

## **Supplementary Figure Captions:**

Figure S1: <sup>1</sup>H NMR of Mo[L<sup>a</sup>]<sub>2</sub> in CDCl<sub>3</sub>.

**Figure S2:** <sup>13</sup>C NMR of Mo[L<sup>a</sup>]<sub>2</sub> in CDCl<sub>3</sub>.

**Figure S3:** Molecular orbital diagrams of Mo[L<sup>a</sup>]<sub>2</sub>: (i) HOMO-1, (ii) HOMO, (iii) LUMO,

(iv)LUMO+1, and (v)LUMO+2.

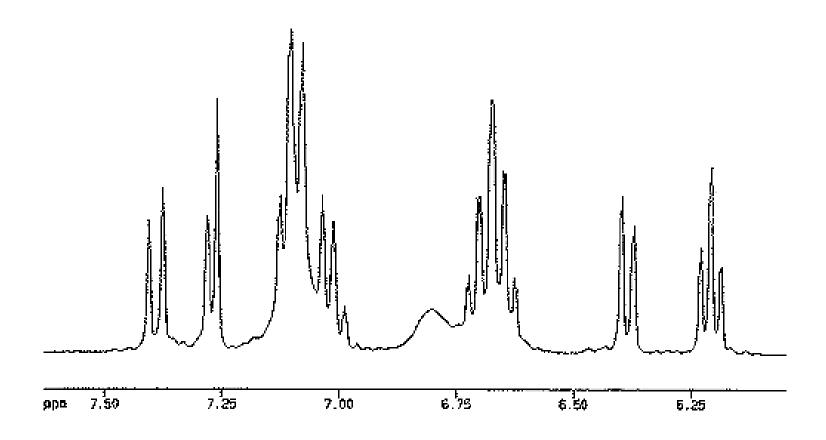


Figure S1

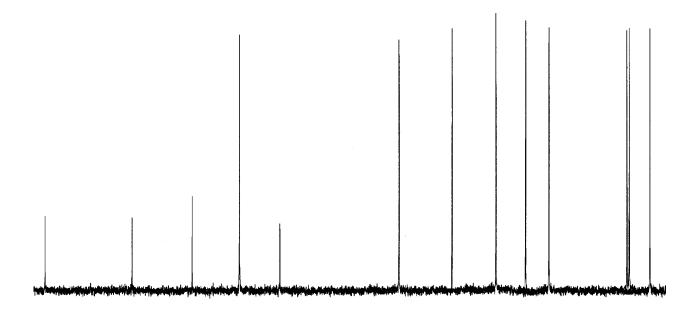
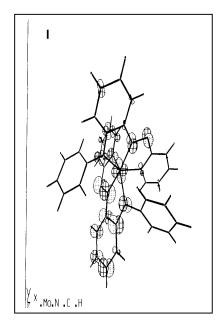
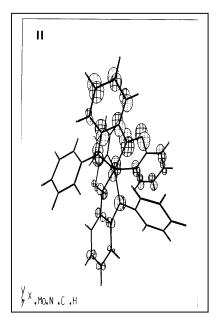
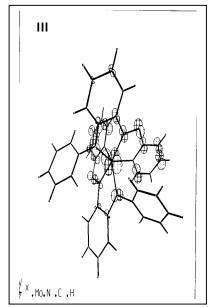
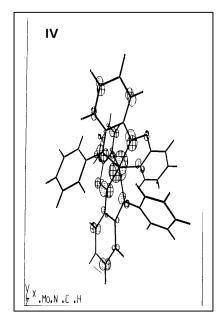


Figure S2









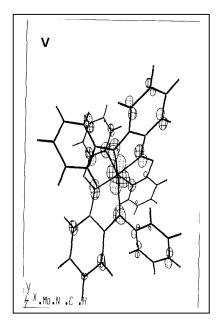


Figure S3