CRYSTAL STRUCTURE OF THE HIGH-SPIN FIVE-COORDINATE COMPLEX CHLORO [N,N-BIS(2-DIPHENYLPHOSPHINOETHYL)-2-METHOXYETHYLAMINE] COBALT(II) HEXAFLUOROPHOSPHATE

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The high-spin complex of cobalt(II) with the tripod ligand N,N-bis(2-diphenylphosphinoethyl)-2-methoxyethylamine (NOP₂), having the formula [Co(NOP₂)Cl]PF₆, has been studied by X-ray analysis using photographic data. The crystals are triclinic, space group P$\bar{1}$, with cell dimensions $a = 13.580 \pm 0.013$, $b = 15.905 \pm 0.009$, $c = 8.593 \pm 0.006$ Å, $\alpha = 93°57' \pm 8'$, $\beta = 106°28' \pm 5'$, $\gamma = 95°48' \pm 6'$. The structure has been solved by three-dimensional Patterson and Fourier syntheses and refined by least-squares techniques to a final R factor of 9.9% for the 1313 independent observed reflections. The complex consists of discrete [Co(NOP₂)Cl]⁺ and PF₆⁻ ions. The cobalt atoms are five-coordinate with an NOP₂Cl donor set; the geometry of the coordination polyhedron can be described as a distorted trigonal bipyramid, with tendency toward a tetrahedron. This geometry appears to strongly favour the high-spin state of this complex.

INTRODUCTION

The quadridentate tripod-like ligand N, N-bis(2-diphenylphosphinoethyl) - 2 - methoxyethylamine (NOP₂), (Ph₂PCH₂CH₂)₂NCH₂CH₂OCH₃, forms nickel(II) and cobalt(II) metal complexes of the general formula [M(NOP₂)X]Y, where X = Cl, Br, I, or NCS, Y = I, PF₆, or BPh₄.[1] The nickel complexes are diamagnetic and square-pyramidal with the oxygen atom of the NOP₂ ligand occupying the apex of the coordination polyhedron at an unusually long distance from the metal atom: 2.62 Å in [Ni(NOP₂)I]I complex[2] and 2.48 Å in [Ni(NOP₂)NCS]PF₆ complex.[3] The cobalt complexes are high or low-spin depending on the nature of X: when X = halogen the complexes are high-spin; when X = NCS the complexes are low-spin.[1] The low-spin cobalt complexes are shown by their X-ray powder diagrams to be isomorphous with the analogous nickel(II) complexes and therefore can also be assigned a square-pyramidal coordination polyhedron.

In order to determine the geometry of a high-spin [Co(NOP₂)X]Y complex, the X-ray analysis of the structure of the [Co(NOP₂)Cl]PF₆ complex was undertaken, using photographic methods.

EXPERIMENTAL SECTION

Crystal Data The preparation and characterization of the [Co(NOP₂)Cl]PF₆ complex were reported elsewhere.[1] This compound crystallizes as violet crystals in the triclinic system.

Cell parameters were determined by a least-squares refinement of 40 2θ values from 0*kl*, *h*0*l*, and *hk*0 Weissenberg photographs taken with FeKα radiation ($\lambda = 1.9373$ Å) and calibrated with NaCl. The results are: $a = 13.580 \pm 0.013$, $b = 15.905 \pm 0.009$, $c = 8.593 \pm 0.006$ Å, $\alpha = 93°57' \pm 8'$, $\beta = 106°28' \pm 5'$, $\gamma = 95°48' \pm 6'$. The space group was assumed to be P$\bar{1}$, which was later confirmed by the determination and refinement of the structure.

The calculated density of 1.393 g.cm⁻³, assuming Z = 2, is in agreement with the observed value of 1.40 $\pm$ 0.01 g.cm⁻³ measured by the flotation technique. The linear absorption coefficient μ(FeKα) was found to be 60.9 cm⁻¹.

