(η^4-allylcarbonyl) structures, where L = CO or $P(Ph)_3$, are similar to this work and support the assessment of the *trans*-lengthening effect exerted by the α-C atom of the dienone on the Fe–CO lengths (Newton, Pantaleo, King & Chu, 1979; Dettlaf, Behrens & Weiss, 1978; Binger, Cetinkaya & Kruger, 1978; Mitsudo, Sasaki, Watanabe, Takegami, Nishigaki & Nakatsu, 1978; Fischer & Ricard, 1982). A closely related structure contains the ligand η^4-vinylketenimine (Mitsudo, Watanabe, Komiya, Watanabe, Takaegami, Nakatsu, Kinoshita & Miyagawa, 1980).

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Structure of (η^5-Cyclopentadienyl)(dimethyldithiocarbamato)(triphenylphosphine)ruthenium(II)

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Abstract. $[Ru(C_3H_6NS_2)(C_5H_5)(C_{18}H_{15}P)]$, M_r = 548·7, triclinic, $P\bar{1}$, a = 10·099 (4), b = 10·373 (3), c = 13·323 (4) Å, α = 98·13 (2), β = 95·91 (3), γ = 115·87 (3)°, V = 1221 (2) Å^3, Z = 2, D_x = 1·49 g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, μ = 8·7 cm^{-1}, $F(000)$ = 560, T = 293 K, R = 0·047 for 1952 unique observed reflections. The dithiocarbamate functions as a bidentate ligand with equal Ru–S distances of 2·395 (3) Å. The two S atoms, the P atom, and the center of the cyclopentadienyl ring approximate a tetrahedral environment for the Ru^{II} ion in contrast to previous Ru-dithiocarbamate structures which have involved six- and seven-coordinate Ru.

Experimental. Complex (I) prepared by reaction of $[Ru(HSC_3H_7)(cp)(PPh_3)_2]^+$ with sodium dimethyldithiocarbamate in CH_2Cl_2. The thin yellow plate-like crystal used for data collection was obtained by evaporation of a diethyl ether solution. Data crystal 0·02 × 0·28 × 0·44 mm mounted on a glass fiber. Intensities measured with an Enraf–Nonius CAD-4 diffractometer using ω–2θ scans of 4–16° min^{-1} in θ. Unit cell determined from least-squares analysis of angle data for 25 reflections with $17 < 2\theta < 22°$. Analytical absorption correction based on crystal-face measurements varied from 0·79 to 1·00. Data collected to $(\sin\theta)/\lambda$ of 0·55 Å^{-1}, $0 < h < 10$, $-10 < k < 10$, $-13 < l < 13$. Three standard reflections ($22\bar{6}$, $41\bar{4}$, 302) decreased 2·2% over 32·0 h of data collection. 3613 reflections measured, 3384 unique (R_{int} = 0·03), 1432 reflections with $I < 3\sigma(I)$ considered unobserved. Solved by Patterson and Fourier methods. Full-matrix least squares minimized $\sum w(\Delta F)^2$. H atoms constrained to idealized positions with C–H = 0·95 Å and isotropic B value of 1·2 times that of the C atom to which it was bonded. Orientation of the methyl H atoms determined from a difference map. All other atoms refined anisotropically for a total of 280

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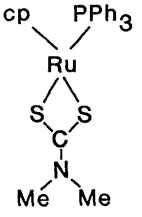
variables. $R = 0.047$, $wR = 0.052$, $S = 1.11$, where non-Poisson $w^{-1} = [\sigma^2(I) + 0.0025I^2]/4F^2$. Final $(\Delta/\sigma)_{max} < 0.03$, $\Delta\rho_{max} = 0.68$ (9) and $\Delta\rho_{min} = -0.53$ (9) e Å^{-3} on final difference map. Atomic scattering factors and anomalous-dispersion correction from *International Tables for X-ray Crystallography* (1974) and programs used were those of Enraf–Nonius (1982) *SDP*.* Tables 1 and 2 give the atom coordinates and selected intramolecular distances and angles; Fig. 1 shows the molecule with the numbering scheme used.



(I)

Related literature. Ru-dithiocarbamate structures previously published include the six- and seven-coordinate complexes reported in a series of papers by Raston & White (1975) and by Pignolet and co-workers (Pignolet & Wheeler, 1980). The chemistry of mononuclear Ru compounds has been reviewed by Bennett, Bruce & Matheson (1982).

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*Lists of structure factors, distances and angles involving C atoms, and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44414 (28 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

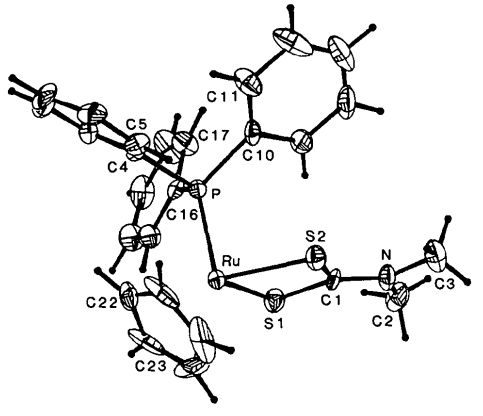

Fig. 1. *ORTEP*II (Johnson, 1976) diagram showing the atom-numbering scheme. Non-H ellipsoids at 30% probability level, H atoms given arbitrary radius.

