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Crystallographic data for some ferrocene derivatives.

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Bis(cyclopentadienyl)iron(II) compounds, better known as ferrocenes, have been the subject of numerous publications in the last few years. Ferrocene itself was discovered only twelve years ago (Kealy & Pauson, 1951) and its structure has been investigated but the results do not all agree (Eiland & Pepinsky, 1952; Dunitz, Orgel & Rich, 1956). The present author's data agree with those published by Dunitz *et al.* Crystal data for ferrocene derivatives have been published in only a few cases (Struchkov, 1956; Struchkov & Khotsyanova, 1958). Table 1 lists the crystal data for fourteen different ferrocene derivatives as determined by the author.

The lattice parameters were obtained from Weissenberg and precession photographs with Mo $K\alpha$ radiation.

Space groups were determined from systematic absence except for $A2/a$ and $C2/m$ which were chosen because of the eight equivalent positions.

Flotation density measurements were made where possible in a mixture of carbon tetrachloride and petroleum ether and are denoted by D_m in the table. Densities calculated from the X-ray data are listed under D_x.

The purity of each crystal was checked by its melting point range.

X-ray powder patterns were made of each compound and all the powder lines could be easily indexed from the crystal data in the table.

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Table 1. *Crystallographic data for ferrocene derivatives*

Compound	a	b	c	β	S.G.	Z	D_m	D_x	m.p.
Ferrocene	10·56 Å	7·597 Å	5·952 Å	121°	$P2_1/a$	2		1·516	
Ethyl ferrocenoate	5·89	11·13	17·91		$P2_12_12_1$	4		1·454	63·0– 64·0 °C
Phenyl ferrocenoate	9·69	10·43	13·54	94° 25′	$P2_1/c$	4	1·482	1·489	124·0–124·5
Benzoylferrocene	13·93	15·19	6·20	99° 40′	$P2_1/n$	4	1·507	1·484	107·8–108·3
1,1′-Dibenzoylferrocene	11·60	25·20	6·28	90° 05′	$P2_1/n$	4	1·420	1·429	104·0–105·0
Benzoylferrocene oxime	7·56	20·59	8·88		$P2_12_12_1$	4		1·462	161·0–162·5
2,4-Dimethoxybenzoylferrocene	7·77	24·26	8·40		$P2_12_12_1$	4	1·445	1·429	132·5–133·5
2,4-Dihydroxybenzoylferrocene	8·41	24·16	13·85		$Pna2$	8	1·523	1·515	176·0–177·0
O-Hydroxybenzoylferrocene	6·14	19·75	11·12		$P2_12_12_1$	4	1·512	1·502	87·5– 88·5
2-Hydroxy-4-methoxybenzoyl-ferrocene	7·42	13·42	14·54	93° 05′	$P2_1/n$	4	1·562	1·540	124·0–125·5
1,1′-Bis(α-hydroxyethyl)-ferrocene	6·13	16·52	12·72	95° 25′	$P2_1/c$	4	1·412	1·420	69·0– 71·0
1,1′-Hydroxymethylferrocene	10·45	7·72	13·36	105° 40′	$P2_1/a$	4		1·575	104·0–105·0
Dimethyl 1,1′-ferrocene-dicarboxylate	13·34	5·96	32·67	104° 20′	$A2/a$	8	1·589	1·594	113·5–114·5
1,1′-Bis(*p*-fluorobenzoyl)ferrocene	12·69	21·11	13·65	91° 45′	$C2/m$	8	1·560	1·564	129·0–130·5
Di(2,3-epoxypropyl) 1,1′-ferrocenedicarboxylate	11·94	5·96	23·88	102°	$P2_1/c$	4		1·543	51·5– 52·5

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Crystal data for dioctadecyl adipate, $C_{42}H_{82}O_4$.

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In soft X-ray spectroscopy there is a great deal of interest in finding a crystal which will disperse X-rays of wavelengths between about 25 and 100Å. Most investigators who do not like the ruled diffraction grating method are turning to artificially fabricated 'crystals' which are built up of many monolayers of a soap film such as barium stearate. This so-called crystal has a $2d$ spacing of approximately 100Å but the monolayer films are rather difficult to make and usually do not give the intensity or peak-to-background ratio which one usually desires. Many attempts have been made to grow organic single crystals with large $2d$ spacings but obstacles such as poor crystal growth, instability in air or vacuum, very low melting point, absence of desired reflections or poor