Data Collection The crystal used for data collection was a parallelepiped of dimensions of 0.12 × 0.08 × 0.50 mm coincident with the [100], [010], and [001] directions, respectively. Multiple-film

equi-inclination Weissenberg photographs $hk0$ through $hk5$ were taken on a Nonius integrating camera with Mn-filtered FeK_α radiation, and the intensities of the spots were measured on a Nonius microdensitometer. The observed independent reflections were 1313, whereas about 1300 reflections had intensities too weak to be measured. The various levels were put on a common scale by means of a Weissenberg photograph containing 30° samples (for ω) from each level (from 0 to 5). Intensities were corrected for Lorentz and polarization factors. No correction was made for absorption; the transmission factors were in the range 0.5–0.6. Atomic scattering factors for Co, Cl, P, F, O, N, and C atoms were taken from ref. 4. From that of cobalt the real part of the anomalous dispersion correction was subtracted according to Cromer.[5] The hydrogen scattering factor was that of ref. 6 taken from the International Tables.

Structure Determination   A   three-dimensional Patterson synthesis showed the positions of the cobalt and chlorine atoms. Three Fourier syntheses showed all the non-hydrogen atoms. At this point the R factor, defined as $\Sigma||F_o| - |F_c|\Sigma|F_o|$, was 21%, assuming $B_{Co} = B_{Cl} = 2.5$ Å^2 and $B = 3.0$ Å^2 for the lighter atoms.

Refinement was undertaken by means of the Busing and Levy full-matrix least-squares program, adapted by Stewart[7] to the IBM 7090 computer. The minimized function was $\Sigma w(|F_o| - |F_c|)^2$, in which w is the weight assigned to the F_o values, in accordance with the scheme: $w = 1$ for $F_o < 40$, and $\sqrt{w} = 40/F_o$ for $F_o > 40$. Three cycles of positional and isotropic thermal parameter refinement of all the non-hydrogen atoms, followed by two cycles of scale factors refinement, lowered R to 12%. At this point the hydrogen atoms were introduced in calculated positions assuming a C–H distance of 1.05 Å and $B_H = 5.0$ Å^2, and were not refined in the subsequent calculations. Three more cycles were performed using isotropic temperature factors for carbon atoms, and anisotropic for the heavier atoms. These cycles were followed by another cycle on scale factors. The refined scale factors were in agreement, within their standard deviations, to those derived from the Weissenberg film. At this point the R factor was 9.9%, and R_w was 12.3%, where $R_w = (\Sigma w(|F_o| - |F_c|)^2/\Sigma w F_o^2)^{1/2}$. A final difference Fourier synthesis showed the highest peak (0.6 e.A^{-3}) in a position close to the metal atom. At the end of refinement the structure factors for non-observed reflections were all lower than the measured data. The final parameters and their standard deviations are in Tables I and II. The table of observed and calculated structure factors is available for inspection in the files of the Editor.

RESULTS AND DISCUSSION

The structure consists of $[Co(NOP_2)Cl]^+$ and PF_6^- ions. The cobalt atoms are five-coordinate, linked

TABLE I

Positional parameters (x10^4), anisotropic temperature factors*, and estimated standard deviations in parentheses

Atom	x/a	y/b	z/c	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Co	2205(3)	2272(2)	3384(4)	4.1(2)	3.8(2)	1.6(2)	0.3(2)	1.4(1)	0.3(1)
Cl	1807(5)	3137(4)	5236(8)	7.7(5)	6.3(4)	4.2(4)	2.0(3)	3.3(3)	0.1(3)
P(1)	1651(5)	2893(3)	841(7)	4.4(3)	3.1(3)	2.4(4)	0.3(2)	1.8(3)	−0.6(2)
P(2)	4061(5)	2266(4)	4584(7)	4.5(3)	4.3(3)	1.2(4)	0.8(2)	1.4(3)	0.1(2)
P(3)	2769(6)	−519(4)	6534(9)	6.0(5)	4.7(4)	2.3(5)	0.6(3)	1.9(4)	0.2(3)
F(1)	2799(11)	467(8)	6399(18)	7(1)	5(1)	7(1)	−0.1(6)	3.0(7)	0.2(6)
F(2)	2754(13)	−1498(9)	6606(17)	13(1)	6(1)	4(1)	2.1(8)	1.6(8)	0.1(6)
F(3)	2164(14)	−460(10)	7865(20)	13(1)	9(1)	6(1)	−1.7(8)	7.2(10)	−1.7(8)
F(4)	1695(11)	−654(9)	5160(18)	6(1)	7(1)	6(1)	0.7(6)	0.8(7)	−0.4(6)
F(5)	3360(12)	−599(11)	5155(19)	7(1)	13(1)	5(1)	4.2(8)	4.0(8)	2.3(8)
F(6)	3831(14)	−382(11)	7889(18)	10(1)	10(1)	4(1)	−1.5(9)	−1.8(8)	1.2(7)
O	1270(10)	1182(8)	3356(17)	4(1)	5(1)	4(2)	−0.1(6)	2.9(6)	1.7(6)
N	2616(15)	1260(10)	1495(20)	7(1)	3(1)	2(1)	0.6(8)	2.6(8)	0.4(7)

