

## New Phenoxy Radical Complexes of Manganese, Gallium, Indium and Iron Based on an H<sub>2</sub>bbpen Ligand Derivative

*Ademir dos Anjos,<sup>a</sup> Adailton J. Bortoluzzi,<sup>a</sup> Miguel S. B. Caro,<sup>a</sup> Rosely A. Peralta,<sup>a</sup>  
 Geraldo R. Friedermann,<sup>b</sup> Antonio S. Mangrich<sup>b</sup> and Ademir Neves<sup>\*,a</sup>*

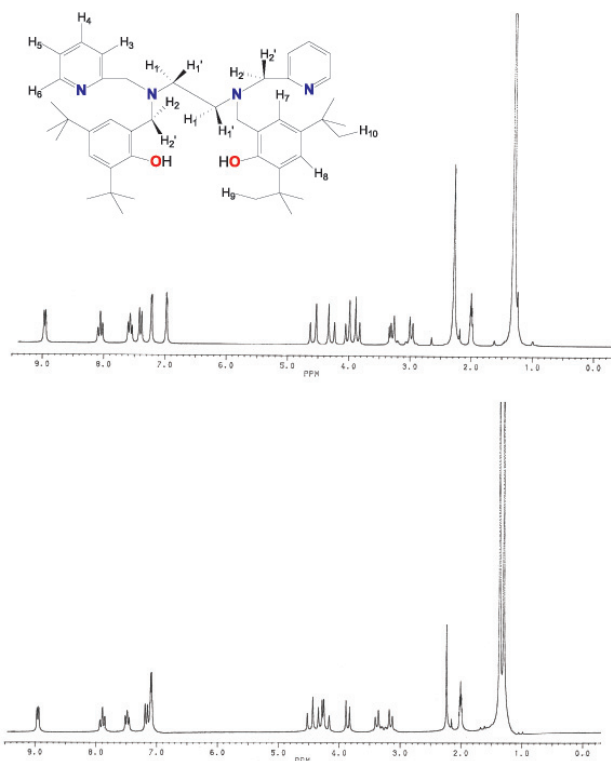
<sup>a</sup>*LABINC, Departamento de Química, Universidade Federal de Santa Catarina,  
 88040-900 Florianópolis-SC, Brazil*

<sup>b</sup>*LABEPR, Departamento de Química, Universidade Federal do Paraná,  
 81531-970 Curitiba-PR, Brazil*

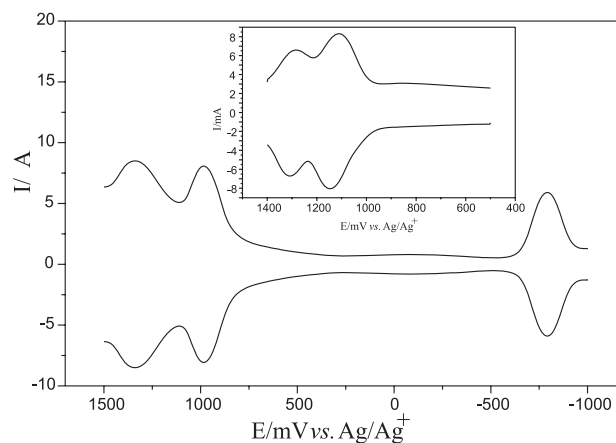
**Table S1.** <sup>1</sup>H NMR chemical shifts (ppm), assignments and multiplicity for complex **2** and **3** in CD<sub>3</sub>CN

