

Table 2. Fundamental frequencies of ferrocene.

Number, species and activity	$\nu$ (cm <sup>-1</sup> )	Ref.
$a_{1g}$	1 3112	7
R	2 815	7
	3 1106	7
	4 311	7
$a_{1u}$	5 1257	9
	6 Ring torsion	
$a_{2g}$	7 1249	5
$a_{2u}$	8 3098	7
IR	9 818	7
	10 1107	7
	11 477	7
$e_{1g}$	12 3089	7
R	13 1001	7
	14 815	7
	15 1414	7
	16 393	7
$e_{1u}$	17 3098	7
IR	18 1006	7
	19 840	7
	20 1414	7
	21 490	7
	22 179	7
$e_{2g}$	23 3103	7
R	24 1197	7
	25 1062	7
	26 1358	7
	27 892	6
	28 600	7
$e_{2u}$	29 3159	9
	30 1189	9
	31 1056	9
	32 1351	9
	33 885	9
	34 569	9

and spectroscopic entropies can be obtained with such a barrier as well as without one.

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## On the Molecular Structure of Perfluorobicyclo(2.2.0) hexa-2,5-diene (Perfluoro-Dewar-benzene)

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We wish in this note to report some preliminary results of an electron-diffraction investigation of gaseous perfluoro-Dewar-benzene (Fig. 1). The compound was kindly supplied by the organic section of the Chemistry Department at the University of Manchester Institute of Science and Technology. The intensity data were recorded with a Balzer diffraction instrument in the same department. The results presented here are based on intensity data from only one nozzle-to-plate distance, *i.e.* about 50 cm. Because of the very limited *s*-range (1.5–16.0 Å<sup>-1</sup>) a precision determination of all the molecular parameters could not be carried out.

However, estimates of the angular parameters were obtained. New, more complete data will be recorded.

A model with  $C_{2v}$  symmetry and the C—F bonds in the plane of the adjacent ring was primarily considered (Fig. 1).

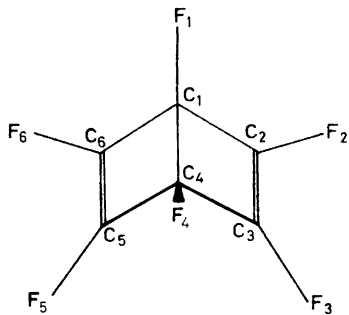


Fig. 1. Numbering of the atoms in  $C_6F_6$ .

Excluding the  $C_1-C_4$  bond, it seems unlikely that the bond lengths in the compound deviate by more than say 0.02 Å from the usual values. The lengths given in Table 1 were therefore assumed for these bonds. With a  $C_1-C_4$  bond somewhat longer than 1.54 Å, quite satisfactory agreement was obtained between the bond distance peaks in the experimental and theoretical radial distribution curves. The independent parameters  $\angle C_1C_4F_4$ ,  $\angle C_3C_2F_2$ , and the dihedral angle between the ring planes ( $\tau$ ) were then refined by least-squares calculations keeping the bond lengths fixed. Refinements were carried out for various  $C_1-C_4$  bond lengths. The angular parameters did not change much with the  $C_1-C_4$  length. The best agreement was obtained with  $C_1-C_4$  about 1.58 Å. The corresponding angles are given in Table 1.

The standard deviations given in the table do not allow for uncertainties in the assumptions. Variation of the bond lengths

Table 1. Perfluoro-Dewar-benzene. Distances (in Å) and angles (in degrees).

$C_1-C_2$	1.50	$\tau$	117.7	(0.9)
$C_2-C_3$	1.32	$C_6C_1C_2$	117.0	(0.9)
$C_1-C_4$	1.58	$C_4C_1F_1$	120.1	(1.6)
$C_1-F_1$	1.38	$C_2C_1F_1$	119.3	(0.3)
$C_2-F_2$	1.34	$C_1C_2F_2$	133.3	(1.0)
$C_4C_1C_2$	85.0	$C_3C_2F_2$	131.7	(1.0)
$C_1C_2C_3$	95.0			

within reasonable limits does not affect the angle parameters considerably. More important changes may occur if the in-plane C—F bonds deviate from the planes of the adjacent rings. By assuming all the angles between the C—F bonds and the ring planes equal and include this angle ( $\delta$ ) as an independent parameter, a somewhat better agreement between experimental and theoretical intensities was obtained.

The best correspondence was achieved if the  $C_{2v}$  symmetry is conserved. However, the values for some of the parameters seem unreasonable. For example the dihedral angle refined to about 103°, and  $\delta$  became 25°. Compared to the original model a better correspondence was also obtained with the neighbouring fluorine atoms on different sides of the ring plane, giving  $C_2$  symmetry only. Except for  $\delta$  which refined to about 12° there were only small changes in the angular parameters compared to the values given in Table 1.

Though it seems unlikely that the angle  $\delta$  should be significantly different from zero, we cannot exclude these models on the basis of the present electron-diffraction data. However, theoretical intensity curves calculated for the three models show considerable differences for  $s$  above 14 Å<sup>-1</sup>, where the quality of the present data becomes poor. We are therefore quite confident that the correct model can easily be determined when better experimental data have been obtained.

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