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Supporting Information

Identification of intermediates of a molecular ruthenium catalyst for water oxidation using *insitu* electrochemical X-ray absorption spectroscopy

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Figure S1. Illustration of in situ electrochemical cell. The cell contains a Kapton film as a window, which allows X-ray pass through. The working electrode (WE), reference electrode (RE), and counter electrode (CE) are glassy carbon foam, Ag/AgCl, and Pt respectively.



Figure S2. (a) k^2 -weighted and (b) k^3 -weighted EXAFS data $k^2\chi(k)$ of complex 1 in 0.1 M HNO₃ under no controlled potential (black line), under potential P1 (blue line) and potential P2 (red line).

Table S1. Best-fit parameters obtained from the EXAFS Ru K-edge of complex 1 in 0.1 M HNO_3 under no controlled potential and under potentials P1 and P2

Fit	Shell, N ^a	R ^b , Å	$\sigma^2 (10^{-3})^c$	R-factor	Reduced χ -square
No	Ru—N, 4	2.17	4	0.01	165
potential	Ru—O, 2	2.42	2		
P1	Ru—N, 4	2.12	13	0.03	382
	Ru—O, 3	2.17			
P2	Ru—O3, 1	2.02	10	0.07	233
	Ru—O2, 2	2.10			
	Ru—N3, 4	2.15			

^acoordination number per Ru center, ^bRu-backscatter distance, ^cDebye-Waller factor. R-factor and reduced χ -square are the goodness of the fit parameters. Amplitude reduction factor $S_0^2 = 1$ was used in all the fits.



Figure S3 (a). Normalized XANES at Ru K-edge and (b) Fourier transformed EXAFS spectra of complex 1 in 0.1 M HNO₃ before and after electrolysis.



Figure S4. Normalized XANES at Ru K-edge and working electrode 0.1 M HNO₃ after experiment.

Table S2. Fit parameters obtained from EXAFS Ru K-edge of complex 1 in 0.1 M HNO₃ under no controlled potential, under potential P1 and potential P2.

Fit	Shell, N	R, Å	$\sigma^2(10^{-3})$	ΔE_0	ΔR	Reff	R-factor	Reduced		
								χ-square		
under no controlled potential										
	The crystal structure used for EXAFS fitting is from reference 1^1									
	1-7.3 k-space, 1-2.4 R-space									
1	Ru—N, 6	2.19	25	2.36	0.10	2.09	0.08	609		
2	Ru—N1, 1	2.07	3	7.47	0.16	1.91	0.14	885		
	Ru—N2, 1	2.11			0.16	1.94				
	Ru—N4, 2	2.24			0.17	2.07				

