complexes of $InCl_3$ to have been structurally characterized by single-crystal X-ray studies. The structure consists of discrete molecules of (2), in which the environment of the In atom shows only slight distortions from an ideal trigonal bipyramidal geometry [P—In—P angle of 175.6 (1)°]. This is in agreement with the geometry proposed from the powder diffraction study previously carried out on this compound (Beattie, Ozin & Blayden, 1969). The molecular structure and atomic numbering scheme are shown in Fig. 2, with bond distances and angles in Table 5.

The mean In—Cl distance is 2.49 (1) Å and the mean In—P distance is 2.576 (3) Å. These can be compared to the distances in $InCl_3(PPh_3)_2$, which has a shorter mean In—Cl distance of 2.38 Å and a longer mean In—P distance of 2.71 Å. Taken together these differences suggest that PPh_3 is a weaker ligand than PMe_3, with the stronger In—Cl bonds compensating for the weaker In—P bonds. The extra steric bulk of the PPh_3 ligand may contribute to this weakness. PPh_3 has a Tolman cone angle (Tolman, 1970) of 145°, while PMe_3 has a cone angle of 118°. Comparison of the In—P bond distances in (2) with other known In—P distances suggests that the mean value of 2.576 Å found in (2) is closer to a 'normal' single-bond distance than the longer distance in $InCl_3(PPh_3)_2$. For example, it is similar to the mean In—P values in $In(P^tBu_2)_3$, in the various adducts of InI_3 noted above, and in $[Li(THF)_4]^+$ $[In(PPh_2)_4]^-$ (2.58 Å) (Carrano, Cowley, Giolando, Jones, Nunn & Power, 1988). The mean In—Cl bond distance of 2.49 Å is close to the value of 2.45 Å in $[Et_4N]_2[InCl_5]$ (Brown, Einstein & Tuck, 1969) and $[InCl_4(H_2O)_2]^-$ (Zeigler, Schlimper, Nuber, Weiss & Ertl, 1975). It is, however, somewhat longer than the values of 2.38 Å found in $InCl_3(PPh_3)_2$ and 2.37 Å in $InCl_3(NMe_3)_2$. Clearly, the nature of the axial ligand in these trigonal bipyramidal complexes has a significant effect on the lengths of the equatorial In—Cl bonds.

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Structural Characterization of 1,1,1,2,2,2,3,3,3-Nonacarbonyl-1,2-μ-iodo-1,2,3-[μ_3-(phenylpyridylphosphido)-μ-*P,N*]-*triangulo*-triruthenium

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Abstract. $C_{20}H_9INO_9PRu_3$, $M_r = 868.4$, monoclinic, $P2_1/c$, $a = 10.058$ (1), $b = 14.182$ (3), $c = 17.988$ (3) Å, $\beta = 97.94$ (2)°, $V = 2541$ Å^3, $Z = 4$, $D_x = 2.269$ g cm^{-3}, λ(Mo $K\alpha$) = 0.71069 Å, $\mu = 30.40$ cm^{-1}, $F(000) = 1632$, room temperature, final $R = 0.025$ for 3564 unique observed reflections with I

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$\geq 3\sigma(I)$. The compound consists of an open trinuclear cluster capped by the phenylpyridylphosphido ligand in a μ_3-η^2 fashion. The phosphido group spans the open edge of the metal triangle whereas the pyridyl group is coordinated to the unique Ru center. The bridging I atom spans the same edge as the phosphido group. The environment of each Ru atom is completed by three terminal carbonyl ligands.

Introduction. As part of our efforts to tailor ruthenium carbonyl clusters for applications in homogeneous catalysis (Lugan, Laurent, Lavigne, Newcomb, Liimatta & Bonnet, 1990), we have devised a series of complexes that combine two different kinds of ancillary ligands, namely (i) a face-bridging polydentate group which contributes to the retention of the metal ensemble under catalytic conditions, and (ii) a lightly bridging ligand which is susceptible to the opening of a vacant coordination site on the cluster by simply moving to a terminal position. In the title complex, the above ligand types are respectively represented by a phosphidopyridyl group (Lugan, Lavigne, Bonnet, Réau, Niebecker & Tkatchenko, 1988) and an iodide atom (Han, Geoffroy & Rheingold, 1987; Lavigne, 1990). The formation of this neutral complex is the result of an electrophilic addition of I^+ to the metal—metal bond of an electron-rich polymetallic precursor.

