

Supporting information for

Encapsulated Ruthenium sites in reaction microenvironment-regulated UiO-66 for stable acetylene hydrochlorination

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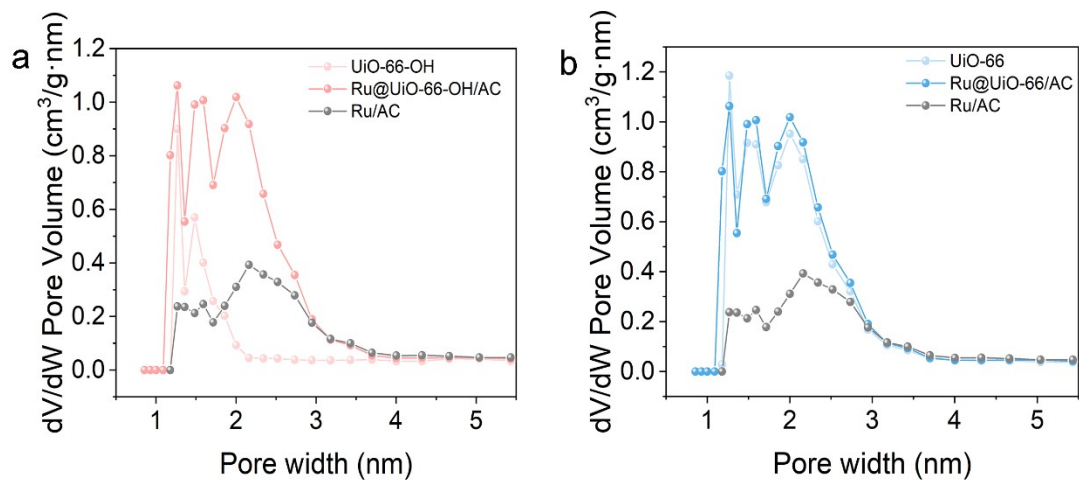


Fig. S1. Pore size distribution image of (a) Ru@UiO-66-OH/AC and (b) Ru@UiO66/AC.

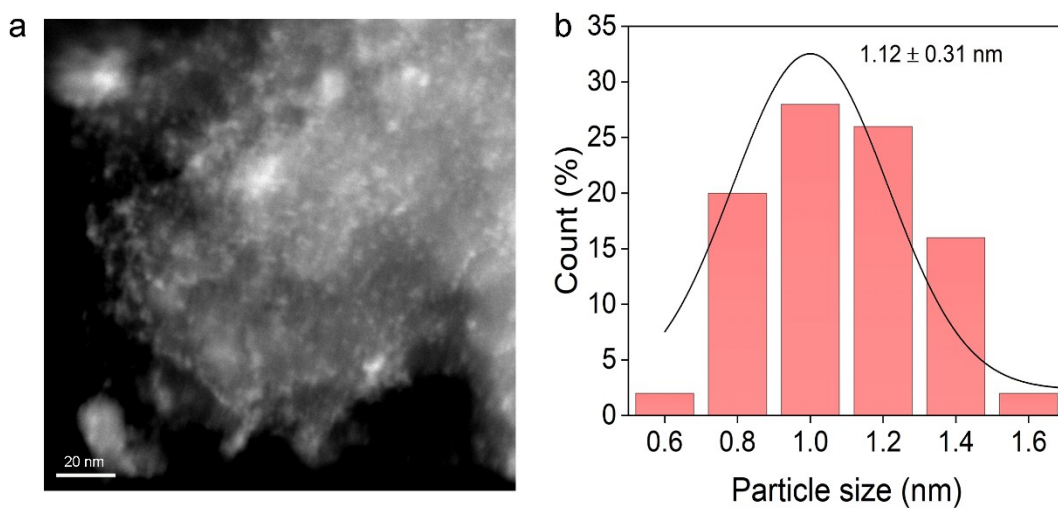


Fig. S2. (a) HADDF-TEM image of fresh Ru/AC and (b) particle size distribution images.