	Ru—O2, 1	2.39			0.18	2.17				
	Ru—O3, 1	2.35			0.18	2.21				
3	Ru—N, 4	2.17	5	7.47	0.23	1.95	0.02	581		
	Ru—O, 2	2.42			0.25	2.17				
4	Ru—N, 4	2.17	5	7.85	0.23	1.95	0.02	381		
	Ru—O, 2	2.42	3		0.25	2.17				
0.8-8 k-space, 1-2.4 R-space										
5	Ru—N, 4	2.17	4	7.67	0.23	1.95	0.01	165		
	Ru—O, 2	2.42	2		0.25	2.17				
	under no controlled potential									
The crystal structure used for EXAFS fitting is from reference 2^2										
1-7.3 k-space, 1-2 R-space										
6	Ru—N, 6	2.18	25	2.57	0.08	2.10	0.06	1337		
7	Ru—N1, 2	2.06	3	7.47	0.14	1.92	0.12	2400		
	Ru—N2, 2	2.22				2.08				
	Ru—O1, 2	2.33				2.32				
-										
8	Ru—N2, 4	2.17	15	6.94	0.08	2.08	0.08	1876		
	Ru—O, 2	2.27		0.77	0.07	2.18	0.00			
9	Ru - N1, 4	2.18	3	8.57	0.25	1.92	0.02	375		
	Ru—O, 2	2.44		8.57		2.18				
under potential P1										
10	D N.C	0.11	I-7.3 K-spa	ce, 1-2	K-space		0.071	5(2)		
10	Ku—N, 6	2.11	12		 D1		0.071	5031		
under potential P1 The emisted structure used for EVAES fitting is from a former 2^2										
	The organ	al structur	a used for I	TATE	fitting i	from rof	2^2			
	The cryst	al structur	e used for I	EXAFS	fitting is	s from ref	erence 2 ²			
11	The cryst $R_{\rm H}$ $N_{\rm 2}$ 2	al structur $1 - \frac{1}{209}$	e used for I -10 k-space	EXAFS , 1-1.86	fitting is 6 R-space	s from ref e	Therefore 2^2	408		
11	The cryst Ru—N2, 2 Ru—O2 1	al structur 1- 2.09 2.14	e used for I -10 k-space 9	EXAFS <u>, 1-1.86</u> 4.61	fitting is 6 R-space 0.09	s from ref e 1.99 2.04	Terence 2 ² 0.03	408		
11	The cryst Ru—N2, 2 Ru—O2, 1 Ru—O3, 1	2.09 2.14 2.14	e used for I -10 k-space 9	EXAFS , 1-1.86 4.61	fitting is 6 R-space 0.09	s from ref e 1.99 2.04 2.04	erence 2 ²	408		
11	The cryst Ru—N2, 2 Ru—O2, 1 Ru—O3, 1 Ru—N3, 2	al structur 2.09 2.14 2.14 2.17	e used for I -10 k-space 9	EXAFS <u>, 1-1.86</u> 4.61	fitting is 6 R-space 0.09	s from ref e 1.99 2.04 2.04 2.04 2.07	erence 2 ² 0.03	408		
11	The cryst Ru—N2, 2 Ru—O2, 1 Ru—O3, 1 Ru—N3, 2	2.09 2.14 2.14 2.17	e used for I -10 k-space 9	EXAFS <u>, 1-1.86</u> 4.61	fitting is 6 R-space 0.09	s from ref e 1.99 2.04 2.04 2.04 2.07	0.03	408		
11	The cryst Ru—N2, 2 Ru—O2, 1 Ru—O3, 1 Ru—N3, 2 Ru—N2, 2	al structur 2.09 2.14 2.14 2.17 2.09	e used for I -10 k-space 9 13	EXAFS , 1-1.86 4.61 5.03	fitting is 6 R-space 0.09 0.10	s from ref e 1.99 2.04 2.04 2.07 1.99	erence 2 ² 0.03 0.03	408		
