis.

Figure SI-8-10 presents their profiles and Table SI-3 presents thermal-analytical data.

The thermal stability of tris-$M_3(V^VO_2)$ complexes have been studied under an oxygen atmosphere. These complexes lose mass exothermally between 100 – 400 ^oC roughly equal to six water molecule. The two/three fragments were also observed upon further increasing the temperature between 410 – 445 ^oC (Table SI-3), suggesting the complete loss of the ligands. The remaining mass loss obtained between 483 – 1013 ^oC (Table SI-3) equals to their corresponding $3KVO_3$/$3NaVO_3$/ $3CsVO_3$.

Table S1 Details of thermogravimetric analytical data of complexes.

Compound	Temp. range	% Weight loss Obs [a] (calcd)	Group lost	Expected) group / residue
$K_3[(V^VO_2)_3\{ptk(inh)_3\}]\cdot 6H_2O$ **7**	100-400	12.8 (10.02)	6 H_2O	$K_3[(V^VO_2)_3\{ptk(inh)_3\}]$
	400-483	52.5 (52.08)	L-3O	$3KVO_3$
	483-987	44.07 (40.46)	$3KVO_3$	
$Na_3[(V^VO_2)_3\{ptk(inh)_3\}]\cdot 6H_2O$ **11**	100-300	10.2 (10.49)	6 H_2O	$Na_3[(V^VO_2)_3\{ptk(inh)_3\}]$
	300-527	67.1 (54.49)	L-3O	$3NaVO_3$
	527-1013	31.7 (35.53)	$3NaVO_3$	
$Cs_3[(V^VO_2)_3\{ptk(nah)_3\}]\cdot 6H_2O$ **16**	100-300	13.8 (10.49)	6 H_2O	$Cs_3[(V^VO_2)_3\{ptk(nah)_3\}]$
	300-539	52.2 (54.49)	L-3O	$3CsVO_3$
	539-987	41.60 (51)	$3CsVO_3$	

[a] Total mass loss considering both temp range given in previous column.

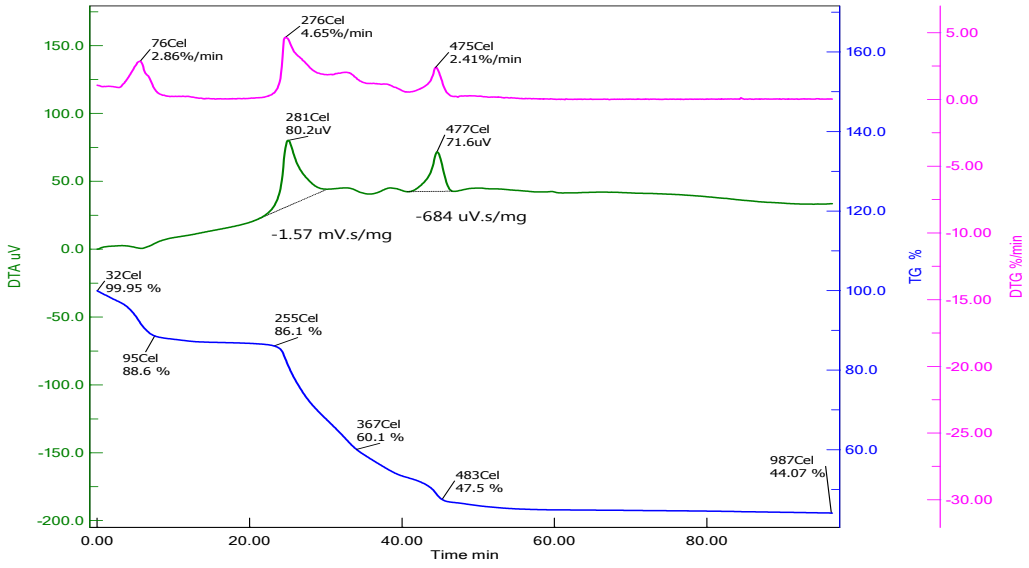

Fig. S1 TGA plots for $K_3[(V^VO_2)_3\{ptk(inh)_3\}]\cdot 6H_2O$ **7**.

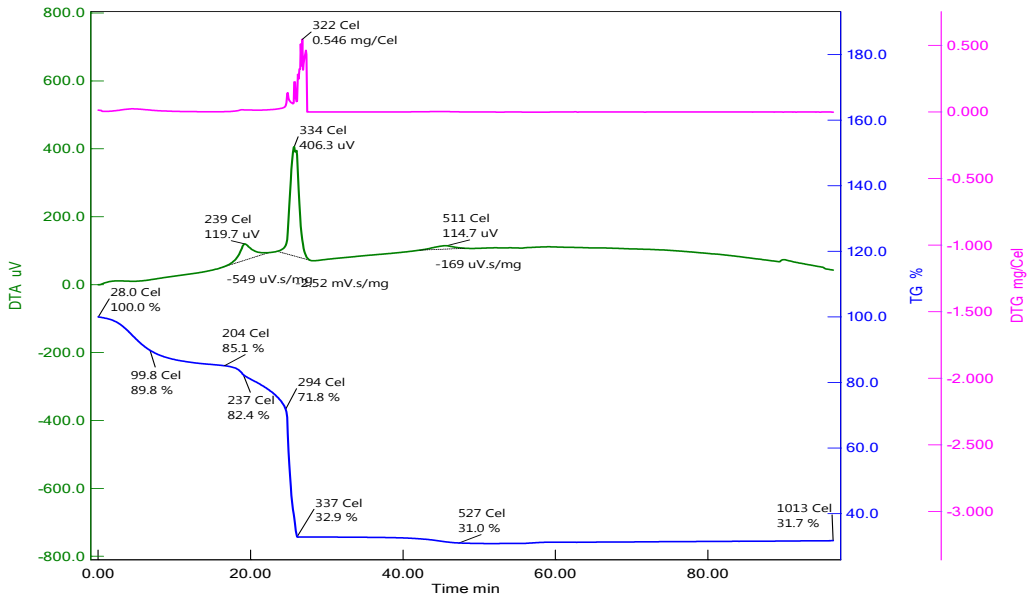

Fig. S2 TGA plots for $Na_3[(V^VO_2)_3\{ptk(inh)_3\}]\cdot 6H_2O$ **11**.

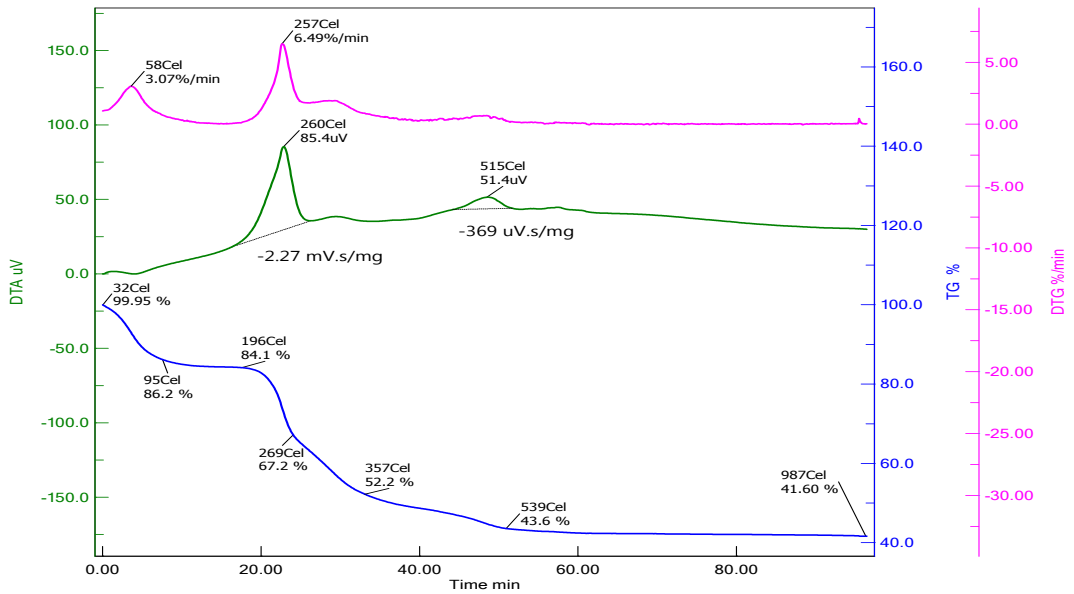

Fig. S3 TGA plots for $Cs_3[(V^VO_2)_3\{ptk(nah)_3\}]\cdot 6H_2O$ **16**.

ES2. Supplementary data of single-crystal X-ray diffraction studies.

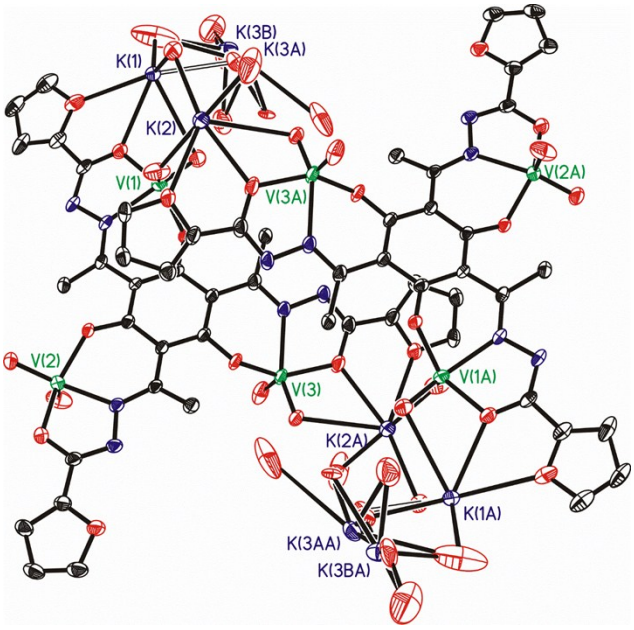

Fig. S4 Dinuclear structure present in **6a**. The complexes are grouped in pairs through K-O-K bridges. Drawing was done with SHELXL package.

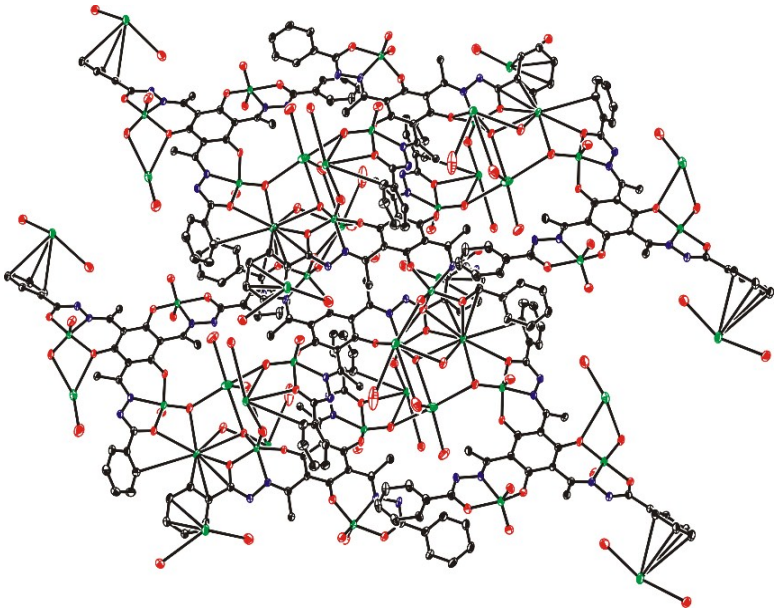

Fig. S5 Polymeric structure present in **13a**. The complexes are grouped through Cs(1)-O-Cs(2) bridges. Cs(3) atoms are bound to carbon atoms of phenyl rings. The drawing was done with SHELXL package.

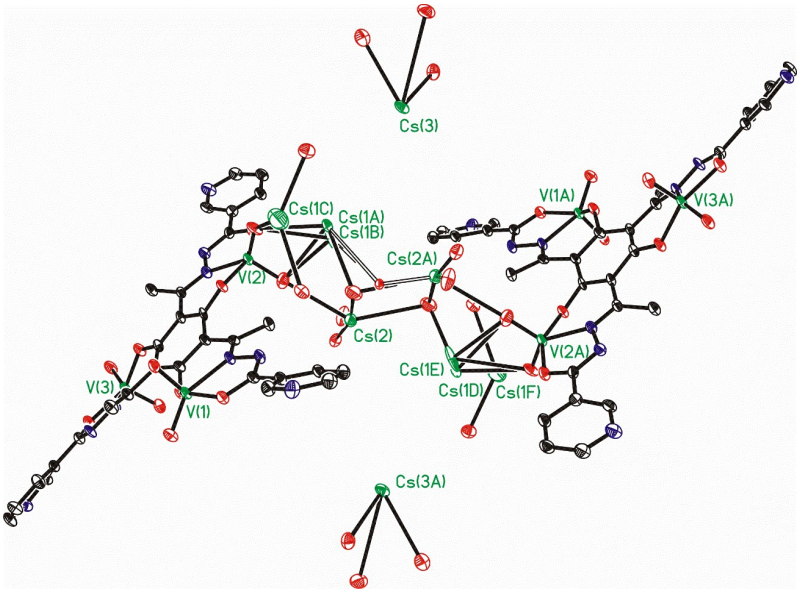

Fig. S6. Dimeric structure present in compound **16a**. The complexes are grouped through disordered atoms Cs-O-Cs bridges. Cs(3) atoms are bound to water molecules and other O-atoms of complexes present in the structure, which do not appear in the view. Drawing was done with SHELXL package.

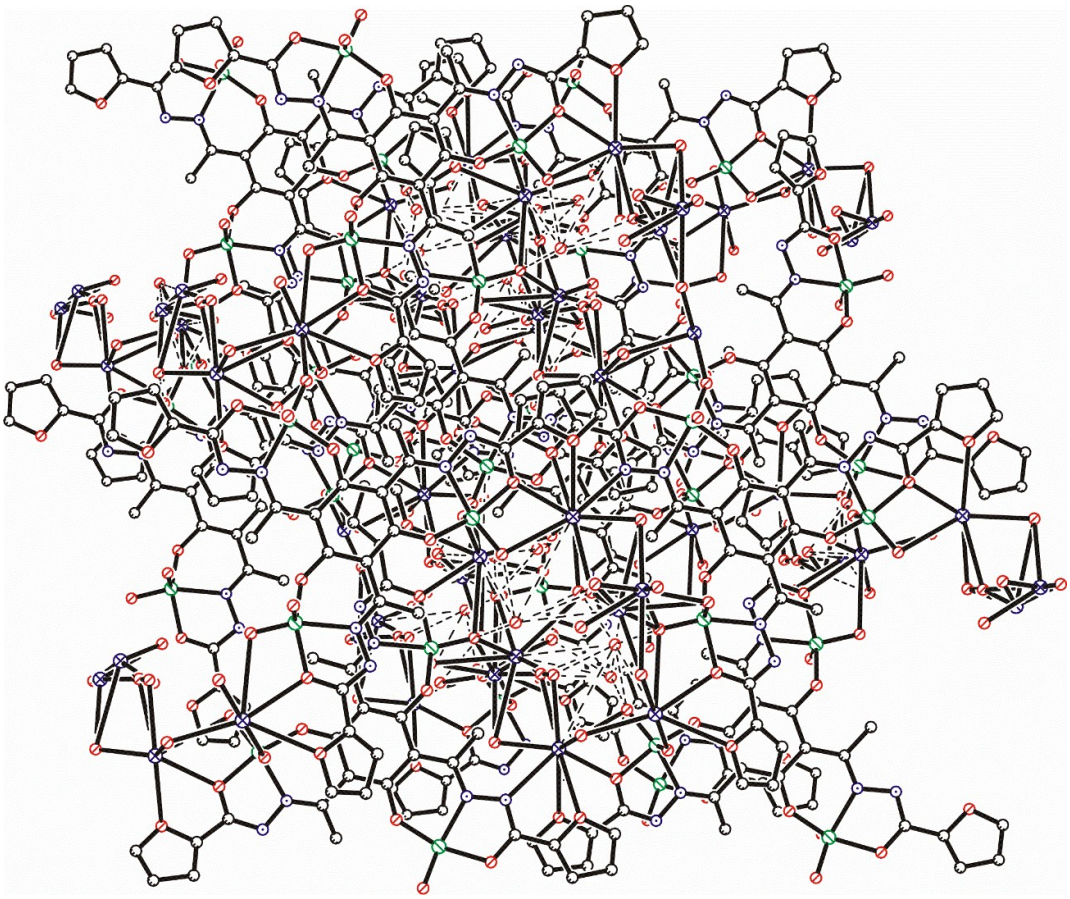

Fig. S7. Crystal packing of **6a**. Drawing was done with SHELXL package in balls and sticks.

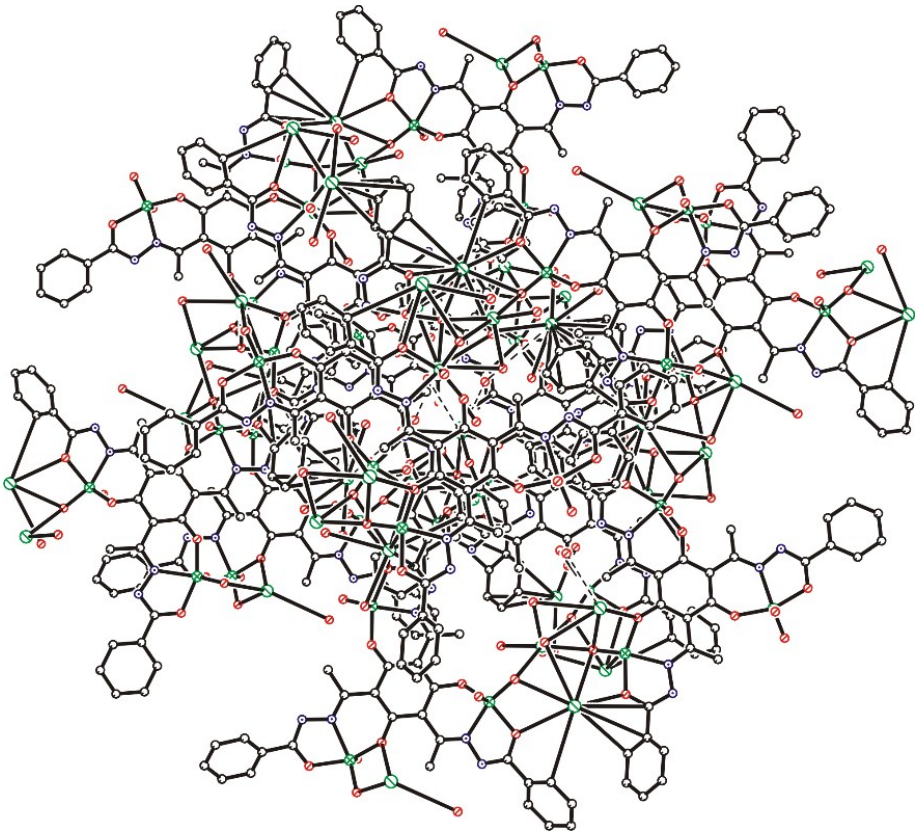

Fig. S8 Crystal packing of **13a**. The drawing was done with SHELXL package in balls and sticks.

