Hindered rotation of some substituted thioureas in complexes of chromium and tungsten carbonyls

Granifo, J.

Costamagna, J.

Garrao, A.

Pieber, M.

We describe a procedure for the preparation of various metal thiourea complexes of the type [M(CO)5L] in which M Cr or W and L TU (thiourea), TMTU (tetramethylthiourea), DptTU (NN?-di-p-totyl thiourea); DtBTU = (NN?-di-t-butyl thiourea). Structural characterization of the compounds was achieved by UV-visible, IR and especially NMR spectroscopy. This study shows evidence of rotamers with NH bonds cis and trans with respect to the thiocarbonyl sulphur group. Also we report the activation free energies for hindered rotation around the CN bonds close to the coalescence temperature in TU, [Cr(CO)5TU] (Cr(CO)5DptTU], DtBTU, [Cr(CO)5DtBTU] and [W(CO)5DtBTU]. @ 1980.