* Anisotropic thermal factors are of the form:
exp $[-\frac{1}{4}(B_{11}h^2a^{*2} + B_{22}k^2b^{*2} + B_{33}l^2c^{*2} + 2B_{12}hka^*b^*\cos \gamma^* + 2B_{13}hla^*c^*\cos \beta^* + 2B_{23}klb^*c^*\cos\alpha^*)]$

TABLE II

Positional parameters (x10³), isotropic temperature factors, and estimated standard deviations in parentheses

Atom	x/a	y/b	z/c	B(Å²)
C(1)	218(2)	44(2)	182(3)	3.8(0.5)
C(2)	110(2)	53(2)	212(3)	4.6(0.6)
C(3)	51(2)	111(2)	428(3)	5.4(0.6)
C(4)	216(2)	143(2)	−23(3)	4.5(0.6)
C(5)	232(2)	237(1)	−44(3)	3.2(0.5)
C(6)	184(2)	399(2)	66(3)	4.4(0.6)
C(7)	153(3)	458(3)	158(5)	9.9(1.0)
C(8)	165(3)	542(3)	152(4)	9.5(0.9)
C(9)	215(3)	575(2)	62(5)	8.5(0.9)
C(10)	262(4)	524(3)	−28(6)	14.1(1.3)
C(11)	241(3)	431(3)	−24(4)	10.1(1.0)
C(12)	29(2)	257(1)	−19(3)	3.8(0.5)
C(13)	−44(2)	232(2)	66(4)	5.9(0.7)
C(14)	−146(3)	208(2)	−13(4)	6.6(0.8)
C(15)	−174(2)	205(2)	−169(4)	5.6(0.7)
C(16)	−115(2)	229(2)	−262(4)	6.7(0.7)
C(17)	−12(2)	259(2)	−186(4)	6.1(0.6)
C(18)	375(2)	126(2)	178(3)	5.2(0.6)
C(19)	434(2)	131(1)	362(3)	3.7(0.5)
C(20)	486(2)	314(2)	406(3)	4.7(0.5)
C(21)	441(2)	381(2)	347(3)	4.8(0.5)
C(22)	502(2)	451(2)	313(4)	6.3(0.7)
C(23)	607(2)	448(2)	352(4)	6.3(0.7)
C(24)	655(3)	384(2)	404(4)	7.7(0.9)
C(25)	594(2)	313(2)	443(3)	6.2(0.7)
C(26)	471(2)	228(2)	679(3)	4.1(0.5)
C(27)	465(2)	292(2)	780(3)	5.5(0.6)
C(28)	520(2)	293(2)	948(3)	5.8(0.6)
C(29)	563(2)	229(2)	2(3)	4.7(0.6)
C(30)	560(2)	161(2)	906(4)	6.0(0.7)
C(31)	511(2)	160(2)	734(4)	5.5(0.7)

TABLE III

Distances (Å) and angles (deg) in the coordination polyhedron with their estimated standard deviations