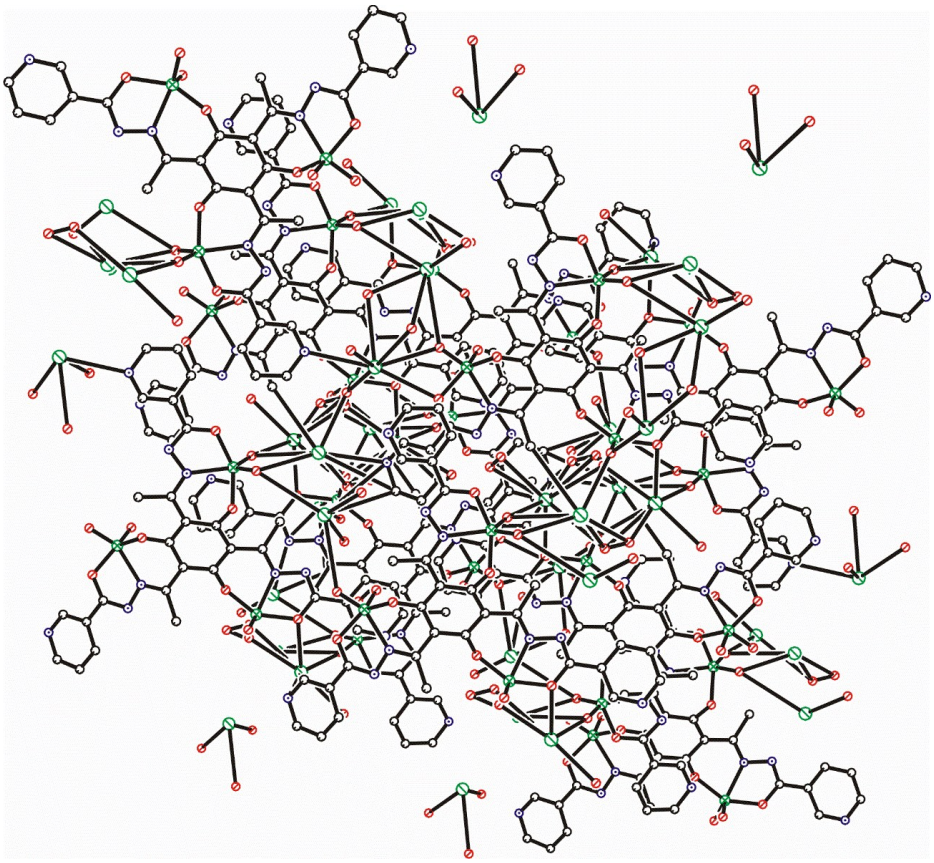

Fig. S9. Crystal packing of **16a**. Drawing was done with SHELXL package in balls and sticks.

Table S2 Hydrogen bonds in compounds $K_{2.7}[\{(V^{V}O_2)_3ptk(fah)_3\}]\cdot 11.5H_2O\cdot MeOH$ **6a**, $Cs_3[\{(V^{V}O_2)_3ptk(bhz)_3\}]\cdot 7H_2O$ **13a** and $Cs_3[\{(V^{V}O_2)_3ptk(nah)_3\}]\cdot 7.3H_2O$ **16a**.

D-H...A (**compound**)	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1W)-H(1WA)...O(2WA) (**6a**)	0.85	2.42	3.232(17)	160.5
O(1W)-H(1WB)...O(6)#7(**6a**)	0.85	1.85	2.700(7)	179.6
O(2WA)-H(2WA)...O(1W) (**6a**)	0.85	2.54	3.232(16)	139.6
O(2WA)-H(2WB)...O(12)#1(**6a**)	0.85	2.04	2.800(9)	148.8
O(2WB)-H(2WC)...O(10W) (**6a**)	0.85	2.44	3.28(2)	169.9
O(2WB)-H(2WD)...O(8W)#1(**6a**)	0.85	2.37	3.094(14)	142.9
O(4W)-H(4WA)...O(1M) (**6a**)	0.85	1.86	2.615(8)	146.4
O(4W)-H(4WB)...N(6)#8(**6a**)	0.85	2.29	2.930(7)	132.4
O(5W)-H(5A)...O(3WB)#4(**6a**)	0.85	1.89	2.510(9)	128.8
O(5W)-H(5A)...O(11W) (**6a**)	0.85	2.58	3.348(12)	150.6
O(5W)-H(5B)...O(10W) (**6a**)	0.85	1.98	2.775(6)	155.7
O(6W)-H(6A)...O(3WA) (**6a**)	0.85	1.96	2.801(8)	169.1
O(6W)-H(6A)...O(3WB) (**6a**)	0.85	2.05	2.656(8)	127.9
O(6W)-H(6B)...O(1M)#9(**6a**)	0.85	1.90	2.726(8)	164.3
O(7W)-H(7A)...O(4W)#1(**6a**)	0.85	2.04	2.830(8)	154.5
O(7W)-H(7B)...O(6W)#7(**6a**)	0.85	1.96	2.708(8)	145.9
O(8W)-H(8D)...O(2WB)#2(**6a**)	0.85	1.79	2.53(2)	143.7
O(8W)-H(8D)...O(2WA)#2(**6a**)	0.85	2.19	2.906(14)	141.1
O(8W)-H(8E)...O(1)#2(**6a**)	0.85	1.84	2.676(6)	166.8
O(9W)-H(9A)...O(13)#10(**6a**)	0.85	2.10	2.951(7)	179.8

O(9W)-H(9B)...O(9)#9(**6a**) 0.85	2.12	2.964(7)	172.6	
O(10W)-H(10A)...O(10)#1(**6a**)	0.85	2.57	3.150(5)	126.9
O(10W)-H(10B)...O(9)#3(**6a**)	0.85	2.32	3.156(5)	168.2
O(11W)-H(11A)...O(3WB)#4(**6a**)	0.85	2.06	2.676(10)	129.2
O(11W)-H(11A)...O(3WC)#4(**6a**)	0.85	2.62	3.208(17)	127.4
O(11W)-H(11B)...O(9W)#4(**6a**)	0.85	1.88	2.699(8)	162.3
O(11W)-H(11B)...O(3WC)#11(**6a**)	0.85	2.01	2.50(2)	115.6
O(2W)-H(2WA)...O(7W)#10(**13a**)	0.85	2.05	2.799(6)	146.9
O(2W)-H(2WB)...O(7W)(**13a**)	0.85	2.02	2.855(7)	166.1
O(3W)-H(3WB)...O(4W)#3(**13a**)	0.85	2.40	2.852(5)	114.1
O(5W)-H(5WA)...N(4)#2(**13a**)	0.85	2.11	2.912(5)	157.0
O(5W)-H(5WB)...O(9)(**13a**)0.85	1.96	2.808(5)	175.0	
O(6W)-H(6WA)...O(2W)#8(**13a**)	0.85	2.07	2.866(6)	155.1
O(6W)-H(6WB)...O(4)#7(**13a**)	0.72	2.23	2.939(5)	170.4
O(4W)-H(4W)...O(3W)#3(**13a**)	0.70	2.16	2.852(5)	166.9
O(1W)-H(1WA)...O(6W)(**13a**)	0.85(6)	2.01(6)	2.824(5)	161(5)
O(1W)-H(1WB)...O(10)(**13a**)0.78(6)	1.95(6)	2.734(5)	172(6)	
O(1W)-H(1WA)...O(2WA) (**16a**)	0.85	2.42	3.232(17)	160.5
O(1W)-H(1WB)...O(6)#7(**16a**)	0.85	1.85	2.700(7)	179.6
O(2WA)-H(2WA)...O(1W) (**16a**)	0.85	2.54	3.232(16)	139.6
O(2WA)-H(2WB)...O(12)#1(**16a**)	0.85	2.04	2.800(9)	148.8
O(2WB)-H(2WC)...O(10W) (**16a**)	0.85	2.44	3.28(2)	169.9
O(2WB)-H(2WD)...O(8W)#1(**16a**)	0.85	2.37	3.094(14)	142.9

O(4W)-H(4WA)...O(1M) (**16a**)	0.85	1.86	2.615(8)	146.4
O(4W)-H(4WB)...N(6)#8(**16a**)	0.85	2.29	2.930(7)	132.4
O(5W)-H(5A)...O(3WB)#4(**16a**)	0.85	1.89	2.510(9)	128.8
O(5W)-H(5A)...O(11W) (**16a**)	0.85	2.58	3.348(12)	150.6
O(5W)-H(5B)...O(10W) (**16a**)	0.85	1.98	2.775(6)	155.7
O(6W)-H(6A)...O(3WA) (**16a**)	0.85	1.96	2.801(8)	169.1
O(6W)-H(6A)...O(3WB) (**16a**)	0.85	2.05	2.656(8)	127.9
O(6W)-H(6B)...O(1M)#9(**16a**)	0.85	1.90	2.726(8)	164.3
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O(8W)-H(8D)...O(2WB)#2(**16a**)	0.85	1.79	2.53(2)	143.7
O(8W)-H(8D)...O(2WA)#2(**16a**)	0.85	2.19	2.906(14)	141.1
O(8W)-H(8E)...O(1)#2(**16a**)	0.85	1.84	2.676(6)	166.8
O(9W)-H(9A)...O(13)#10(**16a**)	0.85	2.10	2.951(7)	179.8
O(9W)-H(9B)...O(9)#9(**16a**)	0.85	2.12	2.964(7)	172.6
O(10W)-H(10A)...O(10)#1(**16a**)	0.85	2.57	3.150(5)	126.9
O(10W)-H(10B)...O(9)#3(**16a**)	0.85	2.32	3.156(5)	168.2
O(11W)-H(11A)...O(3WB)#4	0.85	2.06	2.676(10)	129.2
O(11W)-H(11A)...O(3WC)#4	0.85	2.62	3.208(17)	127.4
O(11W)-H(11B)...O(9W)#4(**16a**)	0.85	1.88	2.699(8)	162.3
O(11W)-H(11B)...O(3WC)#11	0.85	2.01	2.50(2)	115.6

Symmetry transformations used to generate equivalent atoms:

Compound **6a**: #1 x,y,z+1 #2 -x+2,-y+2,-z+2 #3 -x+2,-y+1,-z+2 #4 -x+2,-y+2,-z+3 #5 -x+1,-y+2,z+3 #6 x,y,z-1 #7 -x+1,-y+1,-z+2 #8 x,y-1,z-1 #9 x,y+1,z+1 #10 -x+1,-y+2,-z+2 #11 x+1,y,z

Compound **13a**: #1 x,-y,z-1/2 #2 -x+3/2,-y-1/2,-z #3 -x+1,-y,-z #4 -x+3/2,y-1/2,-z+1/2 #5 x,-y,z+1/2 #6 -x+1,y,-z+1/2 #7 -x+3/2,y+1/2,-z+1/2 #8 -x+2,y,-z+1/2 #9 x+1/2,-y-1/2,z+1/2

#10 -x+2,-y,-z

Compound **16a**: #1 x,y,z+1 #2 -x+2,-y+2,-z+2 #3 -x+2,-y+1,-z+2 #4 -x+2,-y+2,-z+3 #5 -x+1,y+2,z+3 #6 x,y,z-1 #7 -x+1,-y+1,-z+2 #8 x,y-1,z-1 #9 x,y+1,z+1 #10 -x+1,-y+2,-z+2 #11 x+1,y,z

Table S3. IR bands and their tentative assignments in compounds **I-IV** and **1-16**.

Compound	ν (O–H)	ν(N–H)	ν(C=O)	ν (C=N)	ν (C–O)	ν (V=O)
I	3448	3198	1648	1570	---	----
II	3434	3163	1650	1573	---	---
III	3322	3322	1673	1571	---	----
IV	3204	3015	1670	1596	----	---
1	3136	---	---	1543	1291	989
2	3149	---	---	1522	1276	980
3	3137	---	---	1575	1282	943
4	3134	---	---	1567	1279	950
5	3423	--	--	1561	1281	931, 898
6	3432	--	--	1562	1280	923, 892
7	3420	--	--	1549	1282	937, 894
8	3408	--	--	1561	1280	936, 896
9	3404	---	---	1562	1280	930, 882
10	3433	---	---	1567	1288	945, 897
11	3443	---	---	1543	1291	941, 918
12	3426	---	---	1564	1282	935, 906
13	3152	---	---	1563	1275	943, 881
14	3136	---	---	1555	1281	919, 865
15	3128	---	---	1549	1280	912, 855
16	3137	---	---	1560	1278	914, 863

ES3. Supplementary data of UV-Vis spectra.

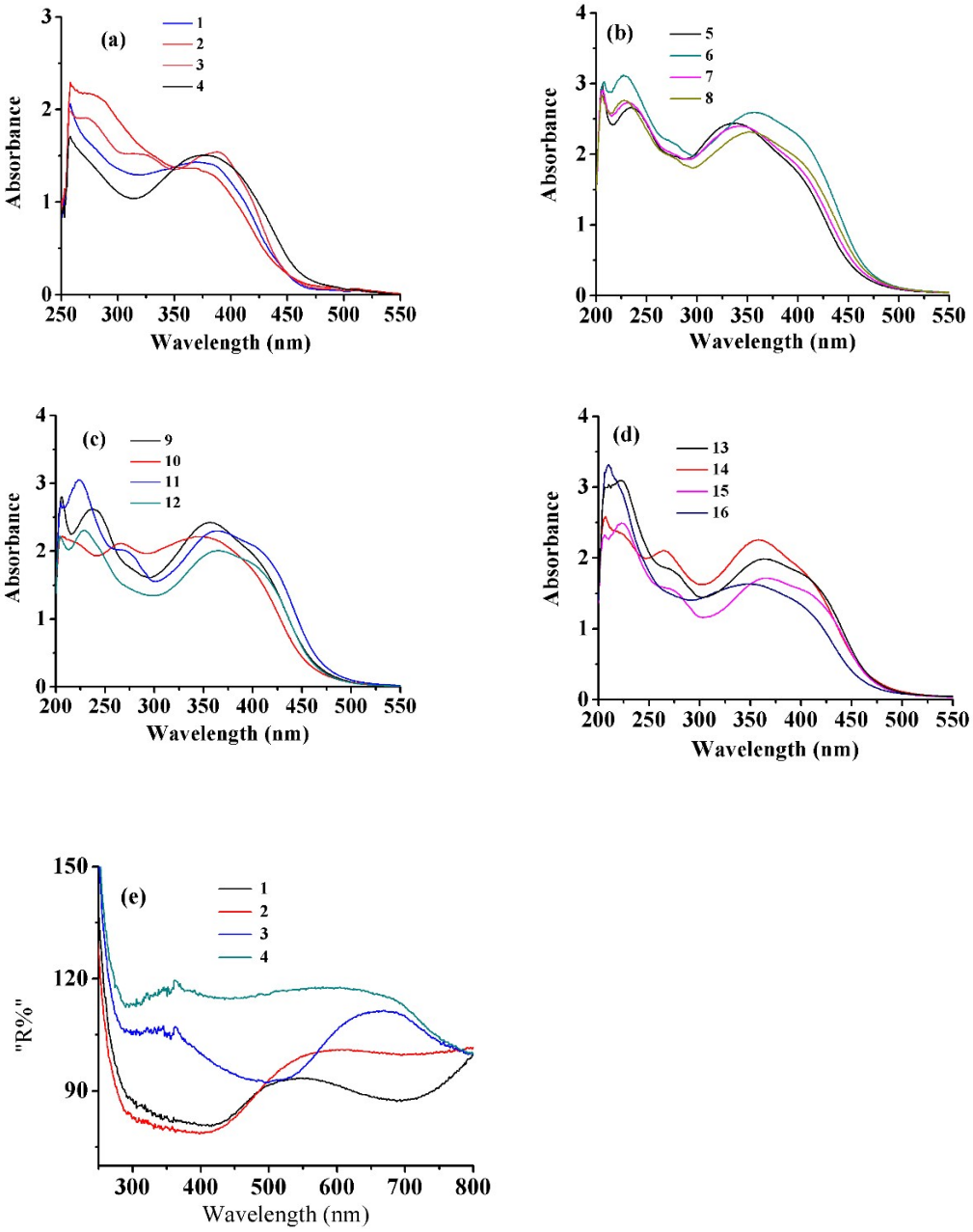


Fig. S10 UV/Vis spectra were recorded in DMSO ($V^{IV}O$-complexes) and MeOH ($V^{V}O_2$-complexes).

Table S4. UV/Vis spectral data for the prepared ligand precursors and vanadium complexes recorded in DMSO and MeOH.

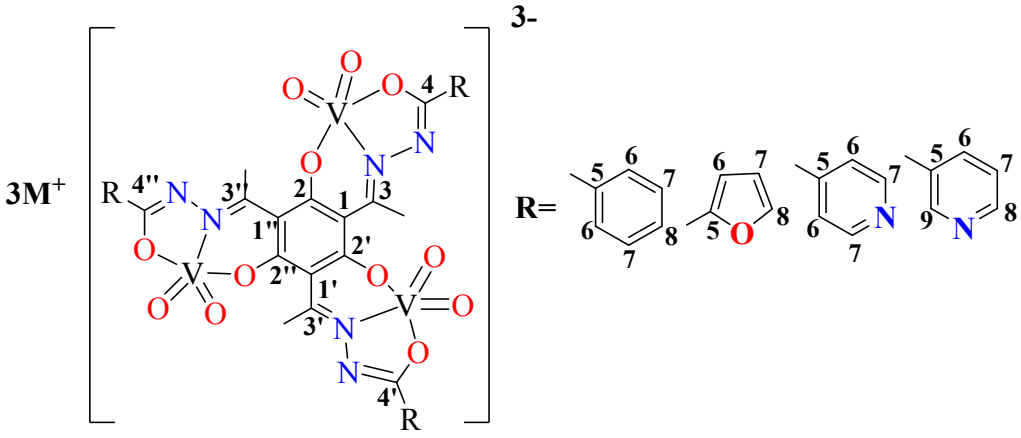
Compound	Conc. (M)	Solvent	λ_{max} /nm (ε/M^{-1} cm^{-1})
I		DMSO	262 (2.13×10^4), 323 (1.87×10^4)
II		DMSO	263 (2.67×10^4), 324 (2.63×10^4)
III		DMSO	262 (2.14×10^4), 321 (1.52×10^4)
IV		DMSO	260 (2.19×10^4), 314 (1.17×10^4)
1	1.16×10^{-4}	DMSO	258 (1.76×10^4), 387 (1.19×10^4)
2	1.21×10^{-4}	DMSO	259 (1.88×10^4), 286 (1.76×10^4), 388 (1.05×10^4)
3	1.16×10^{-4}	DMSO	258 (1.73×10^4), 277 (1.62×10^4), 324 (1.29×10^4), 391 (1.33×10^4),
4	1.16×10^{-4}	DMSO	260 (1.43×10^4), 390 (1.26×10^4)
5	9.31×10^{-5}	MeOH	206 (3.13×10^4), 232 (2.83×10^4), 329 (2.61×10^4), 400 (1.9×10^4)
6	9.57×10^{-5}	MeOH	207 (3.15×10^4), 228 (3.22×10^4), 358 (2.68×10^4), 407 (2.3×10^4)
7	9.27×10^{-5}	MeOH	205 (3.11×10^4), 233 (2.94×10^4), 351 (2.48×10^4), 402 (1.96×10^4)
8	9.27×10^{-5}	MeOH	205 (3.05×10^4), 225 (2.96×10^4), 329 (2.61×10^4), 405 (2.01×10^4)
9	9.74×10^{-5}	MeOH	204 (2.89×10^4), 238 (2.67×10^4), 355 (2.49×10^4), 404 (1.98×10^4)
10	1×10^{-4}	MeOH	208 (2.19×10^4), 269 (2.11×10^4), 342 (2.20×10^4), 384 (1.93×10^4)
11	9.71×10^{-5}	MeOH	203 (2.74×10^4), 223 (3.13×10^4), 278 (2×10^4), 361 (2.34×10^4), 411 (2.03×10^4)
12	9.71×10^{-5}	MeOH	206 (2.23×10^4), 229 (2.37×10^4), 361 (2.05×10^4), 406 (1.82×10^4)
13	7.37×10^{-5}	MeOH	207 (4.07×10^4), 224 (4.20×10^4), 276 (2.41×10^4), 358 (2.67×10^4), 413 (2.25×10^4)
14	7.54×10^{-5}	MeOH	206 (3.44×10^4), 227 (3.07×10^4), 267 (2.78×10^4), 356 (2.97×10^4), 401 (2.45×10^4)
15	7.35×10^{-5}	MeOH	206 (3.15×10^4), 224 (3.40×10^4), 267 (2.12×10^4), 364 (2.35×10^4), 417 (1.93×10^4)
16	7.35×10^{-5}	MeOH	210 (4.51×10^4), 339 (2.19×10^4), 406 (1.74×10^4)

ES4. Supplementary ^{1}H, ^{13}C NMR and ^{51}V NMR data.

Table S5 ^{1}H NMR (400 MHz) data (δ in ppm) of ligand precursors and complexes.

