Table 2. *Selected geometric parameters (Å, °)*

Sn1—C14	2.101 (4)	S1—C1	1.780 (4)
Sn1—C13	2.105 (5)	S1—C15	1.796 (4)
Sn1—O1	2.397 (3)	O2—S2	1.515 (3)
Sn1—O2	2.404 (3)	S2—C7	1.795 (5)
Sn1—Cl2	2.482 (1)	S2—C16	1.807 (4)
Sn1—Cl1	2.486 (1)	C15—C15^i	1.511 (9)
O1—S1	1.517 (3)	C16—C16^{ii}	1.500 (9)
C14—Sn1—C13	165.2 (2)	O2—Sn1—Cl1	172.23 (8)
C14—Sn1—O1	83.7 (2)	Cl2—Sn1—Cl1	98.73 (4)
C13—Sn1—O1	85.3 (2)	S1—O1—Sn1	121.8 (2)
C14—Sn1—O2	84.2 (2)	O1—S1—C1	105.0 (2)
C13—Sn1—O2	85.2 (2)	O1—S1—C15	105.8 (2)
O1—Sn1—O2	86.03 (1)	C1—S1—C15	100.8 (2)
C14—Sn1—Cl2	95.34 (1)	S2—O2—Sn1	127.6 (2)
C13—Sn1—Cl2	94.7 (2)	O2—S2—C7	104.3 (2)
O1—Sn1—Cl2	175.04 (8)	O2—S2—C16	105.4 (2)
O2—Sn1—Cl2	89.03 (8)	C7—S2—C16	99.3 (2)
C14—Sn1—Cl1	94.94 (1)	C15^i—C15—S1	113.0 (4)
C13—Sn1—Cl1	94.2 (2)	C16^{ii}—C16—S2	112.1 (4)
O1—Sn1—Cl1	86.21 (8)		

Symmetry codes: (i) $1 - x, 1 - y, -z$; (ii) $-x, 1 - y, -z$.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989). Cell refinement: *CAD*-4 *Software*. Data reduction: *SDP* (Frenz, 1978). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ORTEP* (Johnson, 1965).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: FG1084). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Phenylimidopentachloroniobate(V) Dianion with *N*-Allylphenylammonium Counterion

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Abstract

Bis[phenyl(2-propenyl)ammonium] pentachloro(phenyl-imido)niobate(V), $(C_9H_{12}N)_2[NbCl_5(C_6H_5N)]$, is a product of the reaction of niobium pentachloride and *N*-allylphenylamine. The coordinated secondary amine loses its allyl group and forms an imino bond to the metal. Unreacted *N*-allylphenylamine behaves as a proton acceptor and is a counterion in the solid state. In the crystalline state, the asymmetric unit consists of two octahedral pentachloro(phenylimido)niobate(V) dianions and four *N*-allylphenylammonium cations.

Comment

Several routes exist for synthesizing alkylimido complexes of early transition metals: (i) azobenzene has been reported to react metathetically with $[Nb_2Cl_6-(Me_2S)_3]$ to form a monomeric phenylimido complex (Cotton, Duraj & Roth, 1984) and (ii) *tert*-butylamide lithium together with LiNMe$_2$ reacts with niobium and tantalum pentahalides to form tris(dimethylamido)–*tert*-butylimido complexes (Nugent & Harlow, 1978). It is also known that even osmium tetraoxide can be used as a metal source and oxoimino derivatives are formed when osmium(VIII) oxide is allowed to react with imido selenium reagents (Chong, Oshima & Sharpless, 1977). Many of the known niobium and tantalum–imido complexes are cyclopentadienyl derivatives, for example, half-sandwich monocyclopentadienyl–methylimido complexes (Williams *et al.,* 1992) and *ansa*-metallocene derivatives with butylimido ligands (Chernega, Malcolm & Suárez, 1995).

The title complex, (I), was prepared by the direct reaction of *N*-allylphenylamine and niobium pentachloride in toluene. The pentachloro(phenylimido)niobium dianion is formed when *N*-allylphenylamine loses its allylic group. Some of the *N*-allylphenylamine molecules form ammonium ions by behaving as proton acceptors and these exist as counterions in the solid state. Two pentachloro(phenylimido)niobium dianions and four *N*-allylphenylammonium ions form the asymmetric unit.

