

S1

## Supporting Information

The derivation of the equation describing the binding of pyridine to **Ru(CO)3**

$$K = \frac{[HL'] [L]}{[HL] [L']} \text{ but since } [L] = \text{constant}$$

$$K' = \frac{[HL']}{[HL] [L']} \text{ and } K = K' [L]$$

Let  $[HL]_o$  be the initial concentration of  $HL$ , and  $[L']_o$  be the initial concentration of  $L'$

$$K' = \frac{[HL']}{([HL]_o - [HL'])([L']_o - [HL'])}$$

$$\Rightarrow K'([HL]_o - [HL'])([L']_o - [HL']) = [HL']$$

$$\Rightarrow K'([HL'])^2 - (K'[HL]_o + K'[L']_o + 1)[HL'] + K'[HL]_o[L']_o = 0$$

Divide by  $K'$

$$\Rightarrow ([HL'])^2 + (-[HL]_o - [L']_o - \frac{1}{K'})[HL'] + ([HL]_o)[L']_o = 0$$

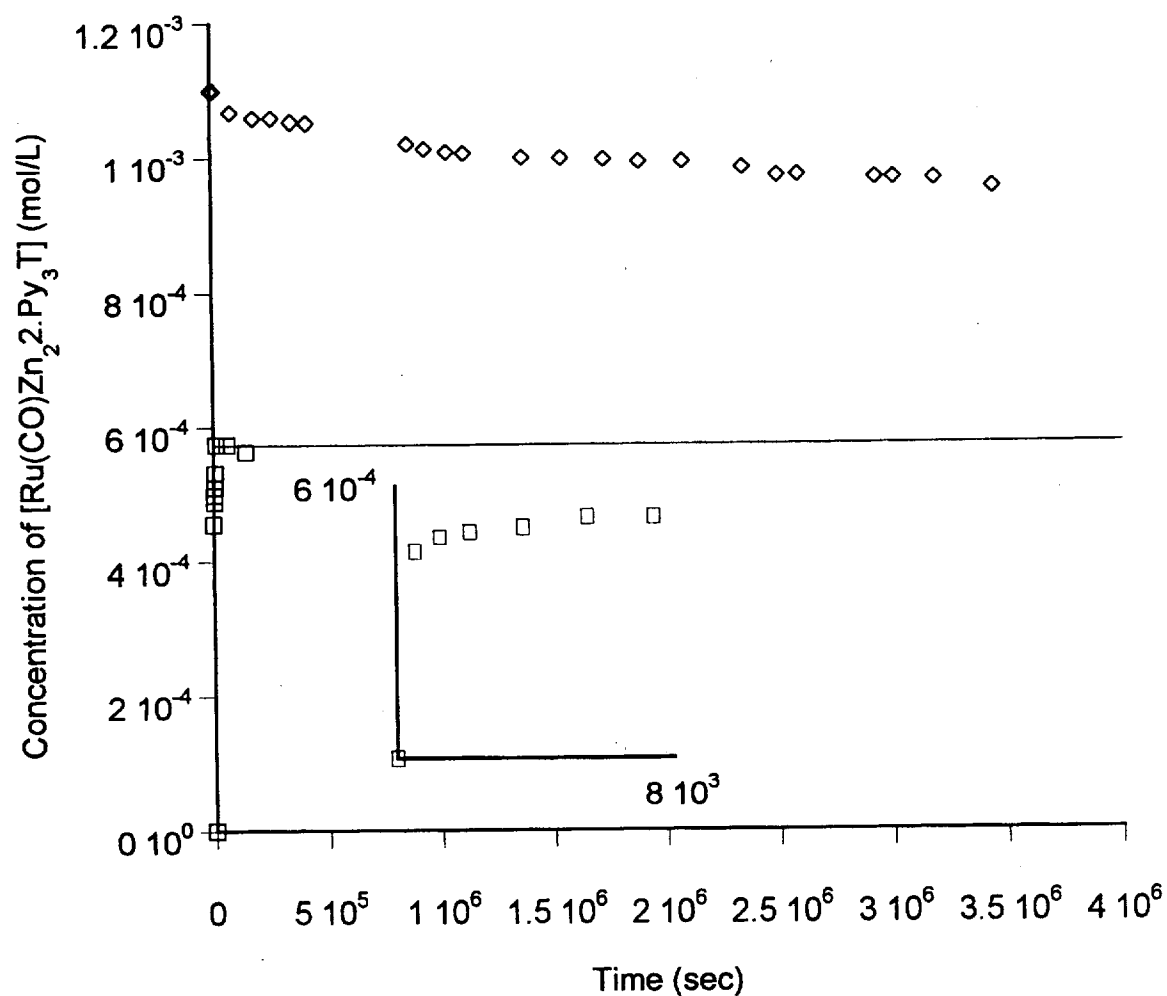
Solve using the Quadratic Equation

$$HL' = \frac{([HL]_o + [L']_o + \frac{1}{K'}) \pm \sqrt{(-[HL]_o - [L']_o - \frac{1}{K'})^2 - 4([HL]_o)[L']_o}}{2}$$

Since we know the initial concentration of host  $[HL]_o$ , then the concentration of the complex  $[HL']$  can be calculated for each initial concentration of ligand  $[L']_o$ , for an arbitrary value of  $K'$ . The error in the calculated curve can then be calculated in each calculated value of  $[HL']$  by averaging  $|[HL'](found) - [HL'](calculated)|$  for each  $[L']_o$ .

S2

**Figure S1.** Graph showing the rate of displacement of  $\text{Py}_3\text{T}$  from  $\text{Zn}_3\text{I}(\text{NO}_2)_6 \cdot \text{Py}_3\text{T}$  into  $\text{Ru}(\text{CO})\text{Zn}_2$  (Reaction A,  $\square$ ) and from  $\text{Ru}(\text{CO})\text{Zn}_2 \cdot \text{Py}_3\text{T}$  into  $\text{Zn}_3\text{I}(\text{NO}_2)_6$  (Reaction B,  $\diamond$ ). The solid line represents the equilibrium value. The inset shows the initial stages of Reaction A.



S3

The 250 MHz proton NMR spectrum of  $\text{Ru}(\text{CO})\text{Zn}_2\text{Py}_3\text{T}$ .