11	The cryst Ru—N2, 2 Ru—O2, 1 Ru—O3, 1 Ru—N3, 2 Ru—N2, 2 Ru—O2, 2	al structur 2.09 2.14 2.14 2.17 2.09 2.14	e used for I -10 k-space 9 13	EXAFS , 1-1.86 4.61 5.03	fitting is 6 R-space 0.09 0.10	s from ref e 1.99 2.04 2.04 2.04 2.07 1.99 2.04	0.03 0.03	408 385		
11 12	The cryst Ru—N2, 2 Ru—O2, 1 Ru—O3, 1 Ru—N3, 2 Ru—N2, 2 Ru—O2, 2 Ru—O2, 1	1.2.09 2.14 2.14 2.17 2.09 2.14 2.17 2.09 2.14 2.15	e used for I -10 k-space 9 13	EXAFS , 1-1.86 4.61 5.03	fitting is 6 R-space 0.09 0.10	s from ref e 1.99 2.04 2.04 2.04 2.07 1.99 2.04 2.04	Terence 2 ² 0.03 0.03	408 385		
11 12	The cryst Ru—N2, 2 Ru—O2, 1 Ru—O3, 1 Ru—N3, 2 Ru—N2, 2 Ru—O2, 2 Ru—O3, 1 Ru—N3, 2	al structur 1- 2.09 2.14 2.17 2.09 2.14 2.17 2.09 2.14 2.17 2.18	e used for I -10 k-space 9 13	EXAFS , 1-1.86 4.61 5.03	fitting is 6 R-space 0.09 0.10	s from ref e 1.99 2.04 2.04 2.04 2.07 1.99 2.04 2.04 2.04 2.07	0.03 0.03	408		
11 12	The cryst Ru—N2, 2 Ru—O2, 1 Ru—O3, 1 Ru—N3, 2 Ru—N2, 2 Ru—O2, 2 Ru—O2, 2 Ru—O3, 1 Ru—N3, 2	2.09 2.14 2.17 2.09 2.14 2.17 2.09 2.14 2.17	e used for I - <u>10 k-space</u> 9 13	EXAFS , 1-1.86 4.61 5.03	fitting is 6 R-space 0.09 0.10	s from ref e 1.99 2.04 2.04 2.04 2.07 1.99 2.04 2.04 2.04 2.07	0.03 0.03	408		
11 12 13	The cryst Ru—N2, 2 Ru—O2, 1 Ru—O3, 1 Ru—N3, 2 Ru—N2, 2 Ru—O2, 2 Ru—O3, 1 Ru—N3, 2 Ru—N3, 2	al structur 2.09 2.14 2.14 2.17 2.09 2.14 2.17 2.09 2.14 2.15 2.18 2.08	e used for I -10 k-space 9 13 10	EXAFS , 1-1.86 4.61 5.03	6 R-space 0.09 0.10 0.08	s from ref e 1.99 2.04 2.04 2.07 1.99 2.04 2.04 2.04 2.04 2.04 2.07 1.99 1.99	erence 2 ² 0.03 0.03 0.03	408 385 417		
11 12 13	The cryst Ru—N2, 2 Ru—O2, 1 Ru—O3, 1 Ru—N3, 2 Ru—N2, 2 Ru—O2, 2 Ru—O2, 2 Ru—O3, 1 Ru—N3, 2 Ru—N3, 2	al structur 2.09 2.14 2.17 2.09 2.14 2.17 2.09 2.14 2.17 2.08 2.12	e used for I -10 k-space 9 13 10	EXAFS , 1-1.86 4.61 5.03	6 R-space 0.09 0.10 0.08	s from ref e 1.99 2.04 2.04 2.04 2.07 1.99 2.04 2.04 2.04 2.07 1.99 2.04	erence 2 ² 0.03 0.03 0.03	408 385 417		
11 12 13	The cryst Ru—N2, 2 Ru—O2, 1 Ru—O3, 1 Ru—N3, 2 Ru—O2, 2 Ru—O2, 2 Ru—O3, 1 Ru—N3, 2 Ru—N2, 1 Ru—O2, 2 Ru—O2, 2 Ru—O2, 1 Ru—O2, 1 Ru—O2, 1	al structur 1.1 2.09 2.14 2.17 2.09 2.14 2.17 2.09 2.14 2.17 2.08 2.12 2.13	e used for I -10 k-space 9 13 10	EXAFS , 1-1.86 4.61 5.03	fitting is6 R-space0.090.100.100.08	s from ref e 1.99 2.04 2.04 2.07 1.99 2.04 2.04 2.07 1.99 2.04 2.04 2.04	erence 2 ² 0.03 0.03 0.03	408 385 417		