Experimental. The title compound, $Ru_3[\mu_3\text{-}\eta^2\text{-}P(C_6H_5)(C_5H_4N)](\mu\text{-}I)(CO)_9$, was prepared by reaction of $[PPN][Ru_3[\mu_3\text{-}\eta^2\text{-}P(C_6H_5)(C_5H_4N)](CO)_9]$ (Lugan, Lavigne, Bonnet, Réau, Niebecker & Tkatchenko, 1988) with iodine in ethanol at room temperature [PPN = bis(triphenylphosphoranylidene)ammonium cation]. Crystals suitable for X-ray diffraction obtained by slow evaporation of an acetone/ethanol solvent mixture at room temperature. Boundary faces {100}, (102), {001}, {011}, {010}, {110}; dimensions 0.28 × 0.40 × 0.43 mm. Enraf–Nonius CAD-4 diffractometer, graphite-monochromatized Mo $K\alpha$ radiation. Cell constants obtained from a least-squares fit to the setting angles of 25 randomly selected reflections in the range $16 < 2\theta(\text{Mo } K\alpha) < 28°$. 4543 data collected in the range $2 < 2\theta(\text{Mo } K\alpha) < 49°$ (h: 0 to 11, k: 0 to 16, l: −21 to 21) using the $\omega/2\theta$ scanning procedure [scan speed: $2° \text{ min}^{-1}$; scan range: $(1.0 + 0.35\tan\theta)°$]. Take-off angle 5.5°. Monitoring of three standard reflections every 2 h showed no intensity fluctuations greater than 1%.

Data reduction, resolution and refinement of the structure were carried out using the *SDP* crystallographic computing package (Frenz, 1985). Lorentz, polarization and absorption corrections applied to the intensity data. Absorption correction applied using the numerical method (Coppens, Leiserowitz & Rabinovich, 1965). Minimum and maximum transmission factors were respectively 0.387 and 0.579. After averaging equivalent reflections, 3564 unique data having $F_o^2 \geq 3\sigma(F_o^2)$ were subsequently used for the structure solution.

The positions of the Ru, P and I atoms were determined by direct methods (*MULTAN*; Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982). All remaining non-H atoms were located by the usual combination of full-matrix least-squares refinements and difference electron density syntheses. Final refinements were conducted using *SHELX*76 (Sheldrick, 1976). All non-H atoms were allowed to vibrate anisotropically, except the C atoms of the phenyl ring which were treated as rigid groups (D_{6h} symmetry, C—C = 1.395, C—H = 0.95 Å). The positions of the H atoms attached to the pyridyl group were idealized (C—H = 0.95 Å). The function minimized was $\sum w(|F_o| - |F_c|)^2$, where $w = 1/[\sigma^2(|F|) + (0.02|F_o|)^2]$. Final $R = 0.025$, $wR = 0.029$, $S = 1.68$ for 274 variable parameters. The residual peaks in the final electron density difference map were in the range 1.01, −0.88 e Å^{-3}; $\Delta/\sigma_{max} = 0.14$. Scattering

Table 1. *Fractional atomic coordinates and isotropic or equivalent isotropic temperature factors* (Å^2 × 10^2) *with e.s.d.'s in parentheses*