Compound	-OH	-CH_3	Ar-H
I	10.45 (br., 3H)	2.45 (s, 9H)	7.90 (d, J = 8.5 Hz 6H), 7.57 (d, J = 8.4 Hz, 6H), 7.45 (m, 3H)
II	11.27 (br., 3H)	2.52 (s, 9H)	7.98 (d, *J* = 2.2 Hz, 3H), 7.36 (d, J = 3.5 Hz,3H), 6.73 (dd, *J* = 3.5, 1.7 Hz,3H)
III	11.54 (br., 3H)	2.56 (s, 9H)	8.80 (d, *J* = 4.8 Hz, 6H), 7.96 (d, *J* = 4.6 Hz 6H)
IV	11.56 (br., 3H)	2.59 (s, 9H)	9.10 (s, 3H), 8.79 (d, J = 6.1, 3H), 8.31 (d, J = 8.0 Hz, 3H), 7.58 (dd, *J* = 7.7, 4.8 Hz, 3H)
5	-	2.80 (s, 9H)	8.02 (d,d, *J* = 6.7 Hz, 3.0 9H), 7.41 (d,d *J* = 6.9, 3.2 Hz 6H)
6	-	2.67 (s, 9H)	7.76 (d, *J* = 1.5 Hz, 3H), 6.90 (d, J = 3.3 Hz,3H), 6.55 (dd, *J* = 3.2, 1.8 Hz,3H)
7	-	2.84 (s, 9H)	8.66 (d, *J* = 5.9 Hz, 6H), 7.89 (d, *J* = 5.9 Hz 6H)
8	-	2.77 (s, 9H)	9.14 (s, 3H), 8.59 (d, J = 7.0, 3H), 8.24 (d, J = 6.2 Hz, 3H), 7.43 (dd, *J* = 7.2, 4.1 Hz, 3H)
9	-	2.82 (s, 9H)	8.01 (d,d, *J* = 6.7 Hz, 3.0 9H), 7.41 (d,d *J* = 6.8, 3.4 Hz 6H)
10	-	2.74 (s, 9H)	7.79 (d, *J* = 4.0 Hz, 3H), 6.96 (d, J = 3.3 Hz,3H), 6.58 (dd, *J* = 3.5, 1.7 Hz,3H)
11	-	2.80 (s, 9H)	8.69 (d, *J* = 6.0 Hz, 6H), 7.79 (d, *J* = 4.5 Hz 6H)
12	-	2.80 (s, 9H)	9.10 (s, 3H), 8.62 (d, J = 7.0, 3H), 8.25 (d, J = 6.2 Hz, 3H), 7.45 (dd, *J* = 7.2, 4.1 Hz, 3H)
13	-	2.79 (s, 9H)	8.00 (d,d, *J* = 6.7 Hz, 3.0 9H), 7.41 (d,d *J* = 6.8, 2.9 Hz 6H)
14		2.73 (s, 9H)	7.79 (d, *J* = 4.0 Hz, 3H), 6.97 (d, J = 8.6 Hz,3H), 6.60 (dd, *J* = 3.3, 1.7 Hz,3H)
15		2.81 (s, 9H)	8.63 (d, *J* = 5.9 Hz, 6H), 7.85 (d, *J* = 6.0 Hz 6H)
16		2.81 (s, 9H)	9.13 (s, 3H), 8.60 (d, J = 7.1, 3H), 8.28 (d, J = 6.3 Hz, 3H), 7.45 (dd, *J* = 7.2, 4.3 Hz, 3H)

Table S6. ^{13}C NMR spectral data of ligand precursors and complexes.



M = Na^+, K^+, Cs^+

Comp.	C3/C3'/C3''	C1/C1'/C1''	C4/C4'/C4''	Other carbons	-CH_3
I	166.49	154.74	152.88	132.29(C5/C5'/C5''),131.70(C8/C8'/C8''),129.08(C7,7/C7',7'/C7'',7''),127.92(C6,6/C6',6'/C6'',6''),127.33(C2/C2'/C2'')	19.74 (C9/C9'/C9'')
II	164.41	153.74	151.37	147.54(C5/C5'/C5''),145.84(C8/C8'/C8''),137.50(C6/C6'/C6''),135.36(C7/C7'/C7''),109.90(C2/C2'C2'')	19.18 C9/C9'/C9'')
III	164.33	156.42	154.61	150.58(C7,7/C7',7'/C7'',7''),140.48(C5/C5'/C5''),121.41(C6,6/C6',6'/C6'',6''),108.89(C2/C2'/C2'')	19.05 (C8/C8'/C8')
IV	165.01	153.18	152.30	150.30(C9/C9'/C9''),149.15(C8/C8'/C8''),135.83(C6/C6'/C6''),128.28(C5/C5'/C5''),123.78(C7/C7'/C7''),109.49(C2/C2'/C2'')	19.50 (C10/C10'/C10'')
5	168.85	164.82	163.56	134.87(C5/C5'/C5''),129.07(C8/C8'/C8''),128.80(C7/C7'C7''),128.10(C6/C6'/C6''),104.25(C2/C2'/C2'')	22.12 (C9/C9'/C9'')
6	170.02	165.03	161.00	149.16(C5/C5'/C5''),144.51(C8/C8'/C8''),112.52(C6/C6'/C6''),111.89(C7/C7'/C7''),109.06(C2/C2'C2'')	21.74 (C9/C9'/C9'')
7	172.70	164.60	163.40	152.40(C7,7/C7',7'/C7'',7''),138.05(C5/C5'/C5''),120.10(C6,6/C6',6'/C6'',6''),103.07(C2/C2'/C2'')	21.85 (C8/C8'/C8')
8	173.00	164.90	163.13	151.90(C9/C9'/C9''),137.20(C8/C8'/C8''),126.30(C6/C6'/C6''),124.11(C5/C5'/C5''),123.32(C7/C7'/C7''),103.70(C2/C2'/C2'')	22.14 (C10/C10'/C10'')
9	171.85	163.90	162.90	133.87(C5/C5'/C5''),129.07(C8/C8'/C8''),128.80(C7/C7'C7''),127.85(C6/C6'/C6''),102.14(C2/C2'/C2'')	21.12 (C9/C9'/C9'')
10	172.02	163.95	163.00	148.89(C5/C5'/C5''),142.51(C8/C8'/C8''),110.36(C6/C6'/C6''),107.27(C7/C7'/C7''),103.01(C2/C2'C2'')	21.74 (C9/C9'/C9'')

11	175.90	165.17	161.68	150.01(C7,7/C7',7'/C7'',7''),141.39(C5/C5'/C5''),123.95(C6,6/C6',6'/C6'',6''),100.05(C2/C2'/C2'')	20.93 (C8/C8'/C8')
12	174.21	164.32	162.12	152.86(C9/C9'/C9''),136.30(C8/C8'/C8''),124.42(C6/C6'/C6''),124.80(C5/C5'/C5''),123.15(C7/C7'/C7''),101.02(C2/C2'/C2'')	21.45 (C10/C10'/C10'')
13	169.82	164.96	162.89	145.21(C5/C5'/C5''),140.87(C8/C8'/C8''),111.45(C6/C6'/C6''),105.67(C7/C7'/C7''),103.82(C2/C2'C2'')	21.35 (C8/C8'/C8')
14	170.15	165.67	162.82	147.45(C5/C5'/C5''),142.89(C8/C8'/C8''),108.92(C6/C6'/C6''),104.38(C7/C7'/C7''),101.72(C2/C2'C2'')	21.32 (C9/C9'/C9'')
15	170.72	166.59	165.88	150.35(C7,7/C7',7'/C7'',7''),141.58(C5/C5'/C5''),122.16(C6,6/C6',6'/C6'',6''),109.05(C2/C2'/C2'')	21.90 (C8/C8'/C8')
16	171.32	166.90	164.12	152.86(C9/C9'/C9''),136.30(C8/C8'/C8''),124.42(C6/C6'/C6''),123.25(C5/C5'/C5''),121.84(C7/C7'/C7''),110.02(C2/C2'/C2'')	22.32 (C10/C10'/C10'')

Table S7.

^{51}V NMR data obtained for some of the $V^{V}O_2$-complexes.

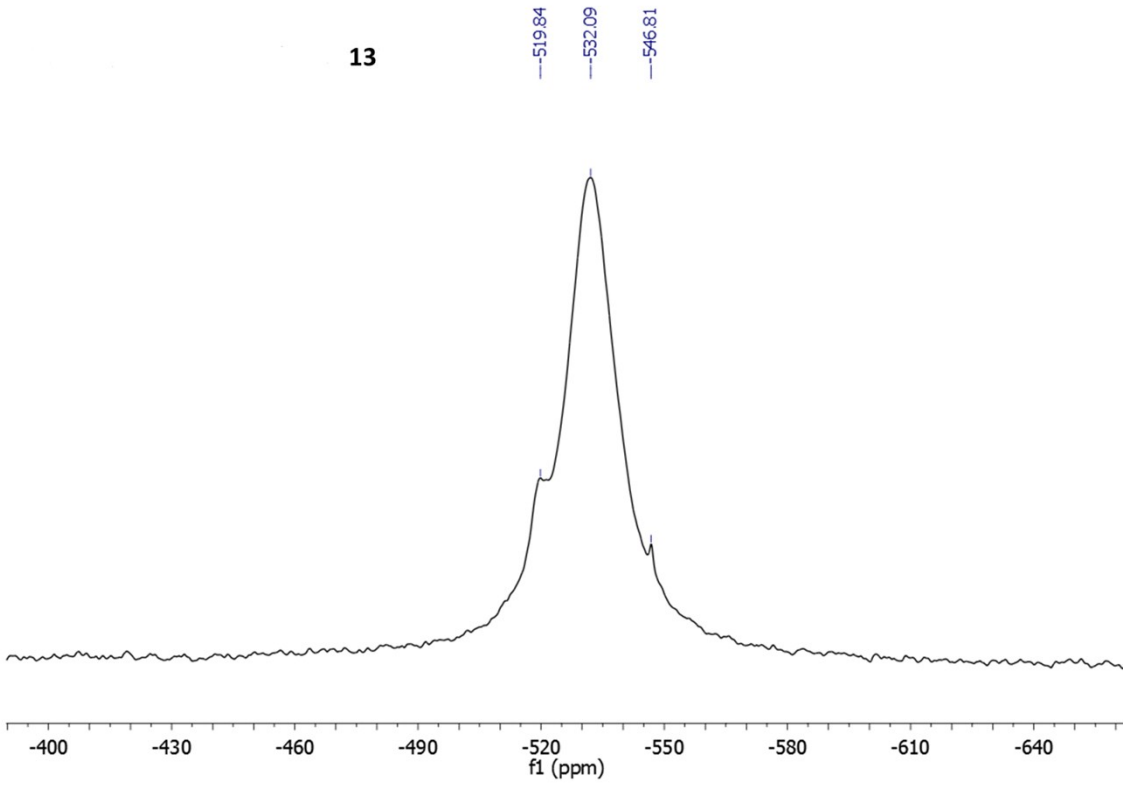


Fig. S11A ^{51}V NMR spectra of a solution of $Cs_3[(V^{V}O_2)_3\{ptk(bhz)_3\}]\cdot 6H_2O$ **13** in MeOH-d_4. Experimental δ_V values: δ_V (main) = -532 ppm; δ_V (minor) = -519 and -547 ppm

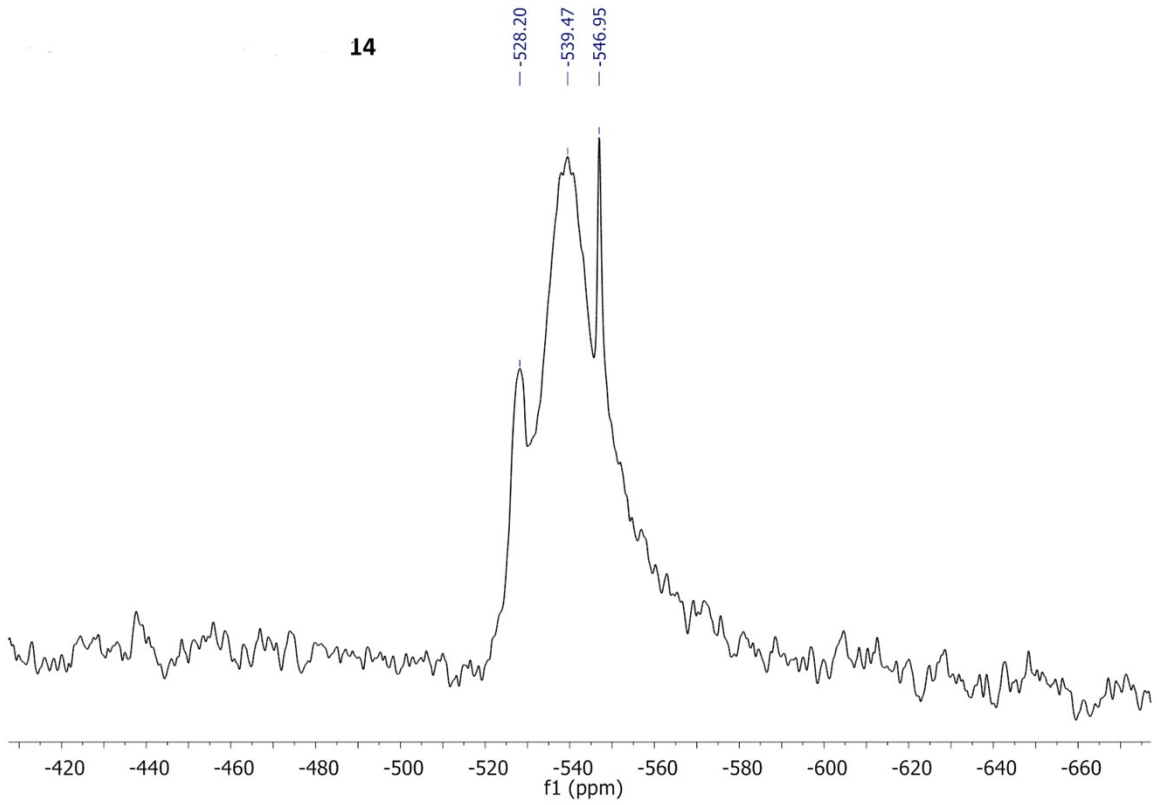


Fig. S11B ^{51}V NMR spectra of a solution of $Cs_3[(V^VO_2)_3\{ptk(fah)_3\}]\cdot 6H_2O$ **14** in MeOH-d_4.

Two ^{51}V NMR spectra were obtained for **14** in MeOH-d_4, with slightly different δ_V results :

δ_V (main) = -539.5 ppm (-537.4 ppm, -538.7 ppm, -542 ppm, obtained in other independent experiments)

δ_V (minor) = -528 and -546 ppm; in three other measurements only one δ_V (minor) = -545 ppm was measured.

Values of δ_V^{calc} obtained by DFT calculations:

^{51}V NMR chemical shifts of anion of **14** : $[(V^VO_2)_3ptk(fah)_3]^{3-}$ are: -526, -535, -548 ppm

Calculations for $K_3[(V^VO_2)_3ptk(fah)_3]$ including the K^+ counter ions: δ_V = -525, -531, -548 ppm.

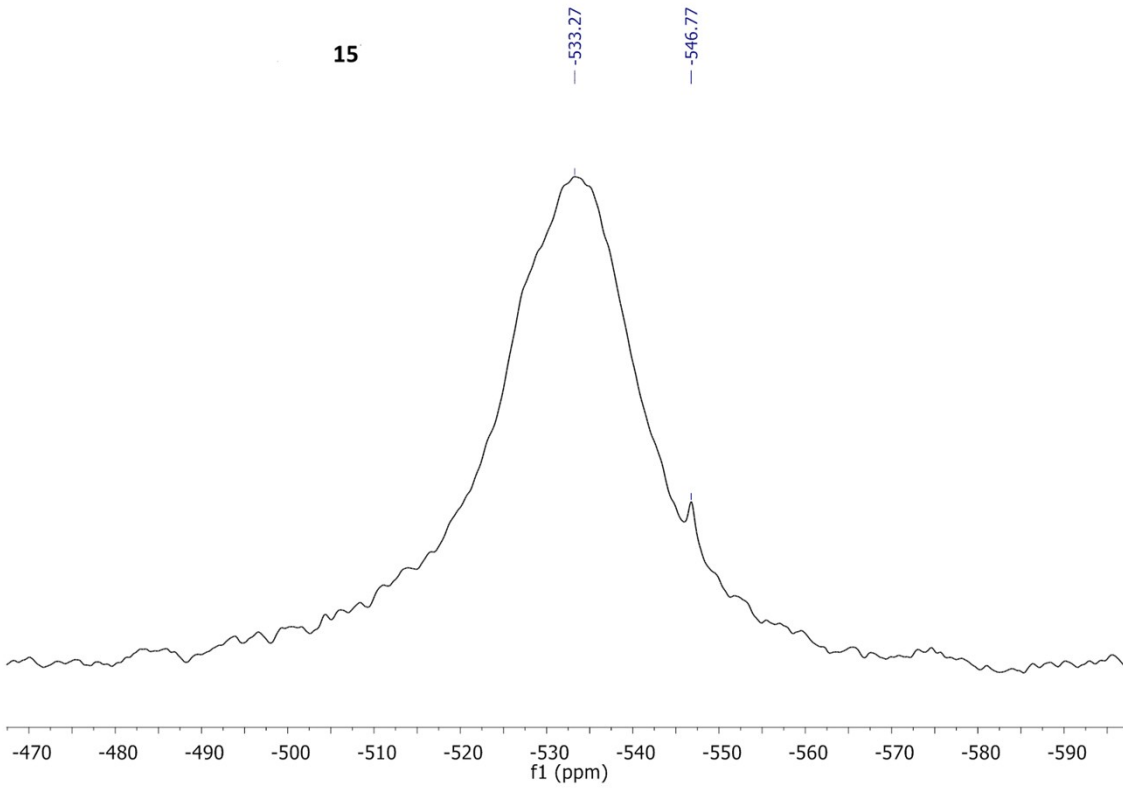


Fig. S11C ^{51}V NMR spectra of a solution of $Cs_3[(V^VO_2)_3\{ptk(inh)_3\}]\cdot 6H_2O$ **15** in MeOH-d_4 by ^{51}V NMR:

δ_V (main) = -533 ppm.

δ_V (minor) = -547 ppm

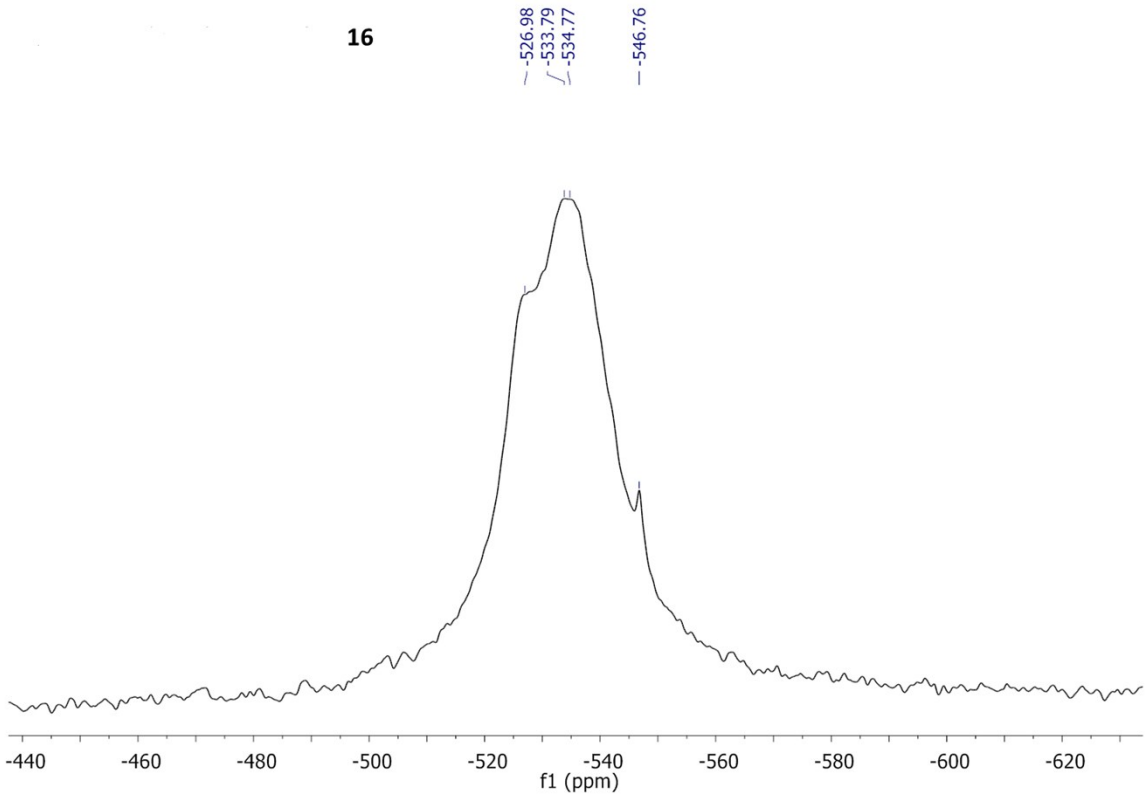


Fig. S11D ^{51}V NMR spectra of a solution of $Cs_3[(V^VO_2)_3\{ptk(nah)_3\}]\cdot 6H_2O$ **16** in MeOH-d_4. Observed ^{51}V NMR chemical shifts:

δ_V (main) = -534 ppm.

