REACTION of Fe₃(CO)₁₂ with Ph₂P(S)CH₂P(S)Ph₂ and CRYSTAL STRUCTURE of

\[ \{\text{Fe}_2(\text{CO})_6(\mu-S-n-	ext{Bu})\}_2(\mu^4-S) \]

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Content Iron-sulfur clusters have been widely studied over the past thirty years primarily as a result of their biological importance, being found at the active site of a number of proteins and shown to facilitate electron-transfer in various organisms [1]. A fairly common structural motif in iron-sulfur cluster chemistry is the \( \mu^4-S \) bridged double butterfly unit, in which two thiolate-bridged units \([\text{Fe}_2(\text{CO})_6(\mu-SR)]\) are linked via a central \( \mu^4 \)-sulfur atom [2]. Such clusters are relatively easily prepared and show long term stability. We herein described the crystal structure of a complex of this type, namely \([\{\text{Fe}_2(\text{CO})_6(\mu-S-n-	ext{Bu})\}_2(\mu^4-S)\] \), which is compared to previously characterized examples [3]. The tetrairon cluster, \([\{\text{Fe}_2(\text{CO})_6(\mu-S-n-	ext{Bu})\}_2(\mu^4-S)\] \), has been prepared and crystallographically characterized. It consists of the expected \( \mu^4-S \) bridged double butterfly structure and is compared with other crystallographically characterized examples of this class of complex.

Small amounts of \([\{\text{Fe}_2(\text{CO})_6(\mu-S-n-	ext{Bu})\}_2(\mu^4-S)\] \) were isolated from the reaction of Ph₂P(S)CH₂P(S)Ph₂ with Fe₃(CO)₁₂ in THF. It is difficult to rationalize its formation, but the butyl groups may result from ring-opening of the THF. Well-formed orange crystals suitable for X-ray crystallography were grown upon slow evaporation of a CH₂Cl₂/hexane solution the results of which are summarized in Figure 1. The molecular dimensions are very similar to those noted in related complexes including \([\{\text{Fe}_2(\text{CO})_6(\mu-SMe)\}_2(\mu^4-S)\] \) [3], \([\{\text{Fe}_2(\text{CO})_6(\mu-SEt)\}_2(\mu^4-S)\] \) [4], the iron-iron vectors and the angles they sub tend at the central sulfur atom being typical. Further, like other crystallographically characterized examples, the n-butyl substituents are both adopt equatorial positions.

References