Table 1. *Final fractional coordinates and B_{eq} thermal factors for non-H atoms*

E.s.d.'s in parentheses are in the units of the least-significant digit. Isotropic equivalent thermal parameter defined as: $\frac{4}{3}[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)]$.

	x	y	z	B_{eq}(Å^2)
Ru	0·29108 (8)	0·22345 (8)	0·34274 (6)	2·71 (2)
S(1)	0·3838 (3)	0·0473 (2)	0·3140 (2)	3·67 (6)
S(2)	0·5285 (3)	0·3178 (2)	0·4552 (2)	3·64 (6)
P	0·3887 (2)	0·3176 (2)	0·2070 (2)	2·62 (5)
N	0·6557 (7)	0·1359 (7)	0·4316 (6)	3·8 (2)
C(1)	0·5383 (9)	0·1627 (8)	0·4058 (7)	3·4 (2)
C(2)	0·654 (1)	−0·001 (1)	0·3857 (8)	5·5 (3)
C(3)	0·787 (1)	0·242 (1)	0·5053 (9)	5·8 (3)
C(4)	0·3156 (9)	0·4392 (8)	0·1634 (6)	2·8 (2)
C(5)	0·327 (1)	0·5556 (9)	0·2353 (7)	3·7 (2)
C(6)	0·279 (1)	0·6518 (8)	0·2043 (8)	4·4 (3)
C(7)	0·209 (1)	0·6274 (9)	0·1053 (8)	5·5 (3)
C(8)	0·196 (1)	0·514 (1)	0·0350 (8)	5·3 (3)
C(9)	0·2476 (9)	0·4171 (8)	0·0620 (7)	3·3 (2)
C(10)	0·5918 (9)	0·4316 (9)	0·2218 (7)	3·3 (2)
C(11)	0·656 (1)	0·579 (1)	0·2193 (9)	5·3 (3)
C(12)	0·811 (1)	0·663 (1)	0·237 (1)	7·8 (4)
C(13)	0·900 (1)	0·600 (1)	0·2572 (9)	7·6 (4)
C(14)	0·839 (1)	0·456 (1)	0·2602 (9)	7·2 (3)
C(15)	0·6841 (9)	0·370 (1)	0·2404 (8)	4·8 (3)
C(16)	0·3469 (8)	0·1825 (8)	0·0890 (6)	2·8 (2)
C(17)	0·440 (1)	0·205 (1)	0·0160 (8)	4·4 (3)
C(18)	0·405 (1)	0·098 (1)	−0·0718 (8)	6·4 (3)
C(19)	0·275 (1)	−0·028 (1)	−0·0905 (8)	5·4 (3)
C(20)	0·181 (1)	−0·052 (1)	−0·0203 (8)	5·0 (3)
C(21)	0·219 (1)	0·0517 (9)	0·0689 (7)	4·0 (3)
C(22)	0·081 (1)	0·229 (1)	0·3019 (8)	5·4 (3)
C(23)	0·050 (1)	0·092 (1)	0·314 (1)	6·8 (4)
C(24)	0·105 (1)	0·102 (1)	0·4127 (9)	8·9 (3)
C(25)	0·167 (1)	0·242 (2)	0·4652 (8)	9·6 (4)
C(26)	0·155 (1)	0·326 (1)	0·393 (1)	6·8 (3)

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

Ru–S(1)	2·394 (3)	S(1)–C(1)	1·711 (9)
Ru–S(2)	2·397 (3)	S(2)–C(1)	1·697 (9)
Ru–P	2·285 (2)	P–C(4)	1·845 (8)
Ru–C(22)	2·159 (10)	P–C(10)	1·838 (9)
Ru–C(23)	2·169 (11)	P–C(16)	1·827 (9)
Ru–C(24)	2·151 (13)	N–C(1)	1·354 (10)
Ru–C(25)	2·195 (12)	N–C(2)	1·455 (12)
Ru–C(26)	2·175 (11)	N–C(3)	1·445 (12)

S(1)–Ru–S(2)	71·88 (9)	C(1)–N–C(2)	121·0 (9)
S(1)–Ru–P	89·82 (9)	C(1)–N–C(3)	121·4 (9)
S(2)–Ru–P	95·18 (9)	C(2)–N–C(3)	117·7 (8)
C(4)–P–C(10)	101·6 (4)	S(1)–C(1)–S(2)	111·2 (5)
C(4)–P–C(16)	102·7 (4)	S(1)–C(1)–N	123·9 (8)
C(10)–P–C(16)	102·3 (4)	S(2)–C(1)–N	124·8 (8)

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