SUPPLEMENTARY MATERIAL TO

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

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**Figure S1.** Optimized geometries of the **H2A** and **H2B** Schiff bases.

 

**Figure S2.** QTAIM molecular graph of the **H2A** and **H2B** Schiff bases. Small green spheres and lines correspond to the bond critical points (BCP) and the bond paths, respectively.

**Table S1**. 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 | υasym(N2-V-N4) |
| 646 (w) | 601 | 88 | 616 (m) | 621 | 7 | υasym(O1-V-O2) |
| 619 | 18 | 637 | 11 | υsym(O1-V-O2)+ υsym(N2-V-N4) |
| 745 (w) | 727 | 51 | 759 (w) | 739 | 39 | Breathing of the pyridine ring |
| 974 (m) | 979 | 88 | 970 (m) | 977 | 92 | υsym(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 | υasym(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 | δip(H1, H4) pyridine ring |
| 1294 | 172 | 1324 (m) | 1300 | 180 | υ(py-C) |
|  | 1329 | 28 | 1323 | 42 | δwag(CH2) cyclohexane ring |
| 1390 (vs) | 1353 | 49 | 1353 | 67 | δ(CH3) Methyl |
| 1400, 1383 | 118, 323 | 1386 (s) | 1400, 1388, 1378 | 103, 149, 246 | υ(C1-O1, C7-O2) |
|  | - | - |  | 1438 | 11 | δsci(CH2) cyclohexane ring |
| 1512 (s) | 1449 | 93 |  | - | - | δsci(CH2) 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 | υsym(CH2) of –CH2OH |
| 2868 | 34 | 2867 | 35 | υasym(CH2) of –CH2OH |
|  | - | - | 2906-2894 | 38-18 | υsym(CH2) cyclohexane ring |
| 2925 (s) | 2893 | 13 |  | - | - | υsym(CH2) butane bridge |
| 2917 | 14 | 2938 (vs,br) | 2914 | 19 | υsym(CH) methyl |
| - | - | 2953-2946 | 42-54 | υasym(CH2) cyclohexane ring |
| 2958-2933 | 21-48 | - | - | υasym(CH2) butane bridge |
| 3163 (s,br) | 2966 |  | 3009 | 20 | υ(C6-H2, C10-H3) |
| 3014, 2961 | 15, 14 | 3015, 2961 | 15, 18 | υasym(CH) methyl |
| 3468 (s) | 3089 | 2 | 3416 (s) | 3090 | 2 | υ(C4-H1, C12-H4) aromatic |
| 3708 | 64 | 3709 | 60 | υ(O-H) of –CH2OH |

*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 S2.** The DPPH and ABTS radicals 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 |