APPLIED ORGANOMETALLIC CHEMISTRY
Appl. Organometal. Chem. 2004; **18**: 371–372
Published online in Wiley InterScience (www.interscience.wiley.com). DOI:10.1002/aoc.648

Crystallographic report

Tricarbonyl(η^5-cyclopentadienyl)(dichloroindium) molybdenum

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Received 27 February 2004; Revised 17 March 2004; Accepted 20 March 2004

In the solid state, [{Cp(CO)$_3$Mo}InCl$_2$]∞ forms a one-dimensional coordination polymer in which the indium atoms are coordinated by four chlorine atoms (In–Cl: 2.448(2)–3.004(2) Å) and a {Cp(CO)$_3$Mo} group (In–Mo: 2.750(1) Å) in a distorted trigonal bipyramidal environment. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; indium; molybdenum

COMMENT

[{Cp(CO)$_3$Mo}InCl$_2$] (**1**) crystallizes as a one-dimensional coordination polymer in which the [{Cp(CO)$_3$Mo}InCl$_2$] units are linked by bridging chlorine atoms (Fig. 1). The indium atoms exhibit a rather distorted trigonal bipyramidal coordination sphere which comprises four chlorine atoms and a {Cp(CO)$_3$Mo} group. The trigonal bipyramids are connected by edge sharing to give strands that are stacked parallel to the crystallographic *a*-axis. This type of supramolecular structure has already been observed for the compounds $(CH_3)_3CH_2InCl_2$ (**2**),[1] $Me_3SiCH_2InCl_2$ (**3**),[2] $(Me_3Si)_2CHInBr_2$[3] and $MesInI_2$[4] (Mes = 1,3,5-trimethylphenyl). As in the case of each of **2** and **3**, the equatorial In–Cl bonds (2.448(2) and 2.481(2) Å) are significantly shorter than the axial In–Cl bonds (2.735(2) and 3.004(2) Å). However, compared with **2** and **3**, this effect is more pronounced in **1**. The In–Mo bond length of 2.750(1) Å is close to the value reported for Na[In{Cp(CO)$_3$Mo}Cl$_3$] (2.739(1) Å).[5]

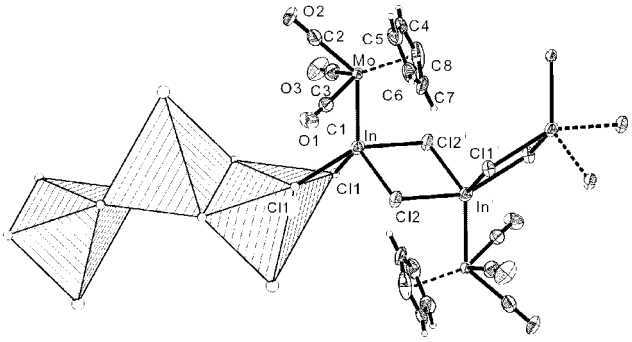

Figure 1. Structure of [{Cp(CO)$_3$Mo}InCl$_2$] in the crystal. Key geometric parameters: Mo–In 2.750(1), In–Cl1 2.481(2), In–Cl2 2.448(2), In–Cl1^i 2.735(2), In–Cl2^i 3.004(2) Å; Cl1–In–Cl2 103.6(1), Cl1–In–Cl1^i 80.3(1), Cl2–In–Cl1^i 86.9(1), Cl2–In–Cl2^i 79.1(1), In–Cl1–In^i 99.7(1), In–Cl2–In^i 100.9(1)°. Symmetry operation i: −x, −y, −z.

EXPERIMENTAL

[{Cp(CO)$_3$Mo}InCl$_2$] was prepared by a redistribution reaction from InCl$_3$ and [{Cp(CO)$_3$Mo}$_3$In][6] in tetrahydrofuran as solvent. Single crystals were obtained by diffusion of *n*-heptane into a solution of [{Cp(CO)$_3$Mo}InCl$_2$] in acetone. Intensity data were collected at 220 K on a STOE IPDS diffractometer for a pale-yellow crystal 0.02 × 0.04 × 0.09 mm^3, $C_8H_5Cl_2InMoO_3$, M = 430.78, monoclinic, $P2_1/n$, a = 6.8457(14), b = 13.709(3), c = 12.803(3) Å, β = 100.44(3)°, V = 1181.6(4) Å^3, Z = 4, 2295 unique data, (θ_{max} = 26.0°), R_1 = 0.076 (all data), wR_2 = 0.094 (all data). Programs used: SHELXL, PLATON, DIAMOND. CCDC deposition number: 231 207.

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Contract/grant sponsor: Deutsche Forschungsgemeinschaft.

REFERENCES

1. Beachley Jr OT, Spiegel EF, Kopasz JP, Rogers RD. *Organometallics* 1989; **8**: 1915.

2. Self MF, McPhail AT, Jones III LJ, Wells RL, Huffmann JC. *Polyhedron*, 1994; **13**: 199.
3. Häußlein M, Hausen HD, Klinkhammer KW, Weidlein J. *Z. Anorg. Allg. Chem.* 1999; **625**: 1608.
4. Leman JT, Ziller JW, Barron AR. *Organometallics* 1991; **10**: 1766.
5. Clarkson LM, Clegg W, Norman NC, Tucker AJ, Webster PM. *Inorg. Chem.* 1988; **27**: 2653.
6. Hsieh ATT, Mays M. *J. Organometal. Chem.* 1972; **37**: 9.