Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Electronic Supplementary Information

Table S1. More relevant geometrical calculated parameters for [VO(oVATPNH2)$_2$

Bond distance (Å)		**Dihedral angle (º)**	
C5-N	1.484	C5-N-V-O1	-179.2
N-V	2.140	C5'-N'-V-O1'	-170.3
O1-C8	1.314	C5-N-V-O1'	-56.9
V-O1	1.912	C5'-N'-V-O1	-47.5
N-C6	1.286	C5-N-C6-C7	178.9
V-O3	1.603	C5'-N'-C6'-C7'	174.3
Bond angle (º)		C1-C5-N-C6	-11.6
C5-N-V	114.6	C1'-C5'-N'-C6'	123.0
C6-N-V	125.1	C1-C5-N-V	173.7
O1-V-N	86.6	C1'-C5'-N'-V	-64.3
O1-V-N'	85.8	C8-O1-V-N	-2.3
N-V-N'	163.6	C8'-O1'-V-N'	-5.6
O1-V-O1'	122.1	C8-O1-V-N'	-171.0
O3-V-O1	119.8	C8'-O1'-V-N	-169.5
O3-V-N	98.0	C6-N-V-O1	6.4
C8-O1-V	135.2	C6'-N'-V-O1'	1.7
C1-C5-N	115.8	C6-N-V-O1'	128.7
C5-N-C6	118.0	C6'-N'-V-O1	124.6
N-C6-C7	127.4	C5-N-V-O3	58.2
		S-C1-C5-N	105.0
		S'-C1'-C5'-N'	-105.8
		C13-O2- C9-C8	-175.3
		C13'-O2'-C9'-C8'	176.0

Table S2. Vibrational spectra of [VO(oVATPNH2)$_2$]. Assignment and comparison with the free ligand (oVATPNH2) data (wavenumbers in cm^{-1}

oVATPNH2 (a)				**VO(oVATPNH2)$_2$**			
IR.	**Raman**	**Calc**	**Assignment**	**IR**	**Raman**	**Calc.**	**Assignment**
3003 vw	3005 w	3153	ν O-H				
2923 sh	2928 m	3045	ν_{as} CH_2	2917 sh		3114/3093	ν_{as} CH_2
1631 vs	1635 vs	1685	ν C=N	1613 vs	1621 vs	1677/1671	ν C=N
1583 sh	1587 m	1660 1618	ν ring (oVA) + δ O-H	1601 sh 1555 m	1558 s	1639/1636	ν ring (oVA)
1462 vs	1472 m	1505	δ_{as} CH_3	1469 s	1474 s	1505	δ_{as} CH_3
	1440 m	1493	δ_{as} CH_3	1452 s,b	1444 vs	1491	δ_{as} CH_3
1415 m,b		1480	δ CH_2	1404 m		1498	δ CH_2
		1460	δ O-H + δ_s CH_3 + δ C-H(oVA)			1477/1471	ν coord. ring + δ CH_2
						1475/1475	δ_s CH_3
				1362 vw	1348 s	1393/1390	ρ_w CH_2 + δ CH (Tph) + δ C-H (Ar-CH)
1333 m-w	1337 s	1355	ρ_w CH_2	1334 m,b		1383/1382	ν ring (oVa) + $\rho_w CH_2$ + δ C-H (Ar-CH)
						1373	ρ_w CH_2
1313 m		1315	ν C-O (ArOH) + δ C-H (oVA)	1301 s,b	1312 m	1370/1349	ν C-O (Ar-O) + δ C-H (Ar-CH) + ρ_w CH_2
						1335	ν C-O(Ar-O) + ρ_w CH_2
1269 s		1286	δ C-H (Tph) + ρ_r CH_2		1272 vw	1307/1301	δ CH (Tph) + ρ_r CH_2
1255 vs	1258 vw	1282	ν C-OCH_3 + δ C-H (oVA)	1247 s,b		1276/1275	ν C-OCH_3 + δ CH (oVa)
1242 sh	1229 m	1168	ν C-CH_2	1226 m,b	1229 m-s	1157/1156	ν C-CH_2
1081 m-s	1088 m	1129	ν O-CH_3 + δ ring (oVA)	1080 m	1083 w	1112/1109	ν O-CH_3 + δ CH (oVa)
				993, m,b	992 mw	1054	ν V=O
853 mw	856 vw	842	γ C-H (Tph)	865 m,s 853 w	859 vw	855	γ C-H (Tph)
832 ms,b	838 w	851	γ O-H				
750 mw	757 w	762	ν S-CH + δ C-C-C(CH_2)	757 w	760 m	751/753	ν S-CH + δ ring(oVa)
736 s	735 m	740	γ C-H (oVA)	742 m	743 w	748	γ C-H (oVA)
725 s		742	δ ring (oVA)	717 m 694 sh	695 vw	764	δ ring [oVA + Tph]
615 vw	620 m	627	δ ring [oVA + Tph]	617 w		625	δ ring [oVA + Tph]
				611 sh	602 m	612	+ δ coord ring
						587	ν_{as} O-V-O + γring (Tph) + γ ring (oVA)
						581	ν_s O-V-O + δ Ar-O-CH_3 + γ ring (Tph)
				461 w,b	467 sh	460/443	ν_{as} N-V-N
					444 w	464/455	ν_s N-V-N

