

Toward a Dodecanuclear Molecular Re(I) Box: Structural and Spectroscopic Properties

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Supporting Information

Table S1 Crystallographic Data for **1** and **2**.

	[(Re(CO) ₃) ₆ (tpeb) ₂ (N ₃ S ₃) ₂] 4CH ₃ CN·toluene 1 ·4CH ₃ CN·toluene	[(Re(CO) ₃) ₁₂ (TTF(py) ₄) ₃ (N ₃ S ₃) ₄] 8CH ₃ CN·12DMF 2 ·8CH ₃ CN·12DMF
Empirical formula	C ₁₀₇ H ₅₆ N ₁₈ O ₁₈ Re ₆ S ₆	C ₁₇₈ H ₁₅₆ N ₄₄ O ₄₈ Re ₁₂ S ₂₄
Formula weight	3191.25	6683.30
Crystal system	Monoclinic	Triclinic
Space group	<i>C2/c</i>	<i>P</i> $\bar{1}$
a (Å)	35.076(1)	14.662(1)
b (Å)	18.413(1)	19.304(1)
c (Å)	24.677(2)	22.801(1)
α (°)		114.181(1)
β (°)	133.677(1)	101.722(1)
γ (°)		93.201(1)
V (Å ³), Z	11527.0(9), 4	5694.2(4), 1
F(000) (e)	6056	3200
μ (Mo-K α) (mm ⁻¹)	6.454	6.648
T (K)	150(2)	150(2)
Reflections collected	42647	52052
Independent reflections (Fo \geq 2 σ (Fo))	13199 (R _{int} =0.034)	26124 (R _{int} =0.022)
Refined parameters	717	1192
Goodness-of-fit on F ²	1.054	1.083
R ^a , R _w ^b (I \geq 2 σ (I))	0.030, 0.073	0.037, 0.091
R ^a , R _w ^b (all data)	0.039, 0.078	0.048, 0.098

$${}^a R = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}, \quad {}^b R_w = \left\{ \frac{\sum w(F_o^2 - F_c^2)^2}{\sum [w(F_o^2)^2]} \right\}^{1/2}.$$

Figure S1. The experimental and simulated powder X-ray diffraction patterns of **1**.

Figure S2. The experimental and simulated powder X-ray diffraction patterns of **2**.

Figure S3. The TGA trace of **1**.

Figure S4. The TGA trace of **2**.

Figure S5. The normalized emission spectra for solid samples of **1** at room temperature (black) and at 77 K (red). Excitation wavelengths are at 300 nm.

Figure S6. The normalized emission spectra for solid samples of **2** at room temperature (black) and at 77 K (red). Excitation wavelengths are at 300 nm.