δ_V (minor) = -527 and -547 ppm

ES5. Supplementary EPR data.

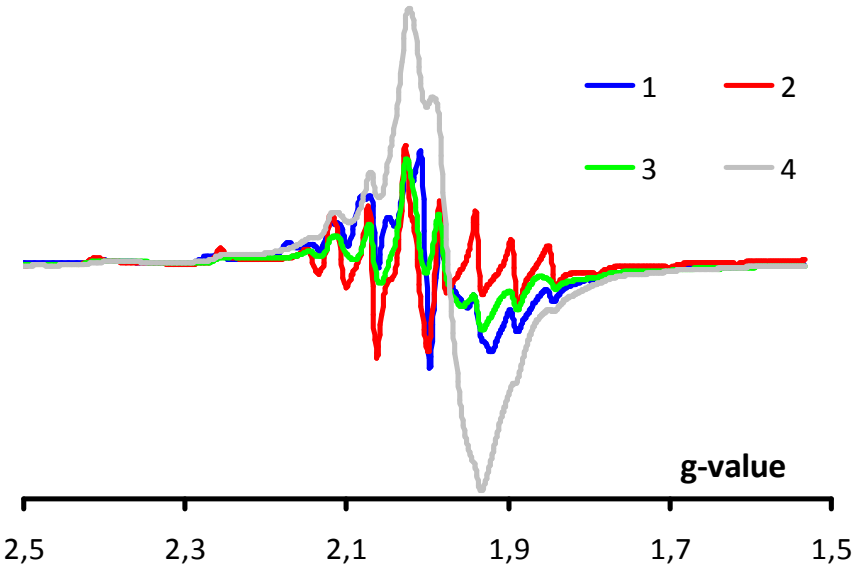


Fig. S12A First derivative EPR spectra of frozen (100 K) solutions (ca. 0.2-0.5 mM) in DMSO of [{$V^{IV}O(H_2O)$}$_3$(ptk(bhz)$_3$)] **1**, [{$V^{IV}O(H_2O)$}$_3$(ptk(fah)$_3$)] **2**, [{$V^{IV}O(H_2O)$}$_3$(ptk(inh)$_3$)] **3** and [{$V^{IV}O(H_2O)$}$_3$(ptk(nah)$_3$)] **4**.

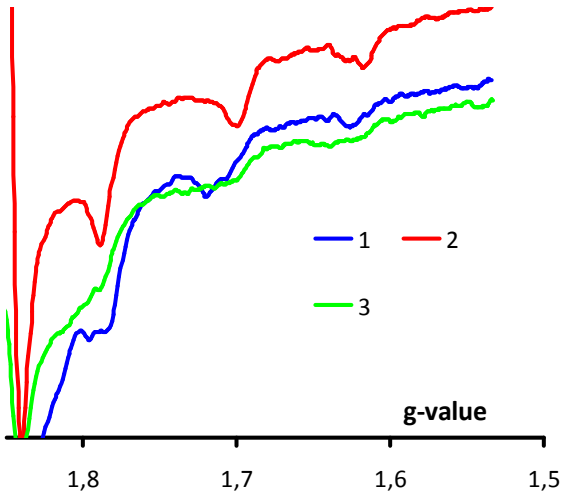


Fig. S12B First derivative EPR spectra of frozen (100 K) solutions (ca. 0.2-0.5 mM) in DMSO of [{$V^{IV}O(H_2O)$}$_3$(ptk(bhz)$_3$)] **1**, [{$V^{IV}O(H_2O)$}$_3$(ptk(fah)$_3$)] **2**, [{$V^{IV}O(H_2O)$}$_3$(ptk(inh)$_3$)] **3** in the high field range.

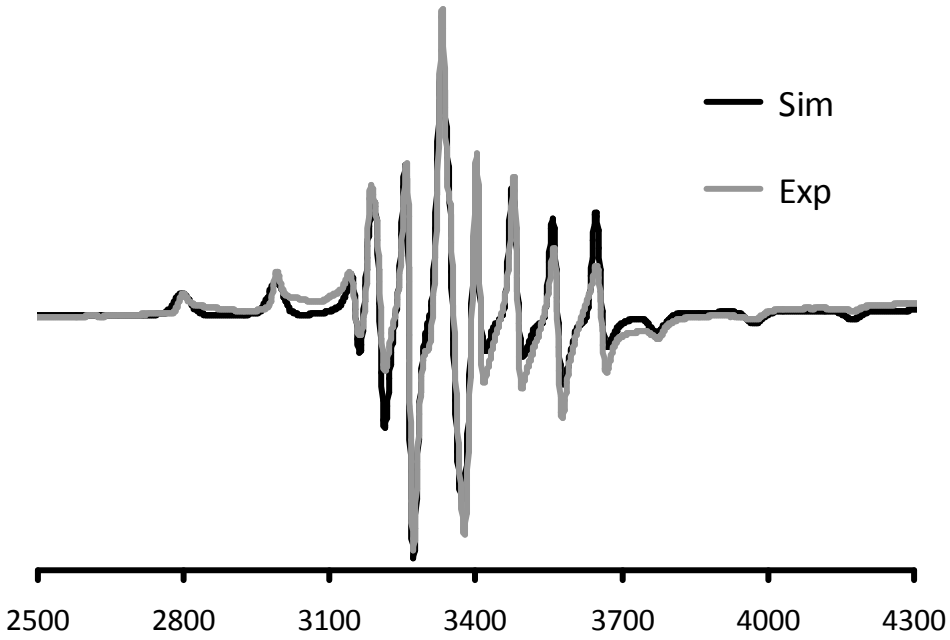


Fig. S12C First derivative EPR spectrum of frozen (100 K) solutions (ca. 0.2-0.5 mM) in DMSO of $[\{V^{IV}O(H_2O)\}_3(ptk(fah)_3)]$ **2** and the simulated spectrum.

ESI-6. UV-Vis spectral changes upon addition of aqueous H_2O_2 solution to V^VO_2-complexes in MeOH.

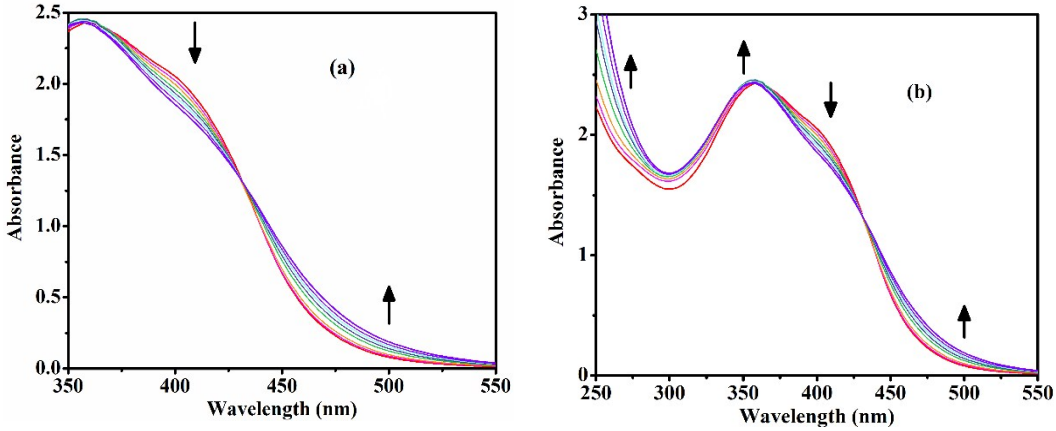


Fig. S13 UV–Vis spectral changes obtained during the titration of $Cs_3[(V^VO_2)_3\{ptk(bhz)_3\}]\cdot 6H_2O$ **13** with H_2O_2. (a) The spectra were recorded upon stepwise additions of one drop portions of an aqueous H_2O_2 solution (1.20 g, 9.02 mmol of 30% H_2O_2) dissolved in 25 mL of MeOH to 10 mL of 1×10^{-4} M solution of **13** in MeOH. (b) Similar titration of 10 mL of 1×10^{-4} M solution of **13** in MeOH with H_2O_2 recorded in the region 250 – 550 nm.

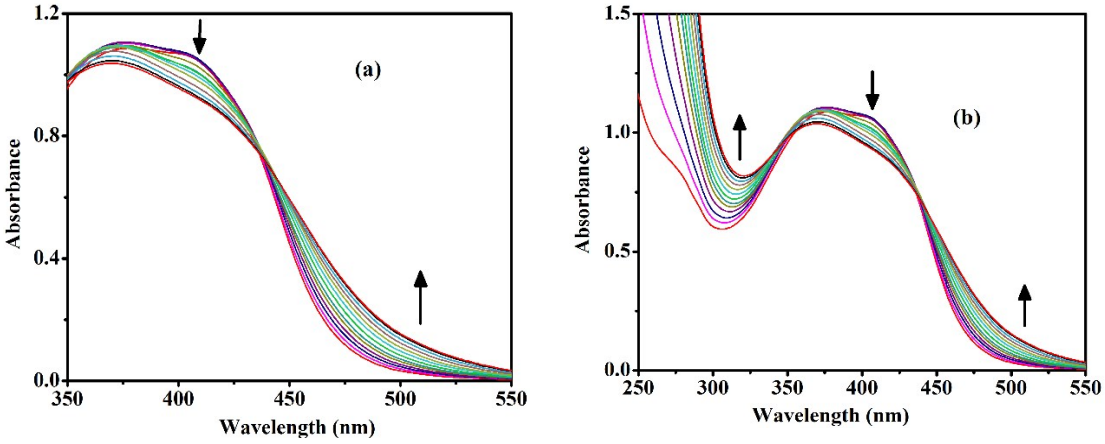


Fig. S14 UV–Vis spectral changes obtained during the titration of $Cs_3[(V^VO_2)_3\{ptk(inh)_3\}]\cdot 6H_2O$ **15** with H_2O_2. (a) The spectra were recorded upon stepwise additions of one drop portions of an aqueous H_2O_2 solution (1.20 g, 9.02 mmol of 30% H_2O_2) dissolved in 25 mL of MeOH to 10 mL of 1×10^{-4} M solution of **15** in MeOH. (b) Similar titration of 10 mL of 1×10^{-4} M solution of **15** in MeOH with H_2O_2 recorded in the region 250 –550 nm.

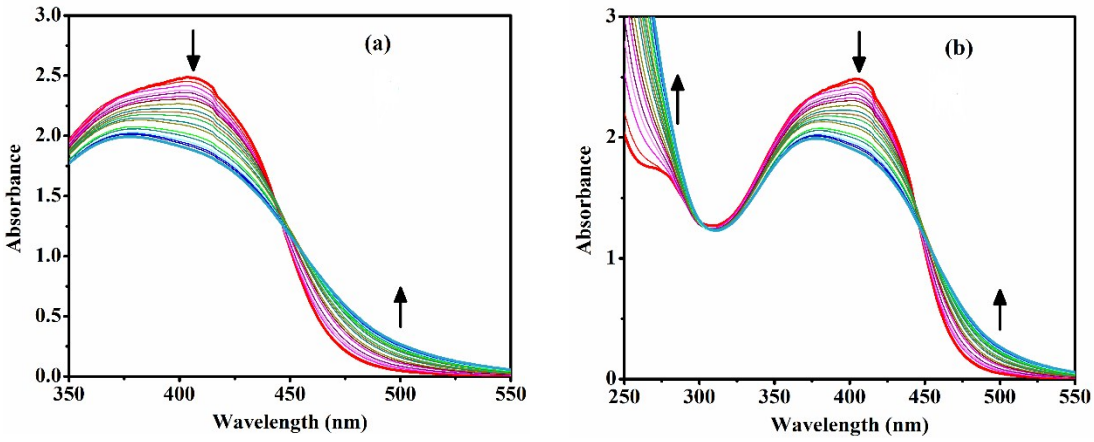


Fig. S15 UV–Vis spectral changes obtained during the titration of $Cs_3[(V^VO_2)_3\{ptk(nah)_3\}]\cdot 6H_2O$ **16** with H_2O_2. (a) The spectra were recorded upon stepwise additions of one drop portions of an aqueous H_2O_2 solution (1.20 g, 9.02 mmol of 30% H_2O_2) dissolved in 25 mL of MeOH) to 10 mL of 1×10^{-4} M solution of **16** in MeOH. (b) Similar titration of 10 mL of 1×10^{-4} M solution of **16** in MeOH with H_2O_2 recorded in the region 250 –550 nm.

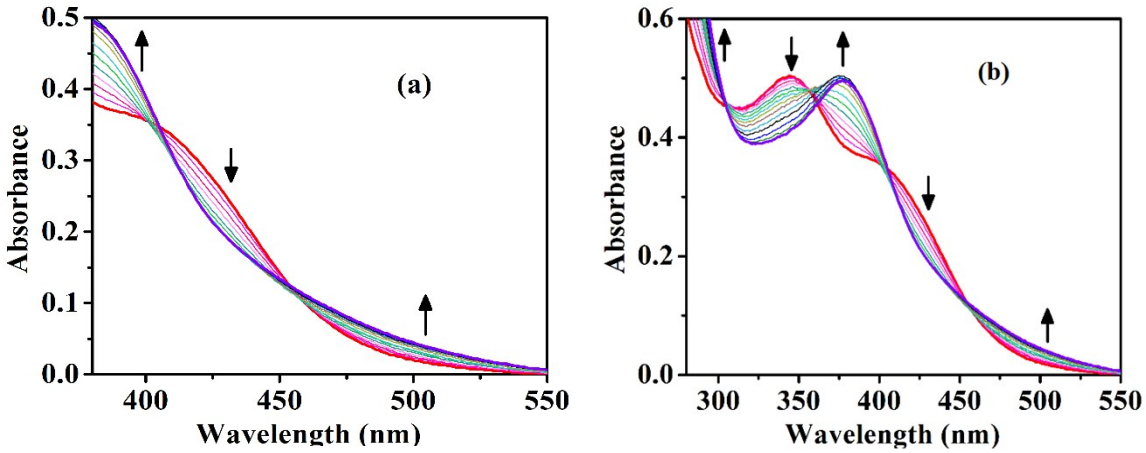


Fig. S16 UV–Vis spectral changes obtained during the titration of $Na_3[(V^VO_2)_3\{ptk(inh)_3\}]\cdot 6H_2O$ **11** with H_2O_2. (a) The spectra were recorded upon stepwise additions of one drop portions of an aqueous H_2O_2 solution (0.601 g, 4.51 mmol of 30% H_2O_2 dissolved in 25 mL of MeOH) to 10 mL of 1×10^{-5} M solution of **11** in MeOH. (b) Data on similar titration of 10 mL of 2×10^{-6} M solution of **11** in MeOH with H_2O_2 recorded in the region 280–550 nm.

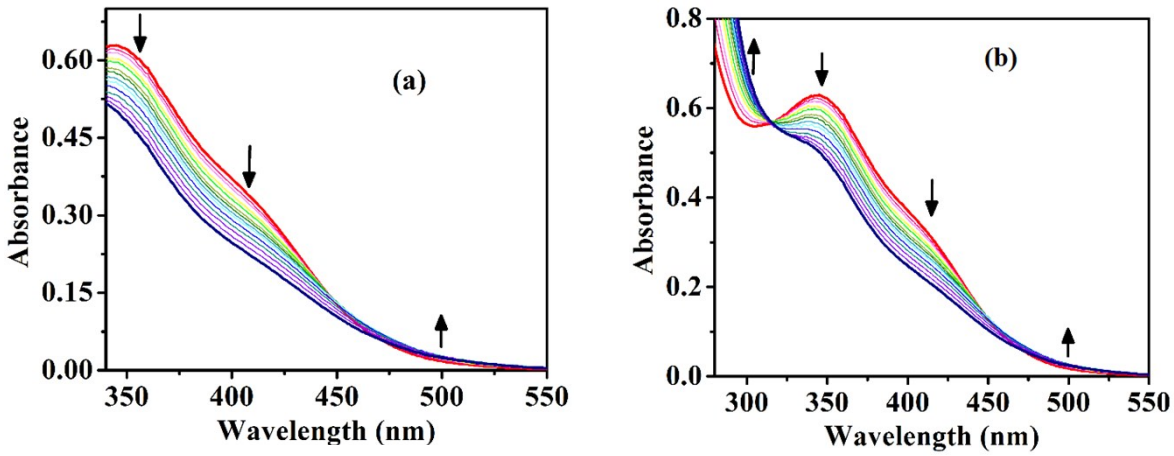


Fig. S17 UV–Vis spectral changes obtained during the titration of $Na_3[(V^VO_2)_3\{ptk(bhz)_3\}]\cdot 6H_2O$ **9** with an aqueous H_2O_2 solution. (a) Spectra recorded upon stepwise additions of one drop portions of H_2O_2 (0.601 g, 4.51 mmol of 30% H_2O_2 dissolved in 25 mL of MeOH) to 10 mL of 1×10^{-5} M solution of **9** in MeOH. (b) Data recorded in the expanded region 280–550 nm of a similar titration of 10 mL of 1×10^{-5} M solution of **9** in MeOH with H_2O_2.

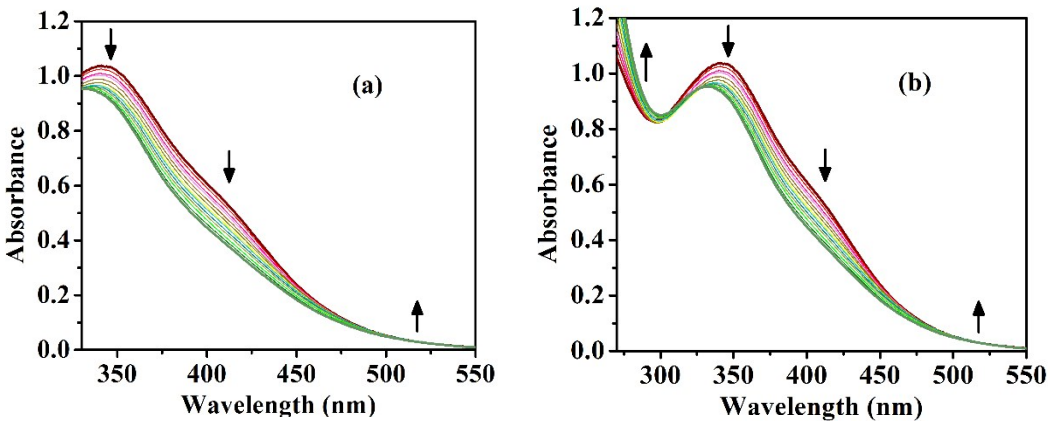


Fig. S18 UV–Vis spectral changes obtained during the titration of $K_3[(V^VO_2)_3\{ptk(fah)_3\}]\cdot 6H_2O$ **6** with H_2O_2. (a) Spectra recorded upon stepwise additions of one drop portions of H_2O_2 (1.202 g, 9.02 mmol of 30% H_2O_2 dissolved in 25 mL of MeOH) to 10 mL of 1×10^{-5} M solution of **6** in MeOH. (b) Data recorded in the expanded region 280-550 nm of similar titration of 10 mL of 1×10^{-5} M solution of **6** in MeOH with H_2O_2.