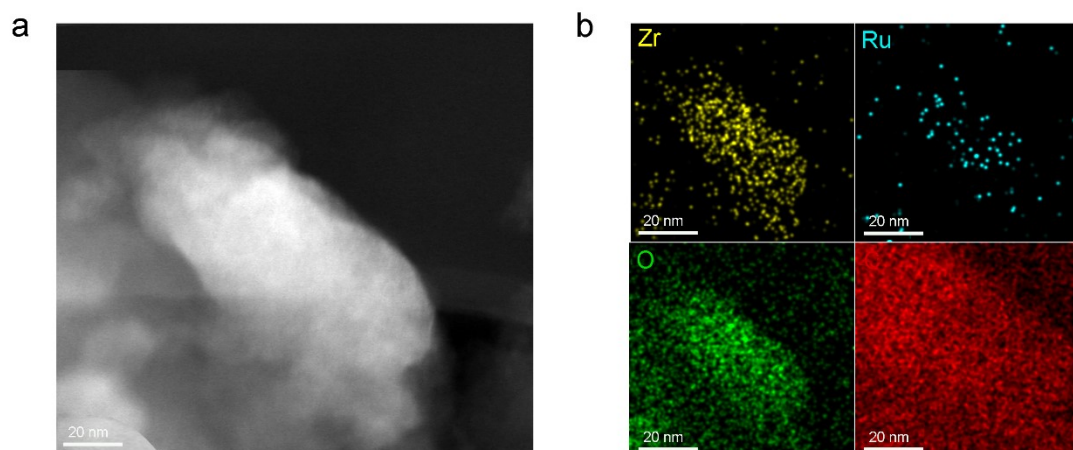


Figure S3. (a) HADDF-TEM image and (b) the relative elemental mapping images of fresh Ru@UiO-66/AC catalyst.

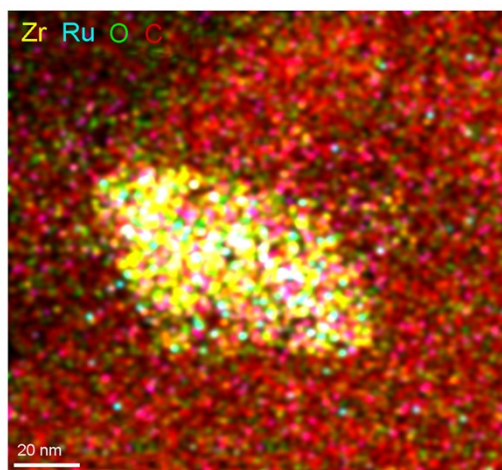


Fig. S4. Overlay image of Ru, O, C and Zr elements.

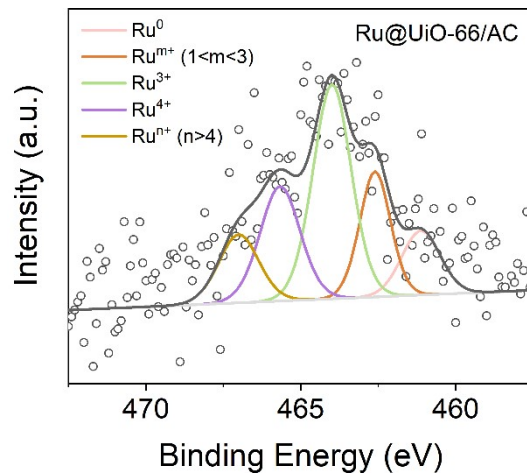


Fig. S5. Ru 3p XPS spectrum of Ru@UiO-66/AC.

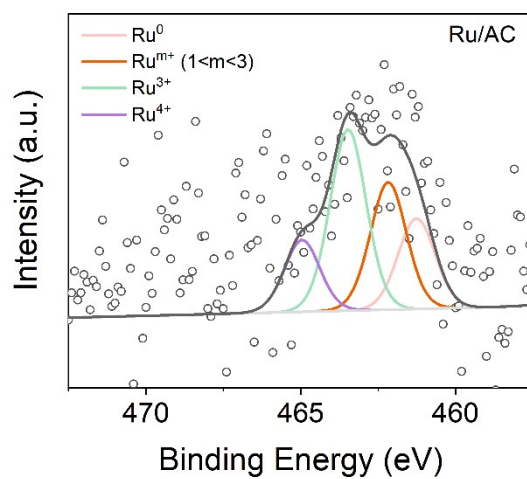


Fig. S6. Ru 3p XPS spectrum of Ru/AC.

