

Supporting Information of

Regioselective Coordination of $\text{Re}_2(\text{CO})_{10}$ to $\text{Y}@\text{C}_{2v}(9)\text{-C}_{82}$:

An Unprecedented η^1 -Complex Stabilized by Intramolecular Electron Transfer

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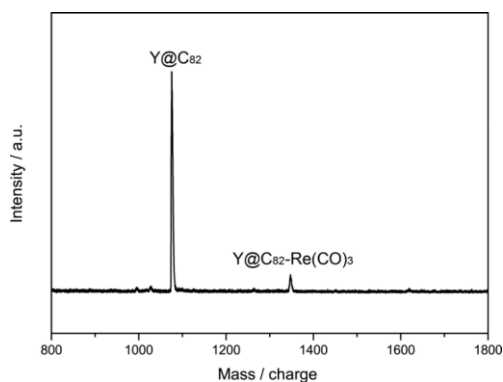


Figure S1. MALDI-TOF mass spectrum of **2**.

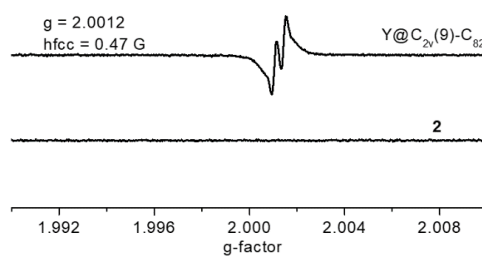
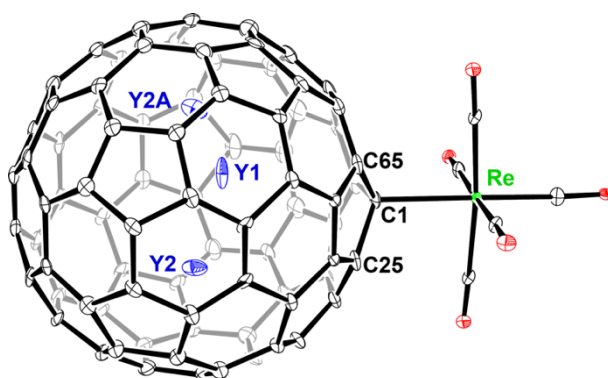


Figure S2. ESR spectra of $\text{Y}@\text{C}_{2v}(9)\text{-C}_{82}$ and **2**.

Table S1. Crystallographic data of **2**.

Empirical formula	[Y@C _{2v} (9)-C ₈₂ -Re(CO) ₅] ₂ ·2CS ₂
Formula weight	2908.21
Temperature	273(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/m
Unit cell dimensions	a = 19.7521(17), α = 90°. b = 11.6727(10), β = 101.072(2)°. c = 19.5544(18), γ = 90°.
Volume	4424.6(7) Å ³
Z	2
Absorption coefficient	4.213 mm ⁻¹
F(000)	2812
Theta range for data collection	1.061 to 25.372°.
Reflections collected	3707
Observed reflections (I > 2σ(I))	3281
Completeness to theta = 25.242°	89.6 %
Refinement method	SHELXL-2016/6 (Sheldrick, 2016)
Data / restraints / parameters	3707 / 595 / 460
Goodness-of-fit on F ²	1.359
Final R indices [I > 2σ(I)]	R1 = 0.0689, wR2 = 0.1708
R indices (all data)	R1 = 0.0810, wR2 = 0.1769

**Figure S3.** The structure of **2** and the disordered Y sites inside the C_{2v}(9)-C₈₂ cage.

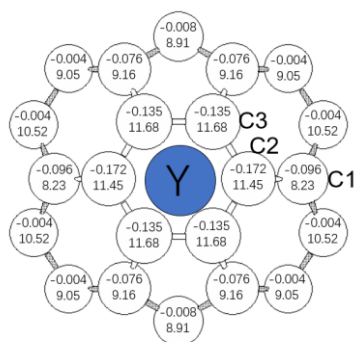


Figure S4. Charge density (upper) and POAV values (lower) of typical cage carbon atoms in $Y@C_{2v}(9)-C_{82}$.