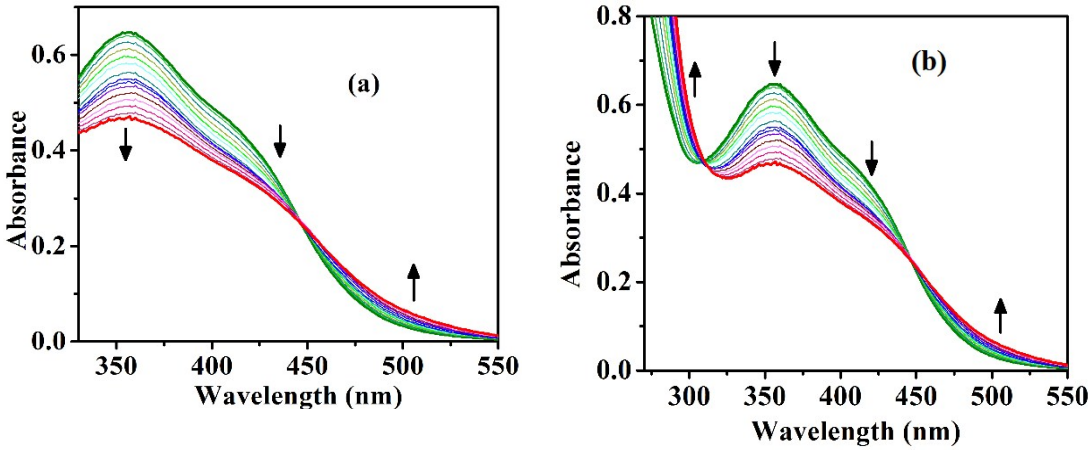


Fig. S19 UV–Vis spectral changes obtained during the titration of $K_3[(V^VO_2)_3\{ptk(nah)_3\}]\cdot 6H_2O$ **8** with an aqueous H_2O_2 solution. (a) The spectra were recorded after stepwise additions of one drop portions of an aqueous H_2O_2 solution (0.601 g, 4.51 mmol of 30% H_2O_2 dissolved in 25 mL of MeOH) to 10 mL of 1×10^{-5} M solution of **8** in MeOH. (b)

Data recorded in the expanded region 280-550 nm of similar titration of 10 mL of 1×10^{-5} M solution of **8** in MeOH with H_2O_2.

ES7. ^{51}V NMR and (^{1}H NMR) spectral changes upon addition of aqueous H_2O_2 solution to $V^{V}O_2$-complexes in MeOH.

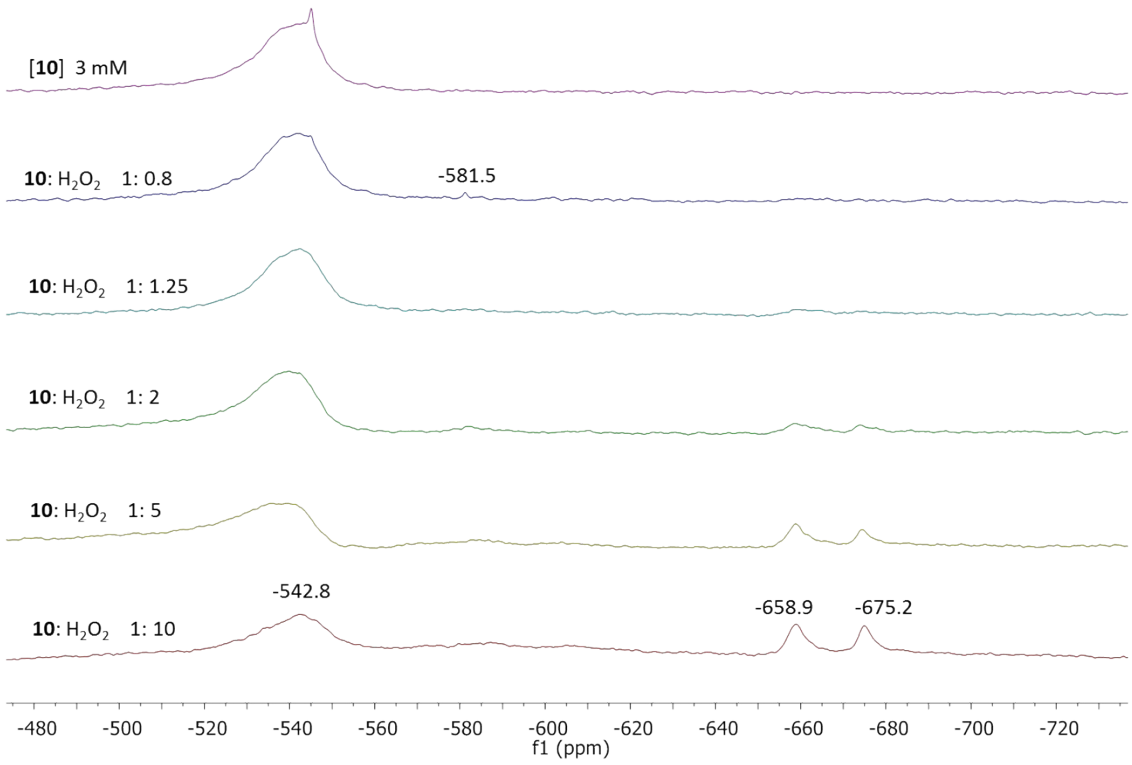


Fig. S20 ^{51}V NMR spectra of a 3 mM solution of $Na_3[(V^{V}O_2)_3\{ptk(fah)_3\}]\cdot6H_2O$ **10** in MeOH/5% D_2O with successive additions of a 1% aqueous solution of H_2O_2. The molar ratios are indicated in the figure.

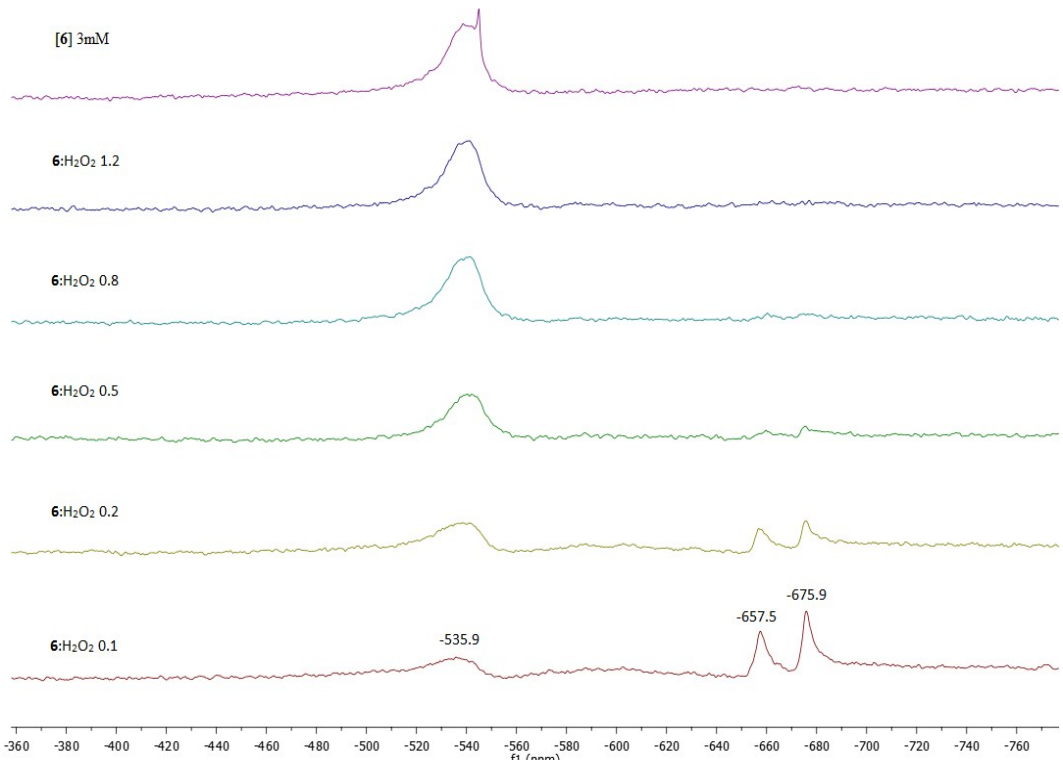


Fig. S21 ^{51}V NMR spectra of a 3 mM solution of $K_3[(V^VO_2)_3\{ptk(fah)_3\}]\cdot 6H_2O$ **6** in MeOH/5% D_2O upon successive additions of a 1% solution aqueous of H_2O_2. The molar ratios are indicated in the figure.

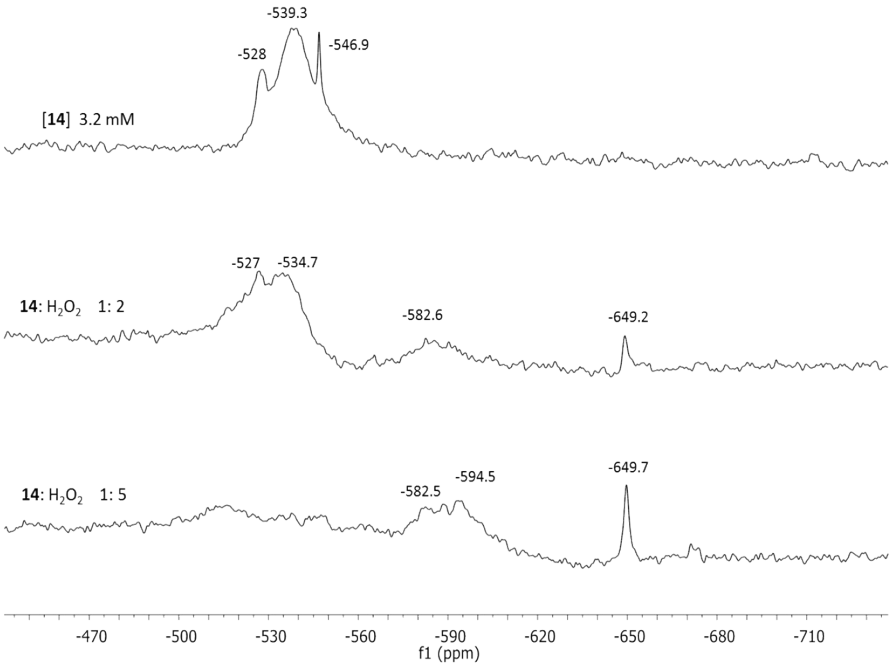


Fig. S22 ^{51}V NMR spectra of a 3.2 mM solution of $Cs_3[(V^VO_2)_3\{ptk(fah)_3\}]\cdot 6H_2O$ **14** in MeOH-d_4 upon successive additions of a 1% aqueous solution of H_2O_2. The molar ratios are indicated.

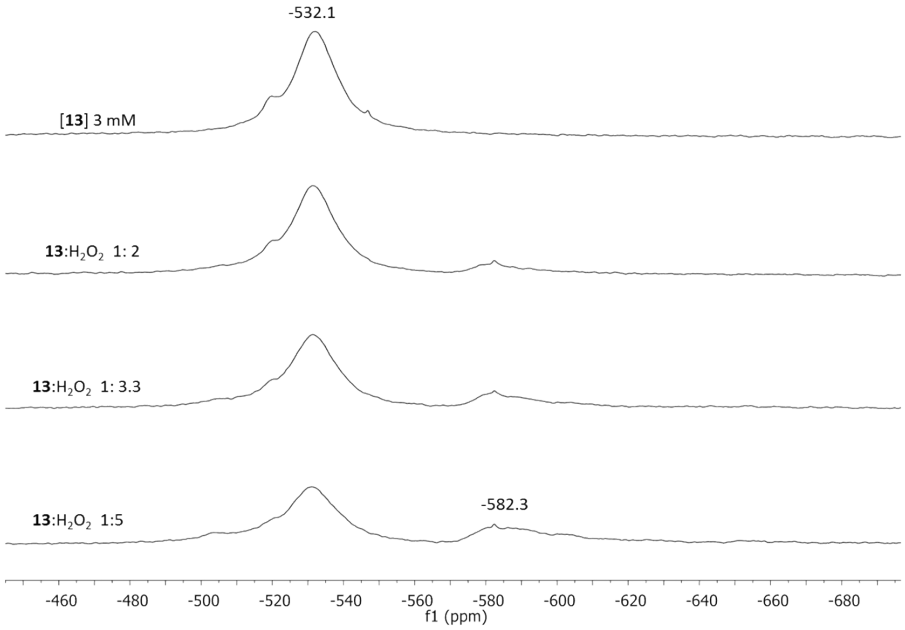


Fig. S23A ^{51}V NMR spectra of a 3 mM solution of $Cs_3[(V^VO_2)_3\{ptk(bhz)_3\}]\cdot 6H_2O$ **13** in MeOH_d_4 upon successive additions of a 1% aqueous solution of H_2O_2. The molar ratios are indicated in the figure.

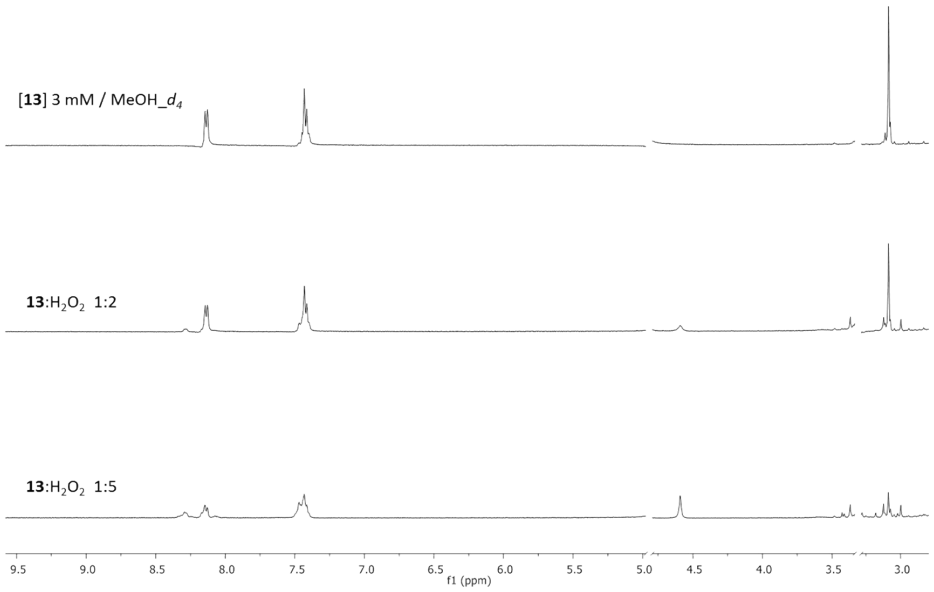


Fig. S23B ^{1}H NMR spectra of a 3 mM solution of $Cs_3[(V^{V}O_2)_3\{ptk(bhz)_3\}]\cdot 6H_2O$ **13** in MeOH-d_4 upon successive additions of a 1% aqueous solution of H_2O_2. The molar ratios are indicated in the figure.

Addition of H_2O_2 probably leads to the hydrolysis of, at least, one of the imine bonds, with consequent release of the corresponding hydrazine. This can be observed by the appearance of new aromatic signals at 8.3 ppm as well as a new -CH_2 signal at 4.6 ppm from the methylene group next to the N-atom. This will provide a set of different signals for the methyl groups for each will suffer a different chemical environment.

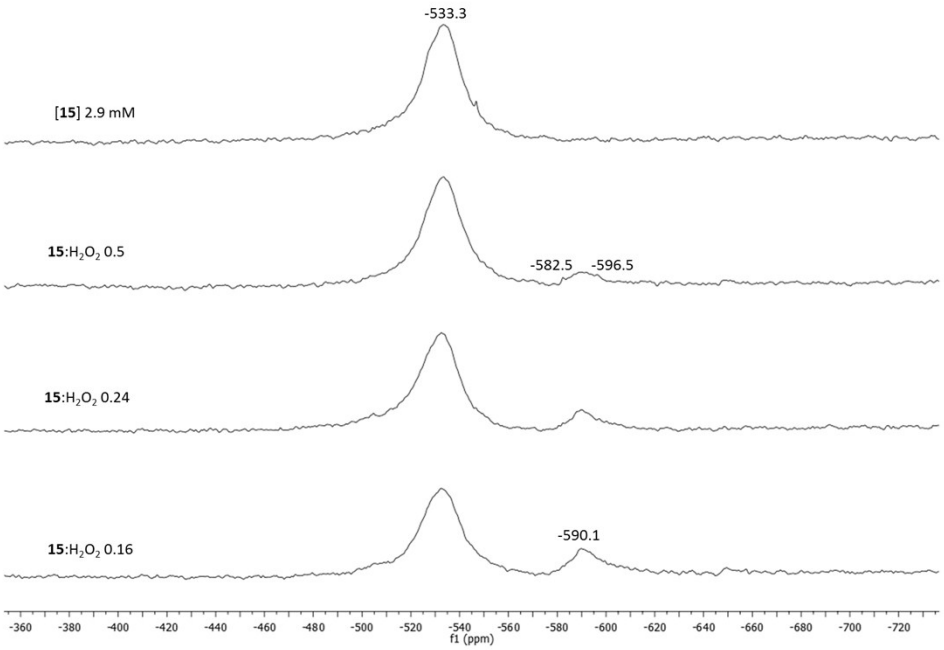


Fig. S24A ^{51}V NMR spectra of a 2.9 mM solution of $Cs_3[(V^VO_2)_3\{ptk(inh)_3\}]\cdot 6H_2O$ **15** in MeOH-d_4 upon successive additions of a 1% aqueous solution of H_2O_2. The molar ratios are indicated in the figure.

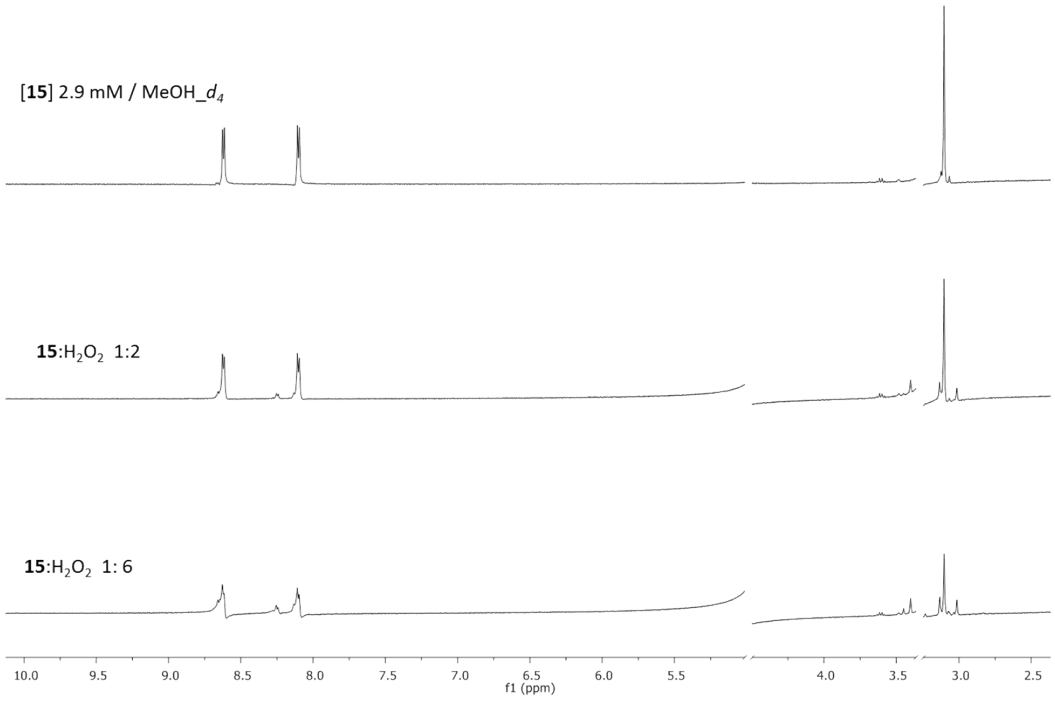


Fig. S24B ^{1}H NMR spectra of a 2.9 mM solution of $Cs_3[(V^{V}O_2)_3\{ptk(inh)_3\}]\cdot 6H_2O$ **15** in MeOH-d_4 upon successive additions of a 1% aqueous solution of H_2O_2. The molar ratios are indicated.

In this case, it is observed that the methyl groups will suffer different chemical environments upon addition of peroxide. Also in the aromatic region a new set of signals appearing at 8.25 and 8.65 ppm revealed that one of the pyridine rings is in a different chemical environment.