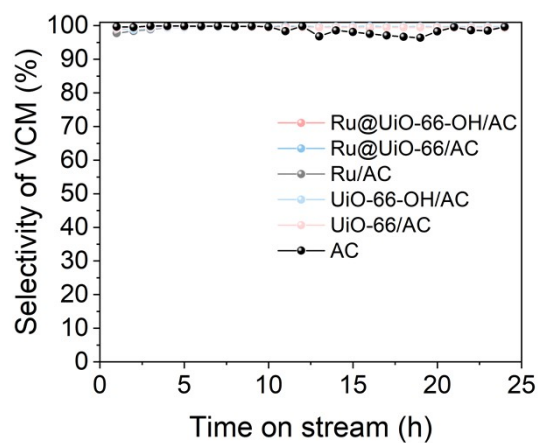


Fig. S7. Selectivity to VCM of Ru-based catalysts and UiO-66-based catalysts.

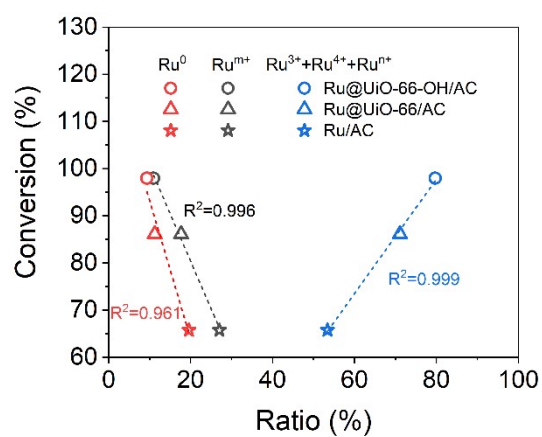


Fig. S8. Relationship between chemical state of Ru species and conversion.

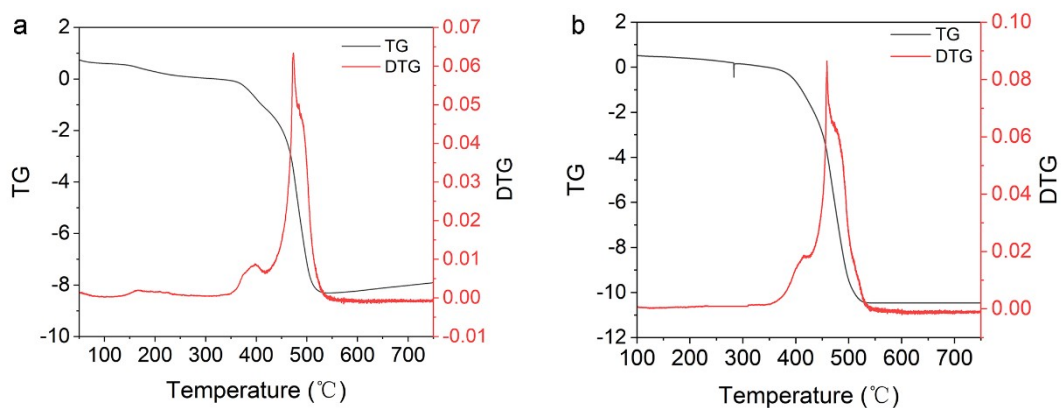


Figure S9. TGA and DTG curves of the fresh (a) Ru@UiO-66-OH/AC and (b) Ru@UiO-66/AC.

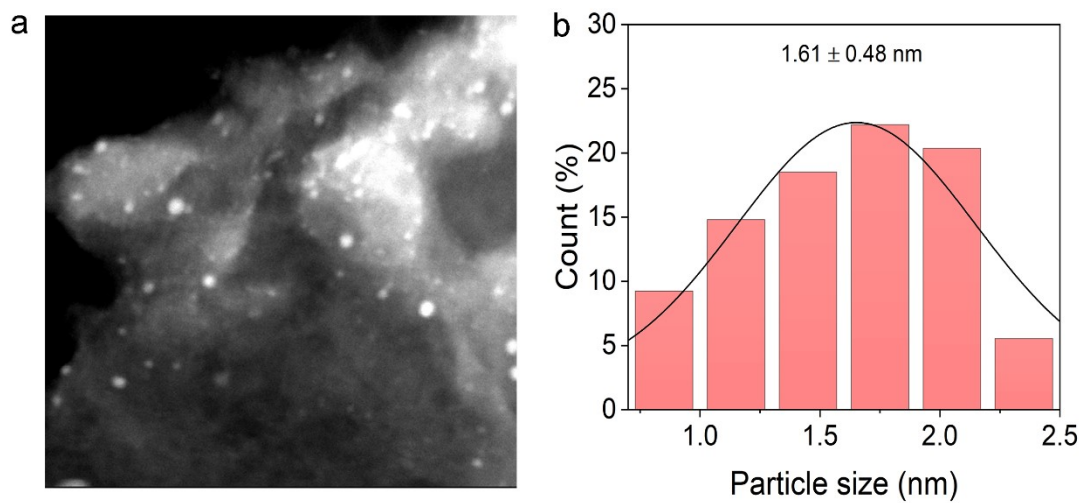


Figure S10. (a) HADDF-TEM image and (b) particle size distribution of used Ru/AC.

