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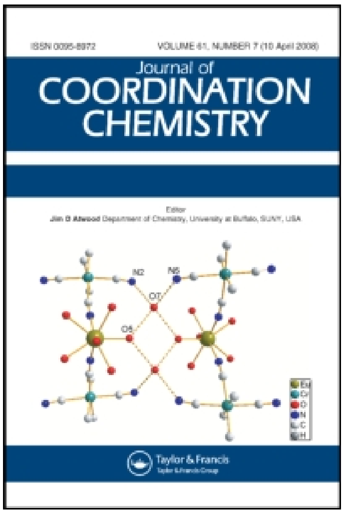

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AN X-RAY STRUCTURAL STUDY OF THE FLUXIONAL MOLECULE [BIS(DIPHENYLPHOSPHINO)METHANE]TRICARBONYLIRON

F. A. Cotton[ab]; K. I. Hardcastle[a]; G. A. Rusholme[a]
[a] Department of Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts [b] Department of Chemistry, The Texas A and M University, College Station, Texas

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AN X-RAY STRUCTURAL STUDY OF THE FLUXIONAL MOLECULE [BIS(DIPHENYLPHOSPHINO)METHANE]TRICARBONYLIRON[1]

F. A. COTTON,[2] K. I. HARDCASTLE[3] and G. A. RUSHOLME[4]

Department of Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

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As part of a broader investigation of fluxional 5-coordinate, neutral complexes of transition metals, the detailed molecular structure of [bis(diphenylphosphino)methane]tricarbonyliron, $(Ph_2PCH_2PPh_2)(CO)_3Fe$, has been determined by X-ray crystallography. The crystals belong to the triclinic system and have the following unit cell dimensions: $a = 12.08(1)$A; $b = 9.63(1)$A; $c = 11.35(1)$A; $\alpha = 101.02(3)°$; $\beta = 90.92(2)°$; $\gamma = 101.13(3)°$. d_{calc} for $Z = 2$: 1.33 g ml^{-1}. d_{obs}: 1.35(2) g ml^{-1}. The structure was solved by Patterson and Fourier methods and refined using 2060 reflections collected with Mo Kα radiation on a manually operated General Electric counter diffractometer. Refinement, in space group $P\bar{1}$, omitting hydrogen atoms, was terminated with $R_1 = 0.063$ and $R_2 = 0.065$. Some important dimensions of the molecule are: Fe–P, 2.209(3)A, 2.225(3)A; Fe–C, 1.74(1)A, 1.77(1)A, 1.77(1)A; $\angle$ P–Fe–P, 73.5(1)°. The coordination geometry is intermediate between trigonal bipyramidal and square pyramidal and would naturally lead to the expectation of very rapid site exchange of the three CO groups.

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INTRODUCTION

It is now well known[5] that five-coordinate complexes generally are stereochemically nonrigid, as manifested by time-average equivalence of all chemically equivalent ligands in nuclear magnetic resonance spectra at room temperature. The most extensively studied systems to date are those derived from pentavalent phosphorus,[6] but it has long been known that $Fe(CO)_5$,[7, 8] and many of its substitution products[9] are stereochemically nonrigid. The isoelectronic species $RCo(PF_3)_x(CO)_{4-x}(R = H, C_nF_{2n+1})$ also appear to be stereochemically nonrigid.[10]

We have undertaken a study of some derivatives of $Fe(CO)_5$ in which two or three CO groups are replaced by bi- or triphosphine ligands. By varying the stereochemical capabilities of these polyphosphine ligands, it is hoped to influence the rates and pathways of fluxional behavior of the five-coordinate complexes in ways which will be informative. This work has been initiated by preparative, nmr (^1H, ^{13}C, ^{31}P), ir and X-ray crystallographic investigation of the series of compounds $[Ph_2P(CH_2)_nPPh_2](CO)_3Fe$, where $n = 1$, 2 and 3. In this paper we report the structure of the compound with $n = 1$. In later reports other structures, preparative procedures and spectroscopic studies will be described.