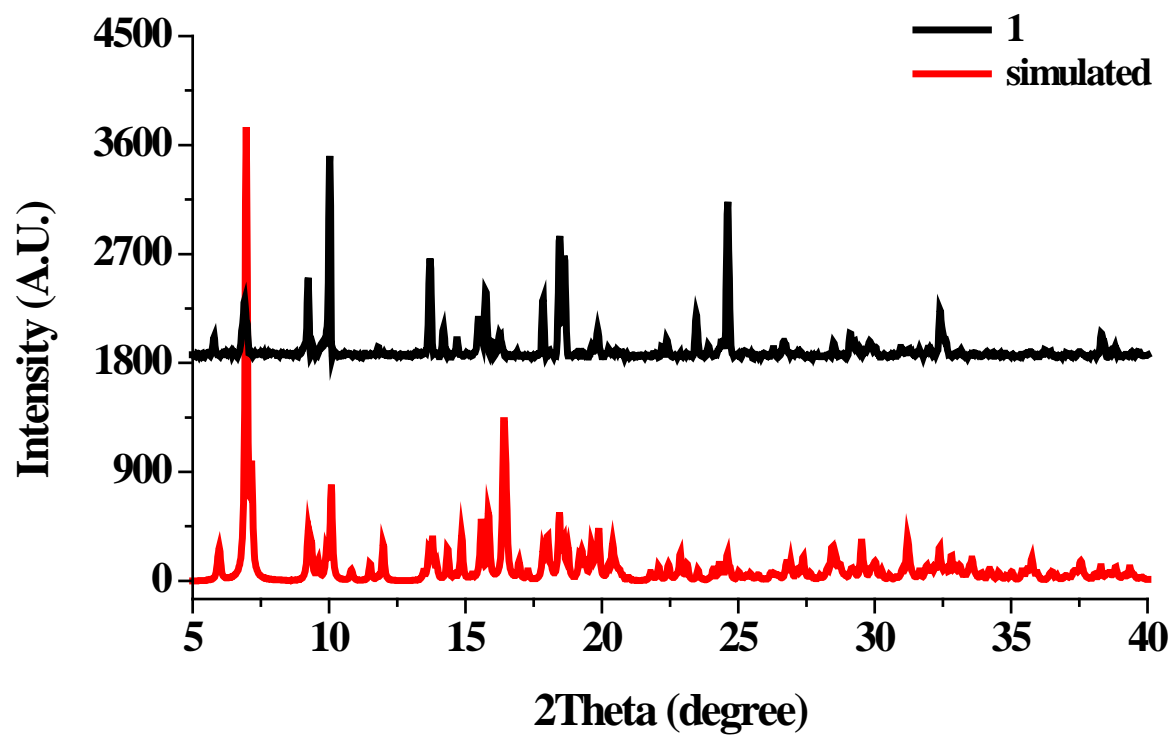


Figure S1

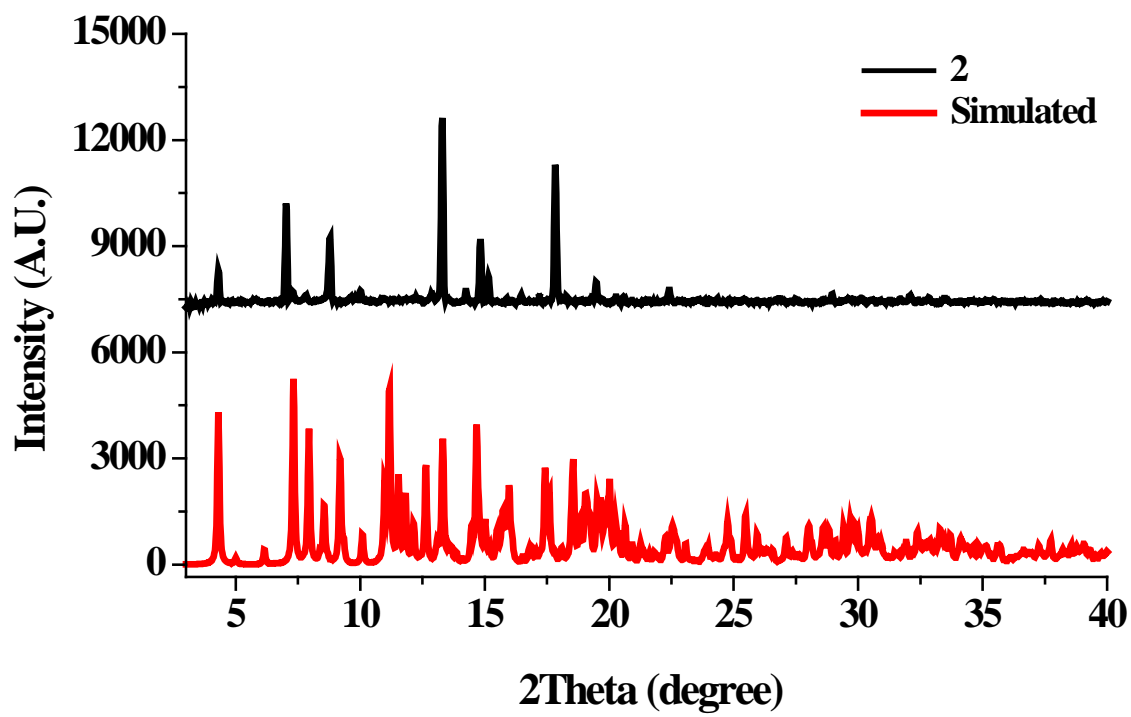


Figure S2