Co–Cl	2.248(8)	Cl–Co–N	176.0(0.5)
Co–P(1)	2.414(7)	P(1)–Co–P(2)	117.3(0.2)
Co–P(2)	2.438(8)	P(1)–Co–O	110.9(0.4)
Co–O	2.03(1)	P(1)–Co–N	77.9(0.4)
Co–N	2.42(2)	P(2)–Co–O	117.0(0.4)
Cl–Co–P(1)	105.5(0.3)	P(2)–Co–N	77.6(0.5)
Cl–Co–P(2)	102.2(0.3)	O–Co–N	75.5(0.6)
Cl–Co–O	101.2(0.4)		

to the four donor atoms of the NOP_2 ligand and to the chlorine atom. The configuration of the coordination polyhedron is "umbrella" type, with the central atom of the tripod ligand, the nitrogen, at an apex of a distorted trigonal bipyramid and the phosphorus and oxygen atoms in the equatorial positions. The other apex is occupied by the chlorine atom (Figure 1). The distances and angles in the coordination polyhedron with their standard deviations are reported in Table III.

The Co–N distance of 2.42 (2) Å is unusually long, the metal atom being displaced from the equatorial plane 0.51 Å toward the chlorine atom. The equation of this plane, calculated by the positions of P(1), P(2), and O atoms, is $-2.780\,x + 4.312y + 2.513z = 1$ (triclinic coordinates). It follows that the Cl–Co–Ligand(equat) angles are larger than the theoretical value of 90° expected for a trigonal bipyramid (Cl–Co–P(1) = 105.5(3)°,
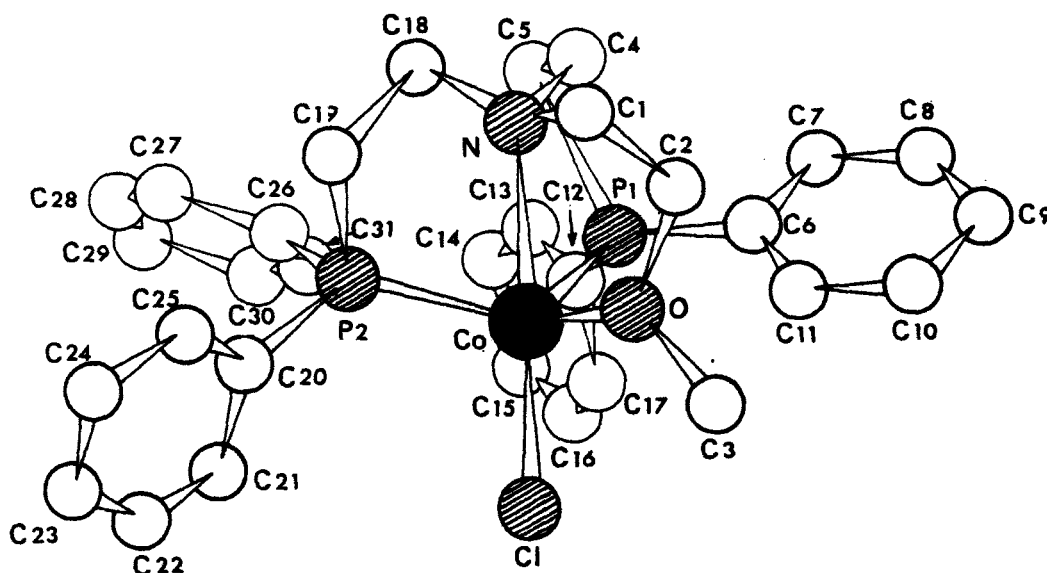

FIGURE 1   A perpective view of the configuration of the complex cation $[Co(NOP_2)Cl]^+$.

Cl–Co–P(2) = 102.2 (3)°, Cl–Co–O = 101.2 (4)°), and the three equatorial angles have values less than 120° (P(1)–Co–P(2) = 117.3 (3)°, P(1)–Co–O = 110.9 (4)°, P(2)Co–O = 117.0 (4)°). The coordination polyhedron, therefore, can be viewed as distorted toward a tetrahedral geometry in which the nitrogen atom is excluded from the donor set. This type of geometry also occurs in the structure of the high-spin complex [Co(NP$_3$)Cl]PF$_6$, where NP$_3$ is the tripod ligand tris(2-diphenylphosphinoethyl) amine.[8] Nevertheless, the perturbation exerted by the nitrogen atom on the cobalt in both these complexes, [Co(NOP$_2$)Cl]PF$_6$ and [Co(NP$_3$)Cl]PF$_6$, is significant, as confirmed by the electronic spectra which are yet indicative of trigonal bipyramidal structures.[8]

