COMMUNICATION

Electronic Supplementary Information

Intermetallic YIr_2 Nanoparticles with Negatively Charged Ir Active Sites for Catalytic Hydrogenation of Cyclohexanone to Cyclohexanol

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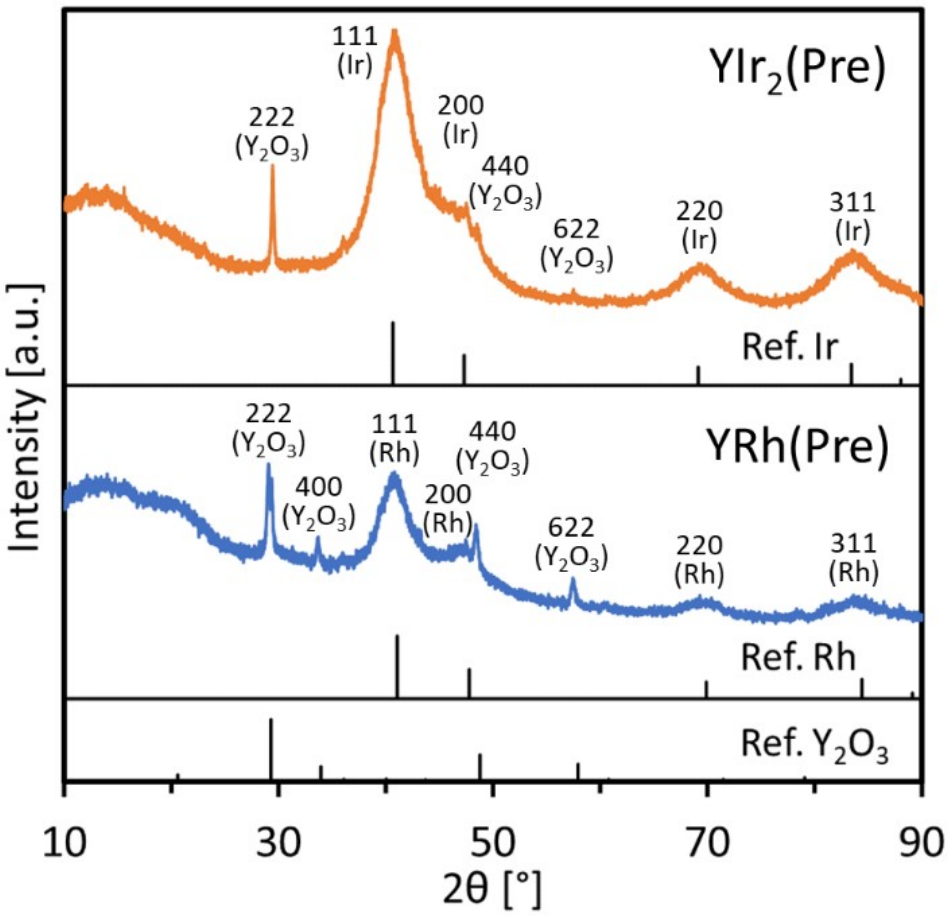


Fig. S1 XRD patterns of YIr_2(Pre) and YRh(Pre).

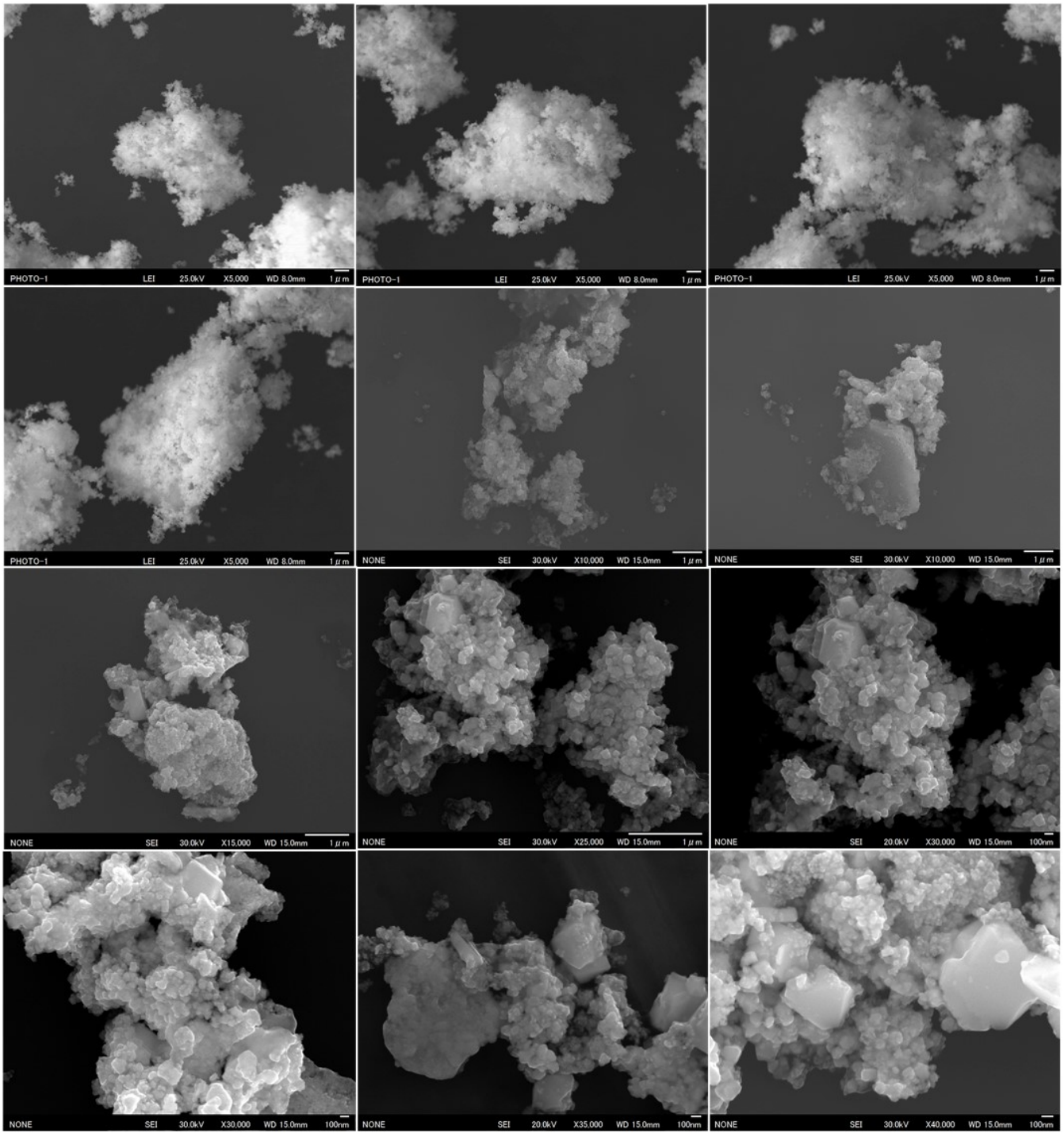


Fig. S2 SEM images of YIr_2(RDT).