EXPERIMENTAL

Collection and Reduction of Data

The $[(C_6H_5)_2PCH_2P(C_6H_5)_2]Fe(CO)_3$ was prepared and characterized by L. J. Kruczynski and will be described elsewhere. A crystal of acicular habit suitable for the X-ray study was selected from several which had been recrystallized from toluene. The overall dimensions of the crystal were 0.38 × 0.13 × 0.21 mm. The crystal was mounted on a glass fiber with the largest crystal dimension parallel to the fiber. Preliminary Weissenberg and precession photographs indicated only $\bar{1}$ symmetry. A suitable reciprocal cell was chosen from the precession films such that the α^*, β^* and γ^* angles were all acute. The unit cell dimensions, $a = 12.08(1)$ A, $b = 9.63(1)$ A, $c = 11.35(1)$ A, $\alpha = 101.02(3)°$, $\beta = 90.92(2)°$ and $\gamma = 101.13(3)°$, were obtained from a least-squares treatment of the angular settings for 30 reflections as measured on a General Electric XRD–5 manual diffractometer equipped with a quarter-circle crystal orienter.

The experimentally measured density, by flotation in $Zn(NO_3)_2$ solutions, was 1.35(2) g ml^{-1}. Using a cell volume of 1270 A^3, a molecular weight of 524.3 a.m.u. and two molecules per unit cell, the calculated density is 1.33 g ml^{-1}.

The crystal was aligned on a eucentric goniometer head so that the b^* axis was coincident with

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the ϕ axis of the orienter. Nb-filtered, Mo Kα radiation was used to collect 2388 independent reflections within the sphere, $2\theta > 40°$. Intensities were measured by a scintillation counter. A $\theta/2\theta$ moving crystal-moving counter technique was employed so that P counts would be obtained in 20 sec (T_P) using a scan range of 1.33° and a take-off angle of 2°. The scan rate was 4°/min, and 10 sec (T_B) background counts, B_1 and B_2, were obtained at each extreme of the $\theta/2\theta$ scan with both the crystal and counter stationary. Four intense reflections were frequently monitored during data collection and each data set collected was scaled to time zero for any change in the intensities of these standard reflections.

The recorded data were used to calculate relative structure factor magnitudes, $|F_o|$, such that $|F_o| = (I/Lp)^{1/2}$, where I is given by $I = P-[(B_1+B_2)T_P/2T_B]$, and Lp = Lorentz-polarization factor. The estimated standard deviations in $|F_o|$, σ_{F_o}, where $\sigma_{F_o} = [\sigma_I^2 + (0.031)^2]^{1/2}$, were also computed; $\sigma_I = [P + (T_P/2T_B)^2(B_1 + B_2)]^{1/2}$. The observed intensities were not corrected for absorption; however, a calculation of A*, the absorption correction, for $\mu = 7.41$ cm^{-1} indicated a maximum variation about a mean intensity value of approximately 9%. Of the 2388 observed reflections, only those 2060 reflections for which $|F_o|^2/\sigma_{|F_o|^2} > 1.0$ were used for the calculations.

Solution and Refinement

A three-dimensional Patterson synthesis was carried out using space group P$\bar{1}$. The Fe–Fe, Fe–P and Fe–C (methylene carbon) vectors were identified and the atom coordinates determined. Two cycles of least-squares refinement of the scale factor and the positional and isotropic temperature

