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Tetracarbonyl(norbornadiene)chromium(0) at 178 K

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Abstract. {(2,3-η,5,6-η)-Bicyclo[2.2.1]hepta-2,5-diene}tetracarbonylchromium(0), $[Cr(C_7H_8)(CO)_4]$, M_r = 256·2, monoclinic, $P2_1/c$, a = 9·570 (4), b = 9·799 (3), c = 10·996 (5) Å, β = 91·08 (3)°, V = 1031·1 (7) Å^3, Z = 4, D_x = 1·65 Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, μ = 1·1 mm^{-1}, $F(000)$ = 520, T = 178 K. The structure was refined to R = 0·029 for 2073 unique observed reflections. The coordination of the Cr atom is pseudo-octahedral, counting each coordinated double bond as one ligand site. The Cr—C(olefin) bond lengths are 2·283–2·310 (2) Å, with Cr—(C=C midpoint) 2·181, 2·201 Å. The Cr—C(carbonyl) bonds *trans* to the olefin are shorter than those *cis* [1·861, 1·866 *cf.* 1·889, 1·904 (2) Å]. The olefinic H atoms (refined freely) each lie *ca* 0·2 Å out of the respective C—C=C—C planes.

Experimental. Crystals were obtained from petroleum ether (313–333 K). A yellow tablet 0·6 × 0·6 × 0·16 mm was mounted in inert oil on a glass fibre, which was transferred to the cold gas stream of the diffractometer (Siemens *R*3*m*/*V* with LT-2 low-temperature attachment). ω scan. 3611 intensities were measured to $2\theta_{max}$ 50° with monochromated Mo $K\alpha$ radiation (quadrant $-h+k\pm l$ and some $+h$ equivalents, index ranges h −12→4, k 0→12, l −14→14). The orientation matrix was refined from setting angles of 50 reflections in the range 2θ 20–23°. 3 standard reflections monitored every 147 reflections showed no intensity variation. An absorption correction based on ψ scans was applied, with transmissions 0·68–0·95. Averaging equivalent reflections gave 2368 unique reflections (R_{int} 0·020), of which 2073 with $F > 4\sigma(F)$ were used for all calculations performed with the program system Siemens *SHELXTL Plus* (Sheldrick, 1987).

The structure was solved by direct methods and submitted to full-matrix anisotropic least-squares refinement on F. Olefinic H atoms were refined freely, other H atoms using a riding model. The final R was 0·029, with wR 0·038. The weighting scheme was $w^{-1} = \sigma^2(F) + 0{\cdot}0003F^2$. 161 parameters; S 1·45; max. Δ/σ 0·002, max. and min. $\Delta\rho$ + 0·29, −0·55 e Å^{-3}, respectively. Scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV). Final atomic coordinates are given in Table 1, with derived bond lengths and angles in Table 2.* The molecule of the title compound in shown in Fig. 1.

Related literature. Structural aspects of tetracarbonyl(diene)chromium(0) complexes have been discussed by Pavkovic & Zaluzec (1989).

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* 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 53701 (15 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Cr	2036·2 (2)	5907·1 (2)	7222·0 (2)	170 (1)
C(1)	2352 (2)	7771 (2)	7048 (2)	239 (5)
O(1)	2503 (2)	8925 (1)	6901 (1)	370 (4)
C(2)	1012 (2)	6415 (2)	8603 (2)	257 (5)
O(2)	362 (2)	6767 (2)	9408 (1)	415 (5)
C(3)	2909 (2)	5791 (2)	5684 (2)	235 (5)
O(3)	3418 (2)	5817 (1)	4758 (1)	368 (4)
C(4)	314 (2)	5922 (2)	6399 (2)	216 (4)
O(4)	−761 (1)	5900 (1)	5925 (1)	303 (4)
C(5)	4207 (2)	5040 (2)	7756 (2)	242 (5)
C(6)	3890 (2)	3548 (2)	7417 (2)	245 (5)
C(7)	3814 (2)	2909 (2)	8700 (2)	294 (5)
C(8)	2749 (2)	3976 (2)	9144 (2)	252 (5)
C(9)	3514 (2)	5307 (2)	8806 (2)	243 (5)
C(10)	1630 (2)	3854 (2)	8130 (2)	233 (5)
C(11)	2327 (2)	3594 (2)	7073 (2)	234 (5)

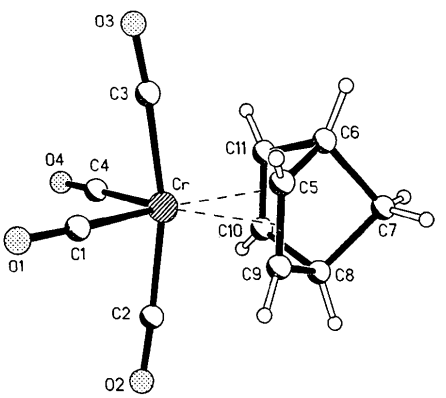

Fig. 1. The molecule of the title compound in the crystal, showing the atom-numbering scheme. Radii are arbitrary.