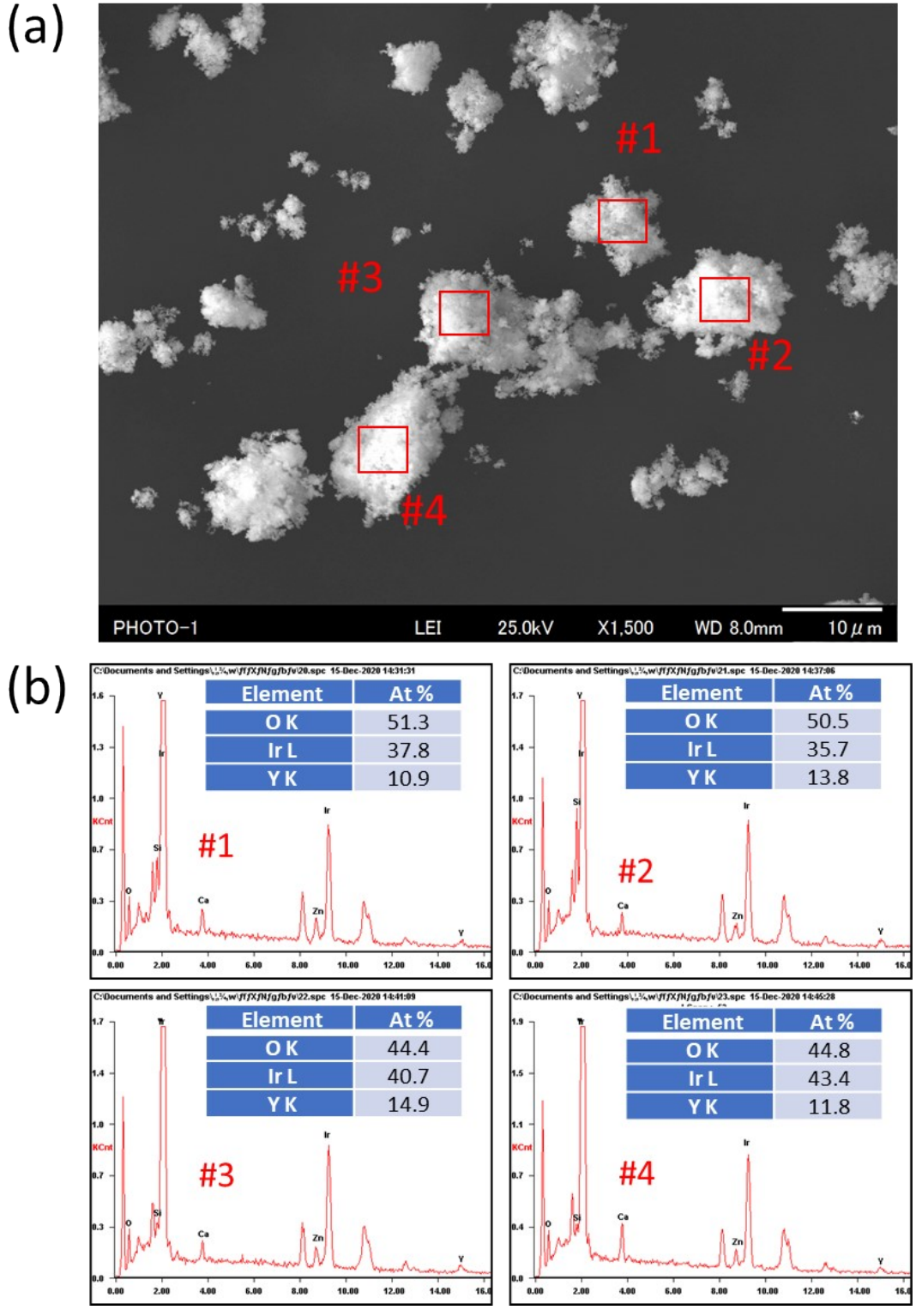


Fig. S3 (a) SEM image and (b) the corresponding EDX spectrum at different positions of #1-#4 for YIr_2(RDT).

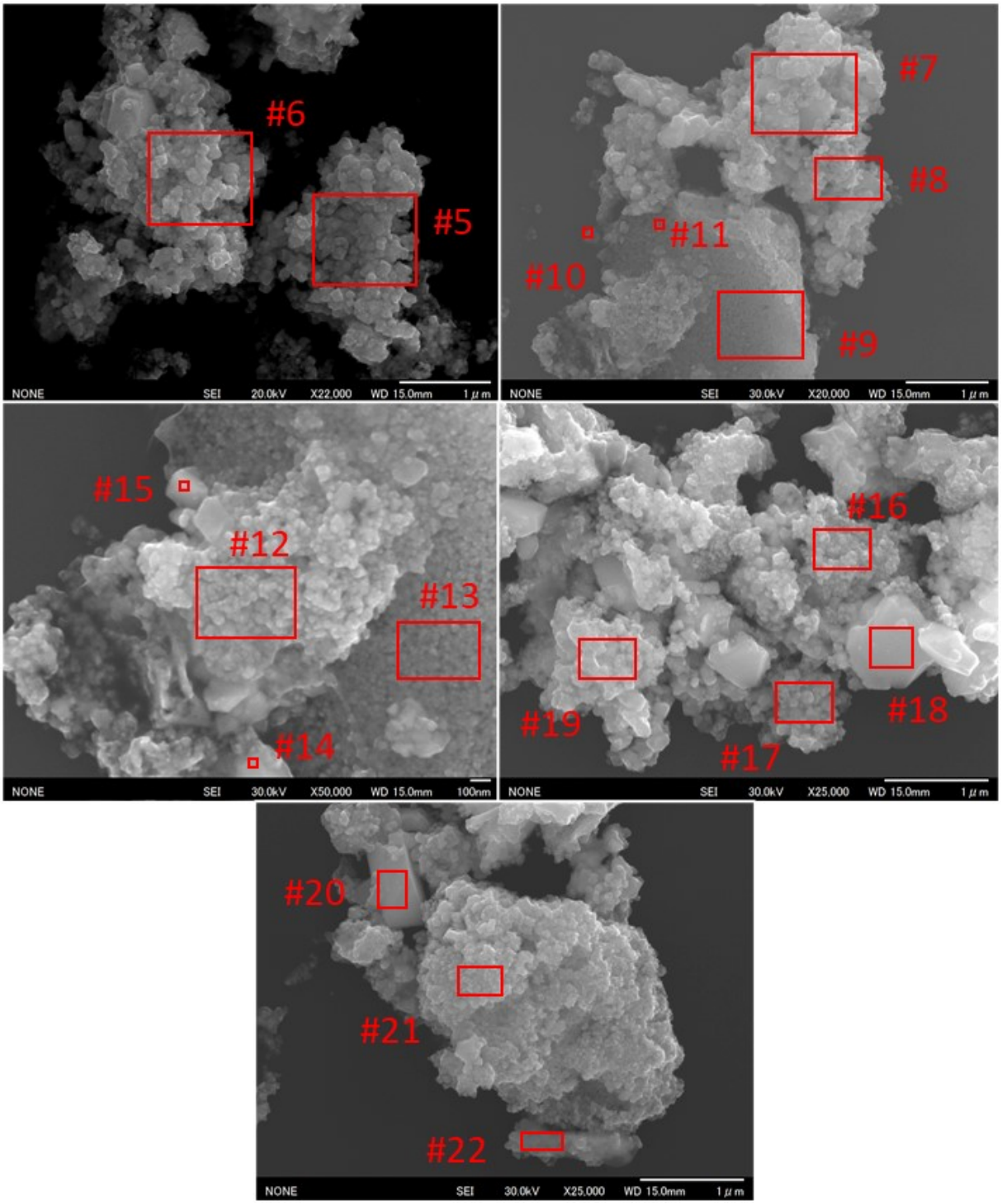


Fig. S4 SEM-EDX of YIr_2(RDT) at different positions of #5-#22.