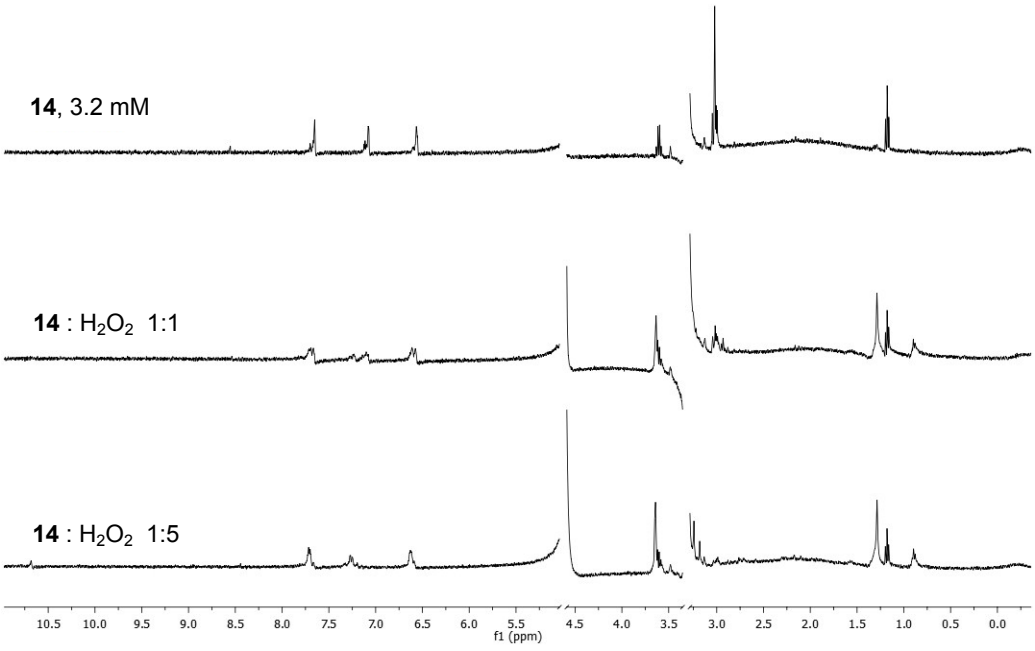


Fig. S25 ^{1}H NMR spectra of a 3.2 mM solution of $Cs_3[(V^{V}O_2)_3\{ptk(fah)_3\}]\cdot 6H_2O$ **14** in MeOH-d_4 upon successive additions of a 1% aqueous solution of H_2O_2. The molar ratios are indicated.

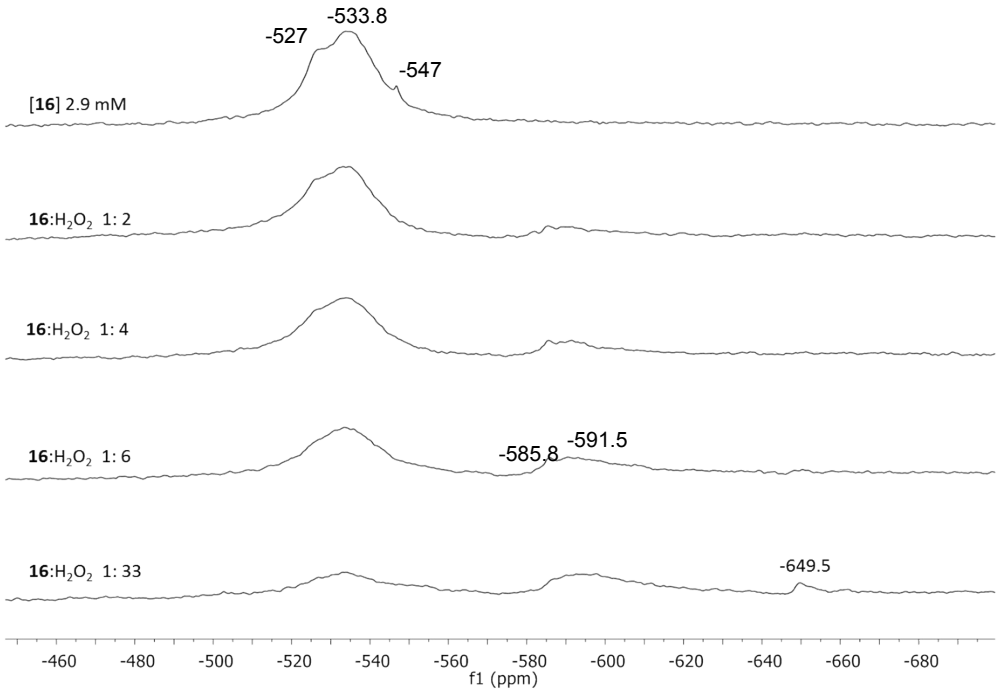


Fig. S26A ^{51}V NMR spectra of a 2.9 mM solution of $Cs_3[(V^VO_2)_3\{ptk(nah)_3\}]\cdot 6H_2O$ **16** in MeOH-d_4 upon successive additions of a 1% aqueous solution of H_2O_2, and finally 5 μL of a 30% solution of peroxide. The molar ratios are indicated.

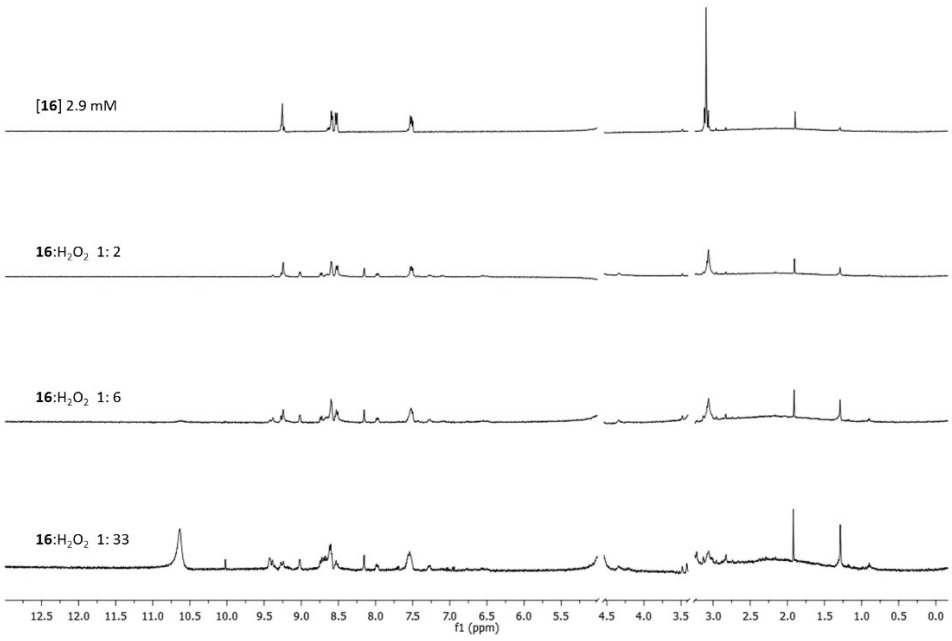


Fig. S26B ^{1}H NMR spectra of a 2.9 mM solution of $Cs_3[(V^{V}O_2)_3\{ptk(nah)_3\}]\cdot 6H_2O$ **16** in MeOH-d_4 upon successive additions of a 1% aqueous solution of H_2O_2, and finally 5 μL of a 30% solution of peroxide. The molar ratios are indicated.

The large excess of peroxide can be observed by the presence of H_2O_2 characteristic signal at 10.6 ppm. This probably leads to quite extensive degradation of the complex and the peaks coming from the free ligand and hydrolysis products can be observed. Notwithstanding, it is clear from the last spectrum of Fig. SI-26 that significant amounts of the original resonances, and those of the corresponding $V^{V}O$-L-$(O)_2$ complex, are clearly visible, thus complex **16** is quite resistant to hydrolysis by excess of H_2O_2 as high as 33, this corresponding to about a molar excess of 11 relative to the V^{V}-ions.

ES8. Catalytic oxidation of dopamine.

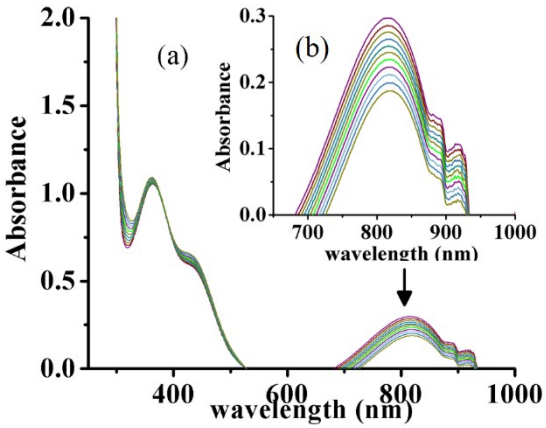


Fig. S27 Spectral changes observed during oxidation of dopamine (2 mL, 2×10^{-4} M), using $Cs_3[(V^VO_2)_3\{ptk(bhz)_3\}]\cdot6H_2O$ **13** (2 mL, 1×10^{-4} M) as pre-catalyst and H_2O_2 (2 mL, 2×10^{-3} M). The spectra were recorded after every 60 seconds for 1 h.

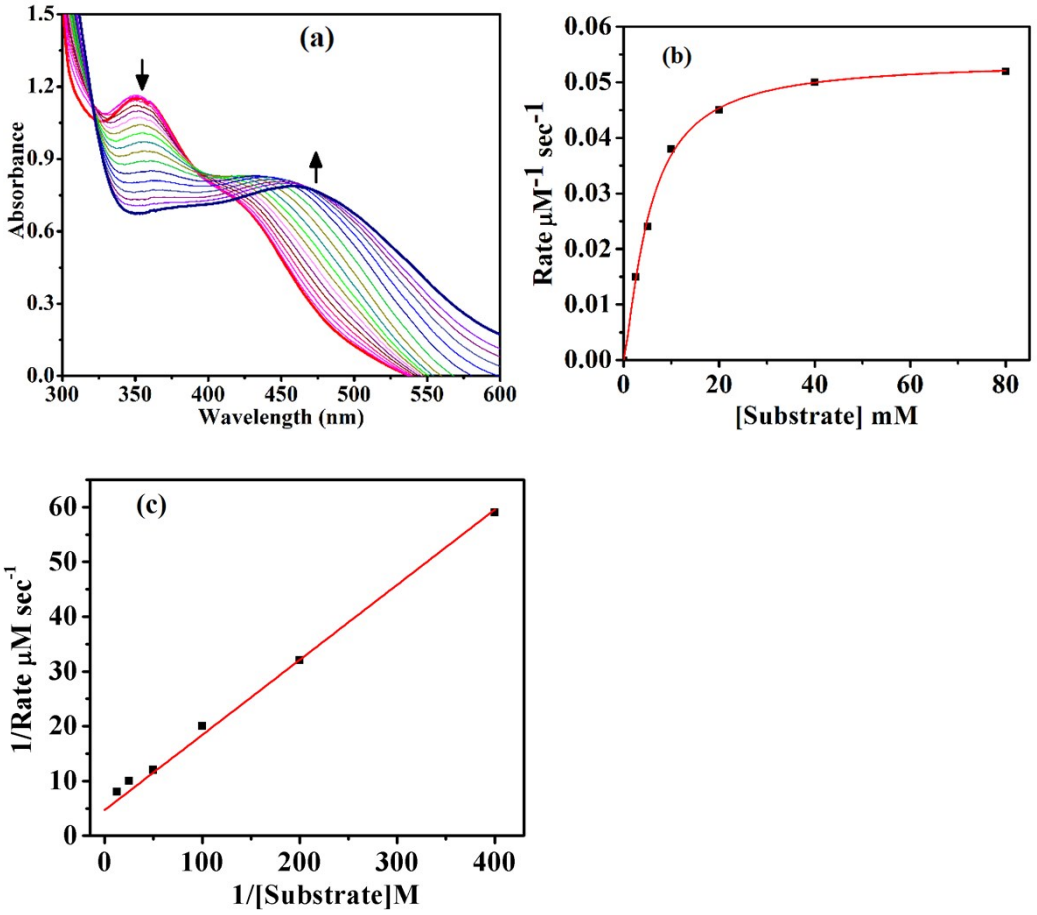


Fig. S28 Spectral changes observed during oxidation of dopamine (2 mL, 2×10^{-4} M), using $Cs_3[(V^{V}O_2)_3\{ptk(bhz)_3\}]\cdot6H_2O$ **13** (2 mL, 1×10^{-4} M) as pre-catalyst and H_2O_2 (2 mL, 2×10^{-3} M). The spectra were recorded after every 60 seconds for 1 h.

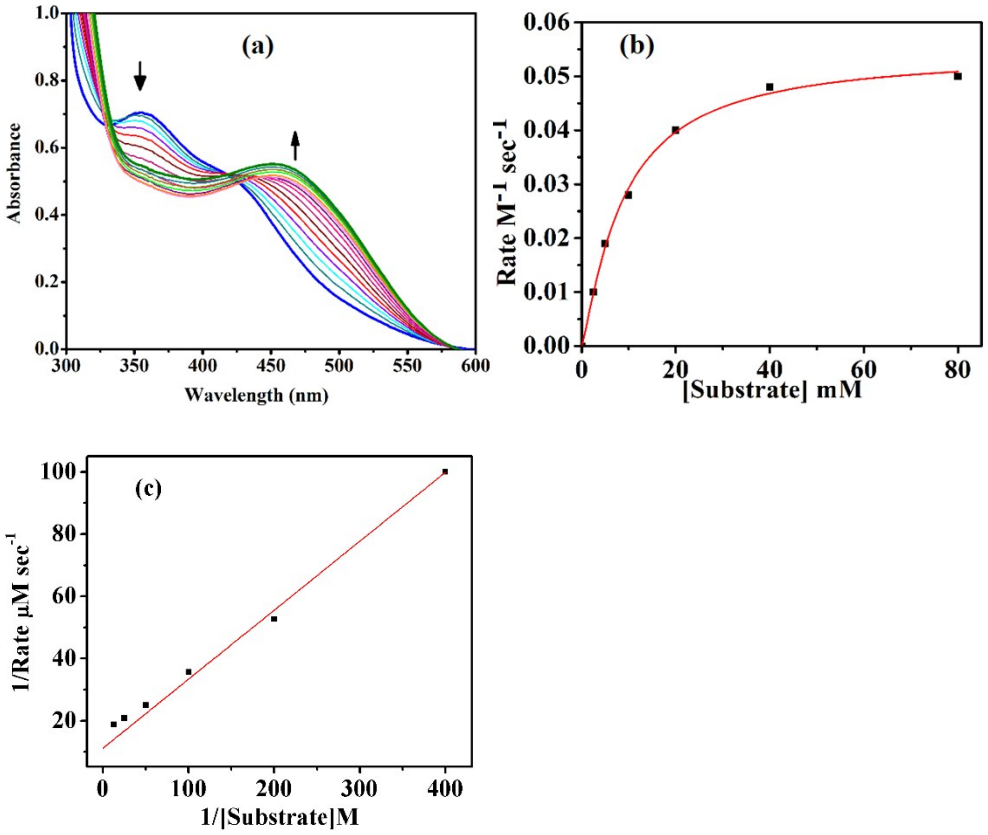


Fig. S29 Spectral changes observed during oxidation of dopamine (2 mL, 2×10^{-4} M) using $Cs_3[(V^VO_2)_3\{ptk(fah)_3\}]\cdot6H_2O$ **14** (2 mL, 1×10^{-4} M) as pre-catalyst and H_2O_2 (2 mL, 2×10^{-3} M). The spectra were recorded after every 60 seconds for 1 h.

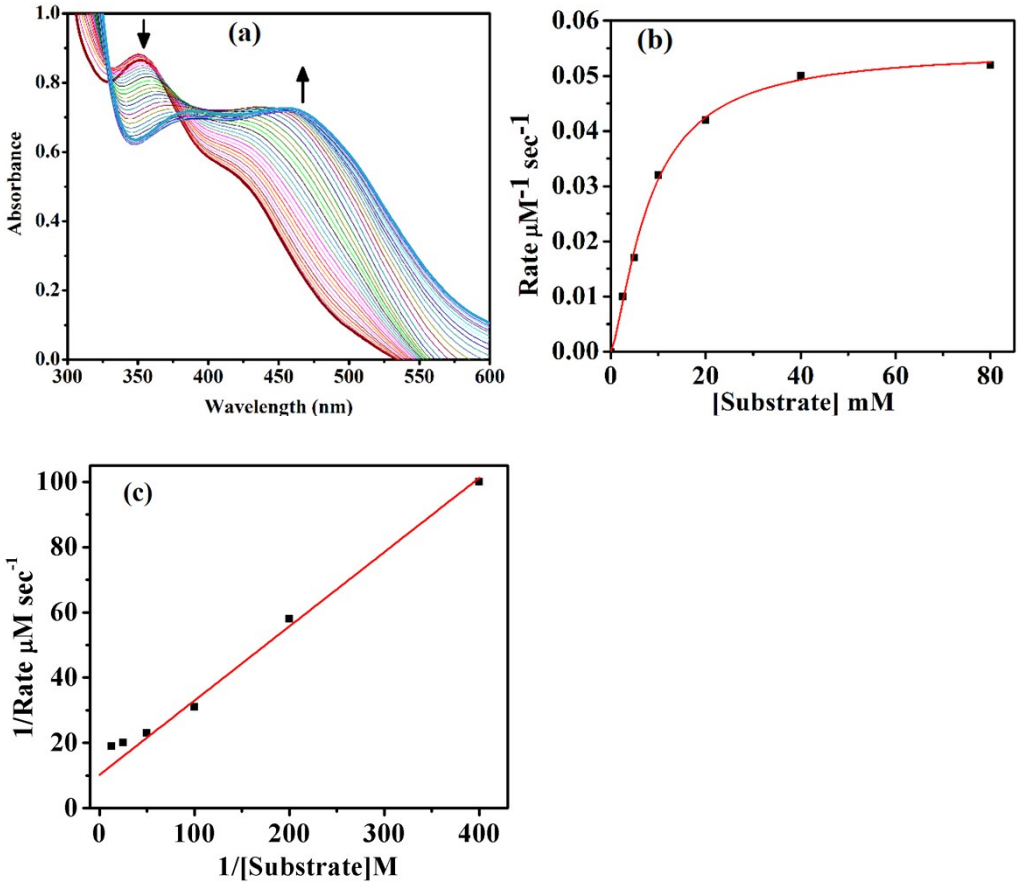


Fig. S30 Spectral changes observed during oxidation of dopamine (2 mL, 2×10^{-4}M), using $Cs_3[(V^VO_2)_3\{ptk(inh)_3\}]\cdot6H_2O$ **15** (2 mL, 1×10^{-4}M) as pre-catalyst and H_2O_2 (2 mL, 2×10^{-3}M). The spectra were recorded after every 60 seconds for 1 h.

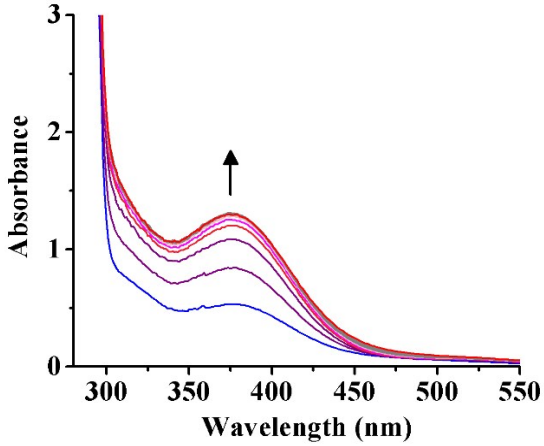


Fig. S31 Spectral changes observed during oxidation of dopamine (2 mL, 2×10^{-4} M), using $V^{IV}OSO_4$ (2 mL, 1×10^{-4} M) as pre-catalyst and H_2O_2 (2 mL, 2×10^{-3} M). The spectra were recorded after every 60 seconds for 1 h.

ES9. Computational section.

Table S8. Cartesian atomic coordinates (in Å) of the calculated equilibrium structures.

