

Metalation of C₆₀ with Pentacarbonylrhenium Radicals. Reversible Formation of C₆₀[Re(CO)₅]₂

Shapley, J. R. *et al.* *J. Am. Chem. Soc.* **1993**, *115*, 6705-6709.

IR-Topic: Quantitative IR, Difference IR

Chem Topic: Fullerene Compounds

Reaction: C₆₀ and Re₂(CO)₁₀ → C₆₀{Re(CO)₅}₂

Method: The spectrum of the starting material is subtracted from spectra taken during the reaction. Difference spectra show positive and negative peaks for product and for starting materials.

Table I. IR Data for C₆₀ and Re₂(CO)₁₀ in Benzene Solution

	band positions, cm ⁻¹ (ε, mm ⁻¹ M ⁻¹)			
C ₆₀	1429 (22)	1183 (12)	578 (40)	528 (102)
Re ₂ (CO) ₁₀	2070 (561)	2011 (1850)	1969 (442)	

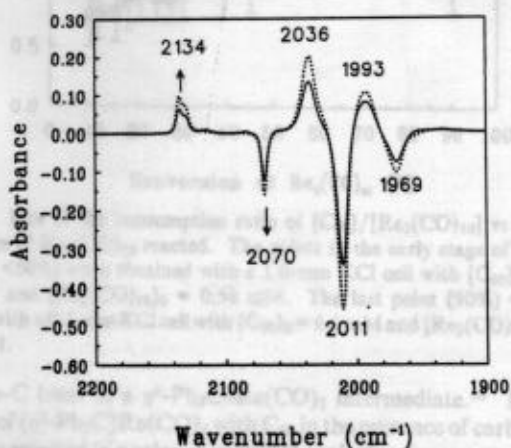


Figure 1. Difference IR (ν_{CO}) spectra of C₆₀ and Re₂(CO)₁₀ in benzene during photolysis. Positive values show the growth of new bands due to P, whereas negative values show the loss of bands due to Re₂(CO)₁₀.

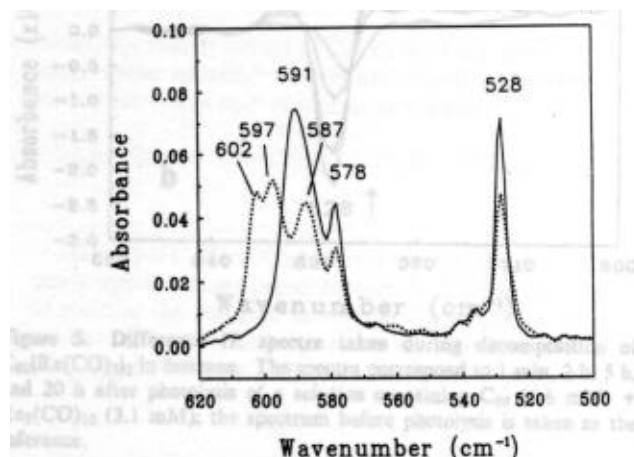


Figure 3. Low-frequency IR spectra of C₆₀ + Re₂(CO)₁₀ in benzene before (solid line) and after (dotted line) ca. 90% reaction.

Observe at 528 for fullerene and at 2070 for the Re-carbonyl. Quantitative evaluation with Beer's Law shows that one C₆₀ reacts with 1 Re-carbonyl. The decomposition reaction in CCl₄ was used to show that there are actually two Re(CO)₅ units connected to the C₆₀. The structure proposed is not based on the IR data! The authors merely review precedent for 1,2 and 1,4 additions and they think 1,4 addition is better here for steric reasons. Probably ok.