(a) Data extracted from ref [21]. vs: very strong, s: strong, m: medium, w: weak, vw: very weak, b: broad, sh: shoulder: Tph: thiophene ring.

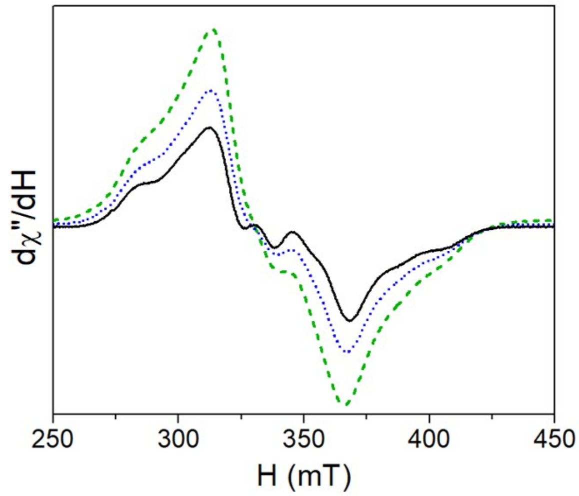

Figure S1. EPR spectra of $[VO(oVATPNH_2)_2]$ (**III**) at different temperatures: 298 K (solid line), 200 K (dotted line) and 120 K (dashed line). Experimental details: modulation frequency = 100 kHz, modulation amplitude = 0.1 mT, time constant = 40.96 ms, conversion time = 81.92 ms, gain = 6,3 x 10^4, power = 2.0 mW, microwave frequency = 9.4223 (298 K), 9.4225 (200 K) and 9.4258 GHz (120 K).