11 12 13	The cryst Ru—N2, 2 Ru—O2, 1 Ru—O3, 1 Ru—N3, 2 Ru—N2, 2 Ru—O2, 2 Ru—O3, 1 Ru—N3, 2 Ru—N2, 1 Ru—O2, 2 Ru—O2, 2 Ru—O3, 1 Ru—O3, 1 Ru—O3, 1 Ru—N3, 2	al structur 1- 2.09 2.14 2.17 2.09 2.14 2.17 2.09 2.14 2.17 2.08 2.12 2.13 2.16	e used for I -10 k-space 9 13 10	EXAFS , 1-1.86 4.61 5.03	fitting is6 R-space0.090.100.10	s from ref e 1.99 2.04 2.04 2.07 1.99 2.04 2.04 2.04 2.04 2.04 2.04 2.04 2.04	erence 2 ² 0.03 0.03	408 385 417		
11 12 13	The cryst Ru—N2, 2 Ru—O2, 1 Ru—O3, 1 Ru—N3, 2 Ru—N2, 2 Ru—O2, 2 Ru—O2, 2 Ru—O3, 1 Ru—N3, 2 Ru—N2, 1 Ru—O2, 2 Ru—O3, 1 Ru—O3, 1 Ru—O3, 1 Ru—O3, 2	al structur 2.09 2.14 2.17 2.09 2.14 2.17 2.09 2.14 2.15 2.18 2.08 2.12 2.13 2.16	e used for I -10 k-space 9 13	EXAFS , 1-1.86 4.61 5.03	6 R-space 0.09 0.10 0.08	s from ref e 1.99 2.04 2.04 2.07 1.99 2.04 2.04 2.07 1.99 2.04 2.04 2.04 2.04 2.04 2.04 2.04	erence 2 ² 0.03 0.03	408 385 417		
11 12 13 14	The cryst Ru—N2, 2 Ru—O2, 1 Ru—O3, 1 Ru—N3, 2 Ru—N2, 2 Ru—O2, 2 Ru—O2, 2 Ru—O3, 1 Ru—N3, 2 Ru—O2, 2 Ru—O3, 1 Ru—O2, 2 Ru—O3, 1 Ru—O3, 1 Ru—O3, 2 Ru—N3, 2	al structur 1- 2.09 2.14 2.17 2.09 2.14 2.17 2.09 2.14 2.17 2.09 2.14 2.15 2.18 2.08 2.12 2.13 2.16 2.09	e used for F -10 k-space 9 13 10	EXAFS , 1-1.86 4.61 5.03 4.61 4.61	6 R-space 0.09 0.10 0.08 0.09	s from ref e 1.99 2.04 2.04 2.07 1.99 2.04 2.04 2.04 2.04 2.04 2.04 2.04 2.04	erence 2 ² 0.03 0.03 0.03 0.03	408 385 417 417		
11 12 13 14	The cryst Ru-N2, 2 Ru-O2, 1 Ru-O3, 1 Ru-N3, 2 Ru-N2, 2 Ru-O2, 2 Ru-O3, 1 Ru-N3, 2 Ru-O2, 2 Ru-O2, 2 Ru-O3, 1 Ru-O3, 1 Ru-N3, 2 Ru-N3, 2	al structur 1- 2.09 2.14 2.17 2.09 2.14 2.17 2.09 2.14 2.15 2.18 2.08 2.12 2.13 2.16 2.09 2.14	e used for F -10 k-space 9 13 10	EXAFS , 1-1.86 4.61 5.03 4.61	6 R-space 0.09 0.10 0.08 0.09	s from ref e 1.99 2.04 2.04 2.04 2.07 1.99 2.04 2.04 2.04 2.04 2.04 2.04 2.04 2.04	erence 2 ² 0.03 0.03 0.03	408 385 417 417		
11 12 13 14	The cryst Ru-N2, 2 Ru-O2, 1 Ru-O3, 1 Ru-N3, 2 Ru-N2, 2 Ru-O2, 2 Ru-O3, 1 Ru-N3, 2 Ru-O2, 2 Ru-O3, 1 Ru-N3, 2 Ru-N3, 2 Ru-N3, 2	al structur 1- 2.09 2.14 2.17 2.09 2.14 2.17 2.09 2.14 2.15 2.18 2.08 2.12 2.13 2.16 2.09 2.14	e used for I <u>-10 k-space</u> 9 13 10 10	EXAFS , 1-1.86 4.61 5.03 4.61	fitting is 6 R-space 0.09 0.10 0.10 0.08 0.09	s from ref e 1.99 2.04 2.04 2.07 1.99 2.04 2.04 2.07 1.99 2.04 2.04 2.07 1.99 2.04 2.04 2.07	erence 2 ² 0.03 0.03 0.03	408 385 417 417		