$$U_{eq} = (U_{11}U_{22}U_{33})^{1/3}.$$

	x	y	z	U_{eq}/U_{iso}
Ru(1)	0.16007 (3)	0.25987 (3)	0.06947 (2)	3.41 (6)
Ru(2)	0.27823 (4)	0.13858 (2)	0.18542 (2)	3.44 (6)
Ru(3)	0.18751 (3)	0.37510 (2)	0.20082 (2)	3.23 (6)
I(1)	0.12720 (3)	0.22118 (2)	0.28796 (2)	4.69 (6)
P(1)	0.3862 (1)	0.28613 (7)	0.19911 (6)	3.0 (2)
C(1)	−0.0057 (5)	0.2234 (4)	0.0971 (3)	5.0 (9)
O(1)	−0.1081 (4)	0.2022 (3)	0.1103 (3)	8.0 (9)
C(2)	0.0777 (5)	0.3550 (4)	0.0014 (3)	4.7 (8)
O(2)	0.0231 (5)	0.4040 (3)	−0.0412 (2)	8.0 (9)
C(3)	0.1588 (5)	0.1587 (4)	0.0002 (3)	5.4 (9)
O(3)	0.1528 (6)	0.0971 (4)	−0.0417 (3)	10. (1)
C(4)	0.3802 (5)	0.1016 (3)	0.1118 (3)	4.6 (8)
O(4)	0.4477 (4)	0.0789 (3)	0.0695 (2)	6.9 (8)
C(5)	0.1415 (5)	0.0415 (4)	0.1601 (3)	5.5 (9)
O(5)	0.0633 (4)	−0.0144 (3)	0.1478 (3)	8.5 (9)
C(6)	0.3870 (5)	0.0730 (3)	0.2646 (3)	4.7 (8)
O(6)	0.4575 (5)	0.0313 (3)	0.3072 (2)	7.5 (8)
C(7)	0.0003 (5)	0.4114 (4)	0.1810 (3)	5.1 (9)
O(7)	−0.1093 (4)	0.4314 (3)	0.1690 (3)	7.8 (9)
C(8)	0.2335 (5)	0.4589 (4)	0.2856 (3)	4.8 (8)
O(8)	0.2595 (4)	0.5182 (3)	0.3281 (2)	7.4 (8)
C(9)	0.2328 (5)	0.4586 (3)	0.1291 (3)	4.0 (7)
O(9)	0.2626 (4)	0.5121 (3)	0.0872 (2)	5.8 (7)
C(11)	0.5323 (3)	0.2903 (2)	0.2725 (2)	3.63 (9)
C(12)	0.5360 (3)	0.3495 (2)	0.3347 (2)	4.9 (1)
C(13)	0.6469 (3)	0.3481 (2)	0.3906 (2)	6.5 (2)
C(14)	0.7541 (3)	0.2876 (2)	0.3843 (2)	6.8 (2)
C(15)	0.7504 (3)	0.2284 (2)	0.3221 (2)	5.9 (1)
C(16)	0.6395 (3)	0.2298 (2)	0.2662 (2)	4.7 (1)
N(1)	0.3613 (4)	0.3031 (3)	0.0519 (2)	3.6 (6)
C(21)	0.4554 (4)	0.3120 (3)	0.1132 (2)	3.2 (7)
C(22)	0.5843 (4)	0.3427 (3)	0.1060 (3)	4.0 (8)
C(23)	0.6190 (5)	0.3600 (4)	0.0359 (3)	6. (1)
C(24)	0.5234 (5)	0.3497 (4)	−0.0248 (3)	6. (1)
C(25)	0.3964 (5)	0.3205 (4)	−0.0155 (2)	4.7 (8)

Table 2. *Selected interatomic distances* (Å) *and bond angles* (°) *with e.s.d.'s in parentheses*

