Nb_6 cluster is bonded to one Cl(1) atom with Nb—Cl(1) distance of 2·667 (1) Å [2·654 (1) Å in $KLuNb_6Cl_{18}$].

2. *Lutetium environment.* The Lu atom is surrounded by six Cl(1) atoms belonging to six different units, forming a distorted octahedron, with Lu—Cl(1) distance of 2·603 (1) Å [$KLuNb_6Cl_{18}$: Lu—Cl(1) = 2·596 (1) Å]. This environment represented in Fig. 2(*b*) is closely similar to that in $KLuNb_6Cl_{18}$, the main difference being that in $CsLuNb_6Cl_{18}$ this chlorine octahedron is less regular owing to the absence of an inversion centre at the Lu atom. The values of the Cl(1)—Lu—Cl(1) angles are 89·93 (2) and 82·95 (2)° [*cf.* 90·33 (3)° in $KLuNb_6Cl_{18}$].

3. *Caesium environment.* The Cs coordination polyhedron is represented in Fig. 2(*c*). The Cs atom is bonded to twelve Cl atoms belonging to six different units: six Cl(1) at a distance of 3·772 (1) Å and six Cl(3) at a distance of 3·800 (1) Å. The Cs-atom site is then approximately a flattened hexagonal antiprism. In $KLuNb_6Cl_{18}$ the K atom is also surrounded by twelve Cl atoms but they belong only to four neighbouring units and the site so created is less regular (Ihmaïne *et al.*, 1988).

When comparing the structures of $CsLuNb_6Cl_{18}$ presented in this paper and the previously reported $KLuNb_6Cl_{18}$ structure, a close similarity appears between the $(Nb_6Cl_{18})^{4-}$ units, which exhibit in these two compounds $\bar{3}$ symmetry and comparable Nb—Nb and Nb—Cl distances. The actual difference is in the stacking of the $(Nb_6Cl_{18})^{4-}$ units: an approximately close-packed cubic arrangement ...*ABCA*... in $KLuNb_6Cl_{18}$ and an ...*AAA*... stacking type in $CsLuNb_6Cl_{18}$. This packing leaves a larger and more regular site for the Cs atom compared to the K-atom site in $KLuNb_6Cl_{18}$, while the Lu-atom site is approximately

the same size in the two structures, but appears somewhat less regular in $CsLuNb_6Cl_{18}$. Obviously the structural modification when Na, K or Rb monovalent cations are replaced by Cs is related to the necessity of formation of a site large enough to accommodate the Cs ion.

Another difference is the multiplicity of the monovalent cation sites. Owing to the chemical formula, the K-atom site in $KLuNb_6Cl_{18}$ is half-occupied (it is vacant in the ternary compound $LuNb_6Cl_{18}$) while in $CsLuNb_6Cl_{18}$ the Cs-atom site is fully occupied.

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The Structure of 1,1,1,2,2,2,3,3,3-Nonacarbonyl-1,2;1,3-(μ_2-dihydrido)-1,3-σ;2-π-[μ_3-η^2-methyl(phenyl)vinylidene]-*triangulo*-triruthenium

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Abstract. [$Ru_3H_2(CO)_9\{\mu_3$-η^2-CC$(CH_3)C_6H_5\}$], $M_r = 673·47$, triclinic, $P\bar{1}$, $a = 9·040$ (4), $b = 10·067$ (4), $c = 12·315$ (5) Å, $\alpha = 102·15$ (3), $\beta = 108·17$ (3), $\gamma = 92·43$ (3)°, $V = 1033·9$ (7) Å^3, $Z = 2$, $D_x = 2·163$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 2·17$ mm^{-1}, $F(000) = 644$, $T = 298$ K, $R = 0·023$ for 3404 measured reflections. The molecular structure consists of a triangle of ruthenium atoms, the two longest edges [Ru(1)—Ru(2) = 2·840 (1), Ru(1)—Ru(3) = 2·821 (1) Å] bridged by hydrides; the triangle is capped by an alkenylidene ligand which is formally σ-bonded to Ru(1) and Ru(3) [Ru(1)—C(10) =

2·057 (5), Ru(3)—C(10) = 2·019 (6) Å], and π-bonded to Ru(2) [Ru(2)—C(10) = 2·167 (4), Ru(2)—C(11) = 2·500 (4) Å]; each Ru atom is also bonded to three terminal carbonyl ligands.

