Electronic Supplementary Data

Crystal structure, configurational and DFT study of nickel(II) complexes with N$_2$O-donor type Schiff base ligand

Yogendra Pratap Singh, Ram N Patel* & Yogendra Singh
Department of Chemistry, APS University, Rewa (MP) 486 003, India
Email: rnp64@ymail.com

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Fig. S1 – IR spectrum of complex (1)

Fig. S2 – IR spectrum of complex (2)
Fig. S3 – Selected molecular orbital excitation of complex (1) and their HOMO- LUMO energy level diagram.

Fig. S4 – Selected molecular orbital excitation of complex (2) and their HOMO- LUMO energy level diagram.
Table S1 – TD-DFT calculated excitations approximate assignments of nickel(II) complexes (1) and (2)

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<tr>
<th>$E$ (eV)</th>
<th>Wavelength (nm)</th>
<th>Oscillator strength ($f$)</th>
<th>Major contribution</th>
<th>Expt wavelength (nm)</th>
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<tr>
<td>Complex (1)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.6984</td>
<td>1229</td>
<td>0.0000</td>
<td>βHOMO-1→βLUMO+1 (23%)</td>
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</tr>
<tr>
<td>1.0109</td>
<td>1036</td>
<td>0.0001</td>
<td>βHOMO→βLUMO+1 (18%)</td>
<td>998</td>
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<tr>
<td>1.2336</td>
<td>857</td>
<td>0.0020</td>
<td>βHOMO-1→βLUMO (44%)</td>
<td>790</td>
</tr>
<tr>
<td>1.4211</td>
<td>761</td>
<td>0.0041</td>
<td>βHOMO→βLUMO (14%)</td>
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<tr>
<td>1.5625</td>
<td>628</td>
<td>0.0005</td>
<td>βHOMO→βLUMO+1 (32%)</td>
<td>620</td>
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<tr>
<td>1.7708</td>
<td>458</td>
<td>0.0027</td>
<td>βHOMO→βLUMO+2 (45%)</td>
<td>382</td>
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<tr>
<td>Complex (2)</td>
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<tr>
<td>0.3933</td>
<td>1187</td>
<td>0.0005</td>
<td>βHOMO→βLUMO (87%)</td>
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<tr>
<td>1.0071</td>
<td>1031</td>
<td>0.0002</td>
<td>βHOMO-1→βLUMO+1 (51%)</td>
<td>998</td>
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<tr>
<td>1.3410</td>
<td>824</td>
<td>0.0007</td>
<td>βHOMO→βLUMO+2 (48%)</td>
<td>790</td>
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<td>1.4270</td>
<td>768</td>
<td>0.0003</td>
<td>βHOMO→βLUMO+3 (15%)</td>
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<tr>
<td>1.6624</td>
<td>745</td>
<td>0.0003</td>
<td>βHOMO-1→βLUMO+1(4%)</td>
<td>621</td>
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<td>1.8195</td>
<td>428</td>
<td>0.0115</td>
<td>βHOMO→βLUMO+2 (94%)</td>
<td>381</td>
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Fig. S5 – Optimized structure of complexes (1) and (2)