11 12 13 14	The cryst Ru—N2, 2 Ru—O2, 1 Ru—O3, 1 Ru—N3, 2 Ru—N2, 2 Ru—O2, 2 Ru—O3, 1 Ru—N3, 2 Ru—O3, 1 Ru—O3, 1 Ru—O3, 1 Ru—N3, 2 Ru—O3, 1 Ru—N2, 2 Ru—O3, 1 Ru—O3, 1 Ru—O	al structur 1- 2.09 2.14 2.17 2.09 2.14 2.17 2.09 2.14 2.17 2.09 2.14 2.15 2.18 2.08 2.12 2.13 2.16 2.09 2.14 2.17 2.09 2.14 2.17	e used for I -10 k-space 9 13 10	EXAFS <u>4.61</u> <u>4.61</u> <u>4.61</u> <u>4.61</u>	6 R-space 0.09 0.10 0.08 0.09	s from ref e 1.99 2.04 2.04 2.07 1.99 2.04 2.04 2.04 2.04 2.04 2.04 2.04 2.04	erence 2 ² 0.03 0.03 0.03 0.03	408 385 417 417		
11 12 13 14 15	The cryst Ru-N2, 2 Ru-O2, 1 Ru-O3, 1 Ru-N3, 2 Ru-N2, 2 Ru-O2, 2 Ru-O3, 1 Ru-N3, 2 Ru-O2, 2 Ru-O3, 1 Ru-N3, 2 Ru-N2, 2 Ru-O2, 2 Ru-O2, 2 Ru-O2, 2 Ru-O3, 1 Ru-N3, 1 Ru-N2, 4 Ru-N2, 4	al structur 1.1 2.09 2.14 2.17 2.09 2.14 2.17 2.09 2.14 2.15 2.18 2.08 2.12 2.13 2.16 2.09 2.14 2.17 2.12 2.13 2.16 2.09 2.14 2.17 2.12 2.13 2.14 2.15	e used for I -10 k-space 9 13 10 10 13	EXAFS , 1-1.86 4.61 5.03 4.61 4.61 5.03	fitting is 6 R-space 0.09 0.10 0.10 0.08 0.09 0.12	s from ref e 1.99 2.04 2.04 2.04 2.07 1.99 2.04 2.04 2.04 2.04 2.04 2.04 2.04 2.04	erence 2 ² 0.03 0.03 0.03 0.03 0.03	408 385 417 417 382		
11 12 13 14	The cryst Ru-N2, 2 Ru-O2, 1 Ru-O3, 1 Ru-N3, 2 Ru-N2, 2 Ru-O2, 2 Ru-O3, 1 Ru-N3, 2 Ru-N2, 1 Ru-O2, 2 Ru-O3, 1 Ru-N3, 2 Ru-N3, 2 Ru-N2, 2 Ru-O3, 1 Ru-O2, 2 Ru-O3, 1 Ru-N3, 1 Ru-N2, 4 Ru-O2, 3	al structur 1- 2.09 2.14 2.17 2.09 2.14 2.17 2.09 2.14 2.15 2.18 2.08 2.12 2.13 2.16 2.09 2.14 2.17 2.12 2.17	e used for I <u>-10 k-space</u> 9 13 10 10 13	EXAFS , 1-1.86 4.61 5.03 4.61 4.61 5.03	fitting is 6 R-space 0.09 0.10 0.08 0.09 0.12	s from ref e 1.99 2.04 2.04 2.07 1.99 2.04 2.04 2.07 1.99 2.04 2.04 2.07 1.99 2.04 2.04 2.04 2.07 1.99 2.04 2.04 2.07 1.99 2.04 2.04 2.07 1.99 2.04 2.04 2.07 1.99 2.04 2.04 2.07 1.99 2.04 2.04 2.07 1.99 2.04 2.04 2.07 1.99 2.04 2.04 2.07 1.99 2.04 2.04 2.07 1.99 2.04 2.04 2.07 1.99 2.04 2.04 2.07 1.99 2.04 2.04 2.07 1.99 2.04 2.04 2.07 1.99 2.04 2.04 2.04 2.07 1.99 2.04 2.04 2.07 1.99 2.04 2.04 2.04 2.07 1.99 2.04 2.04 2.07 1.99 2.04 2.0	erence 2 ² 0.03 0.03 0.03 0.03 0.03	408 385 417 417 382		