(I)
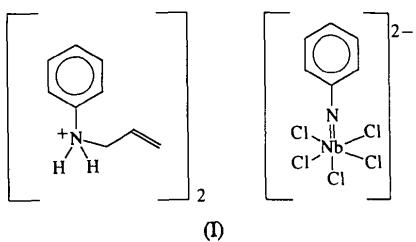
Both pentachloro(phenylimido)niobium units in the asymmetric unit are distorted octahedra, with all the *cis*-positioned N—Nb—Cl angles clearly greater than 90° (Fig. 1). For one octahedron the angles are between 95.0 (2) (N1*A*—Nb1*A*—Cl4*A*) and 97.7 (2)° (N1*A*—Nb1*A*—Cl3*A*), while in the other octahedron they vary between 93.9 (2) (N1*B*—Nb1*B*—Cl3*B*) and 97.2 (2)° (N1*B*—Nb1*B*—Cl1*B*). The Nb—N—C angles are almost linear, with values of 174.0 (5) for Nb1*A*—N1*A*—C1*A* and 172.8 (6)° for Nb1*B*—N1*B*—C1*B*. This supports the theory of the role of the nitrogen lone pair, which donates electron density to the metal center. The bond has been assumed to have triple-bond character (Nugent & Harlow, 1978). The Nb1*A*—N1*A* and Nb1*B*—N1*B* distances are 1.754 (5) and 1.746 (6) Å, respectively. These values are close to the value [1.731 (3) Å] found in the [Nb(N^{t}Bu)Cl$_4$(py)]$^-$ monoanion (Clegg, Errington, Hockless & Redshaw, 1991). The imido H atom has a significant effect on the *trans* positions, the *trans* bond lengths being the longest, with values of 2.692 (2) and 2.655 (2) Å for Nb1*A*—Cl5*A* and Nb1*B*—Cl5*B*, respectively. The equatorial Nb—Cl bond lengths vary between 2.415 (2) and 2.472 (2) Å [Nb1*A*—Cl1*A* and Nb1*A*—Cl3*A*, respectively] for one octahedron, whereas they are between 2.374 (2) and 2.478 (2) Å [Nb1*B*—Cl4*B* and Nb1*B*—Cl1*B*, respectively] in the second octahedron.
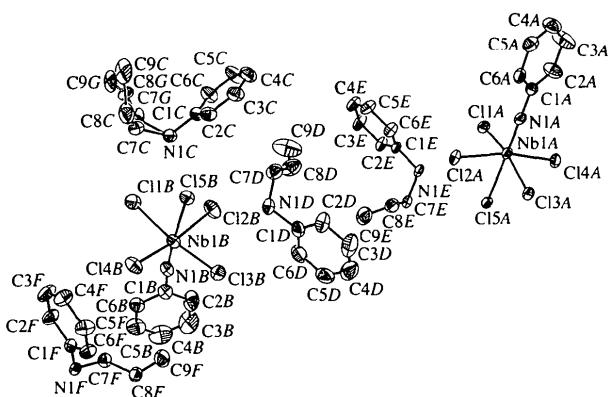
Fig. 1. A view of the asymmetric unit of (I), with ellipsoids drawn at the 30% probability level and H atoms omitted for clarity.

The protonated *N*-allylphenylammonium counterions show disordering in the allylic part, with the terminal C atoms in the chain having large displacement parameters. The disorder is most pronounced in the C7*C*–C9*C*

chain, which can be refined in two orientations, the additional chain being denoted as C7*G*–C9*G*. The refined population parameter of 0.50 (2) indicates equal populations for these different sites. The refinement did not improve C—C bond lengths, but displacement parameters were significantly reduced. Refinement of the other allyl chains gave good results. The double bonds were easily located. Terminal C8—C9 bond lengths vary between 1.202 (14) and 1.292 (12) Å, whereas the C7—C8 bond lengths are between 1.462 (12) and 1.472 (9) Å. C—N bonds in the cations are normal, varying between 1.467 (8) and 1.500 (9) Å for the N1—C1 bonds to the aromatic rings, whereas the allyl group is attached to nitrogen with N1—C7 distances between 1.502 (8) and 1.506 (8) Å.

