

Supplementary Materials

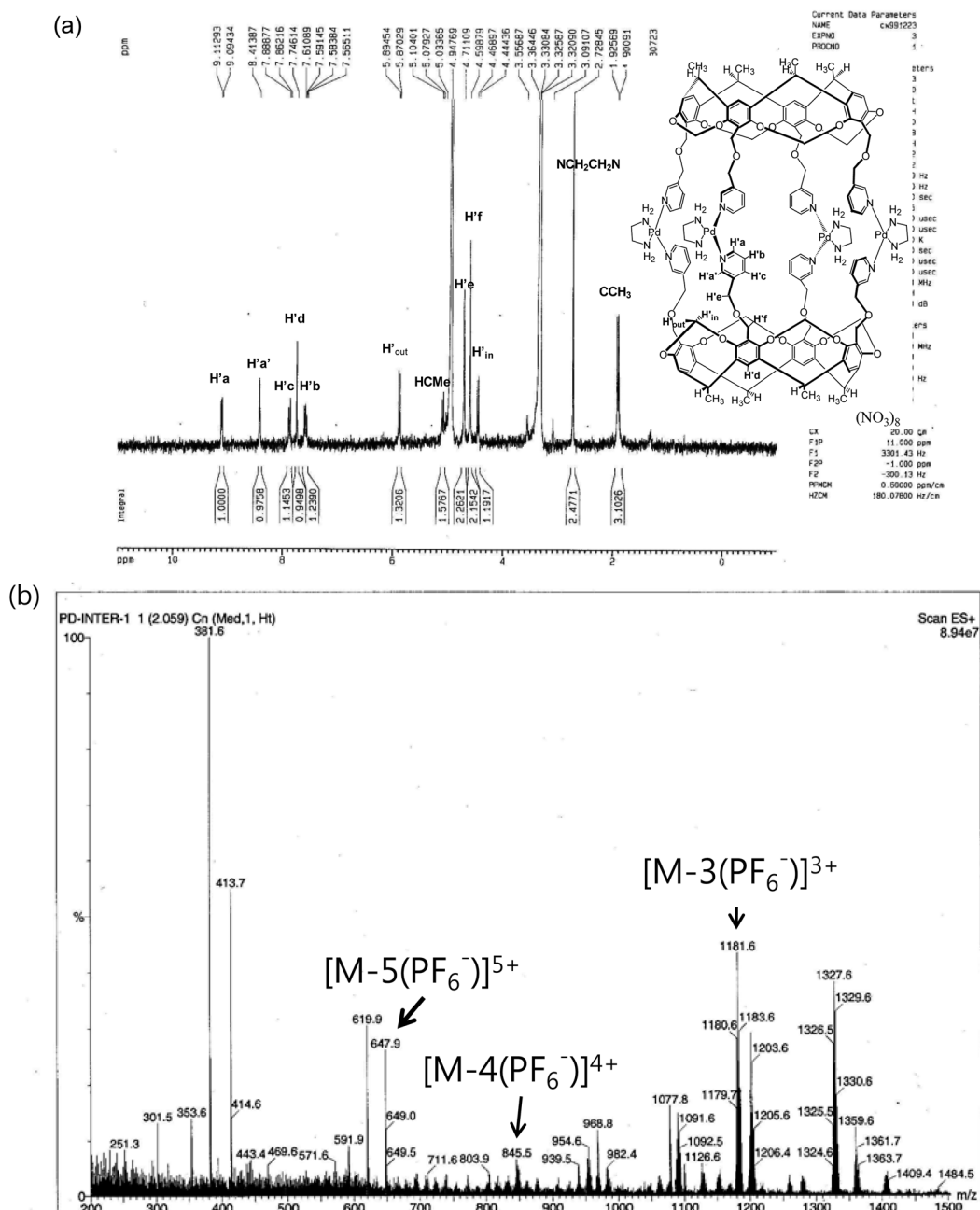
Kinetically Trapped Receptor and its Thermodynamic Conversion
During Metal-mediated Self-assemblyChoon Woo Lim,^{†,*} and Jong-In Hong^{‡,*}[†]Department of Applied Chemistry, College of Applied Science, Kyung Hee University, Gyeonggi-do 449-701, Korea

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Figure S1. (a) ¹H NMR (300 MHz, CD₃OD) spectrum and (b) ESI MS spectrum Pd-inter.

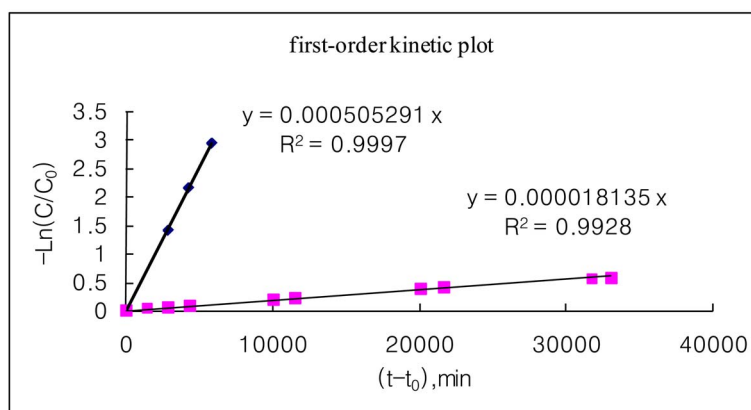


Figure S2. Kinetic data of the conversion of **Pd-intra** into **Pd-inter** in MeOD- d_3 (◆) and in a mixture of MeOD- d_3 /D $_2$ O (1:1, v/v, ■).

^1H NMR experiments were performed using a Bruker Avance 500 spectrometer (500 MHz). Kinetic parameters were evaluated on the basis of time-dependent ^1H NMR measurements using the α - or β -proton of pyridyl groups as probes. The concentration ratio, *i.e.*, the ratio of $[\text{Pd-intra}]_t$ to $[\text{Pd-intra}]_0$, was calculated from the relative integration of the **Pd-intra** signal obtained at a given time and the initial **Pd-intra** signal during ^1H NMR measurements performed at definite time intervals.

If the conversion follows first-order kinetics and the volume of the system remains essentially constant during the conversion process, the first-order rate equation can be written as

$$-dc/dt = kc \quad (1)$$

If the concentration is c_0 at time $t = 0$, and decreases to c at time t , the integration (being carried out between c_0 and c) gives

$$-\int dc/c = k \int dt \quad (2)$$

$$\ln(c_0/c) = kt \quad (3)$$

The graph of t versus $\ln(c_0/c)$ shows a straight line with a slope k . From this graph, we can estimate the rate of conversion of **Pd-intra** into **Pd-inter** at room temperature (298 K).