A QUANTUM CHEMICAL STUDY OF THE STRUCTURE AND CHEMISTRY OF $HZnCH_3$, A TRANSITION METAL COMPOUND WITH $4s^2$ RECOUPLED PAIR BONDING

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A structure was recently reported by Flory et al.[a] for methyl zinc hydride, $HZnCH_3$, a molecule that may be formed via the direct insertion of Zn into one of the CH bonds of methane. The experiments were not able to demonstrate the formation pathway conclusively. The structures, bond energies, and other properties of $HZnCH_3$, ZnH, and $ZnCH_3$ were determined with high level coupled-cluster theory and multireference configuration interaction calculations in order to better understand the nature of the chemistry of $HZnCH_3$. The Zn–H and Zn–C bonds in $HZnCH_3(X^1A_1)$ were found to be formed through recoupling the $4s^2$ pair of $Zn(^1S)$ in a manner that is very similar to the bonding in $HBeCH_3$ and other compounds where the $2s^2$ pair of Be is recoupled. Various formation pathways were characterized, such as the analogous family of exchange reactions $H + CH_4 \rightarrow CH_4 + H$, $Zn + CH_4 \rightarrow ZnCH_3 + H$, and $Be + CH_4 \rightarrow BeCH_3 + H$. Direct insertion may involve an intersystem crossing from the $Zn(^3P) + CH_4$ triplet surface to the singlet surface, which has been explored.

[a] M. A. Flory, A. J. Apponi, L. N. Zack, and L. M. Ziurys, *J. Am. Chem. Soc.* **132**, 17186 (2010).