

Stern-Gerlach Experiments of One-Dimensional Metal-Benzene Sandwich Clusters: $M_n(C_6H_6)_m$ ($M = Al, Sc, Ti$ and V)

Atsushi Nakajima^{1,2}

¹Department of Chemistry, Faculty of Science and Technology, Keio University,
3-14-1 Hiyoshi, Kohoku-ku, Yokohama 223-8522, Japan,

²CREST, Japan Science and Technology Agency (JST), c/o Department of Chemistry,
Keio University, Yokohama 223-8522, Japan,
E-mail; nakajima@chem.keio.ac.jp

A molecular beam of multilayer metal-benzene organometallic clusters $M_n(C_6H_6)_m$ ($M = Al, Sc, Ti$, and V) was produced by a laser vaporization synthesis method, and their magnetic deflections were measured. Multidecker sandwich clusters of transition metal atoms and benzene $Sc_n(C_6H_6)_{n+1}$ ($n = 1-2$) and $V_n(C_6H_6)_{n+1}$ ($n = 1-4$) possess magnetic moments that increase monotonously with n .¹⁻⁴ The ferromagnetic spin ordering of the $V_n(C_6H_6)_{n+1}$ clusters can be reproduced by theoretical calculations.⁵ The magnetic moments of $Al(C_6H_6)$, $Sc_n(C_6H_6)_{n+1}$ and $V_n(C_6H_6)_{n+1}$ are smaller than that of their spin-only values as a result of intra-cluster spin relaxation, an effect that depends on the orbital angular momenta and bonding characters of the orbitals containing electron spin. While $Ti(C_6H_6)_2$ was found to be non-magnetic, $Ti_n(C_6H_6)_{n+1}$ ($n = 2, 3$) possess magnetic moments.⁶ The mechanism of ferromagnetic spin ordering in $M_2(C_6H_6)_3$ ($M=Sc, Ti, V$) is discussed qualitatively in terms of molecular orbital analysis. These sandwich species represent a new class of one-dimensional molecular magnets in which the transition metal atoms are formally zerovalent.

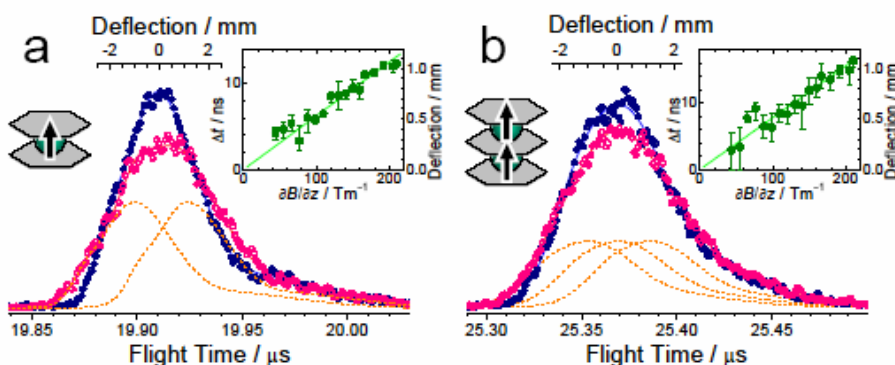


Figure 1. Broadening of TOF peaks of $V(C_6H_6)_2$ and $V_2(C_6H_6)_3$ by the magnetic field gradient at $T = 154$ K. (Filled circle: $\partial B/\partial z = 0$, open circle: $\partial B/\partial z = 205 \text{ Tm}^{-1}$) Solid lines indicate modeled TOF profiles for zero-field profile and simulated broadened profile. Beamlets are shown by dashed lines. Inserts show the deflection magnitude of the outmost beamlet obtained by the ‘beamlet’ model.

- [1] K. Miyajima, A. Nakajima, S. Yabushita, M. B. Knickelbein, and K. Kaya *J. Am. Chem. Soc.* **126** (2004) 13202.
- [2] K. Miyajima, M. B. Knickelbein, and A. Nakajima, *Eur. J. Phys. D.* **34** (2005) 177.
- [3] K. Miyajima, M. B. Knickelbein, and A. Nakajima, *Polyhedron* **24** (2005) 2341.
- [4] K. Miyajima, S. Yabushita, M. B. Knickelbein, and A. Nakajima, submitted to *J. Am. Chem. Soc.* (2007).
- [5] J. Wang, P. H. Acioli, and J. Jellinek, *J. Am. Chem. Soc.* **127** (2005) 2812.
- [6] J. Kua and K. M. Tomlin, *J. Phys. Chem. A* **100** (2006) 11988.