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

Cr—C(1)	1·861 (2)	Cr—C(2)	1·889 (2)
Cr—C(3)	1·904 (2)	Cr—C(4)	1·866 (2)
Cr—C(5)	2·310 (2)	Cr—C(9)	2·299 (2)
Cr—Cent1	2·201	Cr—C(10)	2·283 (2)
Cr—C(11)	2·290 (2)	Cr—Cent2	2·181
C(1)—O(1)	1·152 (2)	C(2)—O(2)	1·145 (2)
C(3)—O(3)	1·137 (2)	C(4)—O(4)	1·145 (2)
C(5)—C(6)	1·538 (3)	C(5)—C(9)	1·368 (3)
C(6)—C(7)	1·547 (3)	C(6)—C(11)	1·536 (2)
C(7)—C(8)	1·546 (3)	C(8)—C(9)	1·544 (3)
C(8)—C(10)	1·536 (3)	C(10)—C(11)	1·375 (3)

C(1)—Cr—C(2)	84·9 (1)	C(1)—Cr—C(3)	83·8 (1)
C(2)—Cr—C(3)	166·5 (1)	C(1)—Cr—C(4)	95·0 (1)
C(2)—Cr—C(4)	85·5 (1)	C(3)—Cr—C(4)	88·2 (1)
C(1)—Cr—C(5)	103·9 (1)	C(2)—Cr—C(5)	111·7 (1)
C(3)—Cr—C(5)	78·2 (1)	C(4)—Cr—C(5)	155·3 (1)
C(1)—Cr—C(9)	103·3 (1)	C(2)—Cr—C(9)	77·3 (1)
C(3)—Cr—C(9)	112·6 (1)	C(4)—Cr—C(9)	153·5 (1)
C(5)—Cr—C(9)	34·5 (1)	C(1)—Cr—C(10)	159·9 (1)
C(2)—Cr—C(10)	77·6 (1)	C(3)—Cr—C(10)	114·7 (1)
C(4)—Cr—C(10)	93·6 (1)	C(5)—Cr—C(10)	74·0 (1)
C(9)—Cr—C(10)	63·3 (1)	C(1)—Cr—C(11)	160·6 (1)
C(2)—Cr—C(11)	112·6 (1)	C(3)—Cr—C(11)	79·7 (1)
C(4)—Cr—C(11)	94·6 (1)	C(5)—Cr—C(11)	62·9 (1)
C(9)—Cr—C(11)	74·2 (1)	C(10)—Cr—C(11)	35·0 (1)
Cr—C(1)—O(1)	177·0 (1)	Cr—C(2)—O(2)	176·9 (2)
Cr—C(3)—O(3)	175·2 (2)	Cr—C(4)—O(4)	177·5 (1)
Cr—C(5)—C(6)	96·6 (1)	Cr—C(5)—C(9)	72·3 (1)
C(6)—C(5)—C(9)	106·8 (1)	C(5)—C(6)—C(7)	100·1 (1)
C(5)—C(6)—C(11)	102·6 (1)	C(7)—C(6)—C(11)	100·0 (1)
C(6)—C(7)—C(8)	93·3 (1)	C(7)—C(8)—C(9)	100·1 (1)
C(7)—C(8)—C(10)	99·9 (1)	C(9)—C(8)—C(10)	102·6 (1)
Cr—C(9)—C(5)	73·1 (1)	Cr—C(9)—C(8)	96·4 (1)
C(5)—C(9)—C(8)	106·4 (2)	Cr—C(10)—C(8)	97·3 (1)
Cr—C(10)—C(11)	72·8 (1)	C(8)—C(10)—C(11)	106·6 (1)
Cr—C(11)—C(6)	97·5 (1)	Cr—C(11)—C(10)	72·2 (1)
C(6)—C(11)—C(10)	106·4 (1)		

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Structure of Poly[nickel(II)-μ-(cyano-*C*:*N*)-{(ethylenediamine-*N*,*N*′)zinc}-tri-μ-cyano(*N*,*C*)]

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Abstract. $[NiZn(C_6H_8N_6)]$, $M_r = 288·26$, orthorhombic, *Pbcn*, $a = 8·878$ (3), $b = 9·911$ (3), $c = 11·106$ (5) Å, $V = 977·3$ (6) Å^3, $Z = 4$, $D_m = 1·97$, $D_x = 1·96$ Mg m^{-3}, λ(Mo $K\bar{\alpha}$) = 0·71069 Å, $\mu = 4·37$ mm^{-1}, $F(000) = 576$, $T = 295$ K, $R = 0·045$ for 812 reflections [$F_o \geq 4\sigma(F_o)$]. The structure is built

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