Crystal structure of [μ-(3,4-η:4,5,6,7-η)-{5,6-di(n-propyl)-3,4,6-decatrien}][bis(η^5-cyclopentadiendiyl)(dimethyl)silan]tricarbonyl-1κ^2*C*:2κ^1*C*-tungstenmolybdenum(W–Mo), $C_{31}H_{42}MoO_3SiW$

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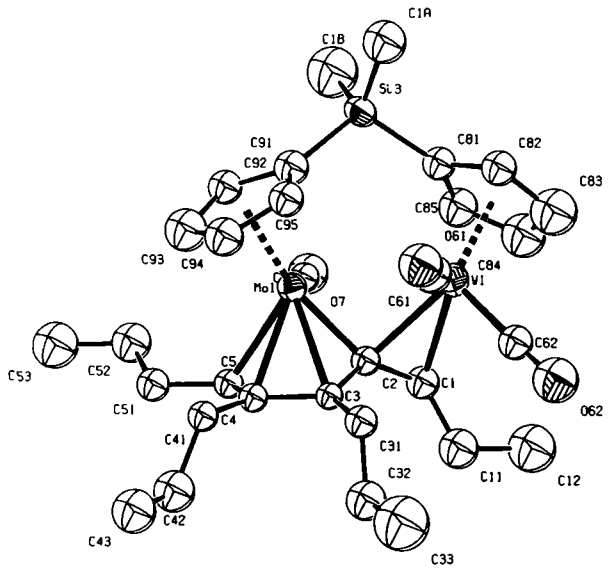

Source of material: The preparation of the crystals (recrystallized from hexane) will be described elsewhere. (see ref. 1).
Application of DIRDIF (see ref. 2) using the automatic Patterson option (PATTY) (see ref. 3) led to the positions of the non-hydrogen atoms.

Table 1. Parameters used for the X-ray data collection

Crystal:	brown plate, size 0.08 x 0.35 x 0.35 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	42.77 cm^{-1}
Diffractometer:	Enraf-Nonius CAD4
Scan mode:	ω (see refs. 3-4)
$T_{measurement}$:	293 K
$2\theta_{max}$:	40°
$N(hkl)_{unique}$:	2799
Criterion for I_o:	$I_o > 2\,\sigma(I_o)$
$N(param)_{refined}$:	170
Programs:	DIFABS, DIRDIF, PATTY, SHELXL-93, PLATON

$C_{31}H_{42}MoO_3SiW$, monoclinic, *C*12/*c*1 (No. 15), a =26.976(6) Å, b =16.141(2) Å, c =16.206(2) Å, β =120.83(3)°, V =6059.3 Å^3, Z =8, $R(F)$ =0.060, $R_w(F^2)$ =0.153.

Table 2. Final atomic coordinates and displacement parameters (in Å^2)

Atom	Site	*x*	*y*	*z*	U_{iso}
C(1)	8*f*	0.4405(9)	0.218(1)	0.422(2)	0.040(6)
H(1)	8*f*	0.4348(9)	0.231(1)	0.362(2)	0.048
C(11)	8*f*	0.486(1)	0.161(2)	0.476(2)	0.058(7)
H(11A)	8*f*	0.474(1)	0.124(2)	0.510(2)	0.070
H(11B)	8*f*	0.519(1)	0.192(2)	0.525(2)	0.070
C(12)	8*f*	0.507(1)	0.108(2)	0.421(2)	0.08(1)
H(12A)	8*f*	0.478(4)	0.068(9)	0.38(1)	0.124
H(12B)	8*f*	0.542(5)	0.08(1)	0.465(2)	0.124
H(12C)	8*f*	0.513(9)	0.143(3)	0.38(1)	0.124
C(2)	8*f*	0.4019(9)	0.258(1)	0.445(2)	0.032(5)
C(3)	8*f*	0.3922(9)	0.248(1)	0.527(1)	0.027(5)
C(31)	8*f*	0.376(1)	0.171(1)	0.559(2)	0.039(6)
H(31A)	8*f*	0.344(1)	0.183(1)	0.569(2)	0.047
H(31B)	8*f*	0.362(1)	0.130(1)	0.508(2)	0.047
C(32)	8*f*	0.426(1)	0.137(2)	0.649(2)	0.059(7)
H(32A)	8*f*	0.438(1)	0.176(2)	0.701(2)	0.071
H(32B)	8*f*	0.458(1)	0.126(2)	0.639(2)	0.071
C(33)	8*f*	0.406(2)	0.055(2)	0.674(3)	0.11(1)
H(33A)	8*f*	0.41(1)	0.063(6)	0.73(1)	0.169
H(33B)	8*f*	0.432(7)	0.012(4)	0.68(2)	0.169
H(33C)	8*f*	0.368(5)	0.042(9)	0.624(9)	0.169
C(4)	8*f*	0.3977(9)	0.331(1)	0.571(1)	0.031(5)
C(41)	8*f*	0.3772(9)	0.341(1)	0.642(1)	0.033(6)
H(41A)	8*f*	0.3514(9)	0.295(1)	0.632(1)	0.040
H(41B)	8*f*	0.3551(9)	0.392(1)	0.627(1)	0.004
C(42)	8*f*	0.425(1)	0.343(2)	0.747(2)	0.064(8)
H(42A)	8*f*	0.450(1)	0.296(2)	0.760(2)	0.077
H(42B)	8*f*	0.448(1)	0.393(2)	0.759(2)	0.077
C(43)	8*f*	0.405(1)	0.342(2)	0.814(2)	0.073(9)
H(43A)	8*f*	0.437(2)	0.35(1)	0.878(3)	0.109
H(43B)	8*f*	0.387(8)	0.289(5)	0.81(1)	0.109
H(43C)	8*f*	0.377(6)	0.385(8)	0.798(9)	0.109
C(5)	8*f*	0.4210(9)	0.395(1)	0.549(1)	0.032(6)
H(5)	8*f*	0.4339(9)	0.386(1)	0.507(1)	0.038
C(51)	8*f*	0.427(1)	0.479(1)	0.591(2)	0.040(6)
H(51A)	8*f*	0.461(1)	0.479(1)	0.655(2)	0.048
H(51B)	8*f*	0.394(1)	0.490(1)	0.598(2)	0.048
C(52)	8*f*	0.433(1)	0.552(2)	0.535(2)	0.060(8)