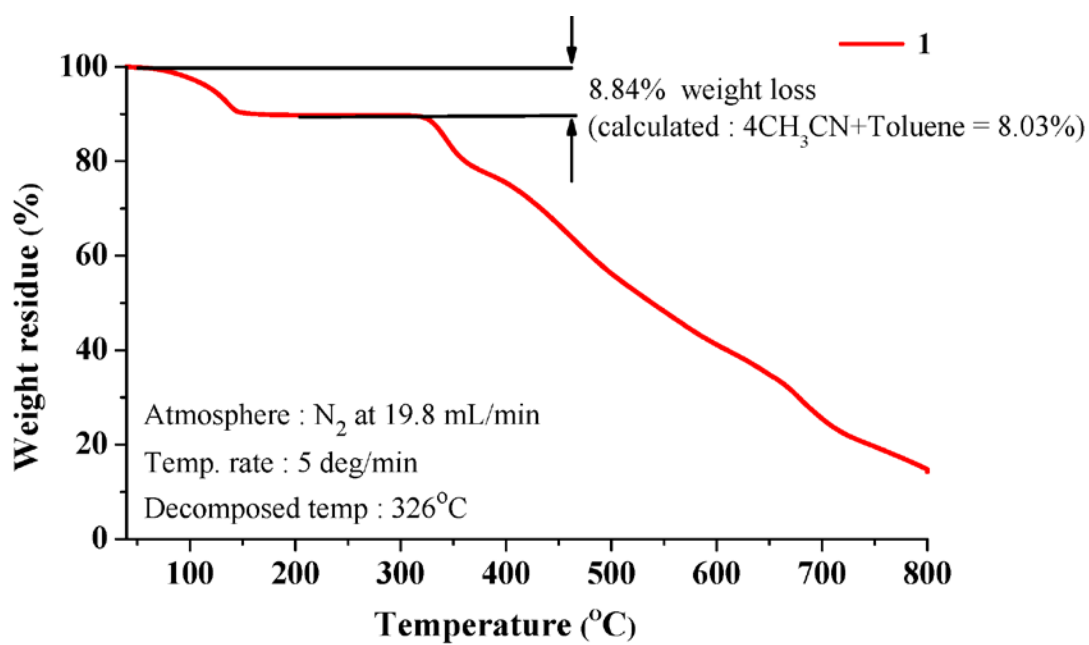


Figure S3

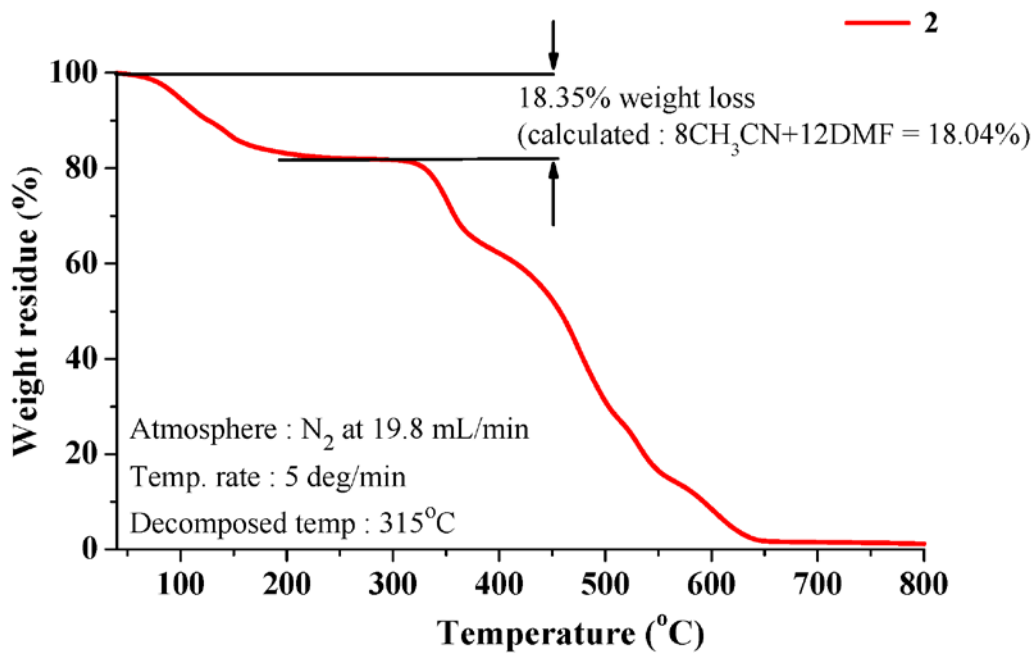


Figure S4

