高スピン多核錯体の開発
Cyanide-Bridged Fe42 High-Spin Nanocage with *S* = 90/2

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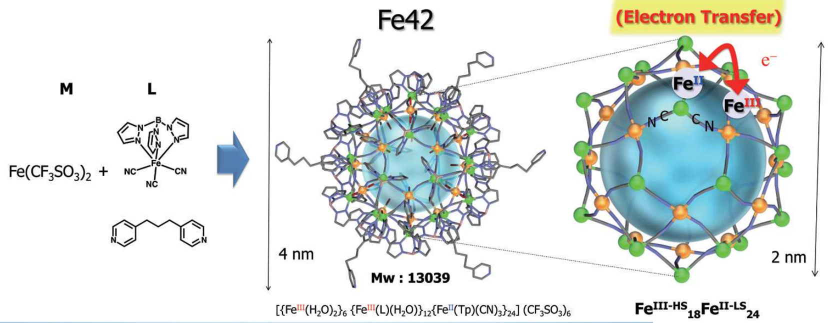
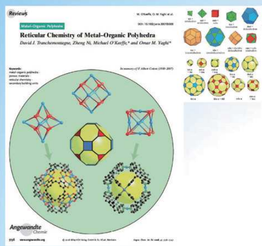
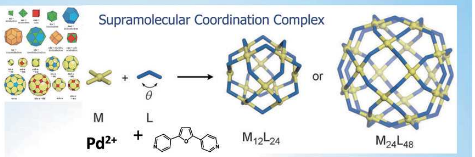


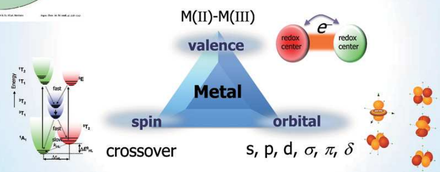
1. **The largest cyanide-bridged metal nanocage reported to date**
2. **Mixed valance state ($Fe^{III}{}_{18}Fe^{II}{}_{24}$)**
3. **High spin cluster [a Record *S* = 90/2]**
4. **Metal-to-metal charge transfer upon reversible coordination bond formation/ cleavage**
5. **Stellated-cuboctahedral structure**

1. Introduction



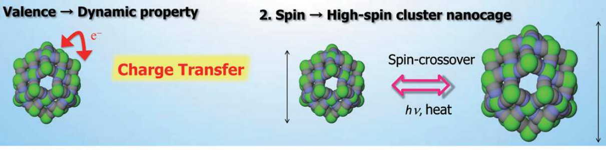


M. O'Keeffe, O. M. Yaghi et al. *Angew. Chem. Int. Ed.* **2008**, 47, 5136.
M. Fujita et al. *Science*, **2010**, 328, 1144.
Angew. Chem. Int. Ed. **2012**, 51, 3161.



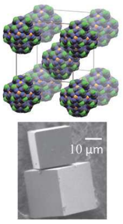
If we could utilize valence, spin and orbital of metals on metal-organic polyhedra....

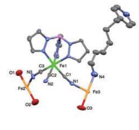
1. Valence → Dynamic property **2. Spin → High-spin cluster nanocage**



2. X-ray Crystal Structures

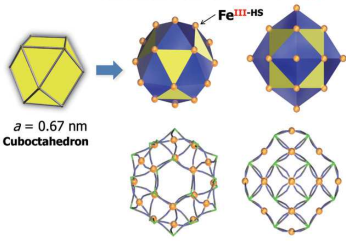
Packing structure Asymmetric unit



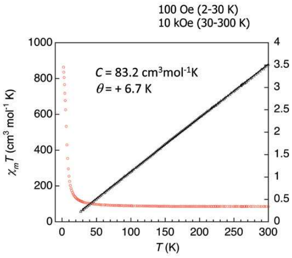


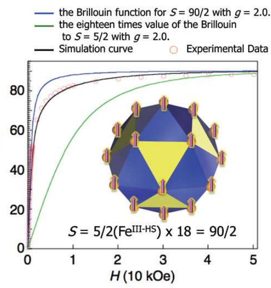
Pn-3n
a = b = c =30.7679(13) Å
α = *β* = *γ* = 90.00 Å
V = 29126.9Å³
T = 100 K
*R*1 = 0.0857

Stellated Cuboctahedral Spin Nanocage

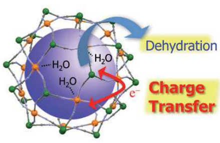


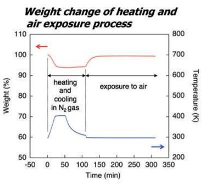
3. Magnetic Properties

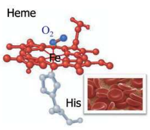




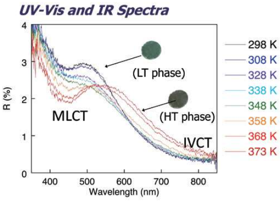
4. Metal-to-Metal Charge Transfer



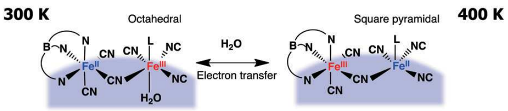


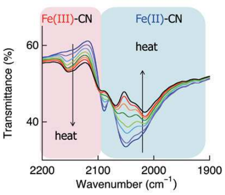


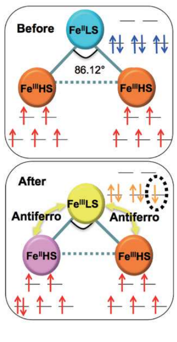
UV-Vis and IR Spectra



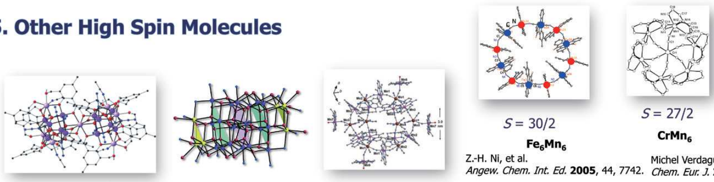
Reversible Coordination Bond Formation/Cleavage







5. Other High Spin Molecules



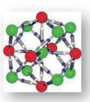
S = 83/2
Mn 19: [$Mn^{III}{}_{12}Mn^{II}{}_7$]
Ayuk M. Ako et al. *Angew.Chem.Int.Ed.* **2006**, 45, 4926.

S = 51/2
Mn 25
Muralee Murugesu et al. *J. Am. Chem. Soc.* **2004**, *126*, 4766.

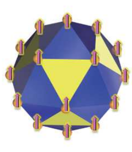
S = 31/2
Mo_8Mn_{14}
X.-Y. Wang et al. *Angew.Chem.Int.Ed.* **2000**, 39, 1605.

S = 30/2
Fe_6Mn_6
Z.-H. Ni, et al. *Angew. Chem. Int. Ed.* **2005**, 44, 7742.

S = 27/2
$CrMn_6$
Michel Verdaguer et al. *Chem. Eur. J.* **2003**, 9, 1677.



S = 39/2
Mn_9Mo_6
Joulia Larionova et al. *Angew.Chem.Int.Ed.* **2000**, 39, 1605.



S = 90/2
Fe_{42}
This study

Acknowledgements