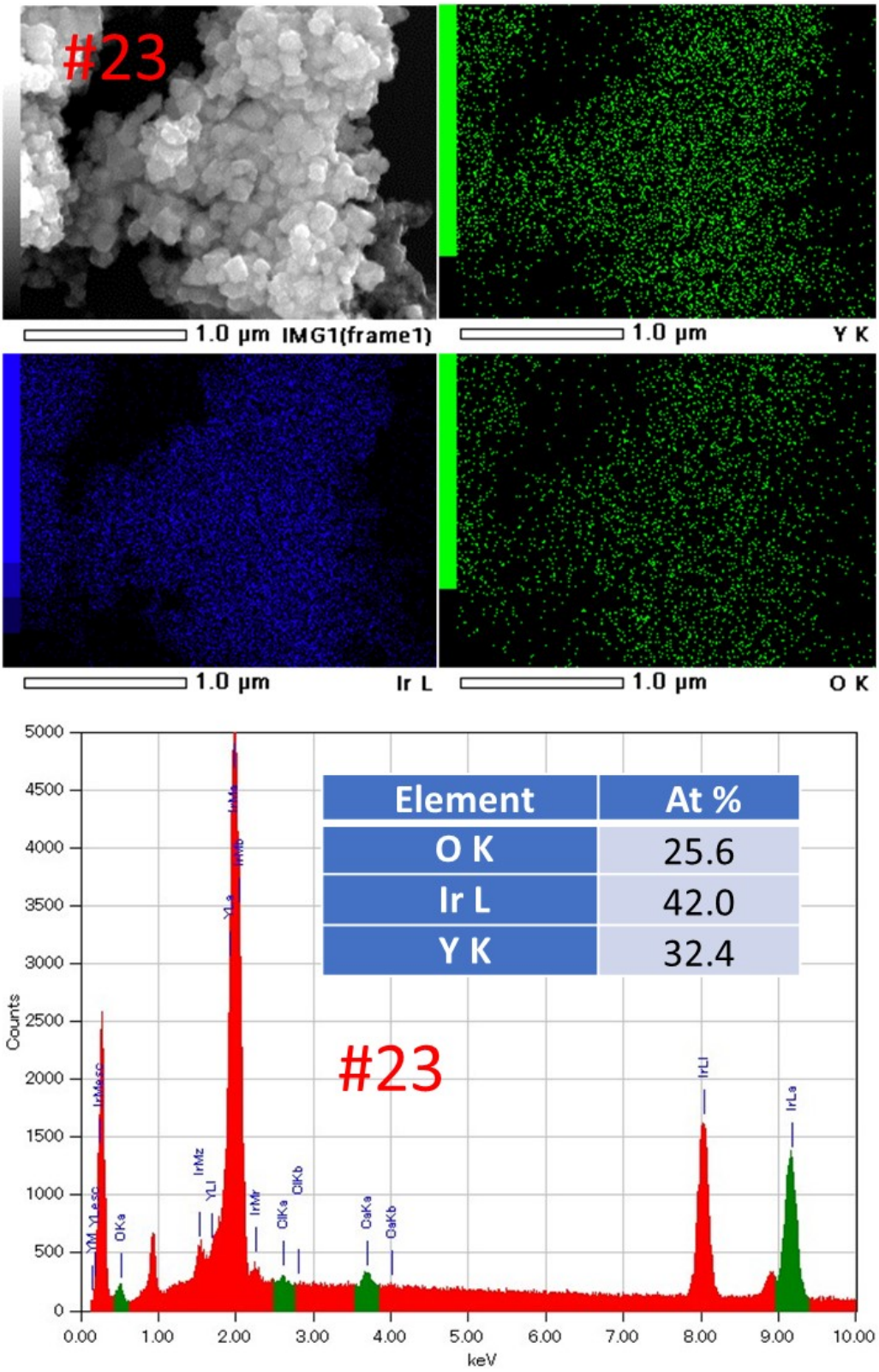


Fig. S5 SEM-EDX of YIr_2(RDT) at a position of #23.

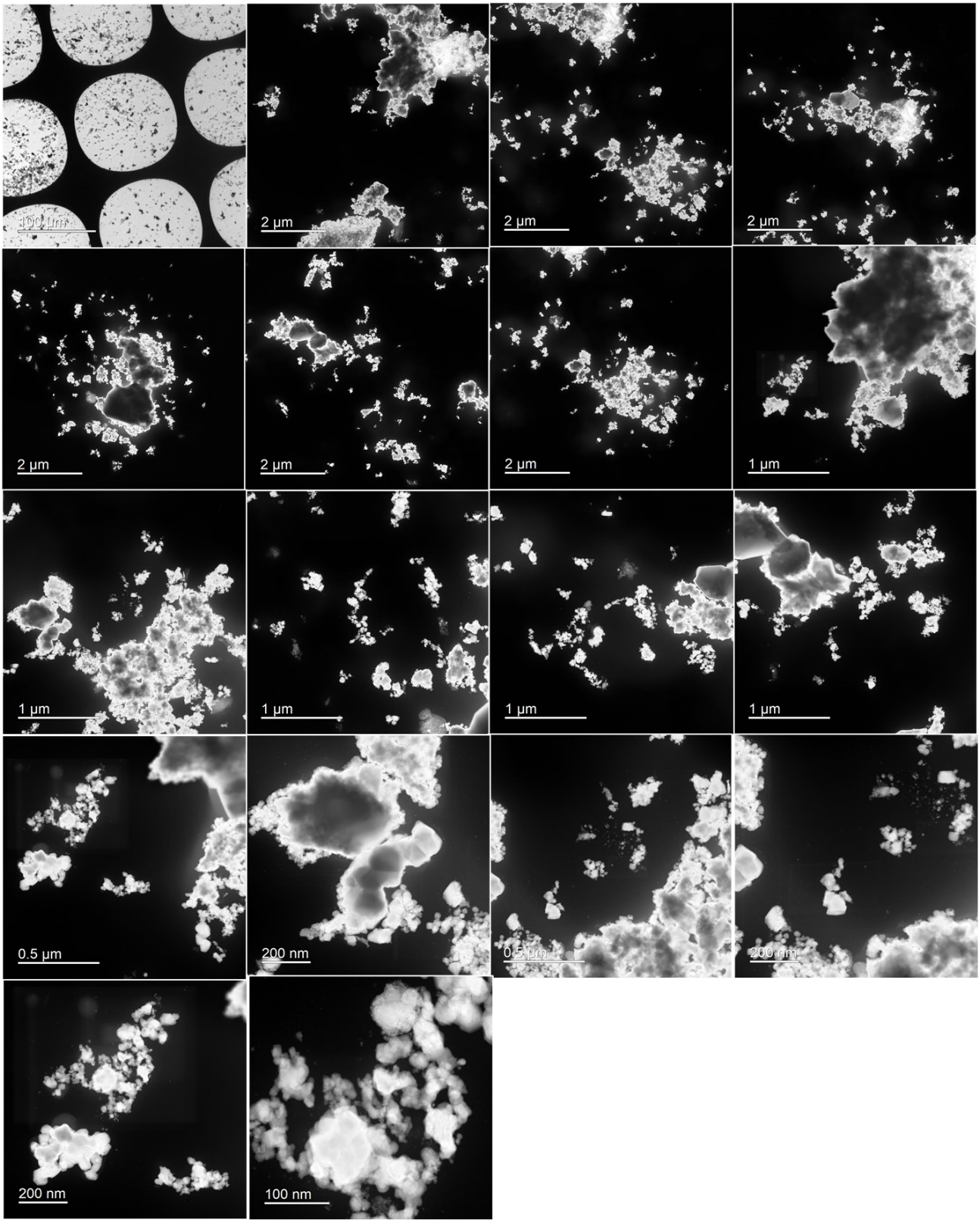


Fig. S6 TEM images of YIr_2(RDT).

