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Neutron Diffraction Study of OsH₃Cl(PPh₃)₃, a Compound Containing a “Stretched” Dihydrogen Ligand. Robert Bau¹, M. Yousufuddin¹, T. Wen², G. Jia², S. Mason³, G. McIntyre³, ¹Dept. of Chemistry, Univ. of Southern California, Los Angeles, CA, USA; ²Dept. of Chemistry, Hong Kong Univ. of Science and Technology, Clear Water Bay, Hong Kong, ³Inst. Laue Langevin, Grenoble, France.

The structure of OsH₃Cl(PPh₃)₃ has been studied by neutron diffraction at 5 K. The compound was suspected to contain a non-classical dihydrogen ligand based on previous ¹H NMR^[1] and X-ray measurements^[2] at low temperature. Our subsequent neutron diffraction study confirms the presence of a dihydrogen ligand, but with an unexpected H-H distance of 1.47(2) Å. This unusually long distance represents a rare example of a “stretched” dihydrogen ligand (intermediate between a true non-classical dihydrogen distance of H-H ~ 0.8 -1.0 Å and a non-bonding dihydride distance of H...H > 1.7 Å) that had been observed only three times before by neutron diffraction.^[3] Experimental details: a crystal with an approximate volume of 0.5 mm³ was mounted on the VIVALDI instrument at the Institut Laue-Langevin in Grenoble, France; R(F) = 0.0896 for 3636 independent reflections with I > 2σ(I).

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