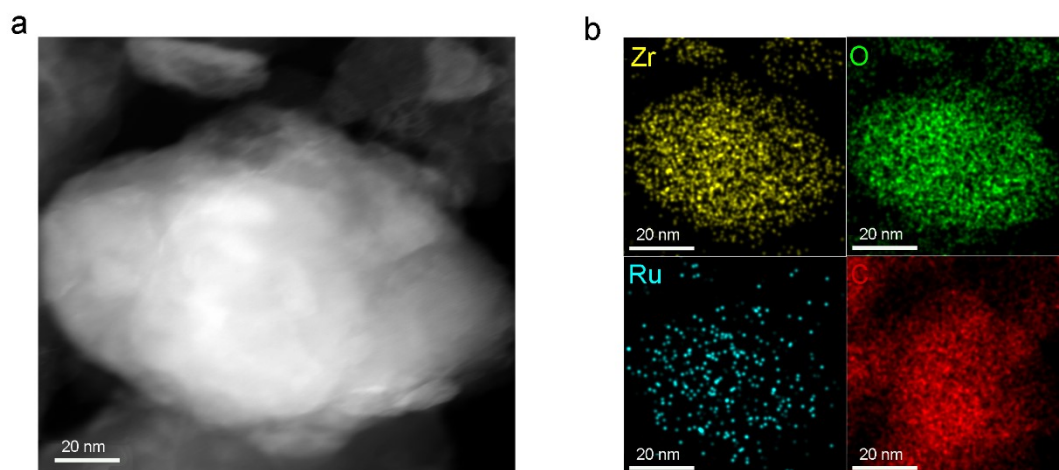


Figure S11. (a) HADDF-TEM image and (b) the relative elemental mapping images of used Ru@UiO-66/AC catalyst.

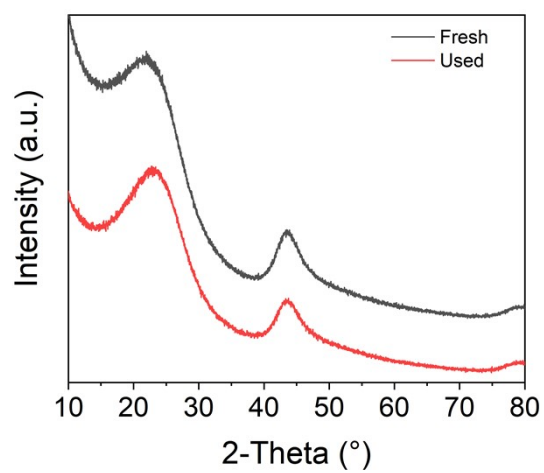


Figure S12. XRD patterns of baseline catalyst.

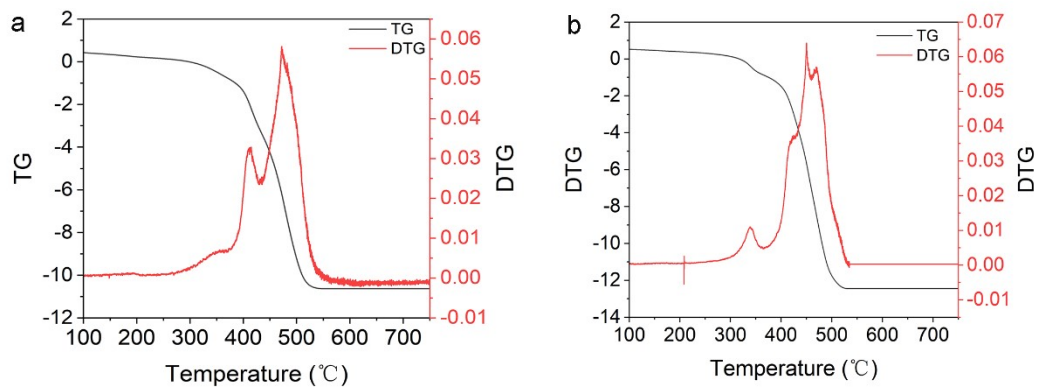


Figure S13. TGA and DTG curves of the used (a) Ru@UiO-66-OH/AC catalyst and (b) Ru@UiO-66/AC catalyst.