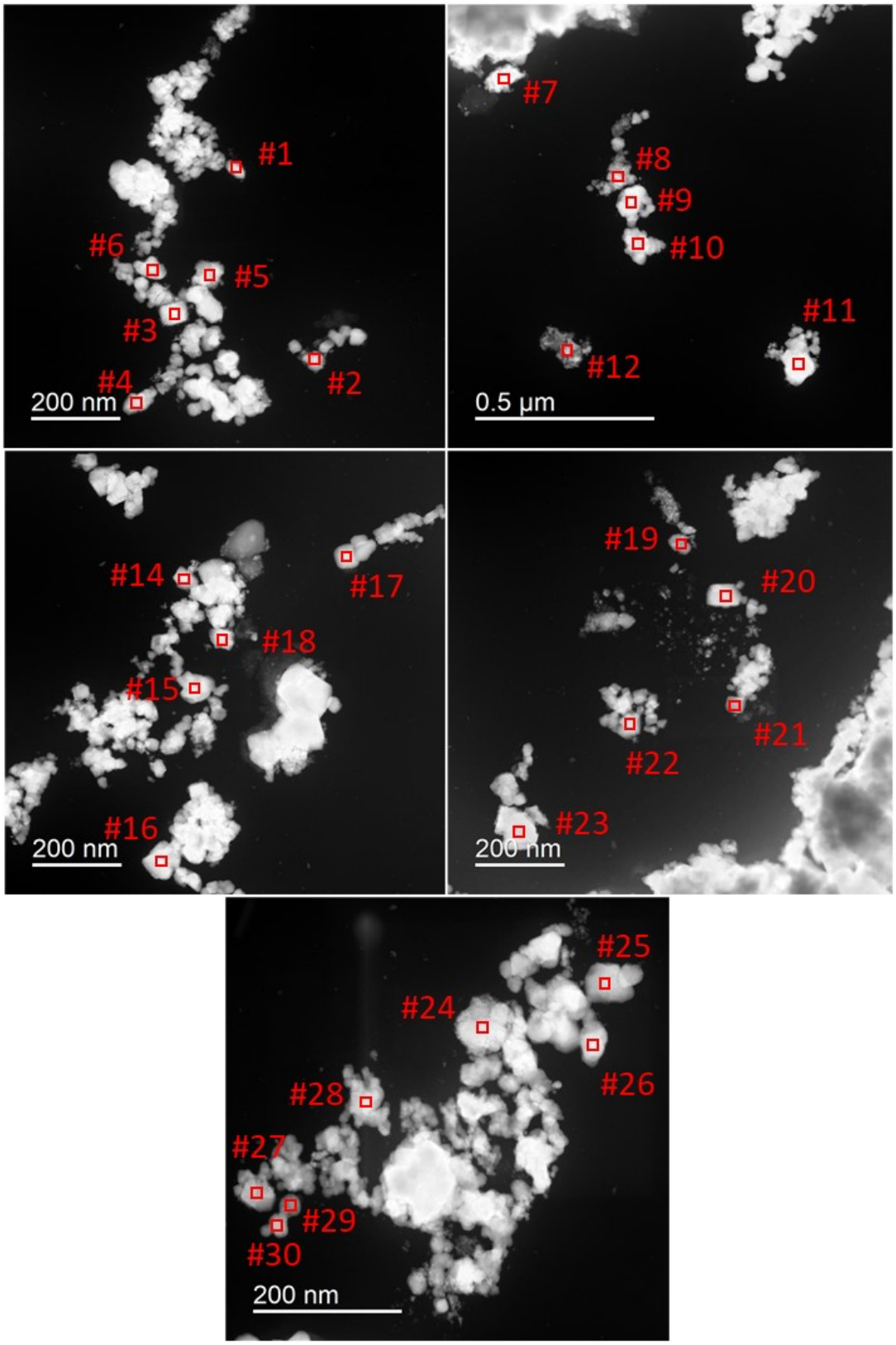


Fig. S7 TEM-EDX of YIr_2(RDT) at different positions of #1-#30.

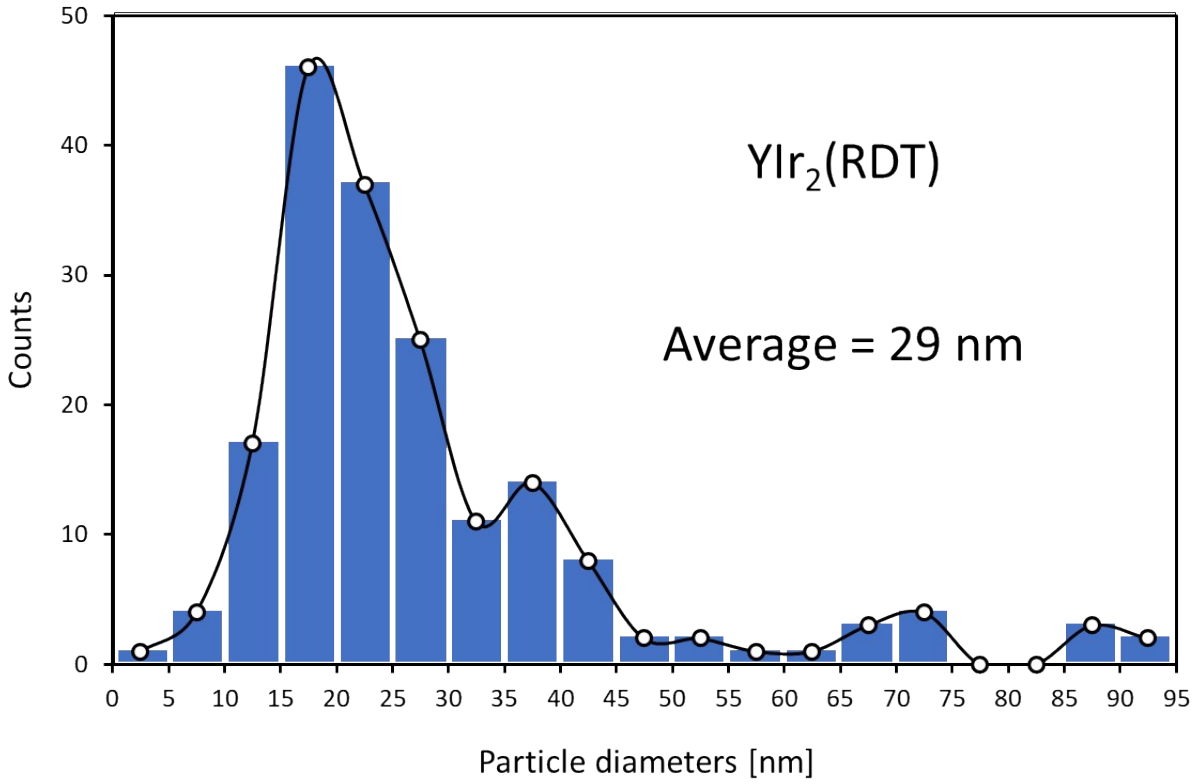


Fig. S8 Particle size distribution on TEM images for $YIr_2(RDT)$.