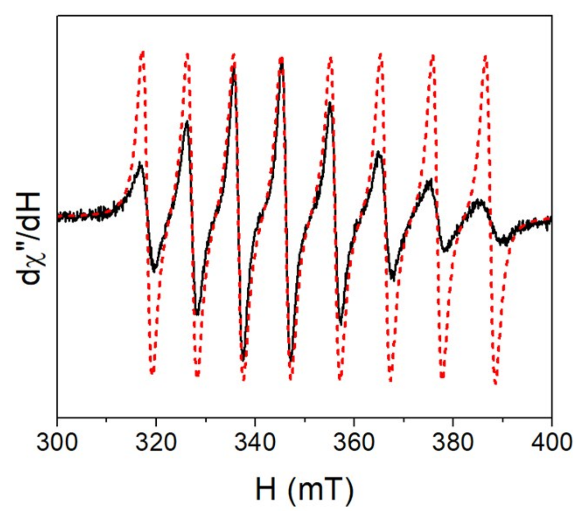

Figure S2. EPR spectrum of $[VO(oVATPNH_2)_2]$ (**III**)solution in a (1:1) (ethanol:DMF) at 298 K (solid line) together with the best fit (dashed line). Experimental details: modulation frequency = 100 kHz, modulation amplitude = 0.1 mT, time constant = 40.96 ms, conversion time = 327.68 ms, gain = 6,3 10^4, power = 20.0 mW, microwave frequency = 9.7624 GHz. Fitting parameters: (a) Lorentzian-type signal, g_{iso} = 1.974; A_{iso} = 9.9 mT (91.2 10^{-4} cm^{-1}) (linewidth H_{iso} = 2.0 mT).