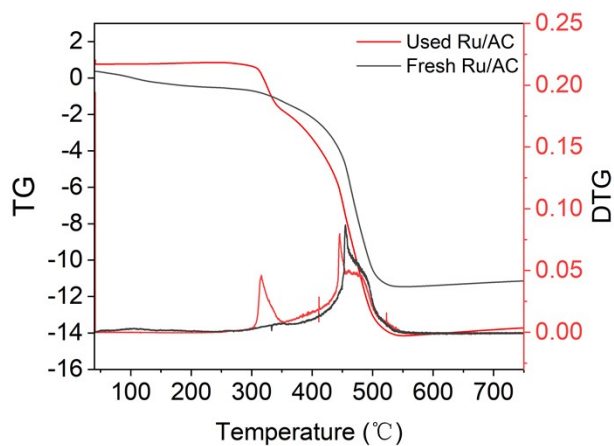


Figure S14. TGA and DTG curves of the fresh and used Ru /AC catalyst.

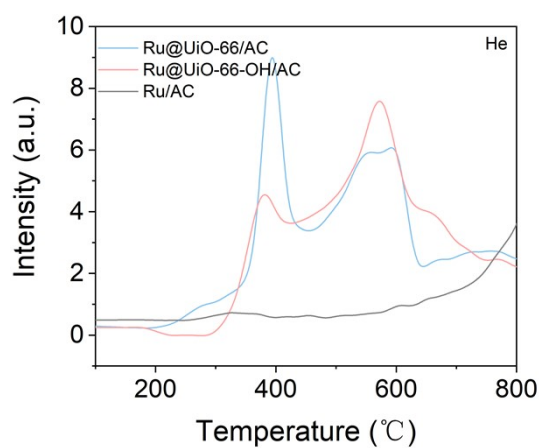


Figure S15. He-TPD profiles of the Ru@UiO-66-OH/AC, Ru@UiO-66/AC and Ru/AC.

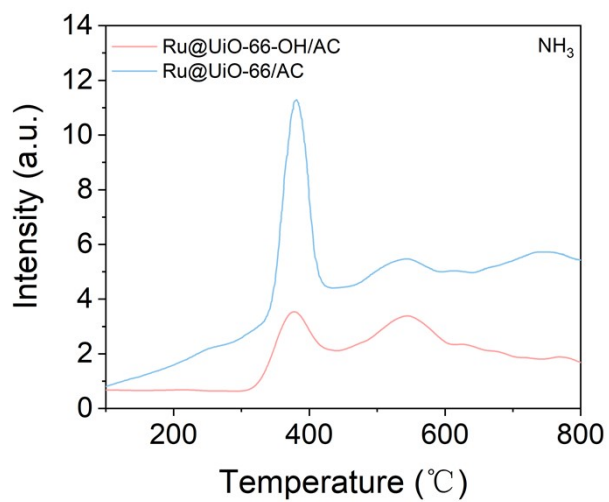


Figure S16. NH₃-TPD profiles of the Ru@UiO-66-OH/AC, Ru@UiO-66/AC and Ru/AC.

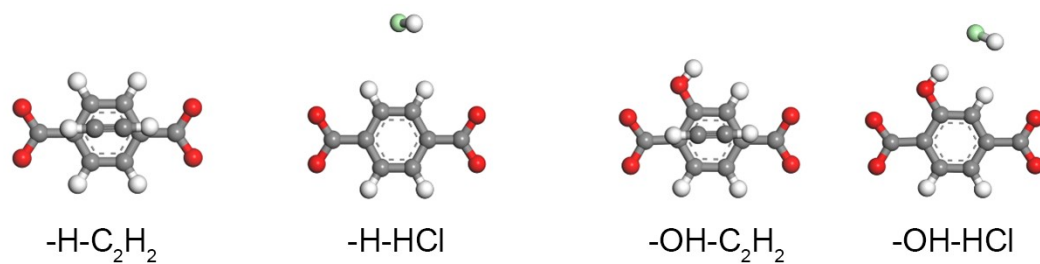


Figure S17. Adsorption models of C_2H_2 and HCl on the unit of linkers. Atom: C, grey; H, white; O, red; Cl, green.

