Supplementary material

The surprisingly high ligation energy of CO to Ruthenium porphyrins

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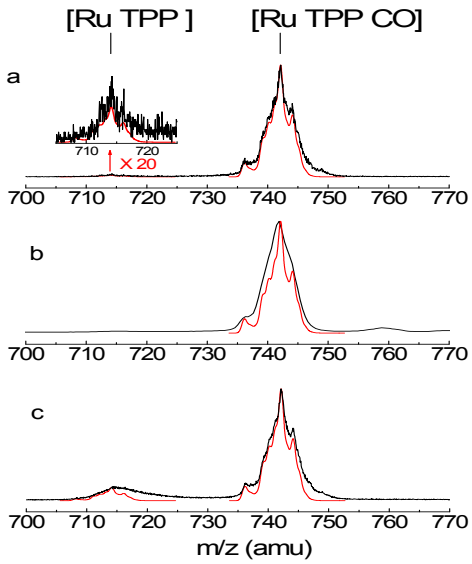
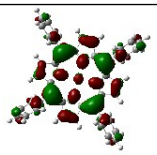
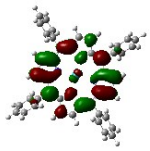
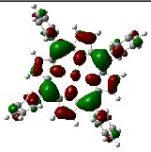
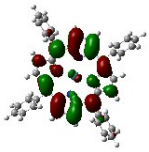
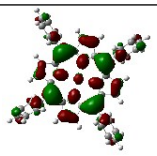
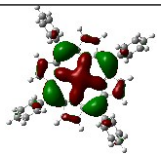
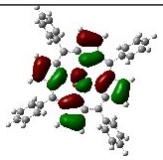
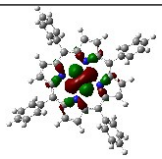
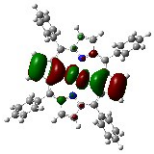
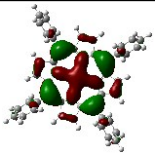
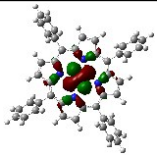
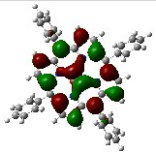
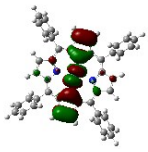
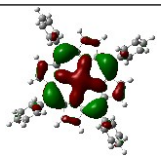
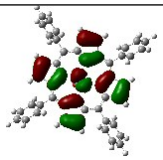
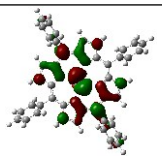
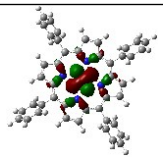
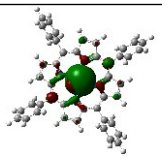


Figure 1 Simulation of the contours of the TOF peaks in red of **(a)** [RuTP-CO] heated at 510°C and ionized at hν=7ev, **(b)** [RuTP-CO] heated at 380°C ionized at hν=7ev and **(c)** [RuTP-CO] heated at 380°C ionized at hν=10ev, respectively. This simulation is obtained with the isotopic distributions of carbon, hydrogen, oxygen and ruthenium convoluted with the mass resolution of m/Δm = 600. In black the experimental traces

Table1- Configuration of the triplet states of [RuTPP]

State	Transition			
	At S_0 minimum		At 5 Å	
	from	to		
T_1				
	$\pi \rightarrow \pi^*$			
T2				
	$\pi \rightarrow \pi^*$			
T3				
	$\pi \rightarrow dz^2, \pi^*$		$\pi, dyz \rightarrow dxy$	
T_4				
	$\pi, dyz \rightarrow dz^2, \pi^*$		$dxy \rightarrow dyz, \pi^*$	
T_5				
	$\pi, dxz \rightarrow dz^2, \pi^*$		$\pi, dyz \rightarrow dyz, \pi^*$	
T_m				
			$dxy \rightarrow dz^2$	

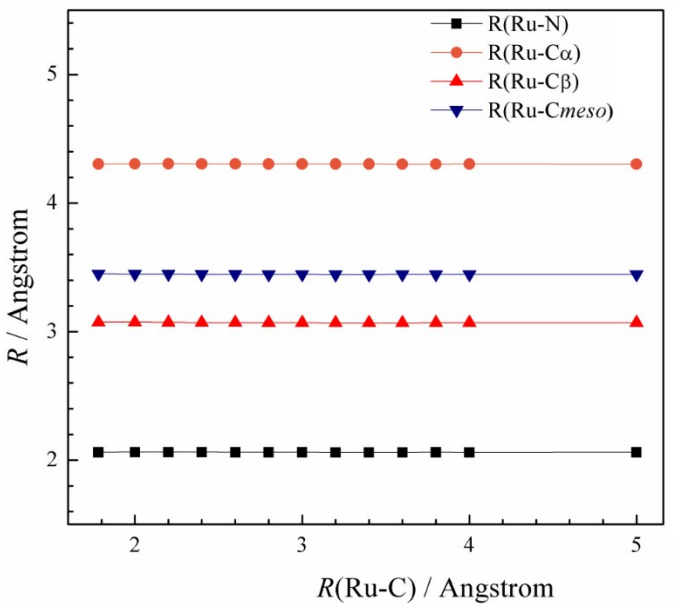


Figure 2. *Evolution of the distances and internal angles between Ru and N, Cα, Cβ, and C meso as a function of the Ru-C coordinate.*