Table 2. (Continued)

Atom	Site	x	y	z	U_{iso}
H(52A)	8f	0.466(1)	0.541(2)	0.527(2)	0.072
H(52B)	8f	0.398(1)	0.553(2)	0.471(2)	0.072
C(53)	8f	0.440(1)	0.634(2)	0.579(2)	0.079(9)
H(53A)	8f	0.403(2)	0.653(6)	0.57(1)	0.118
H(53B)	8f	0.453(8)	0.673(3)	0.55(1)	0.118
H(53C)	8f	0.467(7)	0.631(3)	0.647(3)	0.118
C(61)	8f	0.288(1)	0.160(2)	0.338(2)	0.059(8)
O(61)	8f	0.2507(8)	0.140(1)	0.354(1)	0.072(5)
C(62)	8f	0.363(1)	0.082(2)	0.352(2)	0.043(6)
O(62)	8f	0.3736(9)	0.013(1)	0.381(1)	0.077(6)
C(7)	8f	0.3859(9)	0.392(1)	0.359(2)	0.032(6)
O(7)	8f	0.4147(8)	0.423(1)	0.334(1)	0.060(5)
C(81)	8f	0.288(1)	0.269(2)	0.160(2)	0.041(6)
C(82)	8f	0.272(1)	0.185(1)	0.143(2)	0.046(6)
H(82)	8f	0.236(1)	0.165(1)	0.127(2)	0.055
C(83)	8f	0.318(1)	0.132(2)	0.151(2)	0.08(1)
H(83)	8f	0.317(1)	0.075(2)	0.141(2)	0.098
C(84)	8f	0.363(1)	0.186(2)	0.179(2)	0.071(8)
H(84)	8f	0.399(1)	0.170(2)	0.195(2)	0.085

Table 2. (Continued)

Atom	Site	x	y	z	U_{iso}
C(85)	8f	0.348(1)	0.266(2)	0.182(2)	0.057(7)
H(85)	8f	0.372(1)	0.312(2)	0.196(2)	0.068
C(91)	8f	0.256(1)	0.381(2)	0.274(2)	0.045(6)
C(92)	8f	0.282(1)	0.457(2)	0.327(2)	0.042(6)
H(92)	8f	0.296(1)	0.501(2)	0.306(2)	0.051
C(93)	8f	0.284(1)	0.454(2)	0.416(2)	0.068(8)
H(93)	8f	0.299(1)	0.494(2)	0.463(2)	0.082
C(94)	8f	0.259(1)	0.381(2)	0.419(2)	0.054(7)
H(94)	8f	0.255(1)	0.363(2)	0.470(2)	0.064
C(95)	8f	0.241(1)	0.338(2)	0.334(2)	0.046(7)
H(95)	8f	0.222(1)	0.287(2)	0.319(2)	0.055
C(1A)	8f	0.167(1)	0.322(2)	0.076(2)	0.069(8)
H(1A1)	8f	0.159(2)	0.32(1)	0.011(3)	0.103
H(1A2)	8f	0.142(1)	0.364(5)	0.08(1)	0.103
H(1A3)	8f	0.161(2)	0.270(5)	0.098(8)	0.103
C(1B)	8f	0.259(2)	0.442(2)	0.098(2)	0.10(1)
H(1B1)	8f	0.233(7)	0.487(6)	0.09(2)	0.148
H(1B2)	8f	0.25(1)	0.425(5)	0.038(8)	0.148
H(1B3)	8f	0.298(4)	0.46(1)	0.140(8)	0.148

Table 3. Final atomic coordinates and displacement parameters (in $Å^2$)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
W(1)	8f	0.34231(4)	0.18962(6)	0.30250(7)	0.0387(7)	0.0407(7)	0.0413(7)	−0.0004(5)	0.0192(5)	−0.0054(5)
Mo(1)	8f	0.34098(8)	0.3460(1)	0.4095(1)	0.032(1)	0.034(1)	0.029(1)	0.0010(9)	0.017(1)	0.0011(9)
Si(3)	8f	0.2419(3)	0.3541(4)	0.1534(4)	0.046(4)	0.039(4)	0.030(4)	−0.001(3)	0.014(3)	−0.001(3)

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