

Supplementary Information for

X-Ray Absorption Fine Structure Spectroscopy Studies of Thermal Effect on Ion-Exchange Equilibria

Masami Shibukawa,^{a*} Makoto Harada,^b Tetsuo Okada,^b Yawara Ogiyama,^a Tomomi Shimasaki,^a Asako Inoue,^a Yoshiki Kondo,^a and Shingo Saito^a

^aGraduate School of Science and Technology, Saitama University, 255 Shimo-Okubo, Sakura-ku, Saitama, 338-8570, Japan

^bDepartment of Chemistry, Tokyo Institute of Technology, Meguro-ku, Tokyo, 152-8551, Japan

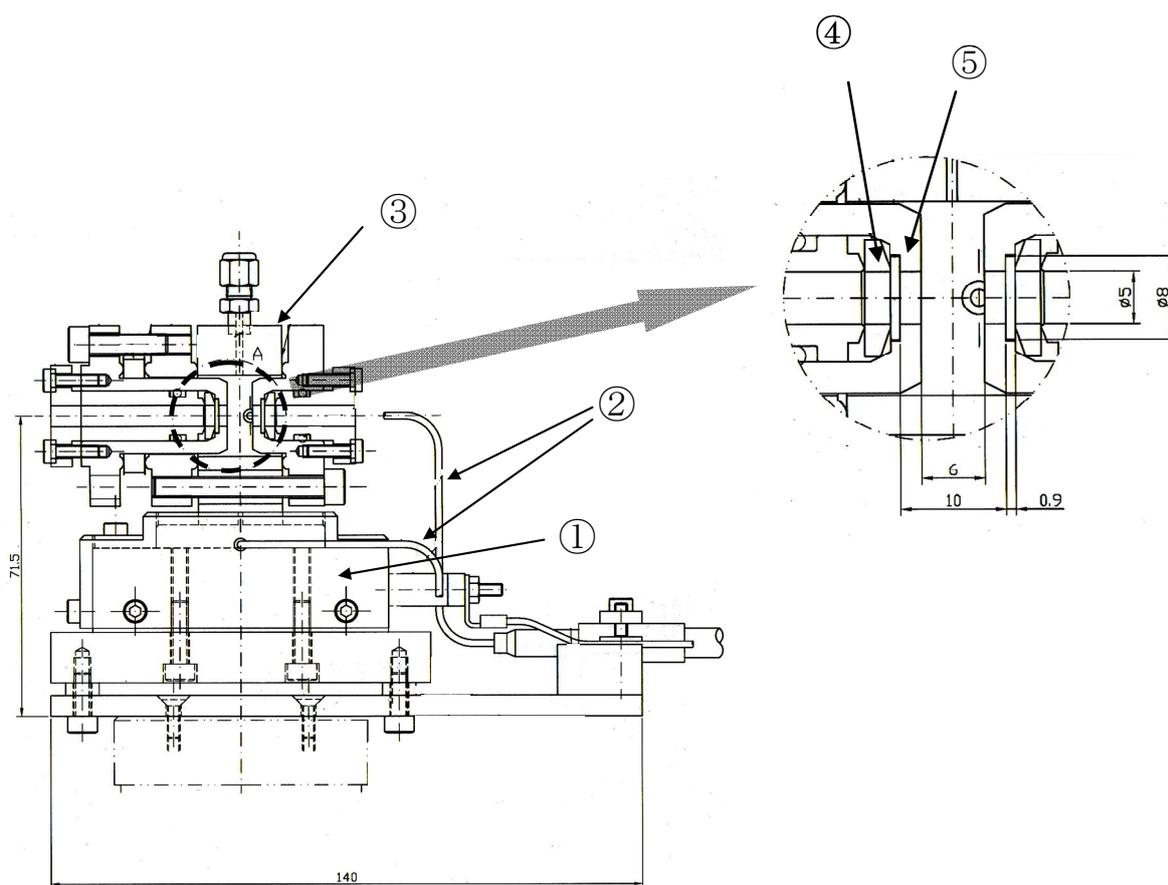


Fig. S1. Structure of the XAFS cell used in this study.

① = heater, ② = thermo couple, ③ = cell, ④ = Ag gasket, ⑤ = Be window

Table S1 Structural parameters of Rb⁺, Sr²⁺, Br⁻, and I⁻ in aqueous solution

Ion	<i>k</i> range of the fit, Å ⁻¹	<i>T</i> , °C	<i>N</i>	<i>r</i> , Å	<i>σ</i> , Å	<i>R</i> ^a
Rb ⁺	1.8 – 5.8	26	4.00	2.88	0.156	0.01
		81	3.48	2.87	0.157	0.02
		96	3.45	2.86	0.159	0.02
		116	3.26	2.86	0.159	0.02
		134	3.10	2.85	0.158	0.02
		153	3.20	2.84	0.165	0.02
		172	2.99	2.83	0.161	0.03
Sr ²⁺	2.8 – 10.2	29	8.00	2.62	0.103	0.04
		77	7.45	2.62	0.107	0.05
		96	7.39	2.61	0.107	0.05
		115	7.04	2.60	0.106	0.05
		134	6.94	2.61	0.108	0.05
		153	6.79	2.62	0.108	0.05
		173	6.70	2.61	0.111	0.06
Br ⁻	1.8 – 6.0	29	6.00	3.27	0.176	0.03
		79	5.78	3.25	0.186	0.03
		99	5.37	3.24	0.183	0.03
		118	5.16	3.24	0.183	0.03
		137	4.67	3.24	0.184	0.03
I ⁻	2.5 – 6.0	27	6.00	3.64	0.159	0.03
		78	5.47	3.65	0.166	0.03
		100	5.21	3.65	0.168	0.03
		119	4.87	3.65	0.169	0.03
		139	4.69	3.65	0.175	0.04
		160	4.48	3.66	0.175	0.03

^a Goodness of fit.

Table S2 Structural parameters of Rb⁺ and Sr²⁺ in water swollen and dried cation-exchange resins

Ion	<i>k</i> range of the fit, Å ⁻¹	resin ^a	<i>T</i> , °C	<i>N</i>	<i>r</i> , Å	<i>σ</i> , Å	<i>R</i> ^b
Rb ⁺	1.3 – 5.8	w	28	4.01	2.91	0.160	0.01
		w	79	3.86	2.88	0.170	0.02
		w	96	3.92	2.88	0.174	0.02
		w	115	3.91	2.86	0.177	0.02
		w	135	3.97	2.87	0.182	0.02
		w	154	3.82	2.86	0.182	0.02
		w	176	3.65	2.85	0.184	0.02
		d	34	3.00	2.94	0.153	0.07
Sr ²⁺	2.8 – 10.2	w	29	7.10	2.58	0.094	0.05
		w	78	7.02	2.61	0.104	0.05
		w	96	7.01	2.60	0.105	0.05
		w	115	7.00	2.61	0.110	0.05
		w	134	6.88	2.60	0.113	0.05
		w	154	6.82	2.59	0.113	0.05
		w	173	6.49	2.59	0.110	0.07
		d	34	5.16	2.51	0.110	0.08

^a w: water swollen resin; d: dried resin

^b Goodness of fit.