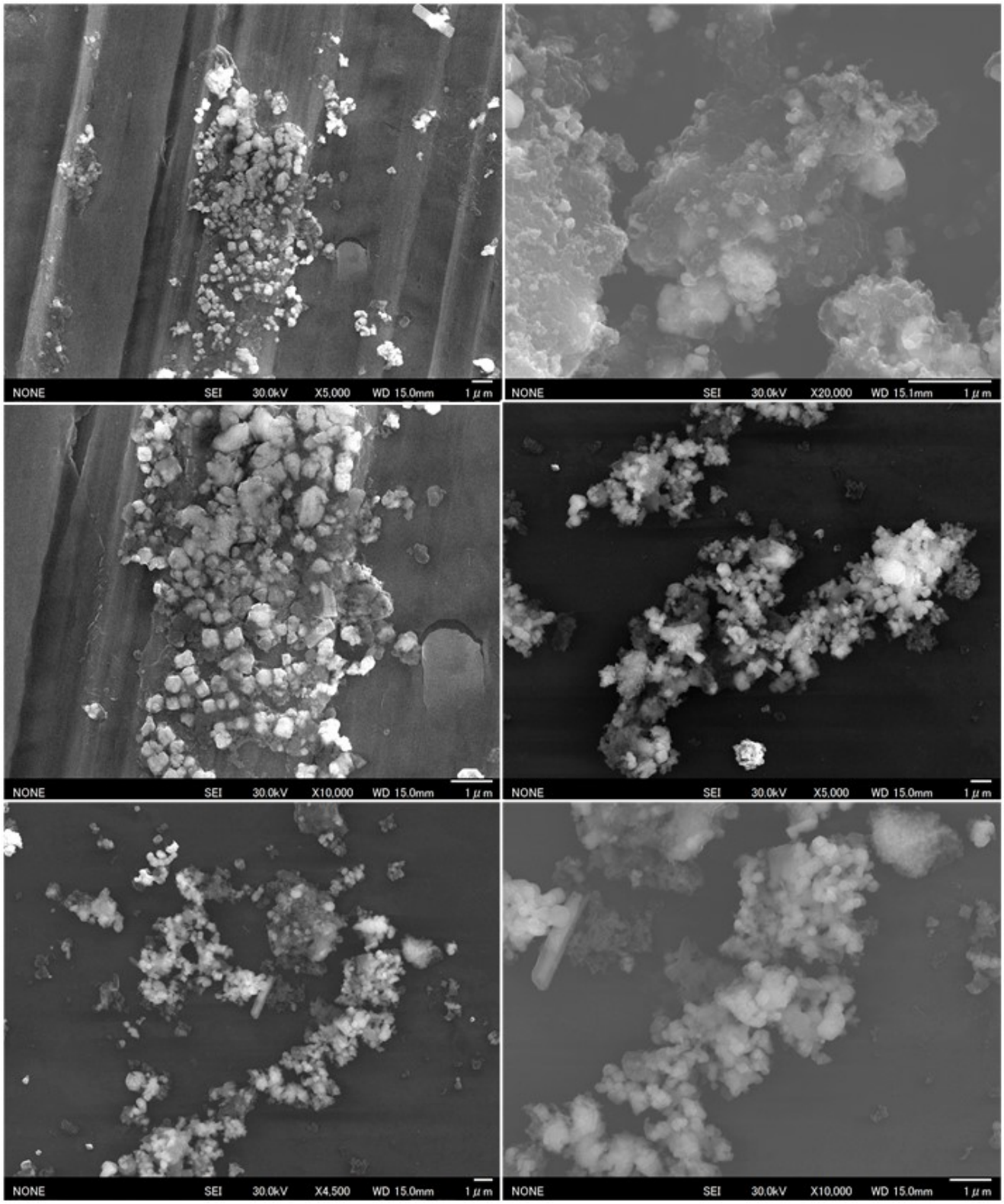
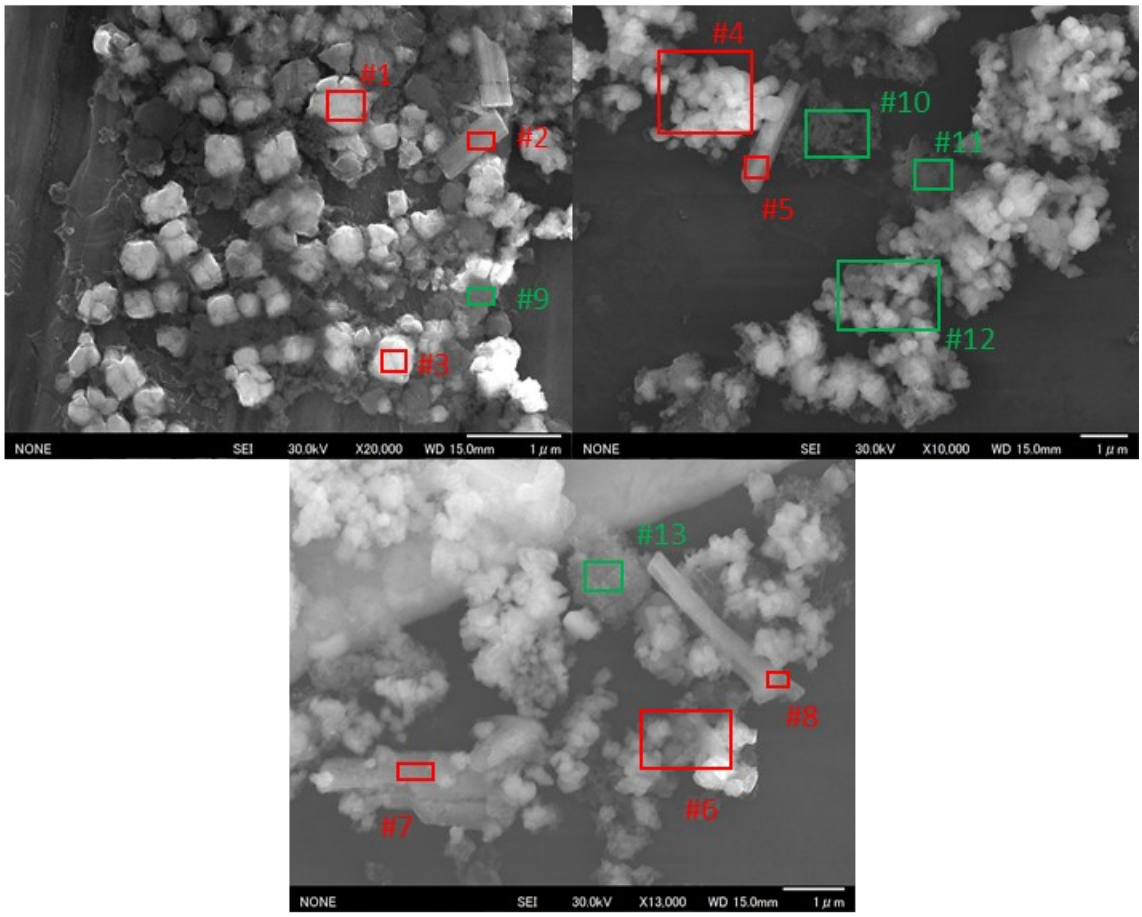


Fig. S9 SEM images of YRh(RDT).

(a)



(b)

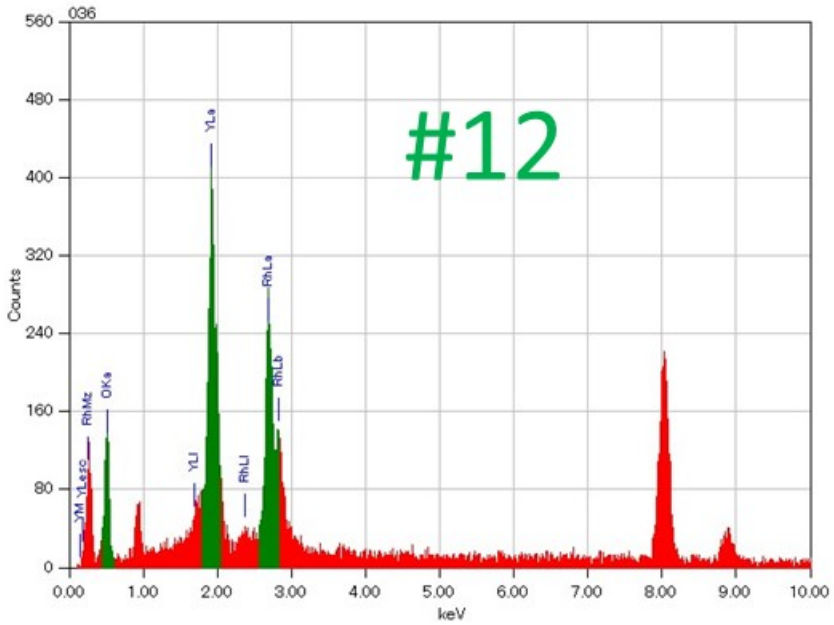


Fig. S10 (a) SEM images and (b) the EDX spectra at a position of #12 for YRh(RDT).