16	Ru—N2, 4	2.12	9	4.89	0.12	1.99	0.03	420
	Ru—O2, 2	2.17				2.04		
17	Ru—N2, 3	2.11	10	4.89	0.11	1.99	0.03	429
	Ru—O2, 3	2.15				2.04		
18	Ru - O2	2.13	14	5.34	0.08	2.04	0.03	392
10	Ru—N3, 4	2.16		0.0.	0100	2.07	0.00	0,1
10	D 02.2	2.11	10	4.61	0.07	2.04	0.02	407
19	Ru—02, 2 Ru—N3, 4	2.11	10	4.61	0.07	2.04	0.03	406
20	Ru—O2, 3	2.11	10	4.61	0.07	2.04	0.03	414
	Ru=N3, 3	2.15				2.07		
21	Ru—N2, 4	2.12	13	5.03	0.12	1.99	0.03	382
	Ru—O3, 3	2.17				2.04		
22	Ru—N2, 4	2.12	8	4.89	0.12	1.99	0.03	419
	Ru—O3, 2	2.17				2.04		
22	Du NO 2	2.11	0	4.80	0.11	1.00	0.02	420
23	Ru = N2, 3 Ru = O3, 3	2.11	9	4.09	0.11	2.04	0.03	429
under potential P1 The effected structure used for EXAES fitting is from reference 2^2								
	The erys	1.	-10 k-space	e, 1-1.92	R-space	e	cremee 2	
24	Ru—N2,4	2.08	5	3.51	0.005	2.08	0.064	597
	Ru—O2,2	2.19		3.69		2.19		
25								
-	Ru—N2,4	2.07	8	3.44	-	2.08	0.064	556
	Ru—N2,4 Ru—O2,3	2.07 2.18	8	3.44 3.61	- 0.005	2.08 2.19	0.064	556
	Ru—N2,4 Ru—O2,3	2.07 2.18	8 under r	3.44 3.61	- 0.005 P1	2.08 2.19	0.064	556
	Ru—N2,4 Ru—O2,3 The cryst	2.07 2.18 tal structur	8 under p e used for I	3.44 3.61 ootential	- 0.005 P1 fitting is	2.08 2.19	0.064	556
26	Ru—N2,4 Ru—O2,3 The cryst	2.07 2.18 tal structur	8 under p e used for I -10 k-space	3.44 3.61 EXAFS 2, 1-1.92	- 0.005 P1 fitting is R-space	2.08 2.19	0.064	556
26	Ru—N2,4 Ru—O2,3 The cryst Ru—N1, 2 Ru—O1, 2	2.07 2.18 tal structur 1 2.06 2.12	8 under p e used for I -10 k-space 7	3.44 3.61 EXAFS 2, 1-1.92 4.07 4.20	- 0.005 P1 fitting is R-space 0.07	2.08 2.19 s from ref 1.99 2.05	0.064 Ference 3 ³ 0.062	556 597
26	Ru—N2,4 Ru—O2,3 The cryst Ru—N1, 2 Ru—O1, 2 Ru—N2, 2	2.07 2.18 tal structur 2.06 2.12 2.14	8 under p e used for I -10 k-space 7	3.44 3.61 EXAFS 9, 1-1.92 4.07 4.20 4.24	- 0.005 P1 fitting is 2 R-space 0.07	2.08 2.19 s from ref e 1.99 2.05 2.07	0.064 Ference 3 ³ 0.062	556
26	Ru—N2,4 Ru—O2,3 The cryst Ru—N1, 2 Ru—O1, 2 Ru—N2, 2	2.07 2.18 tal structur 2.06 2.12 2.14	8 under p e used for I -10 k-space 7	3.44 3.61 Dotential EXAFS 2, 1-1.92 4.07 4.20 4.24	- 0.005 P1 fitting is R-space 0.07	2.08 2.19 s from ref e 1.99 2.05 2.07	0.064 Ference 3^3 0.062	556 597
26	Ru—N2,4 Ru—O2,3 The cryst Ru—N1, 2 Ru—O1, 2 Ru—N2, 2 Ru—N1, 2 Ru—N1, 2 Ru—O1 3	2.07 2.18 tal structur 2.06 2.12 2.14 2.06 2.13	8 under p e used for I -10 k-space 7 11	3.44 3.61 EXAFS <u>5, 1-1.92</u> 4.07 4.20 4.24 4.20 4.20 4.33	- 0.005 P1 fitting is 2 R-space 0.07 0.07	2.08 2.19 s from ref 1.99 2.05 2.07 1.99 2.05	0.064 Ference 3 ³ 0.062	556 597 552
26	Ru—N2,4 Ru—O2,3 The cryst Ru—N1, 2 Ru—O1, 2 Ru—N2, 2 Ru—N1, 2 Ru—O1, 3 Ru—O1, 3 Ru—N2, 2	2.07 2.18 tal structur 2.06 2.12 2.14 2.06 2.13 2.15	8 under p e used for I -10 k-space 7 11	3.44 3.61 EXAFS 2, 1-1.92 4.07 4.20 4.24 4.20 4.33 4.37	- 0.005 P1 fitting is 2 R-space 0.07	2.08 2.19 s from ref 1.99 2.05 2.07 1.99 2.05 2.07	0.064 Ference 3 ³ 0.062	556 597 552
26 27 28	Ru—N2,4 Ru—O2,3 The cryst Ru—N1, 2 Ru—O1, 2 Ru—N2, 2 Ru—N1, 2 Ru—O1, 3 Ru—N1, 4 Ru—N1, 4	2.07 2.18 tal structur 2.06 2.12 2.14 2.06 2.13 2.15 2.1 2.1	8 under p e used for I -10 k-space 7 11 9	3.44 3.61 EXAFS 9, 1-1.92 4.07 4.20 4.24 4.20 4.33 4.37 4.41	- 0.005 P1 fitting is R-space 0.07 0.07	2.08 2.19 5 from ref 2.05 2.07 1.99 2.05 2.07 2.05 2.07	0.064 Ference 3 ³ 0.062 0.061 0.064	556 597 552 605
26 27 28	Ru—N2,4 Ru—O2,3 The cryst Ru—N1, 2 Ru—O1, 2 Ru—N2, 2 Ru—N1, 2 Ru—O1, 3 Ru—N2, 2 Ru—N1, 4 Ru—O1, 2	2.07 2.18 tal structur 2.06 2.12 2.14 2.06 2.13 2.15 2.1 2.12	8 under p e used for I -10 k-space 7 11 9	3.44 3.61 EXAFS 9, 1-1.92 4.07 4.20 4.24 4.20 4.24 4.20 4.33 4.37 4.41 4.45	- 0.005 P1 fitting is R-space 0.07 0.07	2.08 2.19 s from ref 2.05 2.07 1.99 2.05 2.07 2.05 2.07	0.064 Ference 3 ³ 0.062 0.061 0.064	556 597 552 605
26 27 28 29	Ru—N2,4 Ru—O2,3 The cryst Ru—N1, 2 Ru—O1, 2 Ru—N2, 2 Ru—N1, 2 Ru—O1, 3 Ru—N2, 2 Ru—N1, 4 Ru—O1, 2 Ru—N1, 4	2.07 2.18 tal structur 2.06 2.12 2.14 2.06 2.13 2.15 2.1 2.12 2.12 2.09	8 under p e used for I -10 k-space 7 11 9	3.44 3.61 EXAFS e, 1-1.92 4.07 4.20 4.24 4.20 4.24 4.20 4.33 4.37 4.41 4.45 4.32	- 0.005 P1 fitting is 2 R-space 0.07 0.07 0.05 0.09	2.08 2.19 s from ref 2.05 2.07 2.05 2.07 2.05 2.07 1.99 1.99	0.064 Ference 3 ³ 0.062 0.061 0.064 0.062	556 597 552 605 554
26 27 28 29	Ru—N2,4 Ru—O2,3 The cryst Ru—N1, 2 Ru—O1, 2 Ru—N2, 2 Ru—N1, 2 Ru—N1, 2 Ru—N1, 4 Ru—O1, 2 Ru—N1, 4 Ru—O1, 3	2.07 2.18 tal structur 2.06 2.12 2.14 2.06 2.13 2.15 2.1 2.12 2.12 2.12 2.12 2.12	8 under p e used for I -10 k-space 7 11 9	3.44 3.61 00tential EXAFS 0, 1-1.92 4.07 4.20 4.24 4.20 4.24 4.20 4.33 4.37 4.41 4.45 4.32 4.45	- 0.005 P1 fitting is 2 R-space 0.07 0.07 0.07 0.05	2.08 2.19 s from ref 2.05 2.07 1.99 2.05 2.07 2.05 2.07 1.99 2.05 2.07	0.064 Ference 3 ³ 0.062 0.061 0.064 0.062	556 597 552 605 554