Introduction. Transition-metal carbonyl clusters which contain an exposed carbido atom are of particular interest as models for examining the properties of surface carbides (Bradley, 1983), and the reactivity of tetrairon carbido clusters has been studied extensively (Shriver & Whitmire, 1982). It has recently been possible to investigate the chemistry of analogous tetraruthenium carbido clusters because of the discovery of a high-yield route to $Ru_4H_2(CO)_{12}C$ (Cowie, Johnson, Lewis & Raithby, 1986). This cluster reacts with alkynes to form a product in which there is direct coupling between the alkyne and the carbido carbon (Dutton, Johnson, Lewis, Owen & Raithby, 1988). We have extended this work to include the reaction of tetraruthenium carbido clusters with alkenes to establish whether carbon–carbon bond formation also occurs, and herein report the structure of one of the products formed by the reaction of $Ru_4H_2(CO)_{12}C$ with styrene.

Experimental. Reaction of $Ru_4H_2(CO)_{12}C$ with styrene, in toluene, at 333 K for 4 h afforded a mixture of products from which the title compound was separated by thin-layer chromatography, being isolated in 10% yield. The product was recrystallized from CH_2Cl_2/hexane solution and obtained as yellow tablets. Crystal structure determination carried out on a crystal of size 0·22 × 0·36 × 0·52 mm; Nicolet $R3m/V$ diffractometer; unit-cell parameters from angular values of 25 centred reflections in the range $25 < 2\theta < 30°$; 3994 reflections with $2\theta < 50°$ and $h\,-11{\to}11$, $k\,-12{\to}0$, $l\,-15{\to}15$ (hemisphere of data, some repeated); no significant variation for three standard reflections; empirical absorption correction based on 298 azimuthal scan data ($R_{merge} = 0·016$), relative transmission factors 0·409–0·284. 3649 unique reflections ($R_{int} = 0·013$), 3404 with $F > 4\sigma(F)$. Structure solved by automatic direct methods (Ru atoms) and difference Fourier synthesis; full-matrix refinement on F; $w^{-1} = \sigma^2(F) + 0·0012F^2$. Anistropic thermal parameters for all non-hydrogen atoms. The two bridging hydride ligands were located directly and refined freely. The phenyl and methyl H atoms were placed in idealized positions, C—H = 0·96 Å, and allowed to ride on the relevant C atom; each type of H atom assigned a common isotropic temperature factor. Scattering factors including anomalous-dispersion terms from *International Tables for X-ray Crystallography* (1974). 284 parameters, $R = 0·023$, $wR = 0·029$, $S = 1·624$;* max. $\Delta/\sigma = 0·03$; largest peak in final difference map = 0·43,

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* $R = 0·025$, $wR = 0·032$ for all 3649 unique data.

Table 1. *Atomic coordinates* ($\times 10^4$) *and equivalent isotropic displacement parameters* ($Å^2 \times 10^3$)

	x	y	z	U_{eq}*
Ru(1)	3651 (1)	6190 (1)	2287 (1)	29 (1)
Ru(2)	976 (1)	7576 (1)	1553 (1)	30 (1)
Ru(3)	3828 (1)	8700 (1)	1635 (1)	30 (1)
C(1)	2888 (7)	5145 (5)	3171 (5)	40 (2)
O(1)	2439 (6)	4466 (5)	3631 (4)	66 (2)
C(2)	3914 (8)	4579 (6)	1174 (5)	48 (2)
O(2)	4038 (8)	3686 (5)	532 (5)	84 (3)
C(3)	5726 (6)	6478 (5)	3367 (5)	38 (2)
O(3)	6921 (5)	6711 (5)	4041 (5)	69 (2)
C(4)	−735 (6)	6592 (6)	1781 (5)	45 (2)
O(4)	−1762 (6)	5994 (6)	1871 (5)	74 (2)
C(5)	437 (7)	7067 (6)	−96 (5)	45 (2)
O(5)	128 (6)	6771 (5)	−1078 (4)	65 (2)
C(6)	14 (7)	9194 (6)	1423 (6)	49 (2)
O(6)	−560 (6)	10135 (5)	1319 (5)	77 (3)
C(7)	3747 (6)	8517 (6)	16 (5)	41 (2)
O(7)	3674 (6)	8408 (6)	−922 (4)	68 (2)
C(8)	3310 (7)	10497 (6)	1764 (5)	45 (2)
O(8)	2982 (6)	11576 (4)	1770 (5)	65 (2)
C(9)	6025 (7)	9258 (6)	2371 (5)	40 (2)
O(9)	7308 (5)	9517 (5)	2812 (4)	65 (2)
C(10)	3227 (5)	8139 (5)	2936 (4)	28 (2)
C(11)	2402 (6)	8611 (5)	3683 (4)	35 (2)
C(12)	2145 (8)	10099 (6)	4008 (6)	51 (2)
C(13)	2204 (6)	7867 (5)	4549 (4)	34 (2)
C(14)	777 (7)	7587 (7)	4689 (5)	48 (2)
C(15)	648 (7)	6988 (8)	5545 (5)	56 (2)
C(16)	1955 (7)	6645 (7)	6307 (5)	53 (2)
C(17)	3403 (7)	6950 (6)	6217 (5)	48 (2)
C(18)	3515 (6)	7547 (6)	5346 (4)	41 (2)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor.

