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Reactions of the solvent-stabilized compound $[\text{MoOCl}_2(\text{THF})_2]$ with aromatic nitrogen donor ligands: spectroscopic characterization and semiempirical AM1* calculations

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Abstract: Reaction of the solvent-stabilized dioxo-molybdenum(VI) compound $[\text{MoO}_2\text{Cl}_2(\text{THF})_2]$ with PPh_3 yielded the oxomolybdenum(IV) species $[\text{MoOCl}_2(\text{THF})_2]$ (1) by the removal of one oxygen atom as PPh_3O . The complexes $[\text{MoOCl}_2(=\text{NC}_6\text{H}_4\text{CN})]$ 2, $[\text{MoOCl}_2(\text{CNC}_6\text{H}_4\text{OH})]$ 3, $[\text{MoOCl}_2(=\text{NC}_6\text{H}_4\text{NH}_2)]$ 4, and $[\text{MoOCl}_2(=\text{NC}_6\text{H}_4\text{OCH}_3)]$ 5, were synthesized by the reactions of $[\text{MoOCl}_2(\text{THF})_2]$ with $\text{XC}_6\text{H}_4\text{Y}$ ($\text{X} = \text{NH}_2$, $\text{Y} = \text{CN}$; $\text{X} = \text{CN}$, $\text{Y} = \text{OH}$; $\text{X} = \text{Y} = \text{NH}_2$; $\text{X} = \text{NH}_2$, $\text{Y} = \text{OCH}_3$). All the new compounds were characterized by elemental analyses, and FTIR, UV-Vis, and ¹H- and ¹³C-NMR spectra. Geometrical parameters and molecular orbital calculations showed that compounds 2-5 are stabilized by a charge transfer between the Mo center and the phenyl ring.

Key Words: Mo(VI) complexes; oxo-imido complexes; oxomolybdenum complexes; oxygen atom.

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