Experimental

Crystal data

$(C_9H_{12}N)_2[NbCl_5(C_6H_5N)]$	Mo $K\alpha$ radiation
$M_r = 629.66$	$\lambda = 0.71069$ Å
Triclinic	Cell parameters from 25
$P\bar{1}$	reflections
$a = 11.868 (7)$ Å	$\theta = 5$–$25°$
$b = 12.200 (10)$ Å	$\mu = 0.906$ mm^{-1}
$c = 20.746 (11)$ Å	$T = 193 (2)$ K
$\alpha = 96.83 (5)°$	Prismatic
$\beta = 100.85 (5)°$	$0.30 \times 0.27 \times 0.25$ mm
$\gamma = 101.16 (4)°$	Purple
$V = 2857 (3)$ Å^3	
$Z = 4$	
$D_x = 1.464$ Mg m^{-3}	
D_m not measured	

Data collection

Rigaku AFC-7S diffractometer	6988 observed reflections
	$[I > 2\sigma(I)]$
2θ–ω scans	$\theta_{max} = 25°$
Absorption correction:	$h = -14 \rightarrow 13$
ψ scan (North, Phillips	$k = 0 \rightarrow 14$
& Mathews, 1968)	$l = -24 \rightarrow 24$
$T_{min} = 0.70$, $T_{max} = 0.80$	3 standard reflections
8824 measured reflections	monitored every 200
8824 independent reflections	reflections
	intensity decay: 0.8%

Refinement

Refinement on F^2	$(\Delta/\sigma)_{max} = -0.065$
$R(F) = 0.065$	$\Delta\rho_{max} = 0.731$ e Å^{-3}
$wR(F^2) = 0.150$	$\Delta\rho_{min} = -0.861$ e Å^{-3}

S = 1.042
8824 reflections
623 parameters
H atoms riding
$w = 1/[\sigma^2(F_o^2) + (0.058P)^2 + 5.4193P]$
where $P = (F_o^2 + 2F_c^2)/3$

Extinction correction: none
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

	x	y	z	U_{eq}
C9D	−0.0651 (12)	−0.1841 (12)	−0.7693 (7)	0.155 (6)
C7E	−0.4404 (6)	−0.0530 (6)	−0.6312 (3)	0.052 (2)
C8E	−0.3802 (7)	−0.0029 (8)	−0.6797 (4)	0.067 (2)
C9E	−0.3824 (10)	−0.0552 (11)	−0.7380 (5)	0.105 (4)
C7F	−0.4372 (6)	−0.3722 (5)	−1.3430 (4)	0.052 (2)
C8F	−0.4912 (7)	−0.2818 (6)	−1.3177 (4)	0.059 (2)
C9F	−0.4678 (8)	−0.2299 (7)	−1.2586 (4)	0.078 (2)

† Refined occupancy of 0.50 (2).

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters ($Å^2$)