largest trough = −0·67 e Å⁻³; program: MicroVax II version *SHELXTL PLUS* (Sheldrick, 1988).

Discussion. Atomic coordinates and equivalent isotropic thermal parameters are given in Table 1, while associated bond lengths and interbond angles are presented in Table 2. The molecular structure is shown in Fig. 1.*

The three Ru atoms define an isosceles triangle; the two long edges [Ru(1)—Ru(2) and Ru(1)—Ru(3)] are bridged by hydrides, which were located directly in the analysis. Each metal is coordinated to three terminal carbonyl ligands, two in equatorial and one in a pseudo-axial site. The Ru—C—O angles do not deviate from linearity by more than 4·4°. The Ru₃ triangle is capped by an alkenylidene ligand, which coordinates *via* two σ-bonds [Ru(1)—C(10), Ru(3)—C(10)] and a π-bond [Ru(2)—C(10), Ru(2)—C(11)]. The vinylidene ligand carbons C(10) and C(11) are approximately coplanar with the α phenyl and methyl substituent carbons, C(12) and C(13) [the maximum deviation is

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Table 2. *Bond lengths* (Å) *and angles* (°)

Ru(1)–Ru(2)	2·840 (1)		Ru(1)–Ru(3)	2·821 (1)
Ru(1)–C(1)	1·913 (7)		Ru(1)–C(2)	1·966 (6)
Ru(1)–C(3)	1·900 (5)		Ru(1)–C(10)	2·057 (5)
Ru(1)–H(1–3)	1·664 (67)		Ru(1)–H(1–2)	1·819 (46)
Ru(2)–Ru(3)	2·735 (1)		Ru(2)–C(4)	1·926 (6)
Ru(2)–C(5)	1·884 (6)		Ru(2)–C(6)	1·892 (6)
Ru(2)–C(10)	2·167 (4)		Ru(2)–C(11)	2·500 (4)
Ru(2)–H(1–2)	1·785 (54)		Ru(3)–C(7)	1·941 (6)
Ru(3)–C(8)	1·875 (6)		Ru(3)–C(9)	1·910 (5)
Ru(3)–C(10)	2·019 (6)		Ru(3)–H(1–3)	1·790 (58)
C(1)–O(1)	1·111 (9)		C(2)–O(2)	1·099 (8)
C(3)–O(3)	1·117 (6)		C(4)–O(4)	1·133 (9)
C(5)–O(5)	1·123 (7)		C(6)–O(6)	1·110 (9)
C(7)–O(7)	1·117 (8)		C(8)–O(8)	1·137 (8)
C(9)–O(9)	1·109 (7)		C(10)–C(11)	1·379 (8)
C(11)–C(12)	1·515 (8)		C(11)–C(13)	1·475 (8)
C(13)–C(14)	1·379 (9)		C(13)–C(18)	1·383 (7)
C(14)–C(15)	1·352 (11)		C(15)–C(16)	1·370 (9)
C(16)–C(17)	1·374 (10)		C(17)–C(18)	1·363 (9)

