

Location of a 4-coordinate H Atom via Neutron Diffraction

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A four-coordinate H atom has been unambiguously located, by single-crystal neutron diffraction for the first time, in the centre of the tetrahedral metal complex $Y_4H_8(Cp')_4(THF)$ [$Cp'=C_5Me_4(SiMe_3)$]. The core of the molecule consists of a tetranuclear cluster with one interstitial, one face-bridging and six edge-bridging hydride ligands. At the present stage of structural refinement, the four individual Y–H distances to the unique interstitial hydride ligand are 2.184(16), 2.189(16), 2.221(13) and 2.168(12)Å. The compound was prepared via the reaction of $YCp'(CH_2SiMe_3)_2(THF)$ with $PhSiH_3$ and gaseous H_2 , and an initial x-ray analysis suggested the present geometry. [1]

The existence of 4-coordinate hydrogen now completes the series of high-connectivity hydride ligands located in the interstitial cavities of molecular cluster complexes. We had previously reported the existence of 6-coordinate H in the octahedral cavity of $[HCo_6(CO)_{15}]^-$ in 1979, [2] and 5-coordinate H in the square pyramidal cavities of $[H_2Rh_{13}(CO)_{24}]_{3-}$ in 1997, [3] via single-crystal neutron analyses.

[1] Tardif O., Nishiura M., Hou Z., *Organometallics*, 2003, **22**, 1171. [2] Hart D.W., Teller R.G., Wei C.W., Bau R., Longoni G., Campanella S., Chini P., Koetzle T.F., *Angew. Chem. Internat. Edit.*, 1979, **18**, 80. [3] Bau R., Drabnis M.H., Xie Z., Garlaschelli L., Klooster W.T., Koetzle T.F., Martinengo S., *Science*, 1997, **275**, 1099.

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