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Crystallographic report

Tricarbonylacetylcyclopentadienylmolybdenum-tin(IV) trichloride

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The tin atom in $Cl_3SnMo(CO)_3C_5H_4COCH_3$ is in a distorted tetrahedral geometry with the molybdenum atom adopting a 3:4 piano stool geometry. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; tin(IV); molybdenum; cyclopentadienyl; heterobimetallic complex

COMMENT

The heterobimetallic compound $Cl_3SnMo(CO)_3C_5H_4COCH_3$ shows the tin atom to be distorted tetrahedral and the molybdenum atom in a 3:4 piano stool geometry; see Fig. 1. The average Sn–Cl bond distance is 2.353(1) Å, which is slightly shorter than that in the $Ph_2ClSnMo(CO)_3C_5H_4COCH_3$ analogue (2.398(2) Å).[1] Similarly, the Sn–Mo bond distance (2.7307(8) Å) is also shorter than that in the above-mentioned phenyl analogue (2.7683(6) Å).

EXPERIMENTAL

$Cl_3SnMo(CO)_3C_5H_4COCH_3$ was obtained from the reaction between $Ph_3SnMo(CO)_3C_5H_4COCH_3$ and HCl gas as per the literature method;[2] recrystallization was from a CH_2Cl_2/hexane (1/1) solution. Intensity data were collected at 293(2) K on a Bruker Smart 1000 CCD. $C_{10}H_7Cl_3MoO_4Sn$, $M = 512.14$, monoclinic, $P2_1/c$, $a = 7.713(2)$, $b = 12.626(4)$, $c = 16.055(5)$ Å, $\beta = 102.091(5)°$, $V = 1528.7(8)$ Å^3, $Z = 4$, $R = 0.033$ (2198 data with $I \geq 2\sigma(I)$; $\theta_{max} = 26.5°$), $wR = 0.057$ (all 3146 data). Programs used: SMART, SAINT, SHELXL97. CCDC deposition number: 245062.

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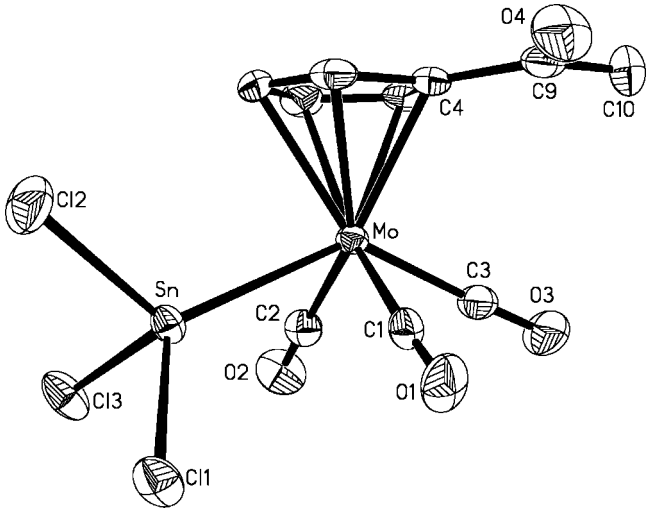

Figure 1. Molecular structure of $Cl_3SnMo(CO)_3C_5H_4COCH_3$; hydrogen atoms are omitted for clarity. Geometric parameters: Sn–Cl1 2.347(1), Sn–Cl2 2.352(1), Sn–Cl3 2.359(1), Sn–Mo 2.7307(8), O4–C9 1.218(6) Å; Cl1–Sn–Cl2 99.16(6), Cl1–Sn–Cl3 97.39(5), Cl2–Sn–Cl3 97.97(7), Cl1–Sn–Mo 121.76(4), Cl2–Sn–Mo 118.63(4), Cl3–Sn–Mo 117.24(4), O4–C9–C4 118.1(5), O4–C9–C10 122.4(5), C4–C9–C10 119.5(5)°.