Ru(2)–Ru(1)–Ru(3)	57·8 (1)		Ru(2)–Ru(1)–C(1)	97·9 (2)
Ru(3)–Ru(1)–C(1)	147·4 (2)		Ru(2)–Ru(1)–C(2)	118·4 (2)
Ru(3)–Ru(1)–C(2)	115·5 (2)		C(1)–Ru(1)–C(2)	94·5 (3)
Ru(2)–Ru(1)–C(3)	141·4 (2)		Ru(3)–Ru(1)–C(3)	95·3 (2)
C(1)–Ru(1)–C(3)	92·9 (3)		C(2)–Ru(1)–C(3)	97·4 (2)
Ru(2)–Ru(1)–C(10)	49·4 (1)		Ru(3)–Ru(1)–C(10)	45·7 (2)
C(1)–Ru(1)–C(10)	102·6 (2)		C(2)–Ru(1)–C(10)	159·9 (2)
C(3)–Ru(1)–C(10)	92·1 (2)		Ru(2)–Ru(1)–H(1–3)	81·1 (20)
Ru(3)–Ru(1)–H(1–3)	36·8 (20)		C(1)–Ru(1)–H(1–3)	172·7 (17)
C(2)–Ru(1)–H(1–3)	79·7 (19)		C(3)–Ru(1)–H(1–3)	92·4 (17)
C(10)–Ru(1)–H(1–3)	82·3 (20)		Ru(2)–Ru(1)–H(1–2)	37·6 (16)
Ru(3)–Ru(1)–H(1–2)	79·3 (18)		C(1)–Ru(1)–H(1–2)	93·8 (20)
C(2)–Ru(1)–H(1–2)	81·6 (17)		C(3)–Ru(1)–H(1–2)	173·3 (19)
C(10)–Ru(1)–H(1–2)	86·9 (16)		H(1–3)–Ru(1)–H(1–2)	80·9 (26)
Ru(1)–Ru(2)–Ru(3)	60·8 (1)		Ru(1)–Ru(2)–C(4)	107·0 (2)
Ru(3)–Ru(2)–C(4)	166·4 (2)		Ru(1)–Ru(2)–C(5)	101·9 (2)
Ru(3)–Ru(2)–C(5)	88·0 (2)		C(4)–Ru(2)–C(5)	101·0 (2)
Ru(1)–Ru(2)–C(6)	151·7 (2)		Ru(3)–Ru(2)–C(6)	94·3 (2)
C(4)–Ru(2)–C(6)	95·9 (3)		C(5)–Ru(2)–C(6)	89·4 (3)
Ru(1)–Ru(2)–C(10)	46·1 (1)		Ru(3)–Ru(2)–C(10)	46·9 (1)
C(4)–Ru(2)–C(10)	120·9 (2)		C(5)–Ru(2)–C(10)	131·6 (2)
C(6)–Ru(2)–C(10)	107·6 (2)		Ru(1)–Ru(2)–C(11)	71·7 (1)
Ru(3)–Ru(2)–C(11)	74·8 (1)		C(4)–Ru(2)–C(11)	96·3 (2)
C(5)–Ru(2)–C(11)	162·6 (2)		C(6)–Ru(2)–C(11)	89·8 (2)
C(10)–Ru(2)–C(11)	33·4 (2)		Ru(1)–Ru(2)–H(1–2)	38·4 (14)
Ru(3)–Ru(2)–H(1–2)	82·3 (18)		C(4)–Ru(2)–H(1–2)	91·0 (19)
C(5)–Ru(2)–H(1–2)	70·9 (17)		C(6)–Ru(2)–H(1–2)	160·1 (18)
C(10)–Ru(2)–H(1–2)	84·4 (14)		C(11)–Ru(2)–H(1–2)	108·0 (15)
Ru(1)–Ru(3)–Ru(2)	61·5 (1)		Ru(1)–Ru(3)–C(7)	114·2 (2)
Ru(1)–Ru(3)–C(7)	106·5 (2)		Ru(1)–Ru(3)–C(8)	148·4 (2)
Ru(2)–Ru(3)–C(8)	95·5 (2)		C(7)–Ru(3)–C(8)	92·1 (3)
Ru(1)–Ru(3)–C(9)	99·2 (2)		Ru(2)–Ru(3)–C(9)	153·4 (2)
C(7)–Ru(3)–C(9)	98·0 (2)		C(8)–Ru(3)–C(9)	93·9 (2)
Ru(1)–Ru(3)–C(10)	46·8 (1)		Ru(2)–Ru(3)–C(10)	51·6 (1)
C(7)–Ru(3)–C(10)	154·3 (2)		C(8)–Ru(3)–C(10)	102·4 (3)
C(9)–Ru(3)–C(10)	102·0 (2)		Ru(1)–Ru(3)–H(1–3)	33·8 (22)
Ru(2)–Ru(3)–H(1–3)	82·3 (20)		C(7)–Ru(3)–H(1–3)	83·5 (20)
C(8)–Ru(3)–H(1–3)	174·3 (18)		C(9)–Ru(3)–H(1–3)	90·4 (17)
C(10)–Ru(3)–H(1–3)	80·4 (21)		Ru(1)–C(1)–O(1)	175·6 (5)
Ru(1)–C(2)–O(2)	178·5 (5)		Ru(1)–C(3)–O(3)	175·9 (5)
Ru(2)–C(4)–O(4)	177·4 (5)		Ru(2)–C(5)–O(5)	179·3 (6)
Ru(2)–C(6)–O(6)	178·4 (6)		Ru(3)–C(7)–O(7)	178·8 (5)
Ru(3)–C(8)–O(8)	175·7 (6)		Ru(3)–C(9)–O(9)	176·4 (6)
Ru(1)–C(10)–Ru(2)	84·5 (1)		Ru(1)–C(10)–Ru(3)	87·6 (2)
Ru(2)–C(10)–Ru(3)	81·5 (2)		Ru(1)–C(10)–C(11)	130·9 (4)
Ru(2)–C(10)–C(11)	86·7 (3)		Ru(3)–C(10)–C(11)	138·4 (4)
Ru(2)–C(11)–C(10)	59·9 (2)		Ru(2)–C(11)–C(12)	110·9 (3)
C(10)–C(11)–C(12)	122·9 (6)		Ru(2)–C(11)–C(13)	118·0 (3)
C(10)–C(11)–C(13)	122·0 (5)		C(12)–C(11)–C(13)	111·6 (5)
C(11)–C(13)–C(14)	123·1 (5)		C(11)–C(13)–C(18)	119·3 (5)
C(14)–C(13)–C(18)	117·2 (6)		C(13)–C(14)–C(15)	121·8 (6)
C(14)–C(15)–C(16)	120·2 (6)		C(15)–C(16)–C(17)	119·6 (7)
C(16)–C(17)–C(18)	119·7 (5)		C(13)–C(18)–C(17)	121·5 (6)
Ru(1)–H(1–3)–Ru(3)	109·5 (34)		Ru(1)–H(1–2)–Ru(2)	104·0 (23)