Complex 2			Complex 3		
Chem. Shift	Mult.	Assign.	Chem. shift	Mult.	Assign.
8.95	d ( <sup>3</sup> J <sub>H6/H5</sub> 5.4 Hz)	2H <sub>6</sub>	8.94	d ( <sup>3</sup> J <sub>H6/H5</sub> 5.2 Hz)	2H <sub>6</sub>
8.05	dd ( <sup>3</sup> J <sub>H4/H5</sub> 7.9 Hz, <sup>3</sup> J <sub>H4/H3</sub> 7.9 Hz)	2H <sub>4</sub>	7.89	dd ( <sup>3</sup> J <sub>H4/H5</sub> 7.8 Hz, <sup>3</sup> J <sub>H4/H3</sub> 7.8 Hz)	2H <sub>4</sub>
7.56	dd ( <sup>3</sup> J <sub>H5/H6</sub> 6.3 Hz, <sup>3</sup> J <sub>H5/H4</sub> 6.3 Hz)	2H <sub>5</sub>	7.48	dd ( <sup>3</sup> J <sub>H5/H6</sub> 6.2 Hz, <sup>3</sup> J <sub>H5/H4</sub> 6.2 Hz)	2H <sub>5</sub>
7.40	d ( <sup>3</sup> J <sub>H3/H4</sub> 7.9 Hz)	2H <sub>3</sub>	7.16	d ( <sup>3</sup> J <sub>H3/H4</sub> 7.9 Hz)	2H <sub>3</sub>
7.22	d ( <sup>4</sup> J <sub>H8/H7</sub> 2.2 Hz)	2H <sub>8</sub>	7.10-7.07	m	2H <sub>8</sub> 2H <sub>7</sub>
6.97	d ( <sup>4</sup> J <sub>H7/H8</sub> 2.2 Hz)	2H <sub>7</sub>	4.47	d ( <sup>2</sup> J 18 Hz)	2H <sub>2py</sub>
4.57	d ( <sup>2</sup> J 19 Hz)	2H <sub>2py</sub>	4.31	d ( <sup>2</sup> J 12 Hz)	2H <sub>2ph</sub>
4.27	d ( <sup>2</sup> J 19 Hz)	2H <sub>2py</sub>	4.20	d ( <sup>2</sup> J 18 Hz)	2H <sub>2py</sub>
4.02	d ( <sup>2</sup> J 13 Hz)	2H <sub>2ph</sub>	3.85	d ( <sup>2</sup> J 12 Hz)	2H <sub>2ph</sub>
3.85	d ( <sup>2</sup> J 13 Hz)	2H <sub>2ph</sub>	3.35	d ( <sup>2</sup> J 10.4 Hz)	2H <sub>1</sub>
3.27	d ( <sup>2</sup> J 10 Hz)	2H <sub>1</sub>	3.15	d ( <sup>2</sup> J 10.4 Hz)	2H <sub>1</sub>
2.96	d ( <sup>2</sup> J 10 Hz)	2H <sub>1'</sub>	1.36	s	18H <sub>9</sub>

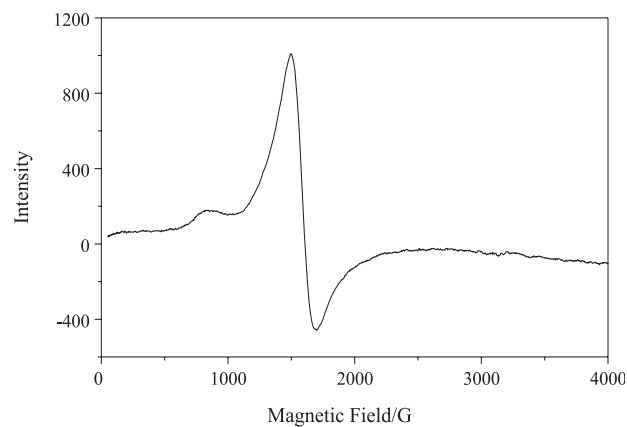
\*e-mail: ademir@qmc.ufsc.br



**Figure S1.**  $^1\text{H}$  NMR spectra of complex 2 (top) and complex 3 (bottom) in  $\text{CD}_3\text{CN}$ . Inset: schematic representation for  $^1\text{H}$  NMR interpretation.



**Figure S2.** Square wave voltammogram of complex 4 in  $\text{CH}_2\text{Cl}_2$  ( $0.1 \text{ mol dm}^{-3}$   $[(\text{TBA})\text{PF}_6]$ ); glass carbon working electrode. Conditions: see Table 4. Inset square wave voltammogram of complex 3.



**Figure S3.** X-band EPR spectrum of complex 4 in  $\text{CH}_2\text{Cl}_2$  at 77K.