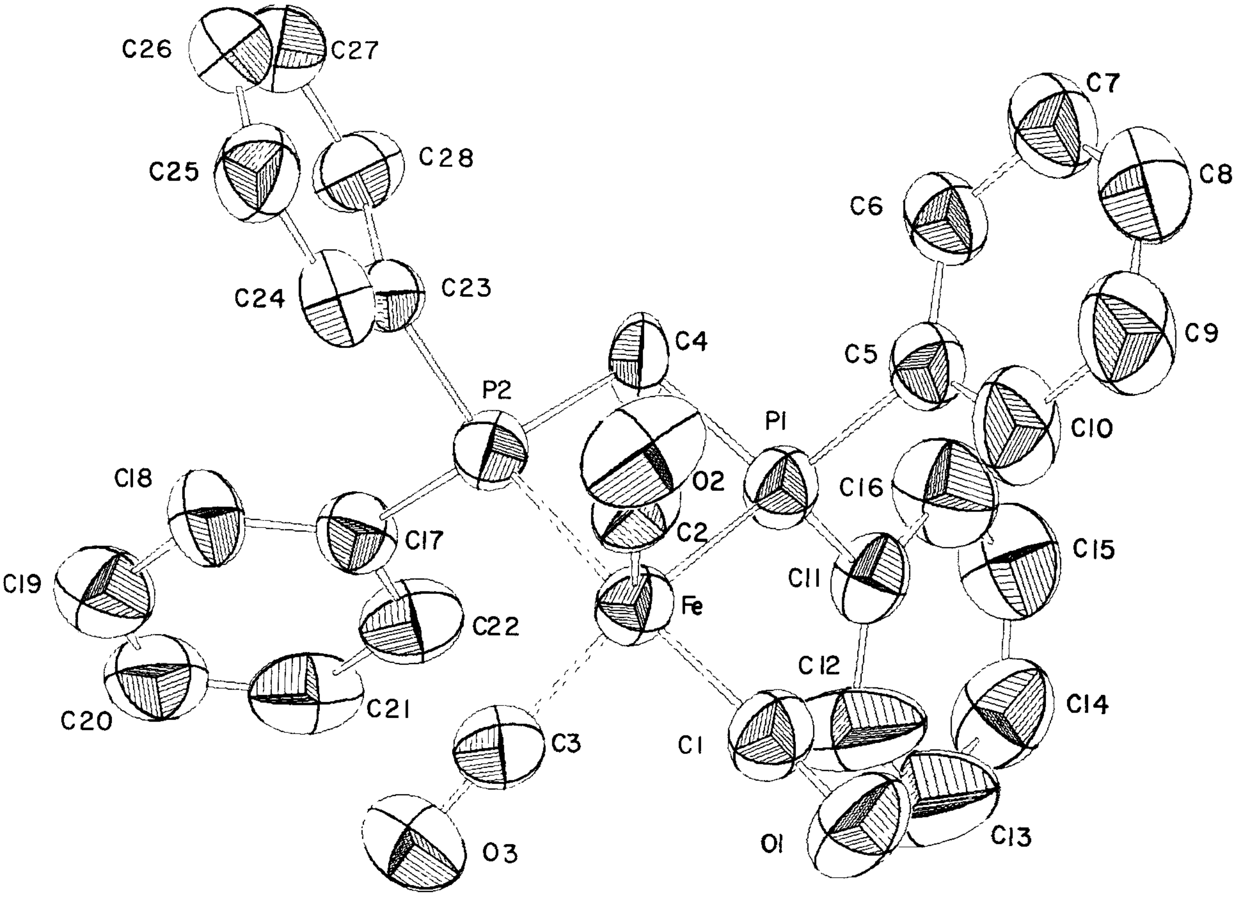

FIGURE 1 A view of the molecule (hydrogen atoms omitted) in which each atom is represented by an ellipsoid proportional to its thermal vibration amplitudes. The numbering scheme is defined.