Braunstein, 1983) there are relatively few examples of X-ray structures containing this ligand coordinated to a trimetal unit (Raithby & Rosales, 1985). In fact, this appears to be the first example of a structurally characterized trinuclear cluster containing this type of ligand in which one of the substituent R groups is not hydrogen. The C(10)–C(11) distance lies within the range 1·32–1·42 Å (Raithby & Rosales, 1985) found in other alkenylidene-containing clusters, and is not significantly different from the value of 1·406 (19) Å found in the other triruthenium cluster, $Ru_3Au_2\{\mu_3$-η^2-CC(H)C(CH$_3$)$_3\}(CO)_9\{P(C_6H_5)_3\}_2$, to have been structurally characterized (Bruce, Horn, Shawkataly & Snow, 1985), and is consistent with this bond retaining multiple-bond character. The C(10)–C(11)–C(12) and C(10)–C(11)–C(13) angles are close to 120°, also consistent with multiple-bond character for C(10)–C(11). The two Ru–C(10) σ-bonds and the Ru–C π-interaction distances in the title compound are similar in length to the equivalent values of 2·040 (14) and 2·102 (17) Å, and 2·190 (14) and 2·243 (15) Å, respectively, found in $Ru_3Au_2\{\mu_3$-η^2-CC(H)C(CH$_3$)$_3\}(CO)_9$-$\{P(C_6H_5)_3\}_2$ (Bruce, Horn, Shawkataly & Snow, 1985). The Ru(1)–C(10) and Ru(3)–C(10) interactions exert an electronic influence on the pseudo-axial *trans* carbonyl ligands. The Ru(1)–C(2) and Ru(3)–C(7) distances are *ca* 0·06 Å longer than the Ru–C distances for the equatorial carbonyls bonded to Ru(1) and Ru(2), and *ca* 0·07 Å longer than the Ru(2)–C(5) bond which is pseudo-*trans* to the C(10)–C(11) π-interaction. These distances are consistent with there being less back donation to the axial carbonyls C(2)O(2) and C(7)O(7), suggesting that there is a

0·13 Å for C(11)], and this C$_4$ plane makes an angle of 56·6 (8)° with the Ru$_3$ triangle, while the phenyl substituent ring makes an angle of 65 (1)° with the C$_4$ plane.