Ru(1)—Ru(2)	2.835 (1)	Ru(3)—C(8)	1.939 (5)
Ru(1)—Ru(3)	2.855 (1)	Ru(3)—C(9)	1.855 (5)
Ru(2)···Ru(3)	3.498 (1)	P(1)—C(21)	1.818 (3)
Ru(1)—N(1)	2.179 (4)	P(1)—C(11)	1.835 (3)
Ru(1)—C(1)	1.877 (6)	N(1)—C(21)	1.355 (5)
Ru(1)—C(2)	1.930 (5)	O(1)—C(1)	1.130 (7)
Ru(1)—C(3)	1.898 (5)	O(2)—C(2)	1.121 (6)
Ru(2)—I(1)	2.803 (1)	O(3)—C(3)	1.151 (7)
Ru(2)—P(1)	2.355 (1)	O(4)—C(4)	1.134 (7)
Ru(2)—C(4)	1.859 (5)	O(5)—C(5)	1.117 (7)
Ru(2)—C(5)	1.955 (5)	O(6)—C(6)	1.135 (6)
Ru(2)—C(6)	1.913 (4)	O(7)—C(7)	1.130 (6)
Ru(3)—I(1)	2.802 (1)	O(8)—C(8)	1.142 (6)
Ru(3)—P(1)	2.368 (1)	O(9)—C(9)	1.138 (6)
Ru(3)—C(7)	1.937 (5)		
Ru(2)—Ru(1)—Ru(3)	75.86 (1)	Ru(3)—Ru(1)—C(3)	165.2 (2)
Ru(2)—Ru(1)—N(1)	88.50 (9)	N(1)—Ru(1)—C(1)	173.0 (2)
Ru(2)—Ru(1)—C(1)	86.3 (2)	N(1)—Ru(1)—C(2)	92.1 (2)
Ru(2)—Ru(1)—C(2)	172.1 (2)	N(1)—Ru(1)—C(3)	92.3 (2)
Ru(2)—Ru(1)—C(3)	89.3 (2)	C(1)—Ru(1)—C(2)	92.4 (2)
Ru(3)—Ru(1)—N(1)	88.47 (9)	C(1)—Ru(1)—C(3)	92.3 (2)
Ru(3)—Ru(1)—C(1)	85.8 (2)	C(2)—Ru(1)—C(3)	98.5 (2)
Ru(3)—Ru(1)—C(2)	96.3 (2)		
Ru(1)—Ru(2)—I(1)	91.17 (1)	I(1)—Ru(2)—C(6)	91.1 (2)
Ru(1)—Ru(2)—P(1)	71.22 (3)	P(1)—Ru(2)—C(4)	91.9 (2)
Ru(1)—Ru(2)—C(4)	82.2 (1)	P(1)—Ru(2)—C(5)	161.8 (2)
Ru(1)—Ru(2)—C(5)	92.6 (1)	P(1)—Ru(2)—C(6)	98.4 (2)
Ru(1)—Ru(2)—C(6)	168.9 (2)	C(4)—Ru(2)—C(5)	94.3 (2)
I(1)—Ru(2)—P(1)	81.02 (3)	C(4)—Ru(2)—C(6)	94.5 (2)
I(1)—Ru(2)—C(4)	171.6 (1)	C(5)—Ru(2)—C(6)	98.2 (2)
I(1)—Ru(2)—C(5)	91.2 (2)		
Ru(1)—Ru(3)—I(1)	90.77 (1)	I(1)—Ru(3)—C(9)	168.5 (2)
Ru(1)—Ru(3)—P(1)	70.70 (3)	P(1)—Ru(3)—C(7)	160.1 (2)
Ru(1)—Ru(3)—C(7)	91.1 (2)	P(1)—Ru(3)—C(8)	103.1 (2)
Ru(1)—Ru(3)—C(8)	170.9 (2)	P(1)—Ru(3)—C(9)	92.4 (2)
Ru(1)—Ru(3)—C(9)	78.1 (1)	C(7)—Ru(3)—C(8)	95.9 (2)
I(1)—Ru(3)—P(1)	80.82 (3)	C(7)—Ru(3)—C(9)	91.6 (2)
I(1)—Ru(3)—C(7)	91.7 (2)	C(8)—Ru(3)—C(9)	95.8 (2)
I(1)—Ru(3)—C(8)	94.8 (2)		
Ru(2)—I(1)—Ru(3)	77.21 (1)		
Ru(2)—P(1)—Ru(3)	95.51 (4)		
Ru(1)—C(1)—O(1)	176.7 (5)	Ru(2)—C(6)—O(6)	174.2 (5)
Ru(1)—C(2)—O(2)	173.8 (5)	Ru(3)—C(7)—O(7)	179.1 (5)
Ru(1)—C(3)—O(3)	177.4 (5)	Ru(3)—C(8)—O(8)	170.3 (5)
Ru(2)—C(4)—O(4)	176.7 (4)	Ru(3)—C(9)—O(9)	177.4 (5)
Ru(2)—C(5)—O(5)	177.9 (5)		
P(1)—C(21)—N(1)	111.5 (3)		

factors and anomalous-dispersion corrections were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV) except those of H which were taken from Stewart, Davidson & Simpson (1965). Final atomic coordinates and equivalent isotropic thermal parameters are given in Table 1.* Selected interatomic distances and angles are given in Table 2. A perspective view of the complex is given in Fig. 1.

