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SUPPLEMENTARY MATERIAL TO

Oxovanadium(IV) complexes of the pyridoxal Schiff bases: Synthesis, experimental and theoretical characterizations, QTAIM analysis and antioxidant activity

PARISA GHORBANI[1], S. ALI BEYRAMABADI[2]*, MASOUD HOMAYOUNI-TABRIZI[3]** and PARICHEHREH YAGHMAEI[1]

[1]Department of Biology, Science and Research Branch, Islamic Azad University, Tehran, Iran, [2]Department of Chemistry, Mashhad Branch, Islamic Azad University, Mashhad, Iran and [3]Department of Biology, Mashhad Branch, Islamic Azad University, Mashhad, Iran

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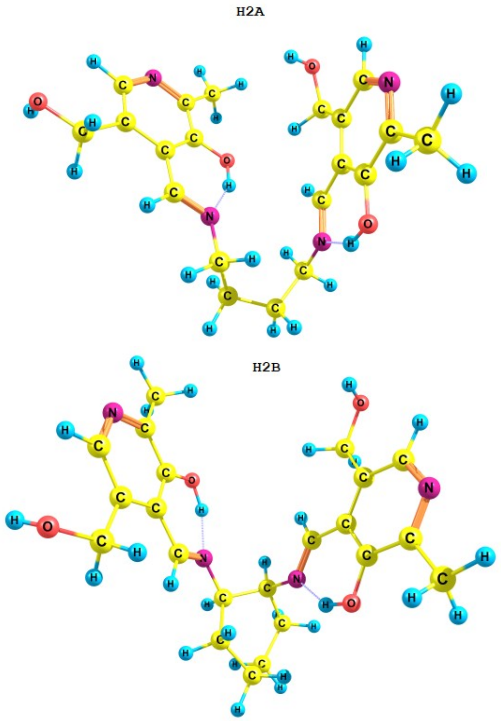

Fig. S-1. Optimized geometries of the H_2A and H_2B Schiff bases.

*,** Corresponding authors. E-mail: (*)beiramabadi@yahoo.com, beiramabadi6285@mshdiau.ac.ir; (**)mmhomayouni6@gmail.com