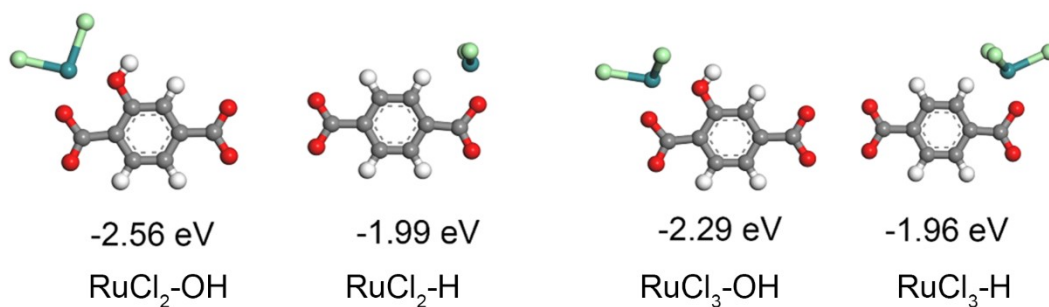


Figure S18. Formation models and energies between RuCl_x species and the relative linkers. Atom: C, grey; H, white; O, red; Cl, green.

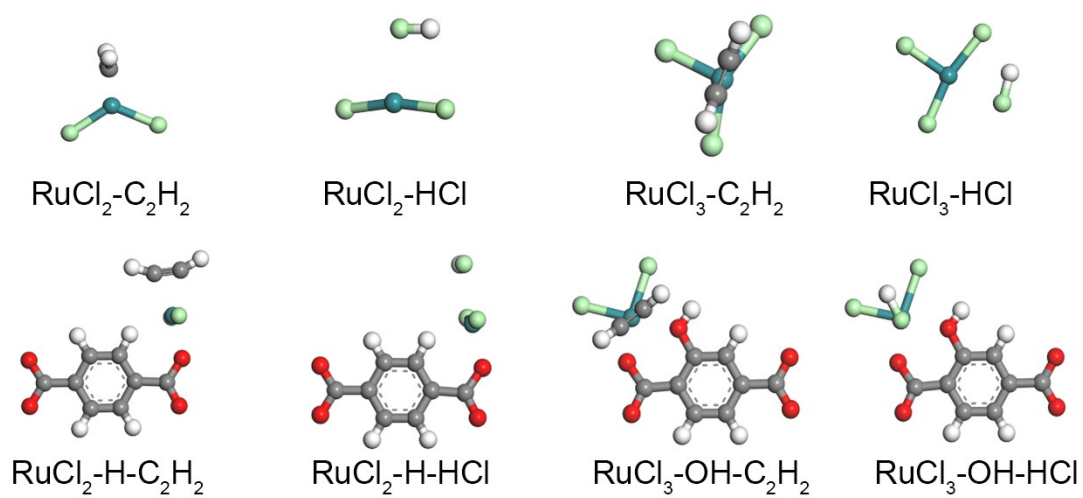


Figure S19. Adsorption models of C_2H_2 and HCl on the relative Ru sites. Atom: C, grey; H, white; O, red; Cl, green.

Table S1. The relative content of Ru species in Ru@UiO-66-OH/AC and Ru@UiO-66/AC catalysts.

Catalyst		Ru@UiO-66-OH/AC	Ru@UiO-66/AC	Ru/AC
Ru ⁰⁺	Binding			
	energy	460.98	461.12	461.26
	(eV)			
	Ratio	9.33	11.23	19.58
Ru ^{m+} (1<m<3)	Binding			
	energy	462.52	462.6	462.17
	(eV)			
	Ratio	10.95	17.68	27.01
Ru ³⁺	Binding			
	energy	463.77	463.99	463.47
	(eV)			
	Ratio	36.73	37.50	38.41
Ru ⁴⁺	Binding			
	energy	465.48	465.67	464.96
	(eV)			
	Ratio	33.05	21.08	14.99
Ru ⁿ⁺ (n>4)	Binding			
	energy	467.26	467.01	/
	(eV)			
	Ratio	9.94	12.51	/