$$U_{eq} = (1/3)\sum_i\sum_j U_{ij}a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Nb1A	−0.27892 (5)	0.30579 (5)	−0.45346 (3)	0.0407 (2)
Nb1B	−0.18452 (6)	−0.30352 (6)	−1.08294 (3)	0.0549 (2)
Cl1A	−0.25495 (15)	0.13279 (13)	−0.41239 (9)	0.0505 (4)
Cl2A	−0.20993 (15)	0.24425 (14)	−0.55114 (9)	0.0533 (4)
Cl3A	−0.34548 (14)	0.45621 (13)	−0.51033 (8)	0.0471 (4)
Cl4A	−0.3905 (2)	0.35338 (15)	−0.37191 (9)	0.0541 (4)
Cl5A	−0.48483 (13)	0.17306 (12)	−0.52253 (8)	0.0418 (4)
Cl1B	−0.0481 (2)	−0.4334 (2)	−1.08540 (11)	0.0744 (6)
Cl2B	−0.1834 (2)	−0.3313 (2)	−0.96749 (11)	0.0857 (7)
Cl3B	−0.2849 (2)	−0.1510 (2)	−1.06521 (11)	0.0750 (6)
Cl4B	−0.1436 (2)	−0.2490 (2)	−1.18372 (10)	0.0742 (6)
Cl5B	0.0079 (2)	−0.14905 (14)	−1.02175 (9)	0.0547 (4)
N1A	−0.1436 (5)	0.3872 (4)	−0.4066 (3)	0.0481 (13)
N1B	−0.3143 (5)	−0.4037 (5)	−1.1193 (3)	0.057 (2)
N1C	0.1481 (5)	−0.3125 (5)	−0.9477 (3)	0.0565 (15)
N1D	−0.1281 (5)	−0.0430 (5)	−0.9081 (3)	0.060 (2)
N1E	−0.3575 (4)	−0.0400 (4)	−0.5647 (3)	0.0456 (13)
N1F	−0.3795 (4)	−0.3417 (4)	−1.3989 (3)	0.0469 (13)
C1A	−0.0382 (6)	0.4443 (5)	−0.3645 (4)	0.049 (2)
C2A	−0.0261 (8)	0.4543 (8)	−0.2971 (4)	0.084 (3)
C3A	0.0817 (10)	0.5100 (11)	−0.2557 (5)	0.113 (4)
C4A	0.1746 (8)	0.5517 (8)	−0.2825 (5)	0.087 (3)
C5A	0.1620 (7)	0.5428 (6)	−0.3489 (5)	0.065 (2)
C6A	0.0570 (6)	0.4902 (6)	−0.3906 (4)	0.053 (2)
C1B	−0.4237 (7)	−0.4718 (6)	−1.1469 (4)	0.061 (2)
C2B	−0.5150 (10)	−0.4734 (10)	−1.1143 (6)	0.105 (4)
C3B	−0.6243 (12)	−0.5441 (14)	−1.1423 (8)	0.144 (6)
C4B	−0.6393 (11)	−0.6096 (12)	−1.2037 (9)	0.135 (5)
C5B	−0.5520 (10)	−0.6072 (9)	−1.2357 (6)	0.101 (3)
C6B	−0.4439 (7)	−0.5404 (6)	−1.2081 (4)	0.067 (2)
C1C	0.1988 (6)	−0.2380 (6)	−0.8825 (4)	0.054 (2)
C2C	0.2320 (6)	−0.1233 (6)	−0.8811 (4)	0.060 (2)
C3C	0.2737 (7)	−0.0554 (7)	−0.8203 (4)	0.071 (2)
C4C	0.2862 (8)	−0.1007 (8)	−0.7632 (4)	0.077 (2)
C5C	0.2574 (9)	−0.2139 (9)	−0.7660 (4)	0.093 (3)
C6C	0.2122 (8)	−0.2862 (7)	−0.8260 (4)	0.076 (2)
C1D	−0.2215 (7)	0.0180 (8)	−0.8945 (4)	0.067 (2)
C2D	−0.1875 (9)	0.1252 (8)	−0.8615 (5)	0.089 (3)
C3D	−0.2776 (14)	0.1816 (12)	−0.8528 (7)	0.125 (4)
C4D	−0.3889 (14)	0.1296 (15)	−0.8752 (7)	0.125 (5)
C5D	−0.4230 (10)	0.0221 (17)	−0.9067 (6)	0.141 (6)
C6D	−0.3355 (11)	−0.0358 (11)	−0.9157 (5)	0.103 (4)
C1E	−0.2616 (6)	−0.1003 (5)	−0.5662 (3)	0.0430 (15)
C2E	−0.2850 (6)	−0.2142 (6)	−0.5639 (4)	0.058 (2)
C3E	−0.1933 (7)	−0.2696 (7)	−0.5655 (5)	0.075 (2)
C4E	−0.0842 (7)	−0.2120 (6)	−0.5678 (4)	0.066 (2)
C5E	−0.0641 (6)	−0.0999 (6)	−0.5704 (4)	0.064 (2)
C6E	−0.1529 (6)	−0.0409 (6)	−0.5684 (4)	0.058 (2)
C1F	−0.2600 (6)	−0.2706 (6)	−1.3788 (3)	0.048 (2)
C2F	−0.1671 (7)	−0.3222 (6)	−1.3710 (4)	0.069 (2)
C3F	−0.0556 (12)	−0.2579 (7)	−1.3501 (5)	0.084 (3)
C4F	−0.0357 (7)	−0.1427 (7)	−1.3367 (4)	0.070 (2)
C5F	−0.1308 (7)	−0.0911 (7)	−1.3438 (4)	0.069 (2)
C6F	−0.2429 (6)	−0.1555 (6)	−1.3651 (4)	0.057 (2)
C7C†	0.238 (2)	−0.305 (2)	−0.9966 (10)	0.059 (6)
C8C†	0.306 (3)	−0.292 (3)	−0.9967 (17)	0.114 (15)
C9C†	0.439 (3)	−0.286 (3)	−0.9486 (18)	0.122 (12)
C7G†	0.2334 (19)	−0.370 (2)	−0.9731 (16)	0.088 (9)
C8G†	0.3423 (16)	−0.3522 (14)	−0.9643 (10)	0.058 (5)
C9G†	0.434 (3)	−0.286 (3)	−0.9835 (14)	0.099 (10)
C7D	−0.0414 (7)	−0.0565 (8)	−0.8482 (4)	0.075 (2)
C8D	−0.0971 (9)	−0.1151 (10)	−0.8009 (6)	0.101 (3)