While μ_3-η^2-CC(R)R' ligands are known widely throughout cluster chemistry (Sappa, Tiripicchio &
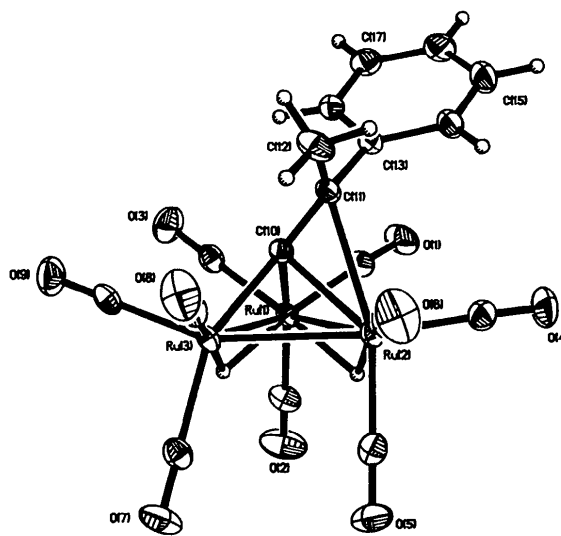

Fig. 1. The molecular structure of the title complex, showing the atom labelling.

component in the bonding between C(10) and Ru(1) and Ru(3) involving the t_{2g} set of orbitals on the metals. The Ru—Ru distances within the Ru$_3$ triangle are all shorter, the unbridged Ru(2)—Ru(3) edge by *ca* 0·11 Å, than the average distance of 2·854 (4) Å for the Ru—Ru edges in Ru$_3$(CO)$_{12}$ (Churchill, Hollander & Hutchinson, 1977). While the metal–metal edge-lengthening influence of a bridging hydride is well established (Churchill, DeBoer & Rotella, 1976), it seems that the $\mu_3\text{-}\eta^2\text{-}CC(CH_3)C_6H_5$ ligand exerts an edge-shortening influence which counterbalances the effect of the hydrides on the Ru(1)—Ru(2) and Ru(1)—Ru(3) edges and causes the considerable shortening of the Ru(2)—Ru(3) edge.

If the $\mu_3\text{-}\eta^2\text{-}CC(CH_3)C_6H_5$ ligand is considered to donate formally four electrons to cluster bonding, then the cluster as a whole has a 48 electron count, consistent with the presence of three formal metal–metal bonds.

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Structure of Bis(3-cyano-2,4-pentanedionato)copper(II)

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Abstract. [Cu(C$_6$H$_6$NO$_2$)$_2$], $M_r = 311·78$, monoclinic, $P2_1/n$, $a = 10·005$ (1), $b = 12·149$ (1), $c = 11·246$ (1) Å, $\beta = 96·748$ (4)°, $V = 1357·5$ (4) Å^3, $Z = 4$, $D_x = 1·525$ g cm^{-3}, $\lambda(Mo\ K\alpha) = 0·71073$ Å, $\mu = 16·2$ cm^{-1}, $F(000) = 636$, $T = 293$ K, $R = 0·033$ for 2046 observed reflections with $I > 3\sigma(I)$. The Cu(CNacac)$_2$ (CNacacH = 3-cyano-2,4-pentanedione) chelate molecules occupy general positions and are associated in infinite zigzag chains parallel to **b**. The CuO$_4$N coordination polyhedron is a distorted square pyramid, with Cu—O distances 1·912 (2)– 1·928 (2) Å and with Cu shifted from the O$_4$ plane towards the apical N atom by 0·114 (1) Å. The CNacac ligands are planar with normal geometry, but are structurally non-equivalent: one coordinates to Cu *via* the cyano group with Cu···N = 2·468 (3) Å, whilst the other takes part in a plane-to-plane coupling with a centrosymmetrically equivalent molecule (distance between ligand planes 3·056 Å).

Introduction. In a preceding paper we have shown that the dipropyl ester of 1-cyano-2,4-propylphosphonic acid (CNpaacH) forms chelate bridges in the structure of Cu(CNpaac)$_2$ (Macicek, Angelova, Petrov & Kirilov, 1988). Spectroscopic investigations of CNpaacH indicated a similarity of its coordination properties to those of β-diketonates (Petrov, 1972*a*). The analogy between O=P—C(CN)—C=O and O=C—C(CN)—C=O fragments focused attention on the simplest cyano-β-diketone derivative – 3-cyano-2,4-pentanedione (CNacacH). The latter, and its metal complexes, are well characterized by various techniques other than crystallographic methods.

The IR and UV spectra of CNacacH (Wierzchowski & Shugar, 1965) indicated that in different solutions the molecule exists exclusively as the *cis*-enol form and that the anion is symmetric with complete charge delocalization. The cyano group was found to cause an electron density rearrangement (due to its large