Two different structures, the square pyramidal and the trigonal bipyramidal tetrahedrally distorted, are associated respectively with the two different spin states in the complexes [Co(NOP$_2$)NCS]$^+$ (low-spin)[1] and [Co(NOP$_2$)Cl]$^+$ (high spin). This appears to be in contrast with the results of the computation of the crystal field stabilization energy for the idealized geometries, the square pyramidal C$_{4v}$ and the trigonal bipyramidal D$_{3h}$. This calculation shows that the high spin state for Co(II) complexes would be favoured by C$_{4v}$ rather than by D$_{3h}$ symmetry.[9] Therefore the tetrahedral distortion seems to be a determining factor in the existence of the high spin state of the [Co(NOP$_2$)Cl]PF$_6$ complex. The same explanation can be given for the different spin states between the square pyramidal complex [Co(NP$_3$)I]I[10] (low spin) and the above mentioned complex [Co(NP$_3$)Cl]PF$_6$ (high spin).[8]

The Co–N distance found in the complex [Co(NOP$_2$)Cl]PF$_6$ (I), unusually long for the distance between cobalt and a bonded nitrogen atom, is remarkably shorter than the analogous distance found in the [Co(NP$_3$)Cl]PF$_6$ (II) complex (2.42 and 2.67 Å respectively). This is in spite of the similarity in the tetrahedral distortion in the two complexes, which is shown by considering the values of the angles about the cobalt atom. The average Cl–Co–Ligand(equat) angle is 102.9° and that between equatorial ligands is 115.1° in complex 1, whereas the same average angles are 104.6° and 113.8° in complex II. The different Co–N distance found in the two complexes is very probably due to the presence in complex I of the relatively short N–C–C–O arm (the expected C–O and C–P distances are 1.43 and 1.87 Å),[11] which brings the nitrogen atom toward the cobalt.

The oxygen atom of the [Co(NOP$_2$)Cl]PF$_6$ complex, in spite of the shorter chain, reaches a position equivalent to that of the two phosphorus atoms with respect to the Co—Cl bond, as shown by the comparable values of the three Cl–Co–Ligand-(equat) angles. The equivalence in these positions is obtained by the displacement of the nitrogen atom from the axis of the bipyramid (Cl—Co—N = 176.0 (5)°) toward the oxygen atom. This is shown by the sum of the N–Co–O and Cl–Co–O angles (176.7°) which is very close to the Cl–Co–N angle. Also some distortions in the chains contribute to bring the phosphorus and oxygen atoms to equivalent positions, as shown by the angles about the nitrogen and the carbon atoms linked to the nitrogen. As a matter of fact, these angles in the phosphorus chains are larger than the theoretical values, whereas they are normal or smaller in the oxygen chain (Figure 2).
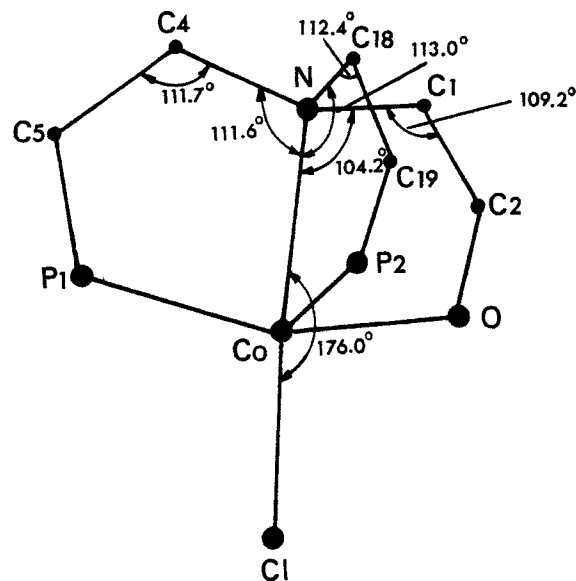
FIGURE 2 A schematic view of the coordination polyhedron and of the ethylenic chains in the [Co(NOP$_2$)Cl]PF$_6$ complex.

