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**Tricarbonyl[(6a,7,8,9,10a- η)-3,3-dimethyl-3H-benzo[*f*]chromene]-
chromium**

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Tricarbonyl[(6a,7,8,9,10a- η)-3,3-dimethyl-3H-benzo[f]chromene]-chromium

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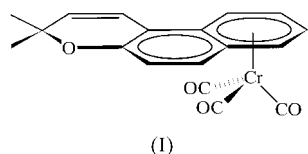
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The title compound, $[\text{Cr}(\text{C}_{15}\text{H}_{14}\text{O})(\text{CO})_3]$, is a chromene complexed with tricarbonylchromium and it exhibits photochromic properties. The molecular geometry is compared to that of two similar complexes. The analysis results indicate that complexation has minor effects on the chromene structure.

Comment

The photochromic properties of 3H-naphthopyrans (2H-benzochromenes) (Becker & Michl, 1966) can be modulated by introducing selected substituents onto the different positions of the aromatic system. Tricarbonylchromium complexation with aromatic rings modifies the reactivity and also the electronic distribution in such structures, which induces modifications of the photochromic properties of 3H-naphthopyrans. Such a behaviour has been found already for indolino-spiropyran (Miyashita *et al.*, 1992) and fulgides (McCabe & Saberi, 1995), and led us to a systematic study of chromenes complexed with tricarbonylchromium. This group improves the photochromic property of the compound by decreasing its fading rate. The red colour is induced by the complexation.



In the three derivatives we have studied [methyl/phenyl (Hanneschlager *et al.*, 1998), diphenyl (Hanneschlager *et al.*, 1999) and dimethyl (the present work)], strong similarities in the geometry are observed; the conformation of the chromene ring is the same, the relative position of the tricarbonylchromium *versus* the complexed phenyl ring is the same, even if in the diphenyl derivative, this group is on the other side of

the chromene group because of the steric hindrance of the axial phenyl group. In all cases, the geometry of the pyranic ring is not significantly affected by the presence of the tricarbonylchromium group, if compared with the non-complexed derivative (Aldoshin *et al.*, 1996). The conformation of the tricarbonyl group is staggered with respect to the phenyl ring and the Cr-atom position is not centred on the phenyl ring: the average distance in the three complexes in the C8–C11 chain is 2.21 (1)  , while this value is 2.30 (1)   for C12–C13. For the three compounds, the crystal packing is essentially governed by van der Waals interactions.

Experimental

The title compound was prepared starting from tripyridine tricarbonylchromium by an exchange reaction with 3,3-dimethyl-3H-naphthopyran (Pozzo *et al.*, 1997; Perez-Encabo *et al.*, 1994). In the case of this compound, as for the previous derivatives, a unique chromium complex was obtained, despite the presence of several aromatic rings in the molecules. Red crystals shaped as square platelets were obtained by evaporation of a (CH_2Cl_2 /hexane 10/90) solution.

Crystal data

$[\text{Cr}(\text{C}_{15}\text{H}_{14}\text{O})(\text{CO})_3]$
 $M_r = 346.29$
 Monoclinic, $P2_1/n$
 $a = 12.190$ (2)  
 $b = 9.147$ (2)  
 $c = 14.612$ (3)  
 $\beta = 104.20$ (2)  
 $V = 1579.5$ (5)  ³
 $Z = 4$
 $D_x = 1.456$ Mg m⁻³
 $D_m = 1.45$ (2) Mg m⁻³

D_m measured by flotation in benzene/chloroform
 Mo $K\alpha$ radiation
 Cell parameters from 25 reflections
 $\theta = 9$ –15  
 $\mu = 0.741$ mm⁻¹
 $T = 293$ (2) K
 Square platelet, red
 0.32   0.30   0.21 mm

Data collection

Nonius CAD-4 diffractometer
 $\omega/2\theta$ scans
 Absorption correction: ψ scans (North *et al.*, 1968)
 $T_{\min} = 0.785$, $T_{\max} = 0.856$
 4663 measured reflections
 4663 independent reflections
 4072 reflections with $I > 2\sigma(I)$

$\theta_{\max} = 30.16$  
 $h = -16 \rightarrow 16$
 $k = 0 \rightarrow 12$
 $l = 0 \rightarrow 20$
 3 standard reflections
 frequency: 60 min
 intensity decay: none

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.073$
 $S = 1.048$
 4663 reflections
 250 parameters

Only coordinates of H atoms refined
 $w = 1/[\sigma^2(F_o^2) + (0.0400P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.002$
 $\Delta\rho_{\max} = 0.42$ e  ⁻³
 $\Delta\rho_{\min} = -0.26$ e  ⁻³

H atoms were refined with $U = 1.2U_{\text{eq}}$ of the connected atom.

Data collection: *CAD-4 Operations Manual* (Enraf–Nonius, 1977); cell refinement: *CAD-4 Operations Manual*; data reduction: *DATARED* (P epe, 1979); program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); software used to prepare material for publication: *PLATON* (Spek, 1990).

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