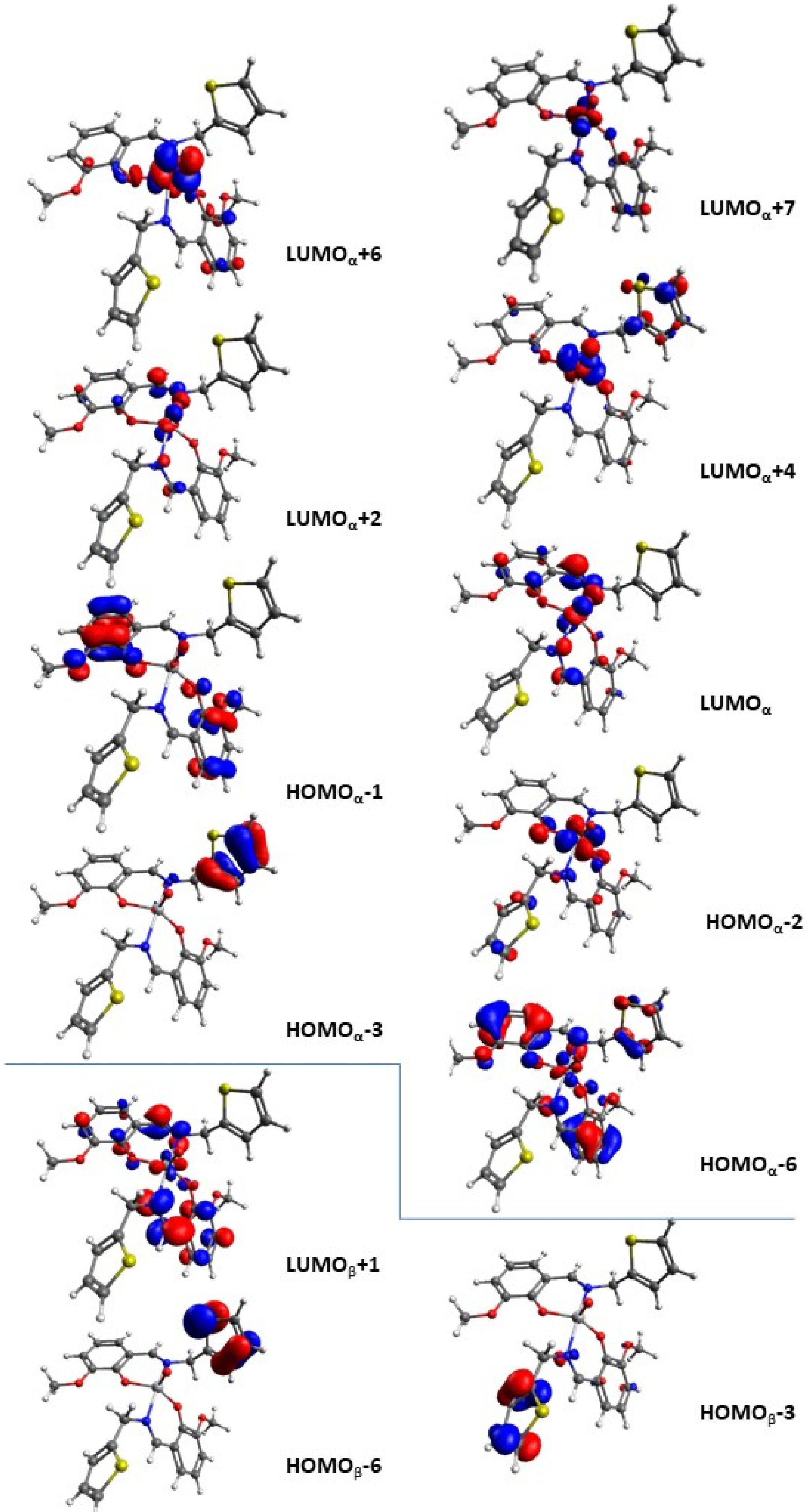

Figure S3. Molecular orbitals involved in the electronic transitions of $[VO(oVATPNH2)_2]$

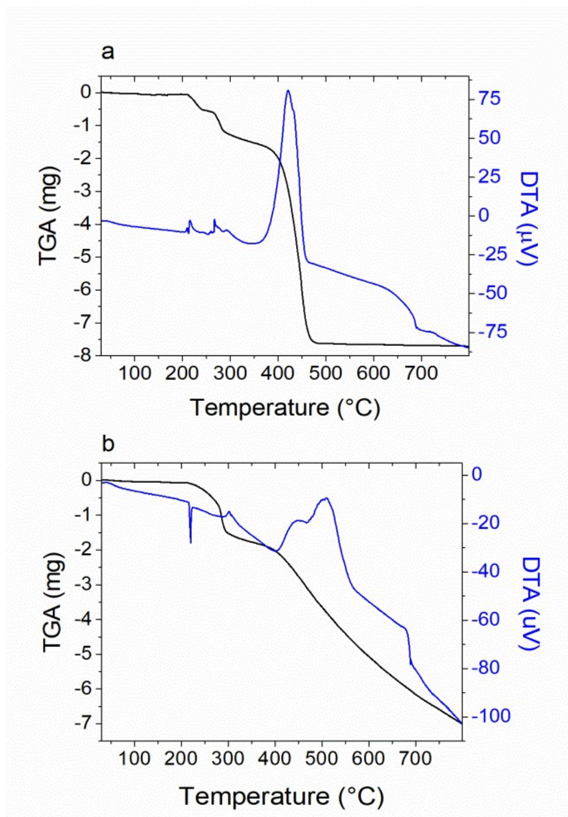

Figure S4. Thermal analysis of the solid complex [VO(oVATPNH2)$_2$] **a**. in oxygen **b**. in nitrogen atmosphere.

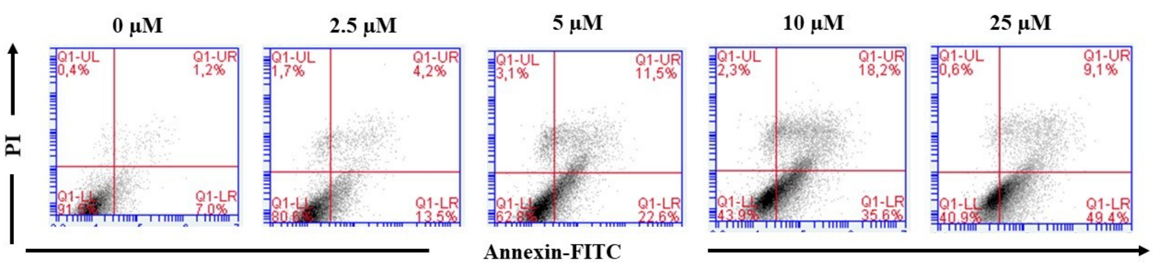

Figure S5. Effect of VO(oVATPNH2)$_2$]. On apoptosis assessed by flow cytometry using annexin V– fluorescein isothiocyanate (FITC)/propidium iodide (PI) staining. The plots are representative of three independent experiments. The numbers in the Q1LR and Q1UR quadrants indicate the proportions of cells that are annexin V positive/PI negative and annexin V positive /PI positive, respectively