The two Co–P distances (2.414 (7) and 2.438 (8) Å) are significantly longer than analogues Co–P distances found in other Co(II) complexes. For example, 2.28 Å (average) was found for the Co–P(equat) distance in the CoCl(QP)BPh$_4$ complex,[12] where QP is the ligand tris-(o-diphenylphosphinophenyl)phosphine, and 2.37 Å (average) was found for the Co–P distance in the [Co(NP$_3$)Cl]PF$_6$

complex.[8] The above mentioned distortions also appear to be a contributing factor in the large distances between the phosphorus atoms and the cobalt (Figure 2).

The distances Co–O (2.04 (1) Å) and Co–Cl (2.248 (8) Å) are in the range of normal values.[8,13,14] Also the distances and angles in the rest of the ligand molecule and in the PF_6^- ion are normal within 2 standard deviations: these values are reported in Table IV.

TABLE IV

Bond lengths (Å) and angles (degrees) in the ligand molecule and in the Hexafluorophosphate ion with estimated standard deviations in parentheses

P(1)–C(5)	1.82(2)	Co–P(1)–C(5)	103(1)
P(1)–C(6)	1.76(2)	Co–P(1)–C(6)	124(1)
P(1)–C(12)	1.81(2)	Co–P(1)–C(12)	112(1)
P(2)–C(19)	1.81(2)	C(5)–P(1)–C(6)	107(1)
P(2)–C(20)	1.84(2)	C(5)–P(1)–C(12)	104(1)
P(2)–C(26)	1.85(2)	C(6)–P(1)–C(12)	105(1)
O–C(2)	1.39(3)	Co–P(2)–C(19)	104(1)
O–C(3)	1.47(3)	Co–P(2)–C(20)	114(1)
N–C(1)	1.45(3)	Co–P(2)–C(26)	125(1)
N–C(4)	1.49(3)	C(19)–P(2)–C(20)	105(1)
N–C(18)	1.48(3)	C(19)–P(2)–C(26)	106(1)
C(1)–C(2)	1.58(3)	C(20)–P(2)–C(26)	101(1)
C(4)–C(5)	1.52(3)	Co–O–C(2)	120(1)
C(6)–C(7)	1.37(5)	Co–O–C(3)	124(1)
C(6)–C(11)	1.33(4)	C(2)–O–C(3)	113(2)
C(7)–C(8)	1.32(6)	Co–N–C(1)	104(1)
C(8)–C(9)	1.27(5)	Co–N–C(4)	112(1)
C(9)–C(10)	1.41(6)	Co–N–C(18)	113(1)
C(10)–C(11)	1.49(6)	C(1)–N–C(4)	112(2)
C(12)–C(13)	1.43(4)	C(1)–N–C(18)	109(2)
C(12)–C(17)	1.38(4)	C(4)–N–C(18)	108(2)
C(13)–C(14)	1.36(5)	N–C(1)–C(2)	109(2)
C(14)–C(15)	1.28(5)	O–C(2)–C(1)	107(2)
C(15)–C(16)	1.33(4)	N–C(4)–C(5)	112(2)
C(16)–C(17)	1.39(4)	P(1)–C(5)–C(4)	106(2)
C(18)–C(19)	1.55(3)	P(1)–C(6)–C(7)	123(2)
C(20)–C(21)	1.35(3)	P(1)–C(6)–C(11)	122(2)
C(20)–C(25)	1.40(4)	C(7)–C(6)–C(11)	114(3)
C(21)–C(22)	1.41(4)	C(6)–C(7)–C(8)	126(4)
C(22)–C(23)	1.39(4)	C(7)–C(8)–C(9)	121(4)
C(23)–C(24)	1.30(5)	C(8)–C(9)–C(10)	120(4)
C(24)–C(25)	1.44(4)	C(9)–C(10)–C(11)	116(4)
C(26)–C(27)	1.32(4)	C(6)–C(11)–C(10)	121(3)
C(26)–C(31)	1.31(4)	P(1)–C(12)–C(13)	123(2)
C(27)–C(28)	1.42(4)	P(1)–C(12)–C(17)	122(2)
C(28)–C(29)	1.28(4)	C(13)–C(12)–C(17)	116(2)
C(29)–C(30)	1.30(4)	C(12)–C(13)–C(14)	122(3)
C(30)–C(31)	1.43(4)	C(13)–C(14)–C(15)	117(3)
P(3)–F(1)	1.58(1)	C(14)–C(15)–C(16)	127(3)
P(3)–F(2)	1.56(2)	C(15)–C(16)–C(17)	118(3)
P(3)–F(3)	1.59(2)	C(12)–C(17)–C(16)	120(3)
P(3)–F(4)	1.58(2)	N–C(18)–C(19)	112(2)
P(3)–F(5)	1.61(2)	P(2)–C(19)–C(18)	107(2)
P(3)–F(6)	1.56(2)	P(2)–C(20)–C(21)	118(2)
		P(2)–C(20)–C(25)	120(2)
		C(21)–C(20)–C(25)	121(2)
		C(20)–C(21)–C(22)	120(2)
		C(21)–C(22)–C(23)	117(3)
		C(22)–C(23)–C(24)	126(3)
		C(23)–C(24)–C(25)	117(3)
		C(20)–C(25)–C(24)	118(3)
		P(2)–C(26)–C(27)	119(2)
		P(2)–C(26)–C(31)	119(2)
		C(27)–C(26)–C(31)	121(2)
		C(26)–C(27)–C(28)	118(2)
		C(27)–C(28)–C(29)	120(3)
		C(28)–C(29)–C(30)	121(3)
		C(29)–C(30)–C(31)	120(3)
		C(26)–C(31)–C(30)	118(3)
		F(1)–P(3)–F(2)	178(1)
		F(1)–P(3)–F(3)	91(1)
		F(1)–P(3)–F(4)	89(1)
		F(1)–P(3)–F(5)	90(1)
		F(1)–P(3)–F(6)	91(1)
		F(2)–P(3)–F(3)	91(1)
		F(2)–P(3)–F(4)	91(1)
		F(2)–P(3)–F(5)	88(1)
		F(2)–P(3)–F(6)	89(1)
		F(3)–P(3)–F(4)	89(1)
		F(3)–P(3)–F(5)	179(1)
		F(3)–P(3)–F(6)	91(1)
		F(4)–P(3)–F(5)	90(1)
		F(4)–P(3)–F(6)	180(2)
		F(5)–P(3)–F(6)	90(1)