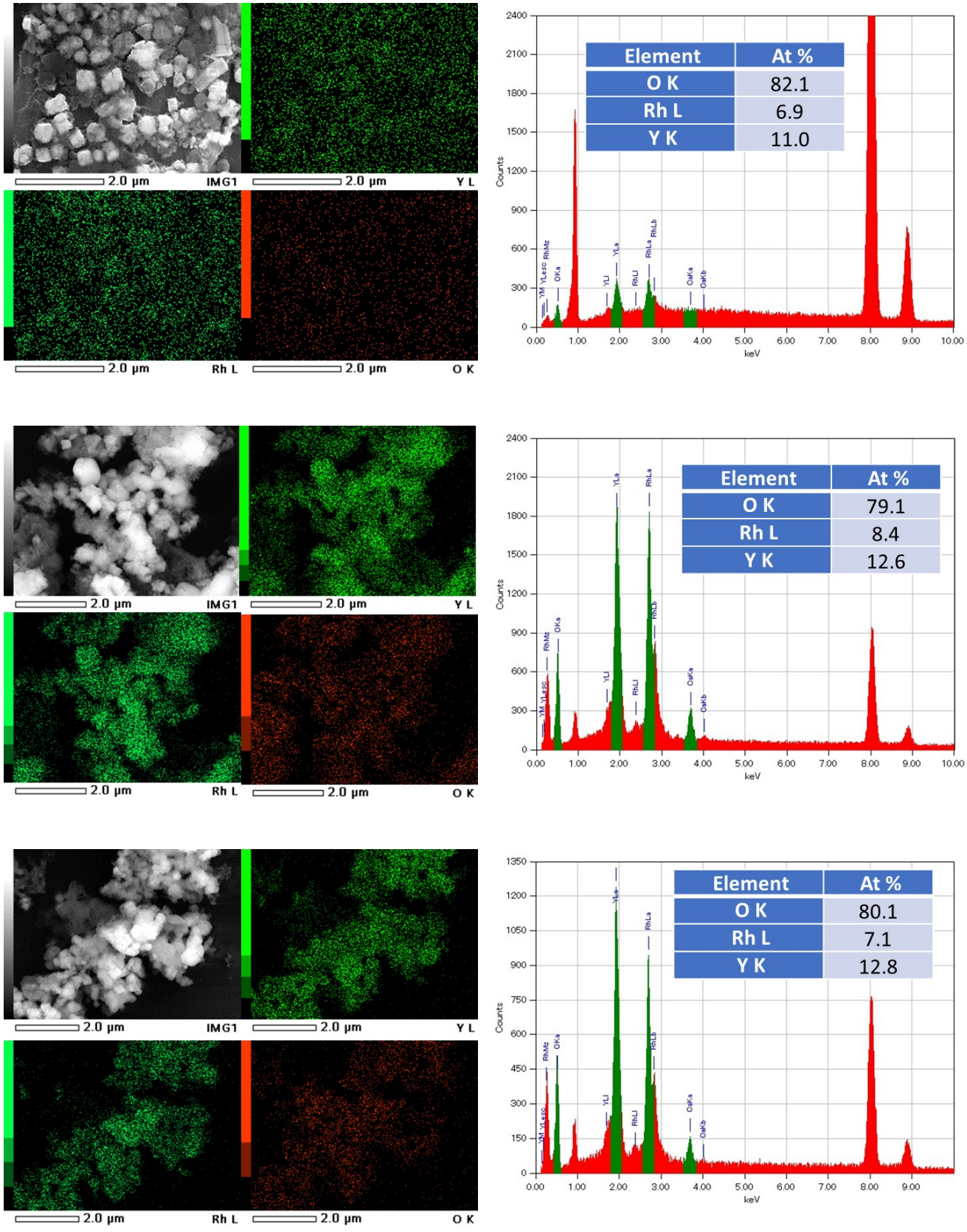


Fig. S11 SEM-EDX of YRh(RDT) at different 3 positions.

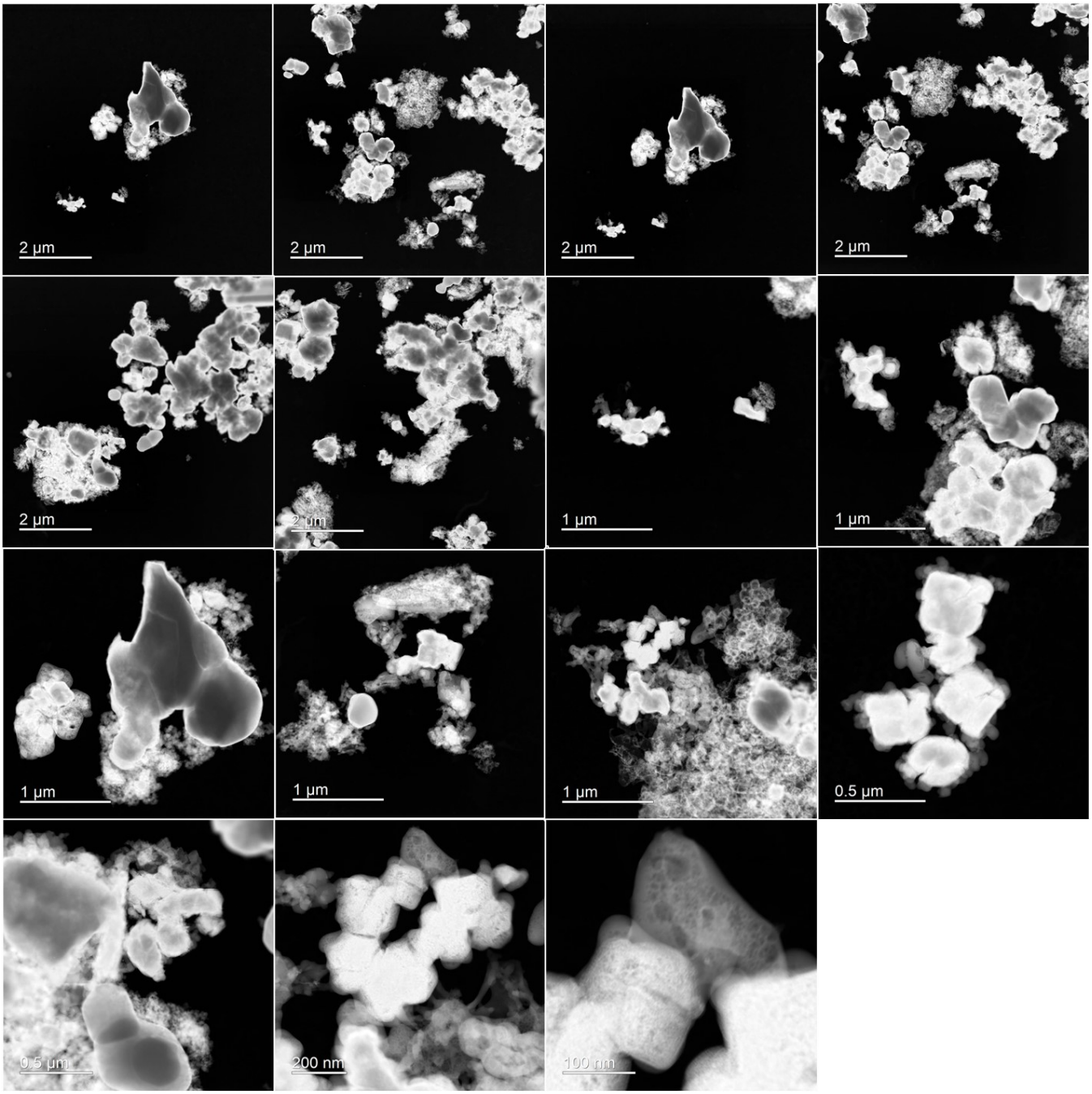


Fig. S12 TEM images of YRh(RDT).