parameters for these four atoms resulted in a conventional R factor,
$R_1 = \Sigma(||F_o| - |F_c||)/\Sigma|F_o| = 0.420$, and a weighted residual
$R_2 = [\Sigma\omega(|F_o| - |F_c|)^2/ - \Sigma\omega|F_o|^2]^{1/2} = 0.504$.
The refinements were all carried out in space group $P\bar{1}$, using full-matrix least-squares methods minimizing $\Sigma\omega(||F_o| - |F_c||)^2$. Scattering factors were those of Cromer and Waber[11, 12] and anomalous dispersion corrections for the real and imaginary parts of the scattering factors were also included in the calculations. The refined coordinates of the Fe, two P atoms and one C atom were then used to generate an observed Fourier map. All remaining non-hydrogen atoms (30) were clearly visible in the Fourier and were included in all further refinements. Two least-squares cycles using 34 atoms and isotropic temperature factors resulted in $R_1 = 0.176$ and $R_2 = 0.223$. At this point, anisotropic thermal parameters were calculated for all 34 atoms using the isotropic values from the previous refinement. Four cycles of fully anisotropic refinement gave convergence and reduced R_1 to 0.063 and R_2 to 0.065. All shifts for the atom parameters were less than 0.2σ, and all thermal parameters were quite reasonable with the possible exception of the B_{33} values for carbons numbered 12 and 13. After the final cycle of refinement the e.s.d. of an observation of unit weight was 2.36 indicating a slight under-estimation of σ_{F_o}. However, the quantity $\omega|F_o - F_c|^2$ showed no dependence upon either $|F_o|$ or $\lambda^{-1}\sin\theta$. A final difference Fourier was computed and all hydrogen atoms except two were clearly visible. No other residual electron density peaks greater than 0.30 eA^{-3} were observed except for one in the vicinity of the Fe atom. The hydrogen atom contributions were not included as our interest

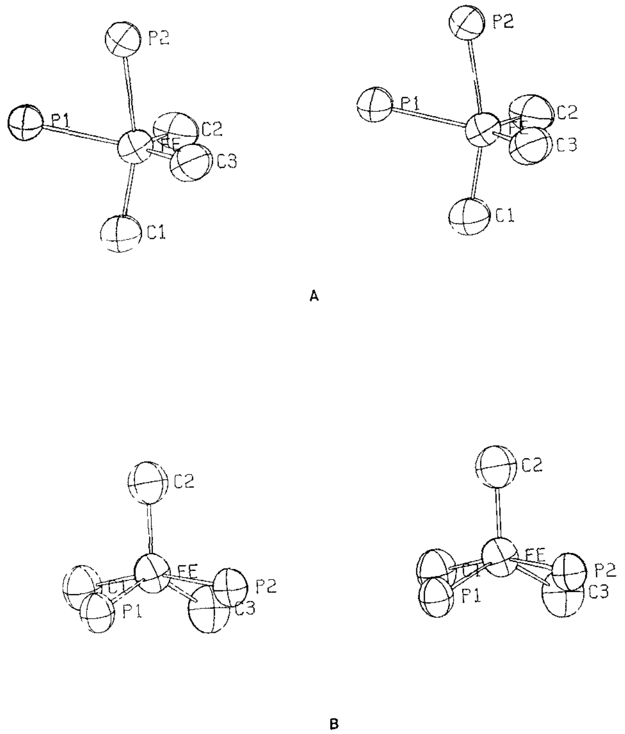

FIGURE 2 Two stereo pairs showing the configuration of the coordination sphere. **A** shows an orientation which emphasizes the distorted trigonal bipyramidal character. **B** shows an orientation which emphasizes the approximate square pyramidal nature of the arrangement.

