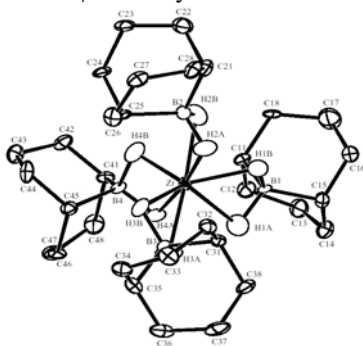


W0396

Synthesis, X-ray and Neutron Structures of $Zr\{(\mu-H)_2BC_8H_{14}\}_4$. Muhammed Yousufuddin^a, Errun Ding^b, Bin Du^b, Edward A. Meyers^b, Sheldon G. Shore^b, Garry J. McIntyre^c, Robert Bau^{a†}, ^aDept. of Chemistry, Univ. of Southern California, Los Angeles, CA 90089, ^bDept. of Chemistry, Ohio State Univ., Columbus, OH 43210, ^cInst. Laue Langevin, 6 rue Jules Horowitz, BP 156, 38042 Grenoble Cedex 9, France.

The complex $Zr(9-BBN)_4$ [9-BBN = $(\mu-H)_2BC_8H_{14}$] has been synthesized via the reaction of $K(9-BBN)$ with $ZrCl_4$ in diethyl ether. The structure of the title compound has been determined by X-ray and neutron



single-crystal diffraction techniques. Each 9-BBN ligand is coordinated to the Zr atom via two B-H-Zr bridges, and these metal-ligand bonding interactions are further augmented by three prominent C-H ...Zr *agostic* interactions. Average molecular parameters derived from the neutron analysis: Zr-H = 2.051(8) Å, B-H = 1.286(7) Å, Zr...B = 2.409(6) Å, Zr-H-B = 87.7(4)°, H-Zr-H = 58.9(3)°. The Zr...H distances corresponding to the three C-H...Zr *agostic* interactions are 2.424(7) Å, 2.663(8) Å, and 2.551(7) Å. The fourth potential C-H...Zr interaction has a Zr...H distance [3.146(7) Å] that is too long to be considered in the *agostic* range. Single crystal X-ray diffraction data were collected on an Enraf-Nonius Kappa CCD diffraction system, and neutron diffraction data

were collected on the quasi-Laue diffractometer VIVALDI at the Institut Laue-Langevin; the final agreement factor for the neutron analysis = 6.52% for 2557 reflections with $I > 2\sigma(I)$.

Neutron structure of $Zr\{(\mu-H)_2BC_8H_{14}\}_4$ showing the eight hydride positions with 50% probability ellipsoids.