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Supplementary Information

$[(\eta^5\text{-}C_5Me_5)Ru]^+$ fragments ligated to polyaromatic hydrocarbons: an experimental and computational approach of pathways for haptotropic migration

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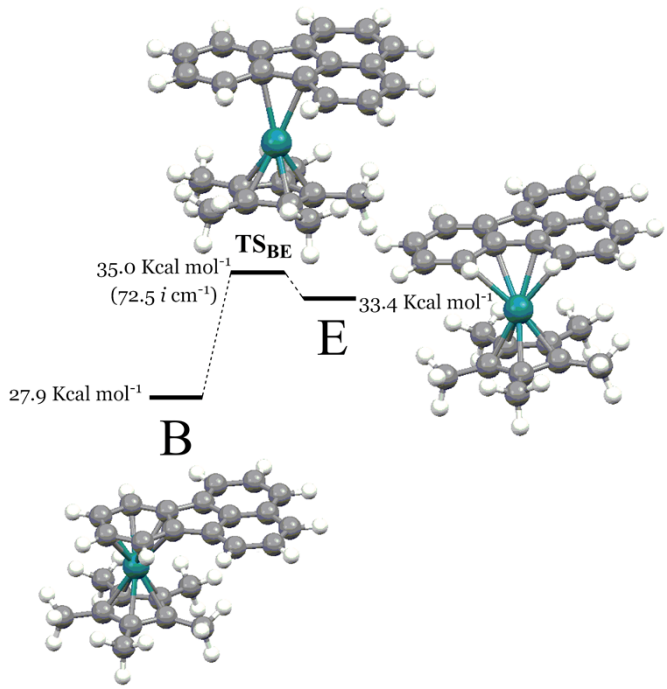

Figure S1. **D** ↔ **E** energy profile for the haptotropic shifts of the [Cp*Ru$^+$] fragment in [Cp*Ru(η^6-fluoranthene)]$^{+,}$ (**3**$^+$).).

Table S1 Computed Distances, relative energies and imaginary frequencies for the isomers and transition states for the interconversion of **1A**$^+$ to **1B**$^+$

Distance	1A$^+$	TS$_{AC}$	1C$^+$	TS$_{CB}$	1B$^+$
Ru-C1	2.233				
Ru-C2	2.232	3.030	3.485	3.800	
Ru-C3	2.233	2.492	2.471	2.910	

Ru-C10a	2.298				
Ru-C3a	2.298	2.262	2.331	2.250	2.334
Ru-C3a[1]	2.318	2.598	3.231	2.612	2.315
Ru-C4		2.862	2.331	2.284	2.247
Ru-C5		3.591	3.137	2.734	2.247
Ru-C5a					2.334
Ru-C5a[1]					2.315
ΔE(ZPE)/ Kcal mol^{-1}	0.0	37.1	33.6	33.9	9.0
ΔG/Kcal mol^{-1}	0.0	36.9	31.5	33.8	9.1
Imaginary Frequencies		134.3*i* 10.0*i*(R)		8.2*i*	

Table S2 Computed Distances, relative energies and imaginary frequencies for the isomers and transition states for the interconversion of **2A**$^+$ to **2B**$^+$ and **2A**$^+$ to **2A**$^+$

Distance / A	**2A$^+$**	**TS$_{AA'}$**	**TS$_{AB}$**	**2B$^+$**
Ru-C1				2.203
Ru-C2			2.861	2.203

Ru-C2a	2.283		2.250	2.307
Ru-C8a				2.308
Ru-C2a[1]	2.275	2.706	2.675	2.312
Ru-C3	2.250		2.390	
Ru-C4	2.215			
Ru-C5	2.226	2.528		
Ru-C5a	2.319	2.196		
Ru-C6		2.517		
Ru-C7				
Ru-C8				
ΔE(ZPE)/ Kcal mol^{-1}	0.0	36.5	35.0	11.0
ΔG/Kcal mol^{-1}	0.0	36.3	33.5	10.9
Im. Freq.		51.2*i* 8.5*i*(R)	164.7*i*	

Table S3 Computed Distances, relative energies and imaginary frequencies for $[(C_5R_5)Ru(fluoranthene)]^+$

Distance / A	**3A$^+$**	**3C$^+$**	**TS$_{AA'}$**	**TS$_{AE}$**	**3E$^+$**	**TS$_{ED}$**	**3D$^+$**	**TS$_{AB}$**	**3B$^+$**	**TS$_{BE}$**
Ru-C1	2.501							3.625		
Ru-C2	2.222									
Ru-C3	2.236	2.491	2.539							
Ru-C3a	2.329	2.216	2.218							
Ru-C3a^1	2.277			3.090		3.115			2.312	3.138
Ru-C10							2.248	2.471		
Ru-C10a							2.272	2.284	2.341	
Ru-C10b	2.269							2.858	2.344	
Ru-C4		2.492	2.463				2.230			
Ru-C5										
Ru-C6				2.589	2.407	2.586				2.581
Ru-C6a				2.295	2.315	2.300			2.344	2.297
Ru-C6b				2.336	2.342	2.332	2.272		2.341	2.338
Ru-C7				2.636	2.400	2.608	2.248			2.622
Ru-C8							2.230			
ΔE (ZPE)/ Kcal mol^{-1}	3.8	43.2	40.1	37.9	33.4	36.7	0	41.2	27.9	35.0
Im. Freq.	-11.9*i*		23.9*i*	69.5*i* 5.5*i*		69.4*i*		128.4*i*	60.1*i*	72.5*i*