TABLE V

Intermolecular contacts < 3.6 Å

$F(1)\cdots O^I$	3.20
$F(1)\cdots C(3^I)$	3.43
$F(1)\cdots C(31^I)$	3.31
$F(4)\cdots O^I$	3.42
$F(4)\cdots C(2^I)$	3.29
$F(4)\cdots C(3^I)$	3.41
$F(5)\cdots C(1^I)$	3.48
$F(6)\cdots C(31^I)$	3.57
$F(1)\cdots C(4^{II})$	3.54
$F(3)\cdots C(1^{II})$	3.59
$F(3)\cdots C(4^{II})$	3.32
$F(2)\cdots C(16^{III})$	3.56
$F(4)\cdots C(16^{III})$	3.17
$F(3)\cdots C(3^{IV})$	3.58
$F(3)\cdots C(14^{IV})$	3.54
$F(4)\cdots C(3^{IV})$	3.18
$F(2)\cdots C(25^V)$	3.49
$F(5)\cdots C(19^V)$	3.33
$F(6)\cdots C(19^V)$	3.50
$C(22)\cdots C(22^{VI})$	3.49

Superscripts refer to the following equivalent positions:

I	x, y, z
II	$x, y, z + 1$
III	$-x, -y, -z$
IV	$-x, -y, 1 - z$
V	$1 - x, -y, 1 - z$
VI	$1 - x, 1 - y, 1 - z$

There are short intermolecular contacts especially between fluorine atoms of the PF_6^- and carbon atoms of the NOP_2 ligand; contacts less than 3.6 Å are reported in Table V. We observe that in these contacts all the phenyl rings of the ligand are involved except for the C_6–C_{11} ring. This feature may be responsible for the high thermal factors found for these atoms (see Table II).

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