TABLE I

Atomic positional parameters and equivalent isotropic temperature factors

Atom	x	y	z	B, A^2
Fe	0.2979(1)	0.4327(1)	0.1453(1)	4.3
P1	0.2012(2)	0.2755(2)	0.2427(2)	4.3
P2	0.2449(2)	0.2273(2)	0.0119(2)	4.2
O1	0.2909(6)	0.6749(7)	0.3388(6)	4.8
O2	0.5389(6)	0.4400(7)	0.1797(6)	5.4
O3	0.2371(6)	0.5963(7)	−0.0290(6)	5.6
C1	0.2937(7)	0.577(1)	0.2627(8)	5.7
C2	0.4440(8)	0.4321(9)	0.1631(8)	7.7
C3	0.2609(8)	0.5295(9)	0.0380(8)	8.4
C4	0.1759(7)	0.1152(8)	0.1166(6)	8.3
C5	0.2738(6)	0.2247(9)	0.3656(7)	4.7
C6	0.2737(7)	0.082(1)	0.3717(7)	5.3
C7	0.3353(8)	0.046(1)	0.4635(9)	6.4
C8	0.3984(9)	0.158(1)	0.5508(9)	7.5
C9	0.398(1)	0.300(1)	0.5448(9)	8.7
C10	0.3377(9)	0.336(1)	0.4510(9)	7.7
C11	0.0613(6)	0.2856(9)	0.2996(7)	4.7
C12	0.0129(9)	0.400(1)	0.286(1)	9.4
C13	−0.099(1)	0.405(1)	0.329(1)	10.9
C14	−0.1552(8)	0.297(1)	0.3823(9)	7.3
C15	−0.1074(9)	0.180(1)	0.3863(9)	7.3
C16	0.005(8)	0.173(1)	0.3465(9)	7.1
C17	0.1389(7)	0.2203(8)	−0.1072(7)	4.6
C18	0.1699(8)	0.2049(9)	−0.2254(8)	5 8
C19	0.088(1)	0.210(1)	−0.3170(9)	7 0
C20	−0.019(1)	0.232(1)	−0.286(1)	6.8
C21	−0.0497(7)	0.2481(9)	−0.168(1)	6.2
C22	0.0296(8)	0.2437(9)	−0.0746(8)	5.7
C23	0.3411(7)	0.1229(8)	−0.0656(6)	4.0
C24	0.4503(7)	0.1889(9)	−0.0894(7)	5.0
C25	0.5239(7)	0.103(1)	−0.1503(8)	6.0
C26	0.4864(9)	−0.046(1)	−0.1841(7)	5.8
C27	0.3770(8)	−0.111(1)	−0.1600(8)	5.8
C28	0.3036(7)	−0.0270(9)	−0.1014(7)	5.3

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required only the first coordinate sphere of the iron atoms. The success of refinement in space group $P\bar{1}$ is taken as sufficient indication that this, rather than P1 is the correct space group.

Computer programs used included: PICK2 (J. A. Ibers) for refining all constants and generating angular settings for data collection; REDUCE (B. G. DeBoer) for data reduction; FORDAP (A. Zalkin) for Patterson and Fourier synthesis; SFIX and SIDIOT (local versions of C. T. Prewitt's SFLS-5), for least-squares refinement of parameters; STAN1 (B. G. DeBoer), for molecular geometry; and ORTEP (C. K. Johnson) for illustrations.

RESULTS

A table of the final values of $|F_o|$ and $|F_c|$ scaled to $|F_c|$ is available.[13]

The molecular configuration and numbering system used are shown in Figure 1. Figure 2 gives only the skeletal atomic configuration around the Fe atom viewed in (A) as a trigonal bipyramidal arrangement and in (B) as a square planar arrangement. Final atomic positional and thermal parameters are given in Tables I and II, respectively. The standard deviations, which are given in parentheses for the last figure quoted, were derived from the inverse matrix of the final least-squares refinement

TABLE II

Anisotropic temperature factors[a]

Atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Fe	4.82(7)	3.57(6)	4.25(6)	0.31(5)	0.53(5)	0.48(5)
P1	5.0(1)	3.9(1)	3.8(1)	0.36(9)	0.46(9)	0.55(9)
P2	4.6(1)	4.0(1)	3.8(1)	0.74(9)	0.36(9)	0.66(9)
O1	9.2(4)	5.9(4)	6.9(4)	1.1(3)	0.9(3)	−1.1(3)
O2	5.9(4)	8.2(4)	9.9(5)	1.7(4)	−0.7(4)	−1.3(3)
O3	11.9(5)	6.7(4)	7.3(4)	2.6(4)	0.5(4)	3.0(3)
C1	6.3(5)	4.6(5)	4.9(5)	0.5(4)	0.3(4)	0.3(4)
C2	5.8(6)	5.3(5)	5.2(5)	1.4(4)	0.2(4)	−0.2(4)
C3	7.3(6)	4.1(5)	5.6(5)	1.0(4)	0.5(4)	0.8(4)
C4	6.9(5)	4.5(4)	2.5(3)	−0.0(4)	1.0(3)	0.4(3)
C5	5.1(5)	5.1(5)	4.2(4)	0.9(4)	1.0(4)	1.3(4)
C6	5.0(5)	6.5(6)	5.1(5)	1.5(4)	1.0(4)	2.3(4)
C7	5.8(5)	8.2(6)	5.9(5)	1.9(5)	1.2(5)	2.7(5)
C8	7.4(6)	9.5(8)	6.1(6)	1.7(6)	0.5(5)	2.5(6)
C9	10.3(8)	9.1(8)	5.8(6)	0.7(6)	−2.2(5)	0.6(6)
C10	9.9(7)	7.4(6)	4.5(5)	−0.1(5)	−2.1(5)	−0.0(5)
C11	4.4(4)	4.8(4)	4.2(4)	0.3(4)	0.4(3)	0.2(4)
C12	7.3(7)	6.1(6)	16(1)	3.1(5)	4.8(7)	3.5(6)
C13	8.7(8)	7.3(7)	18(1)	3.2(6)	4.4(8)	3.2(8)
C14	6.6(6)	7.0(6)	7.5(6)	0.5(6)	2.1(5)	0.5(5)
C15	5.8(6)	8.6(7)	7.6(6)	0.5(5)	1.5(5)	2.5(5)
C16	5.9(6)	7.3(6)	8.3(6)	0.4(5)	2.2(5)	3.2(5)
C17	5.2(5)	4.1(4)	4.2(5)	0.7(3)	−0.7(4)	0.6(3)
C18	7.1(5)	6.5(5)	3.9(5)	1.6(4)	−1.0(4)	1.0(4)
C19	7.8(7)	6.9(6)	6.8(6)	2.8(5)	−0.5(6)	1.4(5)
C20	8.2(7)	5.1(5)	6.9(6)	1.9(5)	−1.5(5)	0.5(5)
C21	5.2(5)	4.6(5)	8.6(7)	1.2(4)	−1.2(5)	0.5(5)
C22	4.5(5)	5.3(5)	7.1(6)	1.3(4)	0.0(5)	0.7(4)
C23	4.8(5)	3.7(4)	3.6(4)	1.2(3)	−0.4(3)	0.5(3)
C24	4.9(5)	6.2(5)	3.9(4)	0.5(4)	0.1(4)	1.8(4)
C25	5.9(5)	7.6(6)	5.0(5)	2.3(5)	0.9(4)	1.2(5)
C26	7.3(6)	5.8(6)	4.8(5)	2.4(5)	0.2(4)	1.2(4)
C27	6.1(6)	6.0(5)	5.5(5)	2.0(5)	0.3(4)	1.2(4)
C28	5.6(5)	4.9(5)	5.3(5)	1.9(4)	−0.4(4)	−0.0(4)

[a] The form of the temperature factor expression is:

$$\exp[-1/4(B_{11}h^2a^{*2} + B_{22}k^2b^{*2} + B_{33}l^2c^{*2} + 2B_{12}hka^*b^* + 2B_{13}hla^*c^* + 2B_{23}klb^*c^*)].$$

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cycle. Bond lengths and angles are given in Tables III and IV, while Table V gives the equations of the various molecular planes, and the distances of pertinent atoms from these mean planes.

TABLE III

Bond distances (Å)

Fe–P_1	2.209(3)	Fe–P_2	2.225(3)
P_1–C_4	1.867(7)	P_2–C_4	1.857(7)
Fe–C_1	1.74(1)	C_1–O_1	1.16(1)
Fe–C_2	1.77(1)	C_2–O_2	1.14(1)
Fe–C_3	1.77(1)	C_3–O_3	1.15(1)
P_1–C_5	1.828(8)	P_2–C_{17}	1.829(9)
C_5–C_6	1.39(1)	C_{17}–C_{18}	1.39(1)
C_6–C_7	1.40(1)	C_{18}–C_{19}	1.44(1)
C_7–C_8	1.41(2)	C_{19}–C_{20}	1.40(1)
C_8–C_9	1.38(1)	C_{20}–C_{21}	1.39(1)
C_9–C_{10}	1.41(2)	C_{21}–C_{22}	1.43(1)
C_{10}–C_5	1.40(1)	C_{22}–C_{17}	1.43(1)
P_1–C_{11}	1.832(8)	P_2–C_{23}	1.812(8)
C_{11}–C_{12}	1.37(1)	C_{23}–C_{24}	1.40(1)
C_{12}–C_{13}	1.45(2)	C_{24}–C_{25}	1.43(1)
C_{13}–C_{14}	1.37(2)	C_{25}–C_{26}	1.39(1)
C_{14}–C_{15}	1.37(1)	C_{26}–C_{27}	1.40(1)
C_{15}–C_{16}	1.39(1)	C_{27}–C_{28}	1.41(1)
C_{16}–C_{11}	1.38(1)	C_{28}–C_{23}	1.40(1)