under potential P2											
The crystal structure (Ru ^{IV} dimer) used for EXAFS fitting is from reference 1											
1-7.6 k-space, 1-1.92 R-space											
30	Ru—N, 6	2.10	9	1.14	-	2.10	0.016	1981			
					0.002						
31	Ru—O3, 1	2.01	9	7.47	0.050	1.96	0.025	3418			
	Ru—O2, 2	2.09			0.052	2.03					
	Ru—N3, 4	2.13			0.053	2.08					
32	Ru—O3, 1	2.00	6	7.07	0.042	1.96	0.018	3414			
	Ru—O2, 1	2.08			0.044	2.03					
	Ru—N3, 4	2.13			0.045	2.08					
under potential P2											
The crystal structure (Ru ^{IV} dimer) used for EXAFS fitting is from reference 1											
1-10 k-space, 1-1.92 R-space											
33	Ru—O3, 1	2.02	10	8.01	0.063	1.96	0.079	233			
	Ru—O2, 2	2.10			0.065	2.03					
	Ru—N3, 4	2.15			0.067	2.08					

N, coordination number for per Ru center. R, Ru-backscatter distance. σ^2 , Debye-Waller factor. ΔE_0 , the energy shift parameter. ΔR , change in half-path length. Reff, initial half path length. R-factor and Reduced χ -square are the goodness of the fit parameters. Amplitude reduction factor $S_0^2 = 1$ was used in all fits.

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