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	<p>the peak corresponding to the fragment <math>2[M-6H_2O-H]^+</math>, relative abundance= 62%. Here M represents the formula of <b>3</b>.</p> <p><b>Figure V-10.</b> The calculated isotope patterns of <b>2</b> &amp; <b>3</b>: (a) for the peak at <math>m/z = 352</math> corresponding to the fragment <math>[M-6H_2O]^+</math>; (b) <math>m/z = 458</math> for the peak corresponding to the fragment <math>[M-2H]^+</math>; (c) <math>m/z = 702</math> for the peak corresponding to the fragment <math>2[M-6H_2O-H]^+</math>. Here M has the usual meaning.</p> <p><b>Figure V-11.</b> IR spectrum (KBr) of <math>H_2L \cdot 1.5H_2O</math> (<b>1</b>)</p> <p><b>Figure V-12.</b> IR spectrum (KBr) of <b>2</b></p> <p><b>Figure V-13.</b> IR spectrum (KBr) of <b>3</b></p> <p><b>Figure V-14.</b> Fluorescence emission spectra of <b>2</b> (<math>CH_3OH</math>, <math>1.1 \times 10^{-3} M</math>), <b>2R</b> (<math>CH_3OH</math>, <math>1.4 \times 10^{-3} M</math>).</p> <p><b>Figure V-15.</b> Fluorescence emission spectra of <b>3</b> (<math>CH_3OH</math>, <math>5.8 \times 10^{-4} M</math>), <b>3R</b> (<math>CH_3OH</math>, <math>5.8 \times 10^{-4} M</math>).</p> <p><b>Figure IV-16.</b> CD spectral data in <math>CH_3OH</math> of (a) <b>2</b> (<math>1.3 \times 10^{-3} M</math>); (b) <b>3</b> (<math>1.1 \times 10^{-3} M</math>).</p> <p><b>Figure V-17.</b> Cyclic voltammetry data of <b>2</b> in DMSO (0.1M TBAP; scan rate, <math>100 mV s^{-1}</math>).</p> <p><b>Figure V-18.</b> Cyclic voltammetry data of <b>3</b> in DMSO (0.1M TBAP; scan rate, <math>100 mV s^{-1}</math>).</p> <p><b>Figure V-19.</b> Absorption spectral changes recorded at 2 min interval during the reaction of (<b>2</b>) (<math>5.8 \times 10^{-5} M</math>) with Im (<math>4.8 \times 10^{-3} M</math>) in <math>CH_3OH</math> at 311K</p> <p><b>Figure V-20.</b> Absorption spectral changes recorded at 4.5 min interval during the reaction of (<b>3</b>) (<math>4.8 \times 10^{-5} M</math>) with Im (<math>4.68 \times 10^{-3} M</math>) in <math>CH_3OH</math> at 313K</p> <p><b>Figure V-21.</b> Absorption spectral changes recorded at 1.5 min interval during the reaction of (<b>2</b>) (<math>3.5 \times 10^{-5} M</math>) with <math>NaBH_4</math> (<math>2.35 \times 10^{-3} M</math>) in <math>CH_3OH</math></p> <p><b>Figure V-22.</b> Absorption spectral changes recorded at 1.5 min interval during the reaction of <b>3</b> (<math>4.8 \times 10^{-5} M</math>) with <math>NaBH_4</math> (<math>2.55 \times 10^{-3} M</math>) in <math>CH_3OH</math>.</p> <p><b>Figure V-23.</b> Absorption spectral changes recorded at 15 second interval during the reaction of <b>2R</b> (<math>3.5 \times 10^{-5} M</math>) with <math>K_3Fe(CN)_6</math> (<math>3.68 \times 10^{-3} M</math>) in <math>CH_3OH</math> at 298K.</p> <p><b>Figure V-24.</b> Absorption spectral changes recorded at 15 second interval during the reaction of <b>3R</b> (<math>4.8 \times 10^{-5} M</math>) with <math>K_3Fe(CN)_6</math> (<math>2.68 \times 10^{-3} M</math>) in <math>CH_3OH</math> at 298K.</p> <p><b>Figure V-25.</b> Absorption spectral changes recorded at 2 min interval at 303K during the reaction of (<b>2R</b>) (<math>3.5 \times 10^{-5} M</math>) with bromobenzene (<math>3.54 \times 10^{-3} M</math>) in <math>CH_3OH</math> saturated with <math>O_2</math>.</p> <p><b>Figure V-26.</b> Frontier molecular orbitals of <b>2</b> and <b>3</b>, showing their energies (eV) and compositions (%).</p>
Chapter VI	<p><b>Figure VI-1.</b> ORTEP diagram of the complex <b>1</b> with atom numbering scheme (40% probability factor for the thermal ellipsoids); lattice water molecules are omitted for clarity.</p> <p><b>Figure VI-2.</b> Unit cell packing diagram of <b>1</b> viewed along plane 1 0 0.</p> <p><b>Figure VI-3.</b> DFT optimized molecular structure of the compound <b>1</b>.</p> <p><b>Figure VI-4.</b> DFT optimized molecular structure of the compound <b>2</b></p> <p><b>Figure VI-5.</b> DFT optimized molecular structure of the compound <b>3</b>.</p> <p><b>Figure VI-6.</b> DFT optimized molecular structure of the compound <b>4</b>.</p>



<p><b>Figure VI-7.</b> (a) ESIMS data of <b>2</b>; (b) the calculated isotope pattern for the base peak at <math>m/z = 435</math> corresponding to the fragment <math>[\text{Co}(\text{L})(\text{bipy})]^+</math> and (c) for the peak <math>m/z = 391</math> corresponding to the fragment <math>[\text{Co}(\text{L})(\text{bipy}) - \text{CO}_2]^+</math>.</p>
<p><b>Figure VI-8.</b> (a) and (b) ESIMS data of <b>3</b>; (c) the calculated isotope pattern for the base peak at <math>m/z = 434</math> corresponds to the fragment <math>[\text{Ni}(\text{L})(\text{bipy})]^+</math> and (d) for the calculated peak <math>m/z = 390</math> corresponding the fragment <math>[\text{Ni}(\text{L})(\text{bipy}) - \text{CO}_2]^+</math>.</p>
<p><b>Figure VI-9.</b> (a) ESIMS data of <b>4</b>; (b) the calculated isotope pattern for the base peak at <math>m/z = 438.9</math> corresponding to the fragment <math>[\text{Cu}(\text{L})(\text{bipy})]^+</math>.</p>
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<p><b>Figure VI-19.</b> Fluorescence emission spectra of <b>3</b> in DMSO.</p>
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<p><b>Figure VI-24.</b> 300 MHz <math>^1\text{H}</math> NMR spectrum of <b>1</b> in DMSO-<math>d_6</math>. Expansion of the region <math>\delta 2.5-0.7</math> of Figure VI - 23 is shown pterin ligand and a coordinated DMSO molecule.</p>
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## **LIST OF APPENDICES**

- Appendix A:** List of Publications
- Appendix B:** List of Seminars/Symposium participated
- Appendix C:** Published papers