DISCUSSION

The most interesting feature of the structure is the disposition of the coordinated atoms about the iron atom. It is well known[14] that the two most symmetrical, or regular, arrangements found in five-coordinate complexes are trigonal bipyramidal (*tbp*) and square pyramidal (*spy*). It is also known that in any given case these two may differ little in energy and that the actual arrangement may lie somewhere between the two ideal configurations. That is clearly the case with the molecule studied here. Figure 2, which shows only the iron atom and the five coordinated atoms, P(1), P(2), C(1), C(2), C(3), is designed to emphasize this fact. The upper part (A) presents a stereo view of the molecule in which its stereochemical kinship to the *tbp* is made evident. The distortions from the ideal *tbp* are quite significant, however. There is first the small P–Fe–P angle (73.5° rather than 90°) which is an inescapable consequence of the steric constraint inherent in the $Ph_2PCH_2PPh_2$ ligand itself. (A recent structural study of the molybdenum analogue reports a similarly small P–Mo–P angle of 67.3°.[15]) In addition the two "axial" ligand atoms, P(2) and C(1) subtend an angle of only 161.0°. The three ligand atoms in the "trigonal plane" and the iron atom are essentially coplanar, but the ligand-iron-ligand angles, 109.1°, 115.7° and 134.2° all deviate markedly from the ideal value of 120°. Table IV lists the various angles as they relate to the idealized *tbp* geometry.

In part (B) of Figure 2 the perspective is chosen to emphasize as much as possible the relationship of the actual configuration to that of an ideal *spy* arrangement. It should be kept in mind that there is no unique set of ideal angles in this case; there is only the requirement that all four (apex ligand)-iron-(basal ligand) angles be equal and all four (basal ligand)-iron-(basal ligand) angles be equal. It can

TABLE IV

Bond angles (degrees)

Trigonal Bipyramidal		*Square Pyramidal*	
apex to trigonal plane		apex to basal plane	
P1–Fe–P2	73.5(1)	P1–Fe–C2	109.1(3)
C2–Fe–P2	99.2(3)	P2–Fe–C2	99.2(3)
C3–Fe–P2	89.8(3)	C1–Fe–C2	97.3(4)
		C3–Fe–C2	115.7(4)
apex to trigonal plane			
P1–Fe–C1	92.3(3)	basal plane	
C2–Fe–C1	97.3(4)	C1–Fe–C3	91.6(4)
C3–Fe–C1	91.6(4)	C3–Fe–P2	89.8(3)
		P2–Fe–P1	73.5(1)
trigonal plane		P1–Fe–C1	92.3(3)
P1–Fe–C2	109.1(3)		
C2–Fe–C3	115.7(4)		
P1–Fe–C3	134.2(3)		
Fe–P2–C4	97.6(2)	Fe–C1–O1	178(1)
Fe–P1–C4	97.9(2)	Fe–C2–O2	176(1)
P1–C4–P2	90.8(2)	Fe–C3–O3	178(1)
Fe–P1–C5	118.5(3)	Fe–P2–C17	118.3(3)
Fe–P1–C11	124.3(3)	Fe–P2–C23	124.7(3)
C4–P1–C5	106.5(4)	C4–P2–C17	107.2(4)
C4–P1–C11	104.8(4)	C4–P2–C23	104.4(4)
Angles within phenyl groups at atom specified			
C5	119.9(8)	C17	121.8(8)
C6	121.4(8)	C18	118.6(8)
C7	118.9(9)	C19	120.0(9)
C8	120(1)	C20	121.2(9)
C9	122(1)	C21	120.2(9)
C10	118.6(9)	C22	118.2(8)
C11	119.8(8)	C23	120.5(7)
C12	119(1)	C24	119.7(8)
C13	120(1)	C25	119.4(8)
C14	119(1)	C26	120.8(8)
C15	121(1)	C27	120.3(8)
C16	120.3(9)	C28	119.4(8)