Hacac

C	-1.963739	-1.290583	0.102927
C	-2.684564	-2.595485	0.302450
C	-2.835045	2.404449	-0.420564
C	-2.110088	1.119004	-0.245215
C	-2.732889	-0.085923	-0.061182
O	-0.797071	1.246839	-0.283479
O	-0.720269	-1.290687	0.084509
H	-3.919339	2.265943	-0.382676
H	-2.561937	2.858325	-1.381636
H	-2.533337	3.112146	0.362023
H	-2.402053	-3.288537	-0.499367
H	-3.774075	-2.487710	0.317824
H	-2.352349	-3.049606	1.243785
H	-3.818535	-0.123452	-0.039127
H	-0.423559	0.324208	-0.155193

$[VO(acac)_2]$

C	-1.602812	-1.561698	0.282339
C	-2.363135	-2.851017	0.284659
C	4.210736	2.170642	-0.810061
C	3.490114	0.900212	-0.482715
C	4.170050	-0.320783	-0.508930
C	3.515390	-1.544654	-0.343351
C	4.262450	-2.828923	-0.525004
C	-2.414688	2.148614	0.001015
C	-1.628018	0.883205	0.143606
C	-2.286140	-0.342315	0.280845
O	-0.361251	1.024325	0.099247
O	-0.333353	-1.680869	0.252767
O	2.249115	1.032930	-0.220210
O	2.277087	-1.672227	-0.066033
O	1.216802	-0.200635	2.137825
V	1.027696	-0.290715	0.588272
H	3.732866	2.643700	-1.676901
H	5.272225	2.012127	-1.022991
H	4.106234	2.869484	0.028714
H	5.320666	-2.673781	-0.755948
H	3.795373	-3.407288	-1.331778
H	4.171518	-3.429816	0.387962
H	-3.495128	1.982908	0.050158
H	-2.163076	2.624360	-0.954973
H	-2.115632	2.848610	0.790583

H	-2.100778	-3.426463	-0.611771
H	-3.446806	-2.703060	0.316123
H	-2.050588	-3.451017	1.147884
H	5.228506	-0.323842	-0.754593
H	-3.372556	-0.352564	0.297647

2 (doublet)

V	-3.695903	1.251714	1.097476
N	-3.718778	-0.440003	0.013524
O	-4.175942	3.311099	1.160302
C	-1.343304	-0.534170	-0.208536
V	0.678928	-3.947579	-1.015524
N	-4.977964	-0.913966	-0.315521
O	-3.385881	0.880067	2.591501
C	-1.131095	0.865249	-0.076575
V	3.119471	2.550198	0.646230
O	-2.121544	1.693968	0.116295
N	2.204117	-3.000289	-0.108318
C	0.185116	1.411832	-0.197545
O	-5.563743	1.109884	0.626312
N	3.265623	-3.810909	0.263510
C	1.290512	0.524129	-0.138359
C	1.096067	-0.885772	-0.028034
N	1.480805	3.421568	-0.128319
O	-8.185800	0.577707	0.236928
N	1.630211	4.762535	-0.444828
C	-0.217941	-1.404847	-0.151322
O	0.734972	-3.675509	-2.560079
O	-0.918272	-5.232791	-0.568106
C	-2.669938	-1.069508	-0.455051
O	-0.450013	-2.696564	-0.112481
C	-2.890065	-2.254363	-1.345981
H	-3.264109	-3.109350	-0.766643
H	-1.985884	-2.546203	-1.883150
H	-3.685998	-2.008445	-2.057510
C	-5.866640	-0.036317	0.066691
O	1.760772	-5.432632	-0.399513
C	-7.266957	-0.347197	-0.150478
C	-7.893280	-1.436424	-0.686253
H	-7.397530	-2.318189	-1.071571
O	5.103873	-5.800025	0.836981
C	-9.285831	-1.164781	-0.623578
H	-10.097733	-1.799826	-0.954438
O	2.525416	0.957917	-0.228834
C	-9.399855	0.067422	-0.055704
H	-10.245118	0.692236	0.199153
O	2.949077	2.458510	2.203421

O	5.006847	1.832988	0.090354
C	2.219421	-1.750559	0.288735
C	3.350132	-1.302288	1.162712
H	3.513625	-2.062892	1.934052
H	3.158719	-0.337289	1.633137
H	4.288032	-1.257281	0.593757
O	3.830038	4.232501	0.002740
C	2.939314	-5.053641	0.047873
O	4.583355	6.784579	-0.480524
C	3.888990	-6.115260	0.314864
C	3.793355	-7.464844	0.127224
H	2.936998	-7.984028	-0.283503
C	5.029552	-8.015448	0.561337
H	5.324922	-9.056793	0.561526
C	5.778766	-6.958852	0.979170
H	6.775500	-6.871270	1.390260
C	0.351666	2.833542	-0.443681
C	-0.695223	3.642106	-1.146500
H	-0.205742	4.295787	-1.874996
H	-1.215684	4.296602	-0.435413
H	-1.440054	3.013216	-1.633165
C	2.889706	5.084914	-0.322270
C	3.265320	6.463670	-0.574920
C	2.535088	7.570158	-0.905030
H	1.461642	7.595572	-1.041530
C	3.463229	8.639207	-1.019527
H	3.252208	9.672132	-1.265657
C	4.685055	8.101933	-0.751236
H	5.684936	8.512399	-0.711209
H	-3.727119	3.792988	1.871445
H	-5.133442	3.372036	1.316217
H	-1.513484	-4.756775	0.035737
H	-0.577281	-6.018031	-0.109352
H	5.494093	2.541136	-0.362811
H	4.900819	1.087139	-0.523400

2 (quartet)

V	-3.695904	1.251712	1.097476
N	-3.718778	-0.440005	0.013524
O	-4.175944	3.311096	1.160302
C	-1.343304	-0.534171	-0.208536
V	0.678930	-3.947579	-1.015524
N	-4.977963	-0.913969	-0.315521
O	-3.385882	0.880065	2.591501
C	-1.131096	0.865248	-0.076575
V	3.119469	2.550200	0.646230
O	-2.121545	1.693967	0.116295

N	2.204119	-3.000288	-0.108318
C	0.185115	1.411832	-0.197545
O	-5.563744	1.109880	0.626312
N	3.265625	-3.810907	0.263510
C	1.290512	0.524130	-0.138359
C	1.096068	-0.885771	-0.028034
N	1.480803	3.421569	-0.128319
O	-8.185800	0.577702	0.236928
N	1.630208	4.762536	-0.444828
C	-0.217940	-1.404847	-0.151322
O	0.734974	-3.675509	-2.560079
O	-0.918269	-5.232792	-0.568106
C	-2.669937	-1.069510	-0.455051
O	-0.450011	-2.696564	-0.112481
C	-2.890064	-2.254365	-1.345981
H	-3.264107	-3.109352	-0.766643
H	-1.985882	-2.546204	-1.883150
H	-3.685997	-2.008447	-2.057510
C	-5.866640	-0.036321	0.066691
O	1.760775	-5.432631	-0.399513
C	-7.266957	-0.347202	-0.150478
C	-7.893279	-1.436429	-0.686253
H	-7.397529	-2.318194	-1.071571
O	5.103877	-5.800022	0.836981
C	-9.285830	-1.164787	-0.623578
H	-10.097732	-1.799832	-0.954438
O	2.525415	0.957919	-0.228834
C	-9.399855	0.067416	-0.055704
H	-10.245118	0.692230	0.199153
O	2.949075	2.458512	2.203421
O	5.006846	1.832991	0.090354
C	2.219422	-1.750558	0.288735
C	3.350133	-1.302286	1.162712
H	3.513626	-2.062890	1.934052
H	3.158719	-0.337287	1.633137
H	4.288033	-1.257278	0.593757
O	3.830035	4.232503	0.002740
C	2.939317	-5.053639	0.047873
O	4.583351	6.784582	-0.480524
C	3.888994	-6.115258	0.314864
C	3.793360	-7.464842	0.127224
H	2.937003	-7.984026	-0.283503
C	5.029557	-8.015445	0.561337
H	5.324928	-9.056790	0.561526
C	5.778770	-6.958848	0.979170
H	6.775504	-6.871266	1.390260

C	0.351664	2.833542	-0.443681
C	-0.695225	3.642106	-1.146500
H	-0.205745	4.295787	-1.874996
H	-1.215687	4.296601	-0.435413
H	-1.440056	3.013215	-1.633165
C	2.889703	5.084916	-0.322270
C	3.265316	6.463672	-0.574920
C	2.535083	7.570160	-0.905030
H	1.461637	7.595573	-1.041530
C	3.463223	8.639209	-1.019527
H	3.252202	9.672134	-1.265657
C	4.685050	8.101936	-0.751236
H	5.684931	8.512403	-0.711209
H	-3.727121	3.792986	1.871445
H	-5.133444	3.372033	1.316217
H	-1.513481	-4.756776	0.035737
H	-0.577277	-6.018031	-0.109352
H	5.494091	2.541139	-0.362811
H	4.900818	1.087142	-0.523400

$[(VO)(H_2O)H_4ptk(fah)_3]$

N	3.194993	-2.699116	-0.272209
C	1.694596	-0.896334	-0.461217
N	4.446388	-3.285271	-0.401146
C	0.564177	-1.742166	-0.343059
V	-3.536719	-0.017440	0.830282
O	0.693888	-3.057048	-0.239031
N	0.906335	3.264616	-0.352718
C	-0.763260	-1.234052	-0.341216
O	5.504891	-1.835608	1.039982
N	0.856066	4.598118	-0.092308
C	-0.932678	0.173664	-0.220605
C	0.182536	1.042439	-0.180424
N	-3.076750	-1.757232	-0.068673
O	7.588742	-3.624811	1.318045
N	-4.162632	-2.579909	-0.327960
C	1.476276	0.504971	-0.387349
C	3.046907	-1.456509	-0.631569
O	2.546583	1.283170	-0.448514
C	4.144612	-0.679900	-1.281018
H	4.707925	-0.102228	-0.541038
H	3.749122	0.017646	-2.021809
H	4.836008	-1.381619	-1.762237
C	5.502480	-2.869395	0.406999
O	3.031081	4.888540	-0.754294
C	6.638616	-3.805848	0.366710
C	6.988133	-4.845537	-0.449095

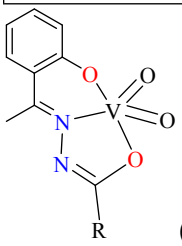
H	6.442357	-5.197246	-1.317124
O	0.520917	7.272240	0.079309
C	8.230066	-5.336356	0.037996
H	8.817802	-6.154024	-0.358923
O	-2.127385	0.721186	-0.185978
C	8.538643	-4.555950	1.109351
H	9.370716	-4.540117	1.800105
O	-3.175927	-0.104008	2.361594
O	-4.608524	1.834334	0.767170
C	-0.005717	2.471041	0.106511
C	-1.126814	2.956519	0.981290
H	-0.780372	3.796582	1.598504
H	-1.463502	2.163492	1.655489
H	-1.997826	3.278922	0.394954
O	-5.284903	-0.682421	0.352108
C	1.961798	5.356901	-0.412908
O	-7.664728	-1.908664	-0.012991
C	1.752365	6.801728	-0.280620
C	2.615842	7.836686	-0.466113
H	3.654200	7.736391	-0.754868
C	1.875904	9.023911	-0.205977
H	2.231216	10.045246	-0.253338
C	0.618219	8.621675	0.118275
H	-0.284980	9.150787	0.390728
C	-1.896299	-2.124004	-0.512917
C	-1.788112	-3.410978	-1.269683
H	-2.679009	-3.531767	-1.892440
H	-1.762174	-4.260490	-0.575828
H	-0.886107	-3.447071	-1.880021
C	-5.260245	-1.929422	-0.061290
C	-6.525399	-2.616575	-0.241925
C	-6.833340	-3.893038	-0.617866
H	-6.114876	-4.667006	-0.855313
C	-8.251352	-3.975671	-0.620912
H	-8.860731	-4.835740	-0.867636
C	-8.697418	-2.745348	-0.247436
H	-9.683220	-2.322971	-0.106604
H	-4.537285	2.256736	1.637296
H	-5.529440	1.527892	0.680103
H	2.258746	2.234894	-0.509858
H	-0.028117	5.056656	0.108637
H	1.676355	-3.250740	-0.153255
H	4.356625	-4.291536	-0.489737

$[\{(VO)(H_2O)\}_2H_2ptk(fah)_3]$

V	3.762093	-0.925662	-0.772098
N	3.712388	0.918182	0.030987

O	3.523035	-0.829096	-2.325154
C	1.328185	1.023765	0.150581
N	4.955116	1.453442	0.330010
O	4.291355	-2.966898	-0.499401
C	1.128688	-0.382000	0.086140
V	-3.064575	-2.103123	0.942965
O	2.135458	-1.216720	0.153055
N	-2.145400	3.416527	-0.227664
C	-0.181857	-0.939483	-0.002559
O	5.596167	-0.694988	-0.213405
N	-3.141961	4.334270	-0.097007
C	-1.301462	-0.066439	0.092519
C	-1.124855	1.340061	0.141230
N	-1.457065	-2.957210	0.082186
O	8.189879	-0.075868	0.236840
N	-1.621548	-4.294384	-0.249644
C	0.183537	1.864819	0.051057
C	2.643824	1.597446	0.377142
O	0.412522	3.159191	-0.110109
C	2.828819	2.905784	1.079920
H	1.930902	3.211002	1.616536
H	3.072715	3.694343	0.357008
H	3.678107	2.823361	1.764136
C	5.865409	0.536790	0.152539
O	-1.733474	6.048144	-0.668177
C	7.251501	0.898266	0.382933
C	7.847046	2.075897	0.734903
H	7.331314	3.011406	0.910159
O	-5.272648	5.991523	-0.278038
C	9.240405	1.809391	0.809795
H	10.031988	2.504196	1.059992
O	-2.534384	-0.518213	0.051102
C	9.385439	0.492332	0.498550
H	10.242346	-0.163361	0.424093
O	-2.842460	-1.991354	2.497952
O	-5.127796	-1.580939	0.752229
C	-2.283013	2.232540	0.273976
C	-3.500710	1.836360	1.058056
H	-3.846137	2.696086	1.649294
H	-3.276122	1.016663	1.745287
H	-4.320856	1.507472	0.405403
O	-3.791249	-3.789624	0.343403
C	-2.856844	5.637849	-0.446655
O	-4.557746	-6.336296	-0.128674
C	-4.030273	6.514155	-0.503569
C	-4.121394	7.845476	-0.769982

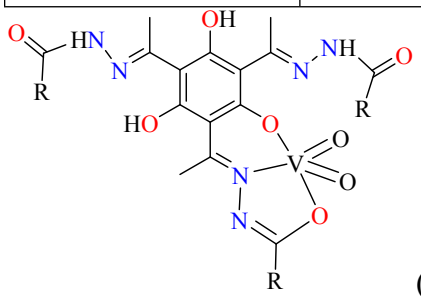
H	-3.283327	8.495403	-0.986516
C	-5.505038	8.170661	-0.706185
H	-5.961970	9.139363	-0.862874
C	-6.151404	7.012781	-0.405732
H	-7.191866	6.759261	-0.253647
C	-0.346809	-2.354845	-0.277248
C	0.676121	-3.136047	-1.045768
H	0.168515	-3.906876	-1.631279
H	1.366552	-3.638574	-0.355844
H	1.258833	-2.482831	-1.700632
C	-2.865845	-4.629990	-0.060638
C	-3.251963	-6.005029	-0.316978
C	-2.544199	-7.099054	-0.726270
H	-1.484346	-7.114754	-0.945189
C	-3.473520	-8.171378	-0.793633
H	-3.276680	-9.197062	-1.078602
C	-4.673652	-7.648878	-0.420610
H	-5.665592	-8.066979	-0.314818
H	-5.458203	-1.243669	1.599042
H	-5.536743	-2.455434	0.617554
H	5.262933	-2.945754	-0.441900
H	4.059296	-3.500782	-1.274440
H	-0.451548	3.628924	-0.276276
H	-4.109818	4.036603	-0.012598



(overall charge -1)

C	-0.067808	-1.260073	-0.915134
C	-0.379350	-2.606813	-0.901849
V	3.150684	-5.677186	0.340027
C	0.467686	-3.575049	-0.329575
C	1.693220	-3.138383	0.253784
C	1.980518	-1.754149	0.248710
N	0.906644	-5.893284	0.057483
N	0.464633	-7.192658	0.081462
C	1.127013	-0.835626	-0.325053
O	2.549103	-3.930125	0.837049
O	3.588626	-5.582104	-1.195053
O	4.440211	-5.735094	1.286961
O	2.669468	-7.581791	0.663322
O	2.181468	-10.243869	0.815567
C	0.058300	-4.973605	-0.302059

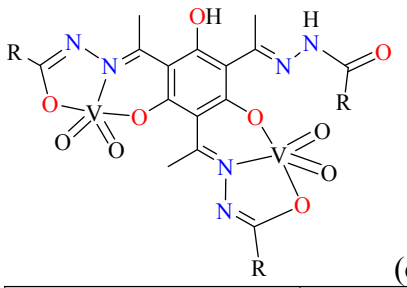
C	-1.346305	-5.325928	-0.701553
H	-1.544498	-6.373578	-0.470453
H	-1.489654	-5.177438	-1.781313
H	-2.074013	-4.688292	-0.184282
C	1.478646	-7.968309	0.391533
C	1.181823	-9.400976	0.446071
C	0.044114	-10.113365	0.193532
H	-0.899221	-9.686697	-0.121519
C	0.366726	-11.479867	0.422993
H	-0.284715	-12.339708	0.321973
C	1.675273	-11.493687	0.797048
H	2.363979	-12.281732	1.071256
H	2.918765	-1.453585	0.712103
H	1.389311	0.223004	-0.321037
H	-0.745884	-0.545046	-1.379090
H	-1.312311	-2.929668	-1.361893



(overall charge -1)

N	3.176410	-2.659391	-0.297850
C	1.700984	-0.827082	-0.484636
N	4.436918	-3.240403	-0.400530
C	0.545442	-1.668082	-0.463921
V	-3.715346	0.330049	0.464651
O	0.670121	-2.991548	-0.385722
N	0.923087	3.342134	-0.357461
C	-0.763710	-1.152903	-0.551113
O	5.436063	-1.997139	1.261240
N	0.809577	4.672886	-0.071739
C	-0.940499	0.252367	-0.438510
C	0.186293	1.115364	-0.290062
N	-3.096812	-1.636423	-0.338501
O	7.424053	-3.893096	1.475318
N	-4.124098	-2.546914	-0.483092
C	1.483376	0.576684	-0.399251
C	3.047066	-1.389154	-0.584806
O	2.562067	1.357457	-0.355282
C	4.208569	-0.586855	-1.080298
H	4.709536	-0.077858	-0.250056
H	3.889717	0.174339	-1.793345
H	4.931751	-1.264054	-1.549691

C	5.437641	-2.948895	0.508071
O	2.995103	5.121293	-0.618477
C	6.562387	-3.906747	0.426881
C	6.970110	-4.827532	-0.496550
H	6.499300	-5.032407	-1.451197
O	0.329043	7.322010	0.246424
C	8.154895	-5.420656	0.023540
H	8.763541	-6.189963	-0.434652
O	-2.108329	0.798318	-0.526345
C	8.375187	-4.812490	1.219961
H	9.137565	-4.921992	1.979452
O	-3.203160	0.455345	1.975805
O	-4.529167	1.640025	0.030829
C	-0.026590	2.534268	0.008252
C	-1.223948	2.999641	0.781898
H	-0.933023	3.808700	1.466912
H	-1.659366	2.193479	1.379034
H	-2.030219	3.355643	0.126983
O	-5.307122	-0.842420	0.528861
C	1.878730	5.493853	-0.298745
O	-7.548488	-2.369928	0.534330
C	1.587405	6.923526	-0.101517
C	2.406055	8.004459	-0.212954
H	3.454509	7.962327	-0.478006
C	1.605919	9.144199	0.083957
H	1.914166	10.182067	0.095450
C	0.360619	8.670441	0.354253
H	-0.574300	9.140675	0.627811
C	-1.918033	-2.027167	-0.740755
C	-1.781055	-3.350005	-1.437243
H	-2.688258	-3.539384	-2.017930
H	-1.680908	-4.166793	-0.711498
H	-0.899594	-3.370750	-2.081146
C	-5.205659	-2.027487	0.043999
C	-6.385367	-2.891562	0.063950
C	-6.577213	-4.189757	-0.313902
H	-5.811939	-4.838924	-0.719196
C	-7.946245	-4.482642	-0.061535
H	-8.465025	-5.417745	-0.235318
C	-8.480912	-3.341053	0.451719
H	-9.470454	-3.069488	0.794644
H	2.265671	2.306320	-0.417666
H	-0.102561	5.074388	0.126997
H	1.639844	-3.192384	-0.256100
H	4.357270	-4.221477	-0.644186



(overall charge -2)