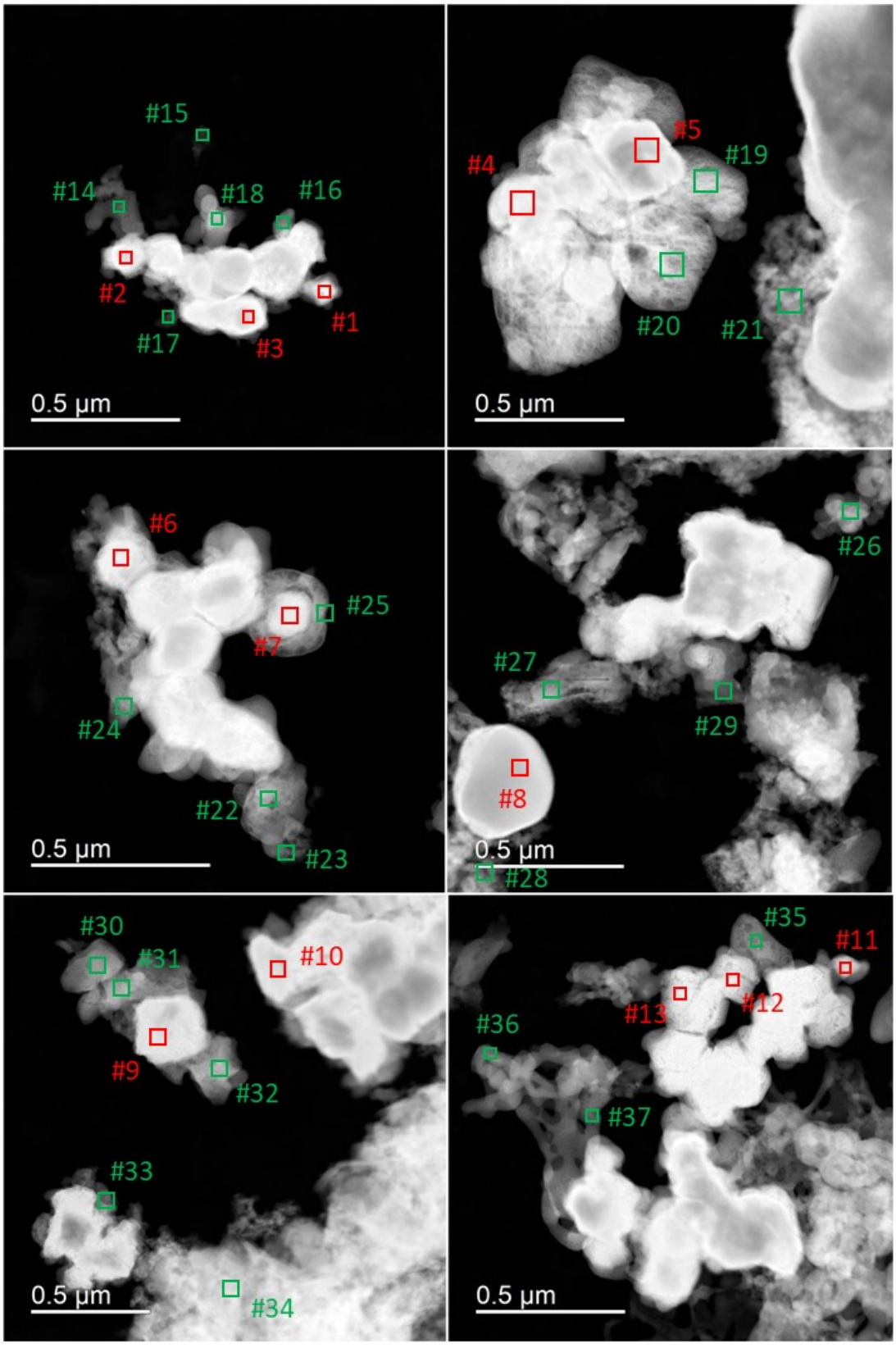


Fig. S13 TEM-EDX of YRh(RDT) at different positions of #1-#37.

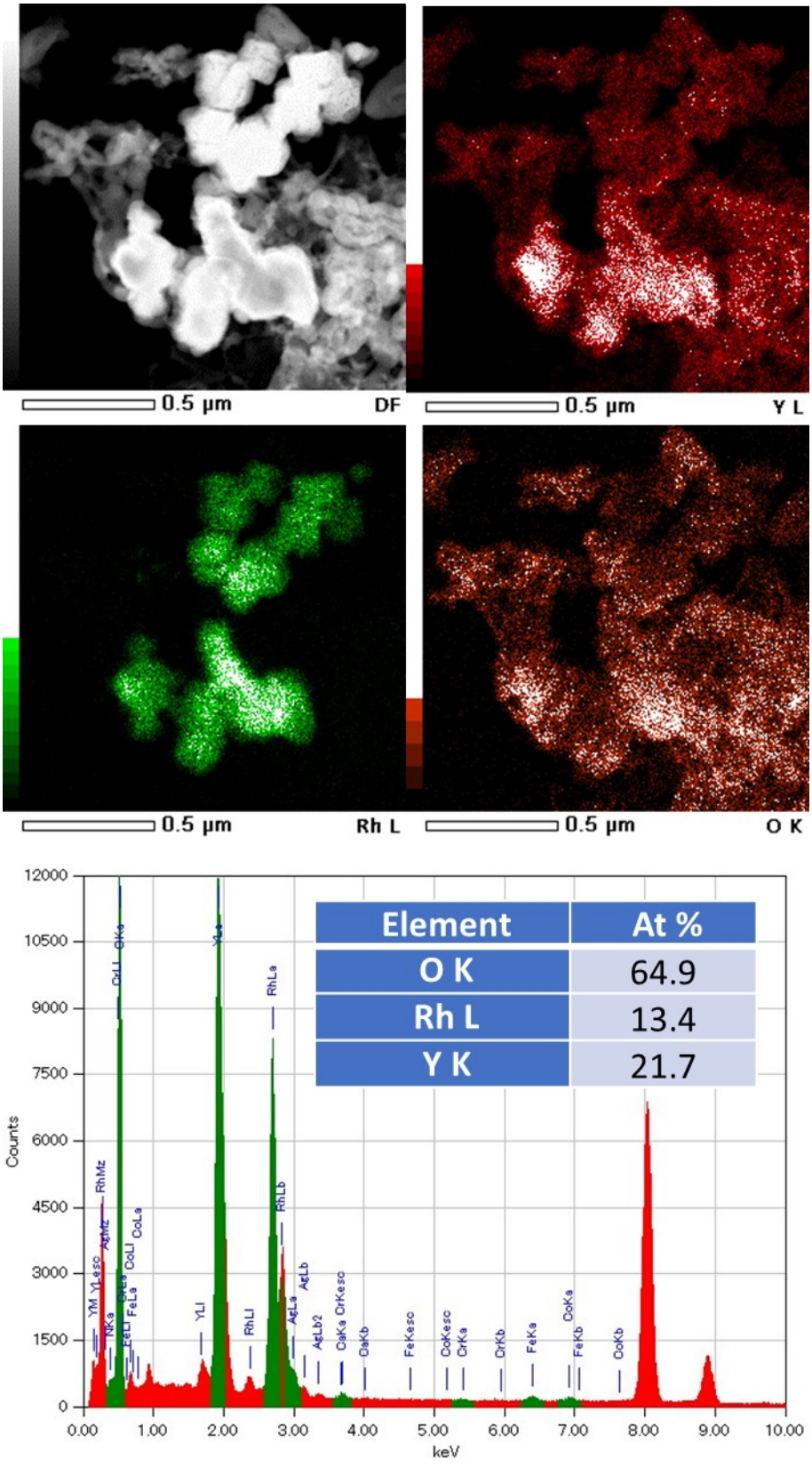


Fig. S14 TEM-EDX of YRh(RDT).