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TABLE V

Least squares planes[a]

Plane	Atoms	Equation
1	C5–C10	$0.8246x - 0.0351y - 0.5646z = 0.1780$
2	C11–C16	$-0.3548x - 0.2349y - 0.9049z = -3.6412$
3	C17–C22	$-0.3170x - 0.9403y - 0.1234z = -2.3135$
4	C23–C28	$-0.2992x + 0.3662y - 0.8811z = -0.3791$
5	Fe, P1, C4, P2	$-0.8484x + 0.4770y - 0.2296z = -1.7568$

Distances (A) of atoms from the least squares planes

Plane 1		Plane 2		Plane 3		Plane 4		Plane 5	
C5	0.01	C11	0.03	C17	−0.01	C23	0.00	Fe	0.03
C6	0.00	C12	−0.01	C18	0.00	C24	0.00	P1	−0.03
C7	0.00	C13	−0.01	C19	0.00	C25	0.00	C4	−0.03
C8	0.00	C14	0.03	C20	0.00	C26	0.00	P2	0.04
C9	0.01	C15	−0.02	C21	0.00	C27	0.00		
C10	−0.01	C16	−0.01	C22	0.00	C28	−0.01		

[a] The equations of the planes are of the form $Lx + My + Nz = D$, where L, M and N are the direction cosines referred to the orthogonal axis system a', b, c^*, where a' is $(b \times c^*)$.

be seen in Table IV that there are substantial deviations from both of these requirements. Again, the steric constraint inherent in the $Ph_2PCH_2PPh_2$ ligand causes the basal angle, P(1)–Fe–P(2) to be substantially smaller than the other three. Also, the angles from the axial ligand atom, C(2), to the basal ligand atoms range from 97.3° to 115.7°.

On the basis of the observed structure, this molecule would be expected to exhibit stereochemical nonrigidity of a very facile character. Only relatively slight bends or twists are needed to carry the structure from the configuration actually observed, in which the three CO groups are all non-equivalent, into configurations in which different pairs become equivalent. The actual configuration is so close to *spy* that bends of only about 10° in the directions of the Fe–C(1)–O(1) and Fe–C(3)–O(3) groups make these CO groups equivalent, and simultaneously make P(1) and P(2) equivalent.

Another set of movements, essentially torsion of the O(3)–C(3)–Fe–C(2)–O(2) group about the P(2)–Fe–C(1)–O(1) axis causes C(2)–O(2) and C(3)–O(3) to become time-average equivalent, simultaneously averaging the environments of the two C(4) protons and the two phenyl groups on each phosphorus atom.

The movements required in all of the above processes are so small, of the order of 10–20° twists or ~ 0.2 A shifts in atomic positions, that they would be expected to occur very rapidly at room temperature and to have such low energies of activation that they would continue to occur rapidly even at the lowest practical temperatures (~ -150°C) of nmr measurement.

Thus, on the basis of the observed structure, we predict that at all temperatures at which nmr measurements can be made two sorts of nmr equivalences should be observed: (1) the three CO groups will appear equivalent; (2) the $Fe(Ph_2PCH_2PPh_2)$ moiety will appear to have C_{2v} symmetry. Nmr studies which are not as yet complete, and will be reported elsewhere when they are, fully support these predictions at room temperature and down to ~ -70°C.

It may be noted that formal consideration of either "turnstyle rotation" or "Berry pseudorotation" is unnecessary because simpler and less extensive deformations, as described, can accomplish the minimum averaging required to produce the equivalences specifically mentioned. While the more elaborate site-exchange pathways may indeed occur, there will be no way to ascertain whether they do or not from nmr observations, since their observable effects are accomplished by simpler processes.

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