Table 2. Selected geometric parameters (Å, °)

Nb1A—N1A	1.754 (5)	Nb1B—Cl4B	2.374 (2)
Nb1A—Cl1A	2.415 (2)	Nb1B—Cl3B	2.423 (2)
Nb1A—Cl2A	2.417 (2)	Nb1B—Cl2B	2.456 (2)
Nb1A—Cl4A	2.421 (2)	Nb1B—Cl1B	2.478 (2)
Nb1A—Cl3A	2.472 (2)	Nb1B—Cl5B	2.655 (2)
Nb1A—Cl5A	2.692 (2)	N1A—C1A	1.384 (8)
Nb1B—N1B	1.746 (6)	N1B—C1B	1.376 (9)
N1A—Nb1A—Cl1A	95.1 (2)	N1B—Nb1B—Cl3B	93.9 (2)
N1A—Nb1A—Cl2A	97.3 (2)	Cl4B—Nb1B—Cl3B	92.01 (9)
Cl1A—Nb1A—Cl2A	89.89 (6)	N1B—Nb1B—Cl2B	96.7 (2)
N1A—Nb1A—Cl4A	95.0 (2)	Cl4B—Nb1B—Cl2B	167.04 (8)
Cl1A—Nb1A—Cl4A	92.41 (6)	Cl3B—Nb1B—Cl2B	88.33 (9)
Cl2A—Nb1A—Cl4A	167.30 (7)	N1B—Nb1B—Cl1B	97.2 (2)
N1A—Nb1A—Cl3A	97.7 (2)	Cl4B—Nb1B—Cl1B	89.68 (9)
Cl1A—Nb1A—Cl3A	167.17 (6)	Cl3B—Nb1B—Cl1B	168.54 (7)
Cl2A—Nb1A—Cl3A	88.29 (6)	Cl2B—Nb1B—Cl1B	87.51 (9)
Cl4A—Nb1A—Cl3A	86.70 (6)	N1B—Nb1B—Cl5B	176.8 (2)
N1A—Nb1A—Cl5A	177.4 (2)	Cl4B—Nb1B—Cl5B	86.48 (7)
Cl1A—Nb1A—Cl5A	82.35 (6)	Cl3B—Nb1B—Cl5B	84.39 (7)
Cl2A—Nb1A—Cl5A	83.02 (6)	Cl2B—Nb1B—Cl5B	80.66 (7)
Cl4A—Nb1A—Cl5A	84.91 (6)	Cl1B—Nb1B—Cl5B	84.40 (7)
Cl3A—Nb1A—Cl5A	84.83 (6)	C1A—N1A—Nb1A	174.0 (5)
N1B—Nb1B—Cl4B	96.2 (2)	C1B—N1B—Nb1B	172.8 (6)

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1993a). Cell refinement: *MSC/AFC Diffractometer Control Software*. Data reduction: *TEXSAN* (Molecular Structure Corporation, 1993b). Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990a). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *SHELXTL/PC* (Sheldrick, 1990b). Software used to prepare material for publication: *SHELXL93*.

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Racemic (α-Ferrocenylphenacyl)triphenyl-phosphonium Iodide

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Abstract

In racemic (α-ferrocenylphenacyl)triphenylphosphonium iodide, $[Fe(C_5H_5)(C_{31}H_{25}OP)]I$, the cations are involved in C—H···I⁻ interactions with short C···I distances of 3.836(7), 3.932(7) and 3.995(7) Å.