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54811 (20 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: PA0254]

Discussion. The neutral complex described here is the result of an electrophilic addition of I^+ to the electron-rich metal—metal bond of the anion $[Ru_3\{\mu_3\text{-}\eta^2\text{-}P(C_6H_5)(C_5H_4N)\}(CO)_9]^-$. The molecular unit possesses approximate C_s symmetry. The compound can be described either as an open cluster or as a bent trinuclear chain of metal atoms. The distances Ru(1)—Ru(2) [2.835 (1) Å] and Ru(1)—Ru(3) [2.855 (1) Å] are in the range of those expected for an Ru—Ru bond in trinuclear clusters (Churchill, Hollander & Hutchinson, 1977). The distance Ru(2)···Ru(3) [3.498 (1) Å] is consistent with the absence of direct metal—metal interaction across this edge, in agreement with the electron counting scheme (50 cluster valence electrons). The phenylpyridylphosphido ligand is bound to the metal triangle in a μ_3-η^2 fashion: the pyridyl group is connected to the central metal atom of the chain [Ru(1)—N(1) = 2.179 (4) Å] whereas the phosphido group is connected to the two terminal Ru atoms, thereby supporting the open edge of the cluster [Ru(2)—P(1) = 2.355 (1); Ru(3)—P(1) = 2.368 (1) Å]. The latter edge is also supported by the I atom [Ru(2)—I(1) = 2.803 (1); Ru(3)—I(1) = 2.802 (1) Å]. The Ru—I distances are within the expected range (Colombié, Lavigne & Bonnet, 1986). The octahedral environment of each metal center is completed by three carbonyl ligands occupying terminal coordination sites. The Ru—C—O bond angles range between 170.3 (5)° for Ru(3)—C(8)—O(8) and 179.1 (5)° for Ru(3)—C(7)—O(7). A comparison of the Ru—C(O) bond lengths within the cluster (average 1.907 Å) clearly shows an important *trans* shortening effect of the I atom (Pidcock, Richards & Venanzi, 1966). Indeed, the two carbonyls *trans* to I(1) exhibit the shortest Ru—C(O) distances, Ru(2)—C(4) [1.859 (5) Å] and Ru(3)—C(9) [1.855 (5) Å]. This is

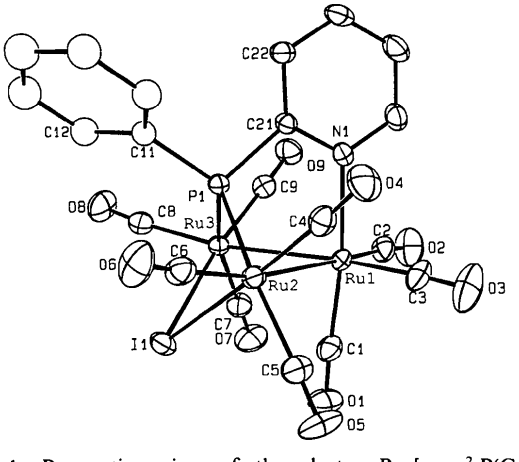

Fig. 1. Perspective view of the cluster $Ru_3[\mu_3\text{-}\eta^2\text{-}P(C_6H_5)(C_5H_4N)](\mu\text{-}I)(CO)_9$. Thermal ellipsoids are drawn at the 30% probability level.

particularly significant if we compare these distances with those of carbonyl ligands occupying coordination sites of comparable symmetry, namely Ru(2)—C(5) [1.955 (5) Å] and Ru(3)—C(7) [1.937 (5) Å] that are *trans* to the opposite bridgehead atom P(1).

Amongst the growing family of edge double-bridged trinuclear complexes of the iron triad (Albers, Robinson & Coville, 1986), the present species is the first involving a phosphorus and an iodide as bridgehead atoms.

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Structure of Di(5-β-methylallyl-2-phenyl-1,3-oxazole)zinc(II) Dichloride

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Abstract. Dichlorobis[5-(2-methylallyl)-2-phenyl-1,3-oxazole-*N*]zinc(II), $[ZnCl_2(C_{13}H_{13}NO)_2]$, M_r = 534.79, orthorhombic, *Fdd*2, a = 26.374 (3), b = 12.220 (2), c = 16.278 (3) Å, V = 5246 (2) Å^3, Z = 8, D_x = 1.350 g cm^{-3}, λ(Mo $K\alpha$) = 0.71069 Å, μ = 11.48 cm^{-1}, $F(000)$ = 2208, T = 300 K, final R = 0.037, wR = 0.034 for 1658 unique reflections with $F > 2\sigma(F)$. The compound consists of two substituted oxazole molecules complexed with one zinc dichloride molecule. The coordination around the Zn atom is a distorted tetrahedron. The oxazole ring is planar and is twisted 26° out of the phenyl-ring plane. The β-methylallyl is disordered.

Introduction. The reaction of *N*-cyanomethylbenzimidates with β-methylallylzinc chloride leads to the

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