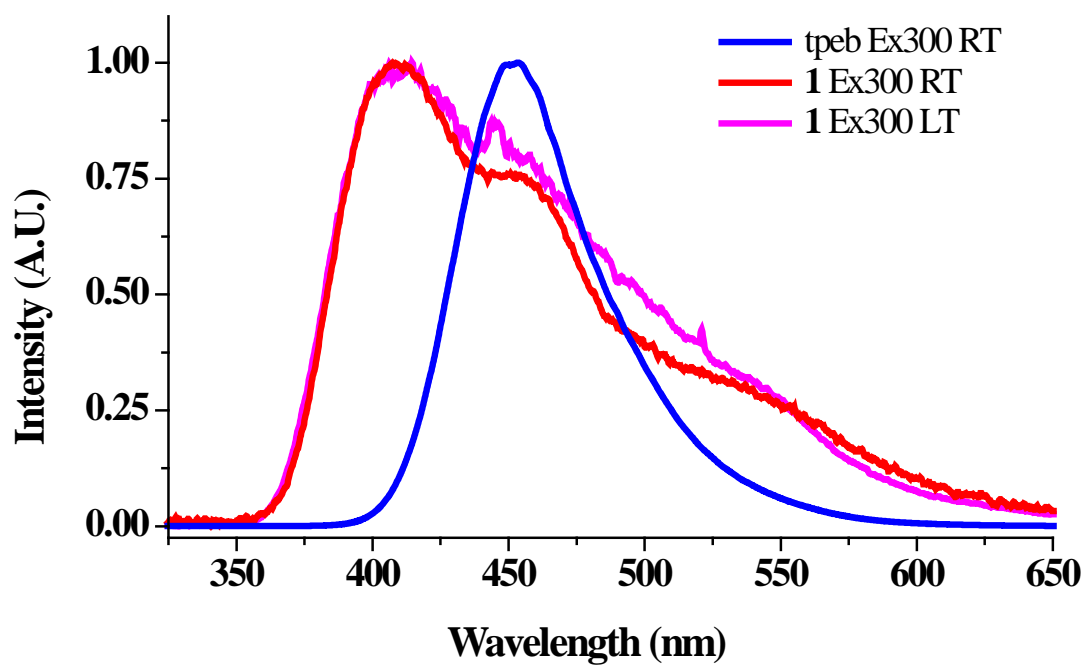


Figure S5

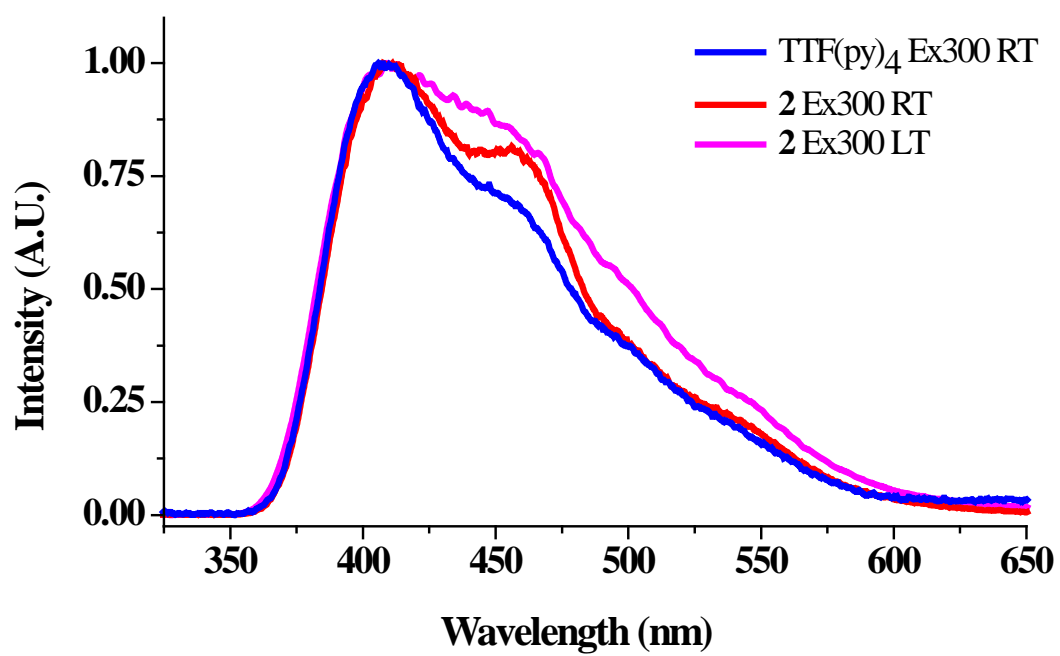


Figure S6