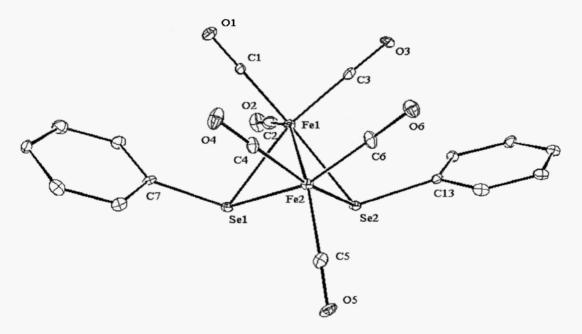
The Molecular Structure of $[Fe_2(\mu-SeC_6H_5)_2(CO)_6]$

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Figure 1. Molecular structure of [Fe₂(μ-SeC₆H₅)₂(CO)₆]. Selected bond lengths (Å) and angles(⁰): Se(1)-Fe(1) 2.4005(18), Se(1)-Fe(2) 2.404(2), Se(2)-Fe(1) 2.3793(19), Se(2)-Fe(2) 2.3884(17), Fe(1)-Fe(2) 2.5363(18), Fe(1)-C(3) 1.793(11), Fe(1)-C(1) 1.800(9), Fe(1)-C(2) 1.821(12), Fe(2)-C(6) 1.778(11), Fe(2)-C(4) 1.798(10), Fe(2)-C(5) 1.821(10), O(1)-C(1) 1.122(12), O(2)-C(2) 1.115(14), O(3)-C(3) 1.136(13), O(4)-C(4) 1.128(12), O(5)-C(5) 1.140(12), O(6)-C(6) 1.164(13), C(7)-Se(1)-Fe(1) 110.6(3), C(7)-Se(1)-Fe(2) 112.8(3), Fe(1)-Se(1)-Fe(2) 63.73(6), C(13)-Se(2)-Fe(1) 111.2(3), C(13)-Se(2)-Fe(2) 113.9(3), Fe(1)-Se(2)-Fe(2) 64.28(6).



COMMENT

Alternative syntheses of the title compound have been reported but it has not previously been crystallographically characterised. Both iron centres have distorted octahedral geometries and are bridged by SePh fragments giving rise to two Fe₂Se rings with a dihedral angle of 92.8°. The Fe-Fe and Fe-Se bond lengths are in the normal ranges /1/ and both the phenyl substituents are in *exo*-positions, as is the case for the

methyl groups in $[Fe_2(\mu-SeMe)_2(CO)_6]$ /2/. This contrasts with $[Fe_2(\mu-p-tolyl)_2(CO)_6]$ which crystallises as its endo-, exo-isomer /3/.

EXPERIMENTAL

Preparation of $[Fe_2(\mu-SeC_6H_5)_2(CO)_6]$:

A solution of the selenophosphaalkene, PhSeP=C(Cl)Bu^t, (0.15 g, 0.51 mmol) and Fe₂(CO)₉ (0.29 g, 0.79 mmol) in hexane (10 ml) was stirred at room temperature for 5 days. After this time, volatiles were removed *in vacuo* and the residue chromatographed (kieselgel / hexane). The title compound was collected as an orange fraction and recrystallised from hexane to give orange plates (0.05 g, 32%). Spectroscopic data for this compound were found to be identical to the literature values /3/.

Crystallography:

Table 1 Crystal data for $[Fe_2(\mu-SeC_6H_5)_2(CO)_6]$

Formula	$C_{18}H_{10}Fe_2O_6Se_2$	Formula weight	591.88
Crystal system	orthorhombic	Crystal size, mm	0.40x0.20x0.03
Space Group	Pca2 ₁	a, Å	7.1053(4)
b, Å	13.8932(9)	c, Å	20.2995(12)
<i>V</i> , Å ³	2003.9(2)	Z	4
Diffractometer	Nonius Kappa CCD	Temperature, K	100(2)
$\mu(Mo-K_{\alpha}), mm^{-1}$	5.11	D _{calcd, g cm} -3	1.962
F(000)	1144	A _{max} o	30.02
Refins meas.	14528	Reflns unique	2966
Reflns with $I > 2\sigma(I)$	2724	$R(F^2), R_w(F^2) (I > 2\sigma(I))$	0.064, 0.131
ρ, e Å- ³	1.64 (near Fe(1))	G.O.F.	1.108
No. obs/No. para	2966/255		
Programs used	SHELX-97 /4/, Ortep-3 /5/		
Deposition number	CCDC 198219		

ACKNOWLEDGEMENTS

We gratefully acknowledge financial support from the University of Wales (MDF)

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