Comment

The structures of (ferrocenylmethyl)triphenylphosphonium iodide and 1,1′-ferrocenediylbis(methylphenylphosphonium iodide) (as the dichloromethane solvate), $[Fe\{(C_5H_4)CH_2P(C_6H_5)_3\}_2]^{2+}.2I^-.CH_2Cl_2$, have recently been found to exhibit extensive three-dimensional networks of C—H···I⁻ interactions (Glidewell, Zakaria, Ferguson & Gallagher, 1994). In a similar way, the structures of (ferrocenylmethyl)trimethylammonium iodide and hexa-*N*-methylferrocene-1,1′-diylbis(methylammonium iodide), $[Fe\{(C_5H_4)CH_2N(CH_3)_3\}_2]^{2+}.2I^-$, are also characterized by such interactions (Ferguson, Gallagher, Glidewell & Zakaria, 1994). In all of these structures there are C···I⁻ distances in the range 3.8–3.9 Å. Such C—H···I⁻ hydrogen bonds are uncommon; for example, in tetraphenylphosphonium iodide (Schweizer, Baldacchini & Rheingold, 1989) and dimethyldiphenylphosphonium iodide (Staples, Carlson, Wang & Fackler, 1995), compounds related to (ferrocenylmethyl)triphenylphosphonium iodide, there are no C···I⁻ distances less than 4.0 Å; however, well documented examples occur in the structures

of benzyltriphenylphosphonium iodide (Archer, Modro & Nassimbeni, 1981), methylphenylphospholanium iodide, $[(CH_3)(C_6H_5)P(CH_2)_4]^+.I^-$ (Alver & Holtedahl, 1967), 3,3-dimethyl-1,1-diphenylphosphetanium iodide, $[(C_6H_5)_2PCH_2C(CH_3)_2CH_2]^+.I^-$ (Mazhar-ul-Haque, 1979), and bis[1 , 2-bis(diphenylphosphino)ethane]-platinum(II) diiodide deuterochloroform solvate, $[\{(C_6H_5)_2PCH_2CH_2P(C_6H_5)_2\}_2Pt]^{2+}.2I^-.2(CDCl_3)$ (Ferguson, Lough, McAlees & McCrindle, 1993). Particularly short C···I⁻ distances (3.67 Å) occur in the fulleride salt $[(C_6H_5)_4P]_2(C_{60})I_{0.35}$ (Penicaud, Perez-Benitez, Gleason, Munoz & Escudro, 1993), but the apparent shortness may be influenced by the low occupancy (35%) of the iodide sites. Here we report the structure of (α-ferrocenylphenacyl)triphenylphosphonium iodide, $[\{(C_5H_5)Fe(C_5H_4)\}CH(COC_6H_5)P(C_6H_5)_3]^+.I^-$, (I), a benzoylated derivative of (ferrocenylmethyl)triphenylphosphonium iodide, which also contains short C···I⁻ distances.
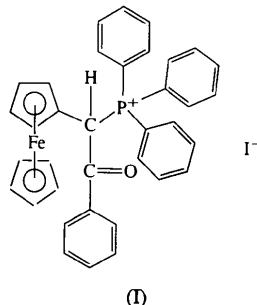
(I)

The structure consists of ion pairs (Fig. 1) within which there is a single short C—H···I⁻ interaction involving C62, characterized by C···I 3.836(7) Å and C—H···I 151°. There are also two further fairly short C—H···I⁻ interactions involving C44 in the cation at $(-\frac{1}{2} + x, y, \frac{1}{2} - z)$ [C···I 3.932(7) Å, C—H···I 134°] and C33 in the cation at $(\frac{3}{2} - x, \frac{1}{2} + y, z)$ [C···I 3.995(7) Å, C—H···I 132°], which serve to generate a continuous network. The cations are chiral, but the space group accommodates equal numbers of *R* and *S* enantiomers. The almost perfectly staggered conformation about the C1—C2 bond is such that O2 and H1 are antiperiplanar, while O2 and P1 are synclinal; despite this, the O···P distance of 3.184(6) Å is significantly shorter than the sum of van der Waals radii (3.45 Å; Bondi, 1984). Since the O atom undoubtedly carries a partial negative charge, the occurrence of an attractive P···O interaction is not surprising. Similar, although stronger, attractive interactions have been observed previously in acyl and sulfonyl ylides of arsenic and antimony (Ferguson, Glidewell, Lloyd, Metcalfe & Ruhl, 1987; Ferguson *et al.*, 1988). The conformation about the C1—P1 bonds departs from perfect staggering by *ca* 14(2)°. The C1—P1 bond [1.845(6) Å] is significantly longer than the corresponding bonds in both (ferrocenylmethyl)triphenylphosphonium iodide [1.813(2) Å] and