The Structure of the Ligand Tri(1-cyclohepta-2,4,6-trienyl)phosphane, $P(C_7H_7)_3$, in the Hexafluoroacetylacetonato Copper(I) Complexes, $(hfac)Cu[P(C_7H_7)_3]_n$ (n=1,2)

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The reaction of $CuCl[P(C_7H_7)_3]$ (1a) with sodium hexafluoroacetylacetonate, Na(hfac), leads to $(hfac)Cu[P(C_7H_7)_3]$ (2a), which in the presence of excess $P(C_7H_7)_3$ (a) gives $(hfac)Cu[P(C_7H_7)_3]_2$ (3a). Whereas the 1:2 compound 3a is a pseudo-tetrahedral copper(I) complex with relatively long Cu-P (224.85(10) and 223.75(10) pm) and Cu-O (212.7(3) and 212.0(3) pm) distances, the 1:1 complex 2a may be described as having a distorted pseudo-trigonal coordination sphere (Cu-P 214.32(11) pm, Cu-O 196.6(3) and 208.1(3) pm), although one of the cyclohepta-2,4,6-trienyl substituents develops a weak additional interaction with the metal through its central C=C double bond (Cu-C 275.1 and 272.9 pm). The molecular geometries of the tri(1-cyclohepta-2,4,6-trienyl) complexes 2a and 3a are compared with those of the known tri(cyclohexyl)phosphane complexes, $(hfac)Cu[P(C_6H_{11})_3]_n$ (n = 1 (2b) and 2 (3b)), and related compounds.

Key words: Copper(I), 1,3-Diketonate Complexes, Olefinic Phosphanes, Crystal Structure