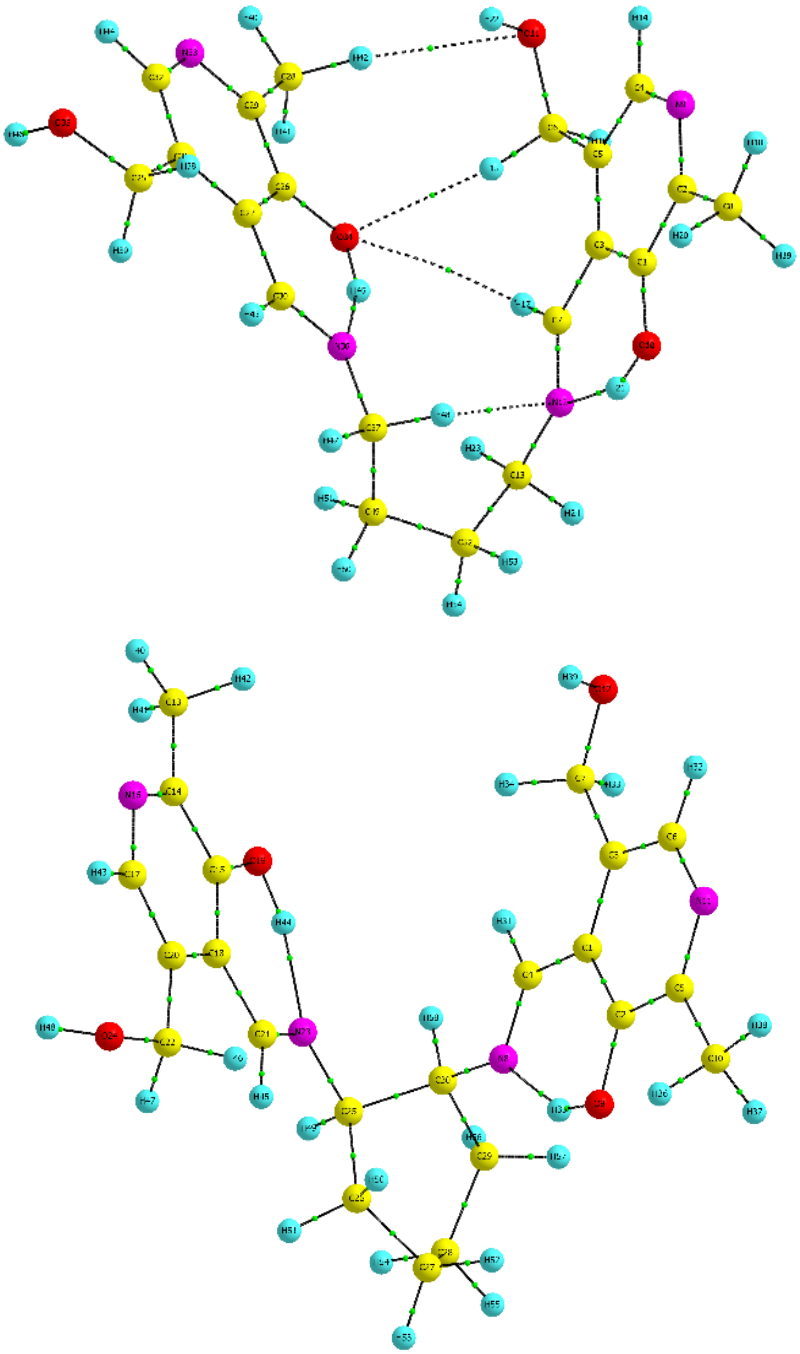

Fig. S-2. QTAIM molecular graph of the **H_2A** and **H_2B** Schiff bases. Small green spheres and lines correspond to the bond critical points (BCP) and the bond paths, respectively.

TABLE S-I. Selected experimental and theoretical IR vibrational frequencies (cm^{-1}) and their computed intensity (km mol^{-1}) for the [VO(**A**)] and [VO(**B**)] complexes

[VO(**A**)]			[VO(**B**)]			Vibrational assignment
Exp.	Theo.		Exp.	Theo.		
	Frequency	IR Intensity		Frequency	IR Intensity	
542 (w)	511	39	556 (w)	539	61	υ_{asym}(N2–V–N4)
646 (w)	601	88	616 (m)	621	7	υ_{asym}(O1–V–O2)
	619	18		637	11	υ_{sym}(O1–V–O2)+ υ_{sym}(N2–V–N4)
745 (w)	727	51	759 (w)	739	39	Breathing of the pyridine ring
974 (m)	979	88	970 (m)	977	92	υ_{sym}(C5–C16–O4, C11–C13–O3)
1023 (m)	1006	19	1058 (vs)	1005	35	υ(C17–N2, C19–N4)
	1013	106		1021	170	υ(V–O5)
	1031	108		1033	118	υ(C16–O4, C13–O3)
	1075	27		1072	42	υ_{asym}(C5–C16–O4, C11–C13–O3)
	–	–		1063	23	υ(C–C) cyclohexane ring
1189 (m)	1176, 1152	128, 142	1133 (s, sh)	1175	183	υ(C=C, C=N) of the pyridine ring
1265 (m)	1242	57		1240	64	δ_{ip}(H1, H4) pyridine ring
	1294	172		1300	180	υ(py–C)
	1329	28	1324 (m)	1323	42	$\delta_{wag}(CH_2)$ cyclohexane ring
1390 (vs)	1353	49	1386 (s)	1353	67	$\delta(CH_3)$ Methyl
	1400, 1383	118, 323		1400, 1388, 1378	103, 149, 246	υ(C1–O1, C7–O2)
	–	–		1438	11	$\delta_{sci}(CH_2)$ cyclohexane ring
1512 (s)	1449	93		–	–	$\delta_{sci}(CH_2)$ butane bridge
	1551–1489	10–86	1545 (m)	1552–1490	19–108	υ(C=C, C=N) of the pyridine rings
1609 (s)	1578	500	1633 (s)	1586	585	υ(C10–N4)
	1595	260		1601	250	υ(C6–N2)
2856 (m)	2847	49	2851 (m, br)	2844	58	$\upsilon_{sym}(CH_2)$ of $-CH_2OH$
	2868	34		2867	35	$\upsilon_{asym}(CH_2)$ of $-CH_2OH$
	–	–		2906–2894	38–18	$\upsilon_{sym}(CH_2)$ cyclohexane ring
2925 (s)	2893	13	2938 (vs, br)	–	–	$\upsilon_{sym}(CH_2)$ butane bridge
	2917	14		2914	19	υ_{sym}(CH) methyl
	–	–		2953–2946	42–54	$\upsilon_{asym}(CH_2)$ cyclohexane ring
	2958–2933	21–48		–	–	$\upsilon_{asym}(CH_2)$ butane bridge
3163 (s,br)	2966			3009	20	υ(C6–H2, C10–H3)
	3014, 2961	15, 14		3015, 2961	15, 18	υ_{asym}(CH) methyl
3468 (s)	3089	2	3416 (s)	3090	2	υ(C4–H1, C12–H4) aromatic
	3708	64		3709	60	υ(O–H) of $-CH_2OH$

Abbreviation: wag, wagging; sci, scissoring; sym, symmetric; asym, asymmetric; ip, in–plane; w, weak; m, medium; s, strong; vs, very strong; sh, shoulder; br, broad.

TABLE S-II. The DPPH and ABTS radical scavenging activities (%) of the [VO(A)] and [VO(B)] complexes together with the BHA.

Concentration (**μg/mL**)	62.5	125	250	500
DPPH radical				
BHA	76.0	81.4	85.9	95.3
[VO(**A**)]	76.0	82.2	87.7	93.8
[VO(**B**)]	81.9	88.1	95.7	97.5
ABTS radical				
BHA	81.7	96.1	93.2	96.1
[VO(**A**)]	85.0	87.2	94.3	97.0
[VO(**B**)]	87.9	92.1	95.5	97.8