

Preliminary communication

FORMATION OF A ZIRCONIUM—MOLYBDENUM BOND VIA METHANE ELIMINATION

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Summary

Reaction of $(\eta^5\text{-C}_5\text{H}_5)_2\text{Zr}(\text{CH}_3)_2$ and $(\eta^5\text{-C}_5\text{H}_5)\text{Mo}(\text{CO})_3\text{H}$ gives $(\text{C}_5\text{H}_5)_2\text{CH}_3\text{Zr—Mo}(\text{C}_5\text{H}_5)(\text{CO})_3$. Some properties of this compound are described.

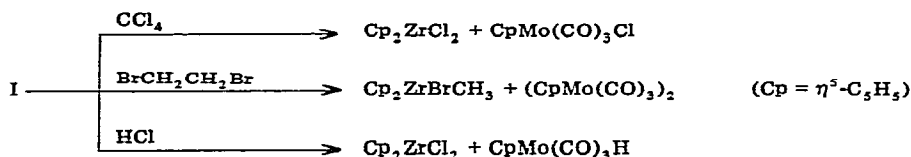
In recent years metal—metal bonding has received much attention, but for Group IVA metals, if we exclude compounds with Group IVB metals [1], the only known compounds containing such a bond are $(\eta^5\text{-C}_5\text{H}_5)(\text{CO})_3\text{MoTi}(\text{O-i-Pr})_3$ [2] and $(\eta^5\text{-C}_5\text{H}_5)(\text{CO})_3\text{MoTi}(\eta^5\text{-C}_5\text{H}_5)_2$ [3]. In this paper, we report the synthesis and some properties of $(\eta^5\text{-C}_5\text{H}_5)_2\text{CH}_3\text{Zr—Mo}(\eta^5\text{-C}_5\text{H}_5)(\text{CO})_3$ (I).

Reaction between molecular amounts of dimethylzirconocene and cyclopentadienylmolybdenum tricarbonylmonohydride in THF at room temperature occurs with rapid evolution of methane. Evaporation of the solvent and washing with pentane affords yellow crystals of I, which are very sensitive to oxygen. The NMR spectrum of I exhibits three singlets at 0.45 (3H), 5.25 (5H) and 5.75 (10H) ppm (C_6D_6 , TMS) relative to methyl, molybdenum-bonded cyclopentadienyl and zirconium-bonded cyclopentadienyl groups. The elementary analysis was satisfactory. Found: C, 47.42; H, 3.80; Mo, 19.94; Zr, 18.89. $\text{C}_{19}\text{H}_{18}\text{O}_3\text{MoZr}$ calcd.: C, 47.39; H, 3.77; Mo, 19.92; Zr, 18.94%.

I reacts rapidly with CCl_4 , $\text{BrCH}_2\text{CH}_2\text{Br}$ and anhydrous HCl giving the products expected from a complex having the postulated metal—metal bonded structure (see Scheme 1).

These products were characterised by spectroscopic methods.

SCHEME 1



The synthetic method is a little less satisfactory for the isoleptic hafnium compound. We are presently investigating the potential of methane and hydrogen elimination reactions for the preparation of metal-metal compounds of the IVA elements.

References

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- 3 M.F. Lappert and A.R. Sanger, *J. Chem. Soc. (A)*, (1971) 1314.