V	3.854258	-1.348009	-0.550576
N	3.766742	0.694425	0.259514
O	3.541403	-1.292062	-2.119475
C	1.377990	0.922542	0.250737
N	4.992659	1.274211	0.531741
O	4.234225	-2.837915	-0.092285
C	1.131952	-0.479633	0.121532
V	-3.480027	-1.898508	0.494643
O	2.100784	-1.327885	0.256940
N	-1.984035	3.480625	-0.250398
C	-0.193155	-0.979834	-0.083240
O	5.742608	-0.702350	-0.396225
N	-3.030330	4.361161	-0.146091
C	-1.274229	-0.067993	-0.081170
C	-1.045747	1.339331	0.049113
N	-1.616755	-2.904247	-0.113610
O	8.316843	0.138550	-0.129389
N	-1.745879	-4.267251	-0.318639
C	0.286750	1.811426	0.102061
C	2.712891	1.412371	0.555796
O	0.557982	3.118453	0.033742
C	2.912435	2.719781	1.271027
H	2.003811	3.043926	1.779361
H	3.201791	3.510788	0.567655
H	3.734916	2.607352	1.983858
C	5.927568	0.463311	0.106905
O	-1.725448	6.243016	-0.376373
C	7.299767	0.961576	0.238805
C	7.804827	2.151360	0.681444
H	7.207447	2.984218	1.028850
O	-5.273311	5.889078	-0.299895
C	9.220826	2.050651	0.578843
H	9.958071	2.802005	0.837350
O	-2.495299	-0.444836	-0.309601
C	9.469716	0.808764	0.081065
H	10.374927	0.272268	-0.171744
O	-3.400482	-1.541475	2.055639
O	-4.898405	-1.452632	-0.118164

C	-2.179930	2.246853	0.131916
C	-3.485691	1.803900	0.729353
H	-3.915592	2.620988	1.327254
H	-3.356039	0.936231	1.380466
H	-4.212734	1.495408	-0.033603
O	-3.892594	-3.835506	0.414619
C	-2.814748	5.695194	-0.301187
O	-4.488717	-6.486661	0.241162
C	-4.053208	6.498446	-0.350467
C	-4.210980	7.846800	-0.447833
H	-3.399862	8.560888	-0.505155
C	-5.615684	8.086681	-0.459256
H	-6.121698	9.041887	-0.528295
C	-6.206944	6.866013	-0.367752
H	-7.235901	6.533408	-0.340090
C	-0.430258	-2.393089	-0.346881
C	0.653695	-3.252534	-0.925706
H	0.199314	-4.081408	-1.473445
H	1.293864	-3.669731	-0.138868
H	1.311633	-2.671032	-1.578104
C	-2.951108	-4.625539	0.026571
C	-3.232379	-6.060679	-0.057355
C	-2.449925	-7.127185	-0.398453
H	-1.405916	-7.062803	-0.676432
C	-3.279116	-8.279876	-0.305115
H	-3.003976	-9.309599	-0.502338
C	-4.501636	-7.828673	0.087306
H	-5.446909	-8.313963	0.292920
H	-0.286744	3.606381	-0.152396
H	-3.983305	4.008249	-0.162306

14 (anion without counterions)

V	0.081414	4.232537	-0.633734
N	1.866644	3.227677	0.136789
O	-1.103254	5.206506	-0.144717
C	1.027812	0.977400	0.058098
V	3.689006	-2.162113	0.385509
N	2.933656	4.065333	0.418236
O	0.017878	4.006357	-2.219972
C	-0.331542	1.377772	-0.030656
V	-3.715500	-2.036777	0.757168
O	-0.672034	2.623057	0.099393
N	1.897626	-3.233516	-0.285678
C	-1.377688	0.400762	-0.133234
O	1.472063	5.655587	-0.401137
N	2.088889	-4.585291	-0.534042
C	-1.034150	-0.977403	-0.070632

C	0.338352	-1.399299	-0.196784
N	-3.754318	-0.007148	-0.055656
O	3.374715	7.579107	-0.041719
N	-5.024904	0.499000	-0.287402
C	1.356205	-0.410365	-0.112735
O	3.628564	-1.993471	1.978788
O	5.084947	-1.609330	-0.197260
C	2.060635	1.945209	0.369873
O	2.606707	-0.717858	-0.266600
C	3.341029	1.505873	1.021169
H	4.112272	1.284424	0.272717
H	3.200748	0.591157	1.602157
H	3.711273	2.314053	1.657691
C	2.612648	5.276899	0.060820
O	4.235988	-4.065009	0.141118
C	3.672821	6.277864	0.222646
C	4.979849	6.174632	0.610048
H	5.471535	5.246843	0.872304
O	2.871970	-7.242612	-0.772210
C	5.514451	7.493680	0.582826
H	6.525014	7.802074	0.827538
O	-1.943533	-1.885620	0.029066
C	4.495534	8.301368	0.180478
H	4.407928	9.366414	0.007463
O	-3.966934	-3.542637	0.244705
O	-3.507597	-1.994609	2.343571
C	0.667382	-2.785935	-0.460858
C	-0.378798	-3.728277	-0.989455
H	0.104683	-4.538496	-1.538014
H	-1.099265	-3.202972	-1.619782
H	-0.964396	-4.164568	-0.170866
O	-5.648884	-1.551630	0.571601
C	3.319024	-4.889598	-0.247295
O	-8.272563	-0.853370	0.323432
C	3.753103	-6.281037	-0.381884
C	4.982114	-6.838824	-0.169910
H	5.858177	-6.287013	0.144794
C	4.846303	-8.230399	-0.445403
H	5.611570	-8.996260	-0.382076
C	3.547110	-8.413077	-0.804704
H	2.966946	-9.278964	-1.097599
C	-2.753427	0.803507	-0.342711
C	-3.051599	2.132011	-0.981218
H	-3.981214	2.053870	-1.550517
H	-2.231088	2.456393	-1.625379
H	-3.180613	2.916889	-0.225797

C	-5.902909	-0.379744	0.105341
C	-7.303801	0.037325	-0.021907
C	-7.880176	1.203304	-0.443903
H	-7.331140	2.076948	-0.770501
C	-9.288121	1.014214	-0.351508
H	-10.068193	1.725912	-0.598930
C	-9.465085	-0.250147	0.120047
H	-10.337281	-0.844997	0.359613

14 (with conuterions K^+ or Na^+. Structure of the trianion was fully optimized without K+ or Na+. Then, alkali metal atoms were added to the indicated position without following optimization.)

V	-5.59382	-2.54087	0.18402	
N	-5.64103	-0.49052	0.94841	
O	-5.54292	-4.06112	0.71076	
C	-3.43176	0.15905	0.26230	
V	-2.43929	4.16659	0.24639	
N	-6.83227	-0.11780	1.54963	
O	-5.79090	-2.49298	-1.40664	
C	-2.98409	-1.17611	0.08075	
V	1.81592	-1.87441	-0.37004	
O	-3.72177	-2.18306	0.43499	
N	-0.75069	3.33888	-0.88098	
C	-1.65051	-1.44587	-0.37560	
O	-7.43827	-2.25358	0.91105	
N	0.12495	4.28569	-1.39320	
C	-0.76169	-0.35388	-0.57266	
C	-1.25564	0.99995	-0.60166	
N	0.05252	-3.12125	-0.71263	
O	-9.93295	-1.84575	1.94033	
N	0.33013	-4.45032	-0.99692	
C	-2.58701	1.23943	-0.16441	
O	-2.12444	4.05276	1.81436	
O	-3.82137	4.95417	-0.00545	
C	-4.69657	0.42800	0.91688	
O	-3.10682	2.42668	-0.21146	
C	-4.92346	1.73462	1.62249	
H	-5.38797	2.47148	0.95518	
H	-3.98264	2.17388	1.96286	
H	-5.59965	1.57017	2.46578	
C	-7.68072	-1.09967	1.42821	
O	-1.33917	5.72583	-0.33541	
C	-9.02569	-0.83145	1.94898	
C	-9.59696	0.29257	2.47746	
H	-9.09153	1.24261	2.59268	
O	1.67675	6.48085	-2.10345	
C	-10.93556	-0.05515	2.81461	

H	-11.69284	0.58360	3.25591	
O	0.49204	-0.54949	-0.79993	
C	-11.08079	-1.36279	2.46614	
H	-11.90208	-2.06584	2.52214	
O	2.99756	-1.19961	-1.23133	
O	2.07294	-1.69720	1.19973	
C	-0.43619	2.07817	-1.11809	
C	0.76059	1.77871	-1.97829	
H	0.97026	2.63519	-2.62142	
H	0.60424	0.87363	-2.56883	
H	1.64720	1.58138	-1.36321	
O	2.50278	-3.72492	-0.70416	
C	-0.27195	5.46416	-1.01673	
O	3.40483	-6.25959	-1.14524	
C	0.52425	6.63279	-1.39491	
C	0.30554	7.95834	-1.14673	
H	-0.54538	8.34641	-0.60234	
C	1.39310	8.66413	-1.73826	
H	1.56421	9.73506	-1.74238	
C	2.18912	7.71579	-2.30161	
H	3.11945	7.75235	-2.85415	
C	-1.22641	-2.79827	-0.67545	
C	-2.25132	-3.83681	-1.03947	
H	-1.80311	-4.55316	-1.73253	
H	-3.14108	-3.38009	-1.47895	
H	-2.59172	-4.38782	-0.15412	
C	1.61855	-4.63167	-0.93039	
C	2.06719	-6.01103	-1.15105	
C	1.38427	-7.17346	-1.37950	
H	0.30600	-7.25313	-1.42784	
C	2.36433	-8.19600	-1.52270	
H	2.19630	-9.25090	-1.71034	
C	3.56950	-7.58234	-1.37015	
H	4.59461	-7.92987	-1.38815	
Alkali metal	-3.02715	7.80880	-0.90072	
Alkali metal	-8.56484	-4.75049	0.76287	
Alkali metal	5.06124	-3.12006	0.06786	

17A

V	-1.468847	-3.931227	-0.516214
N	-2.734551	-2.406905	0.251774
O	-0.112939	-5.004089	0.111060
C	-1.226067	-0.528401	0.119719
V	-2.773837	3.289036	0.411815
N	-4.036878	-2.802126	0.549244
O	-1.269325	-3.624523	-2.049615
C	-0.067538	-1.345114	0.025323

V	4.255733	0.868897	0.642039
O	-0.147684	-2.623212	0.181056
N	-0.747545	3.735975	-0.287440
C	1.230863	-0.742466	-0.103654
O	-3.376093	-4.666013	-0.620571
N	-0.506540	5.077570	-0.547799
C	1.334127	0.676069	-0.062965
C	0.161425	1.508001	-0.183516
N	3.620758	-1.093029	-0.058085
O	-5.870269	-5.743809	-0.303060
N	4.657501	-1.990758	-0.276931
C	-1.112435	0.890227	-0.072171
O	-2.762339	3.120950	2.006530
O	-4.274057	3.195252	-0.165671
C	-2.487166	-1.123916	0.472330
O	-2.207413	1.566745	-0.222162
C	-3.541367	-0.299642	1.155875
H	-4.259224	0.108510	0.432922
H	-3.102260	0.552865	1.678524
H	-4.095566	-0.934914	1.851877
C	-4.247058	-3.966701	0.008905
O	-2.698014	5.265966	0.157748
C	-5.612510	-4.486698	0.148860
C	-6.751834	-3.942495	0.672351
H	-6.821386	-2.948142	1.094262
O	-0.411845	7.842321	-0.807598
C	-7.769655	-4.928299	0.535178
H	-8.808417	-4.852557	0.837436
O	2.481450	1.253911	0.007909
C	-7.176067	-5.996899	-0.063248
H	-7.529655	-6.970438	-0.377998
O	4.953023	2.142086	-0.053875
O	4.132220	1.063905	2.226662
C	0.279308	2.923624	-0.466952
C	1.561283	3.486565	-1.016099
H	1.348365	4.402808	-1.569903
H	2.074503	2.756507	-1.645522
H	2.264711	3.724903	-0.208678
O	5.921465	-0.239835	0.538618
C	-1.572963	5.756712	-0.249336
O	8.171924	-1.766720	0.309187
C	-1.544922	7.213480	-0.389937
C	-2.526179	8.135207	-0.158249
H	-3.525304	7.894583	0.180694
C	-1.959775	9.409737	-0.450456
H	-2.439005	10.380074	-0.379426

C	-0.678974	9.167256	-0.838830
H	0.140681	9.801124	-1.152555
C	2.409809	-1.553010	-0.317496
C	2.265929	-2.917858	-0.928689
H	3.151666	-3.136110	-1.530884
H	1.358898	-2.985272	-1.532899
H	2.181293	-3.693132	-0.157775
C	5.776185	-1.439744	0.098948
C	6.959954	-2.300849	-0.002658
C	7.114055	-3.609316	-0.367723
H	6.304032	-4.265648	-0.658152
C	8.506106	-3.893131	-0.275332
H	9.004144	-4.833383	-0.485666
C	9.095769	-2.738944	0.140176
H	10.117958	-2.456770	0.358071
O	-1.274680	-5.723524	-0.203411

17B

V	-1.824459	-3.812524	-0.499959
N	-2.982166	-2.185765	0.247483
O	-0.550778	-4.985646	0.116623
C	-1.325771	-0.437106	0.133893
V	-2.602846	3.491149	0.316301
N	-4.315726	-2.473739	0.524736
O	-1.593740	-3.501195	-2.028055
C	-0.239233	-1.344527	0.063900
V	4.164008	0.386565	0.924315
O	-0.415623	-2.611791	0.221069
N	-0.516670	3.774092	-0.308482
C	1.105599	-0.845536	-0.052268
O	-3.775881	-4.408011	-0.591499
N	-0.172812	5.091551	-0.576048
C	1.328677	0.561737	-0.004060
C	0.226751	1.486550	-0.148830
N	3.456865	-1.376602	-0.074737
O	-6.349329	-5.288562	-0.301347
N	4.430028	-2.293187	-0.422881
C	-1.093398	0.967527	-0.069011
O	-2.644710	3.379299	1.915052
O	-4.091690	3.473994	-0.296996
C	-2.637754	-0.926309	0.467224
O	-2.131608	1.719869	-0.252395
C	-3.632202	-0.015809	1.129127
H	-4.317925	0.425954	0.394806
H	-3.135855	0.813228	1.637403
H	-4.231665	-0.596520	1.835238
C	-4.604232	-3.629446	0.002106

O	-2.384939	5.442542	-0.010065
C	-6.008534	-4.039943	0.118486
C	-7.116950	-3.394370	0.590457
H	-7.123382	-2.383882	0.977884
O	0.115526	7.838203	-0.906119
C	-8.202934	-4.304893	0.453966
H	-9.240801	-4.139825	0.721638
O	2.522575	1.031673	0.082368
C	-7.676238	-5.434486	-0.092202
H	-8.093650	-6.389105	-0.386167
O	4.900219	1.763283	0.629403
O	3.275170	0.402148	2.505388
C	0.458189	2.888884	-0.428714
C	1.804857	3.355991	-0.907975
H	1.699416	4.317117	-1.413399
H	2.261073	2.614655	-1.568186
H	2.500312	3.471953	-0.068101
O	5.814827	-0.604423	0.313371
C	-1.206640	5.846746	-0.358790
O	7.992051	-2.179883	-0.184414
C	-1.076990	7.293519	-0.539317
C	-2.012540	8.279383	-0.400633
H	-3.043155	8.109221	-0.117984
C	-1.352610	9.506484	-0.700247
H	-1.775434	10.505176	-0.694533
C	-0.067637	9.174190	-0.999075
H	0.805954	9.746976	-1.283441
C	2.204670	-1.737853	-0.313590
C	1.948613	-3.068302	-0.962644
H	2.797890	-3.321608	-1.602447
H	1.018529	-3.062142	-1.534740
H	1.845580	-3.858747	-0.209546
C	5.598781	-1.787844	-0.140365
C	6.741857	-2.666624	-0.410076
C	6.824462	-3.949226	-0.876359
H	5.972499	-4.565943	-1.131732
C	8.210536	-4.267515	-0.938732
H	8.660304	-5.200506	-1.260505
C	8.868526	-3.157188	-0.507038
H	9.914172	-2.911496	-0.372083
O	-1.753957	-5.620943	-0.219748
O	4.551665	-0.219628	2.589227

17C

V	-1.897412	-3.858723	-0.502824
N	-3.001776	-2.191080	0.235485
O	-0.620321	-5.046784	0.077797

C	-1.306817	-0.482475	0.065126
V	-2.441365	3.560793	0.166554
N	-4.336959	-2.437809	0.540118
O	-1.710674	-3.566346	-2.040255
C	-0.240485	-1.415577	0.011831
V	4.198599	0.208362	0.928694
O	-0.446726	-2.676025	0.175583
N	-0.388859	3.710002	-0.403804
C	1.120691	-0.950712	-0.088713
O	-3.856125	-4.425187	-0.506992
N	0.072635	5.002952	-0.646159
C	1.376840	0.450029	-0.042514
C	0.296043	1.394180	-0.220629
N	3.460670	-1.533939	-0.075110
O	-6.448590	-5.229633	-0.156534
N	4.413972	-2.476842	-0.409823
C	-1.040347	0.916010	-0.152761
O	-2.449926	3.321733	1.724649
O	-4.022308	2.988430	-0.580013
C	-2.626138	-0.933515	0.415977
O	-2.041833	1.695710	-0.365942
C	-3.592434	0.018089	1.059734
H	-4.279256	0.448558	0.320397
H	-3.072035	0.854083	1.530944
H	-4.192903	-0.526616	1.793396
C	-4.659230	-3.605097	0.066929
O	-2.001018	5.542293	0.182128
C	-6.070061	-3.978077	0.219496
C	-7.153819	-3.290338	0.689088
H	-7.127538	-2.268510	1.044662
O	0.650259	7.718240	-0.828535
C	-8.264234	-4.176470	0.598162
H	-9.293016	-3.977057	0.877323
O	2.574681	0.897776	0.075973
C	-7.775368	-5.335354	0.078177
H	-8.221349	-6.288097	-0.177493
O	4.970729	1.560121	0.614065
O	3.298465	0.271897	2.502106
C	0.548814	2.774203	-0.528139
C	1.898329	3.194151	-1.044003
H	1.787560	4.064904	-1.692812
H	2.393322	2.372264	-1.562862
H	2.561196	3.472701	-0.214670
O	5.834138	-0.832351	0.356705
C	-0.836670	5.848793	-0.275045
O	7.973237	-2.468379	-0.117862

C	-0.560085	7.282812	-0.382279
C	-1.358727	8.352037	-0.093064
H	-2.372901	8.276395	0.276833
C	-0.590741	9.517840	-0.379394
H	-0.893064	10.553728	-0.271606
C	0.615236	9.069616	-0.821085
H	1.520528	9.561972	-1.152899
C	2.202238	-1.867751	-0.327314
C	1.925741	-3.196407	-0.971568
H	2.773858	-3.467798	-1.605383
H	0.999447	-3.175497	-1.548477
H	1.804780	-3.981510	-0.215591
C	5.591761	-2.006803	-0.106332
C	6.712643	-2.917455	-0.363094
C	6.764438	-4.199866	-0.834344
H	5.898728	-4.790851	-1.104092
C	8.141291	-4.558029	-0.879498
H	8.568029	-5.502100	-1.200276
C	8.825333	-3.469395	-0.433557
H	9.875718	-3.254723	-0.283305
O	-1.842608	-5.667284	-0.212643
O	4.556510	-0.382349	2.605597
O	-4.006670	4.369216	-0.342311

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V	2.945257	-1.239392	-1.122380
N	0.871009	-1.927204	-0.715300
O	4.438267	-0.292245	-0.652907
C	-0.171969	0.229666	-0.701102
N	0.688408	-3.289637	-0.677360
O	2.628166	-0.942242	-2.634790
C	1.048025	0.904974	-0.412136
O	2.166994	0.294543	-0.167532
C	1.023926	2.318974	-0.334510
O	2.970513	-3.249919	-0.964284
C	-0.122902	3.037167	-0.595107
C	-1.311685	2.376404	-0.930661
O	3.035192	-5.966593	-1.033303
C	-1.323391	0.995750	-0.966632
C	-0.224609	-1.217934	-0.661416
C	-1.546823	-1.921282	-0.551489
H	-1.831453	-2.363118	-1.516503
H	-2.342388	-1.249934	-0.217535
H	-1.458390	-2.756684	0.149327
C	1.855246	-3.863774	-0.841571
C	1.848886	-5.327211	-0.862876
C	0.841588	-6.241835	-0.742424

H	-0.203652	-6.000213	-0.599338
C	1.449551	-7.524084	-0.845389
H	0.965219	-8.491998	-0.796252
C	2.778923	-7.290320	-1.020923
H	3.638816	-7.934445	-1.147994
O	4.727398	-1.619361	-0.997677
H	1.964652	2.807218	-0.086033
H	-0.099900	4.126732	-0.550173
H	-2.215319	2.939171	-1.160562
H	-2.248736	0.486603	-1.234141