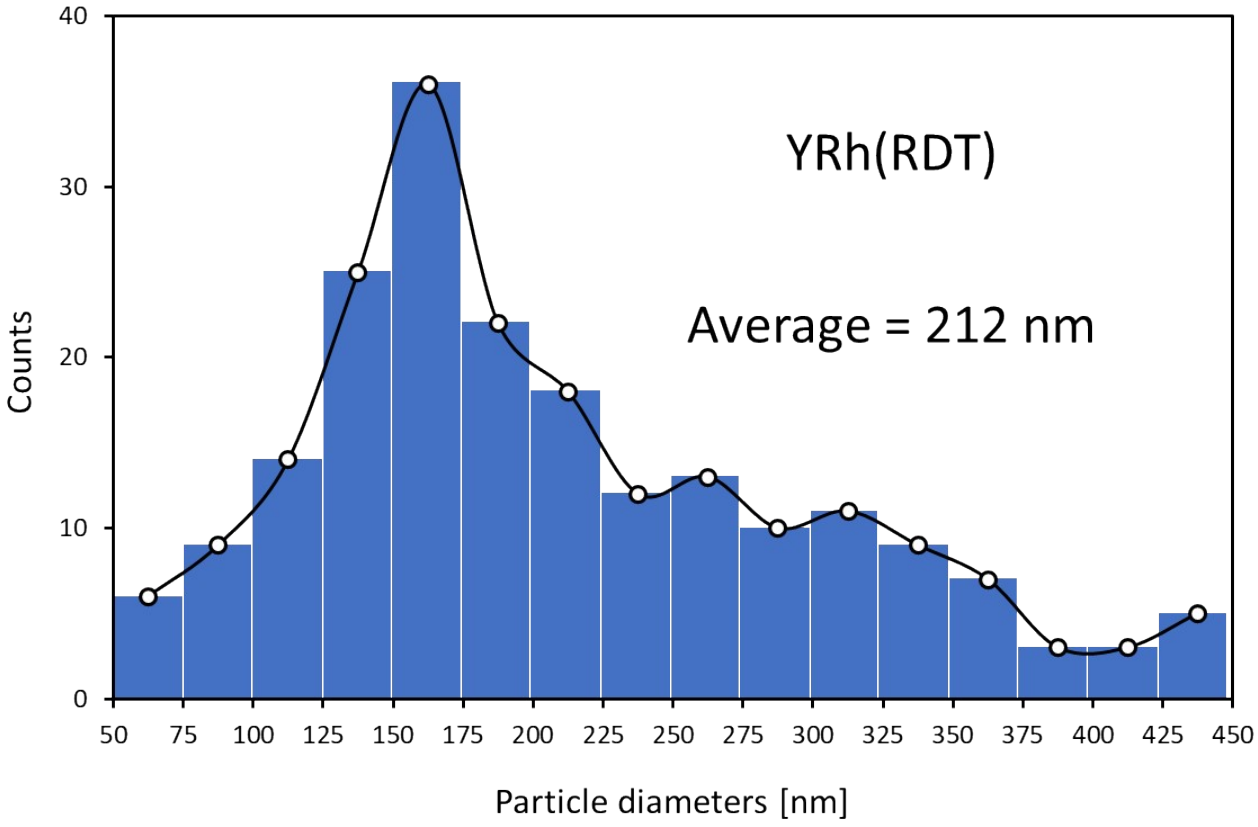


Fig. S15 Particle size distribution on TEM images for YRh(RDT).

Table S1 Summary of the molar ratios measured by SEM-/TEM-EDX for YIr_2(RDT).

Measurement	Position #	Molar ratio [mol%]			Average ratio [mol/mol]
		Y	Ir	O	
SEM-EDX	1	10.9	37.8	51.3	Ir/Y = 1.7/1
	2	13.8	35.7	50.5	
	3	14.9	40.7	44.4	
	4	11.8	43.4	44.8	
	5	33.0	40.4	23.7	
	6	31.9	34.7	30.6	
	7	31.9	38.5	26.6	
	8	36.1	41.1	21.3	
	9	31.8	36.0	28.4	
	10	13.1	27.4	53.8	
	11	25.1	35.1	35.9	
	12	25.3	34.6	35.2	
	13	25.6	38.4	32.2	
	14	24.6	32.5	30.8	
	15	33.0	33.0	30.4	
	16	23.7	42.1	30.4	
	17	24.6	36.8	35.8	
	18	42.5	40.2	14.9	
	19	21.1	30.3	43.9	
	20	31.9	42.1	21.3	
	21	24.5	35.6	34.9	
	22	17.7	34.1	44.7	
TEM-EDX	1	21.7	61.9	5.5	Ir/Y = 3.2/1
	2	25.5	66.4	2.9	
	3	19.1	72.6	2.4	
	4	19.7	71.1	2.2	
	5	26.2	64.0	3.4	
	6	12.2	75.5	3.4	
	7	15.4	46.1	21.1	
	8	17.0	44.4	23.0	
	9	15.7	52.6	12.3	
	10	18.6	51.1	15.4	
	11	22.6	59.5	5.3	
	12	6.2	28.7	45.7	
	13	20.2	56.2	8.8	
	14	20.3	53.9	10.5	
	15	16.1	56.5	9.5	
	16	19.5	46.0	14.4	
	17	13.4	47.7	19.5	
	18	14.8	50.9	17.1	
	19	19.4	62.0	5.8	
	20	19.6	59.1	5.6	
	21	22.4	64.1	5.4	

	22	26.7	65.4	1.9	
	23	14.2	53.5	15.5	
	24	18.0	54.4	11.4	
	25	16.1	53.6	11.2	
	26	17.2	48.7	16.0	
	27	20.7	48.2	17.8	
	28	15.7	47.2	23.7	
	29	17.5	50.1	19.1	

Table S2 Summary of the molar ratios measured by SEM-/TEM-EDX for YRh(RDT).

Measurement	Position #		Molar ratio [mol%]			Average ratio [mol/mol]
			Y	Rh	O	
SEM-EDX	Rh-rich	1	17.7	12.4	69.9	Rh/Y = 0.9/1
		2	9.0	6.8	84.1	
		3	14.7	11.6	73.7	
		4	19.6	13.3	67.1	
		5	8.7	9.3	82.0	
		6	10.7	6.1	83.1	
		7	7.5	16.4	76.1	
		8	10.0	9.5	80.5	
	Y-rich	9	9.5	3.5	87.0	Rh/Y = 0.3/1
		10	12.9	1.0	86.1	
		11	3.8	0.6	95.6	
		12	14.5	7.3	78.2	
		13	12.8	1.7	85.5	
TEM-EDX	Rh-rich	1	46.7	36.7	16.6	Rh/Y = 0.9/1
		2	51.9	38.1	9.9	
		3	47.8	37.4	14.8	
		4	49.2	22.2	28.6	
		5	46.1	23.8	30.1	
		6	54.5	31.4	14.1	
		7	44.8	28.2	27.1	
		8	50.7	42.2	7.1	
		9	28.9	48.3	22.8	
		10	56.4	30.8	12.8	
		11	44.5	22.5	33.0	
		12	24.3	45.3	30.4	
		13	27.2	56.3	16.5	
	Y-rich	14	36.9	0.1	62.9	Rh/Y = 0.005/1
		15	40.1	0.2	59.8	
		16	37.4	0.0	62.6	
		17	40.7	0.3	59.0	
		18	37.7	0.1	62.2	
		19	34.3	0.0	65.7	
		20	30.2	0.0	69.8	
		21	71.1	2.4	26.6	
		22	35.3	0.1	64.6	
		23	36.8	0.5	62.7	
		24	38.1	0.2	61.6	
		25	35.0	0.2	64.8	
		26	31.5	0.2	68.4	
		27	19.8	0.1	80.1	
		28	31.3	0.1	68.7	
		29	37.6	0.2	62.2	
		30	60.6	0.0	39.4	

		31	51.3	0.0	48.7	
		32	35.5	0.0	64.5	
		33	32.9	0.4	66.7	
		34	10.3	0.0	89.7	
		35	38.1	0.1	61.8	
		36	42.7	0.1	57.2	
		37	43.8	0.4	55.8	

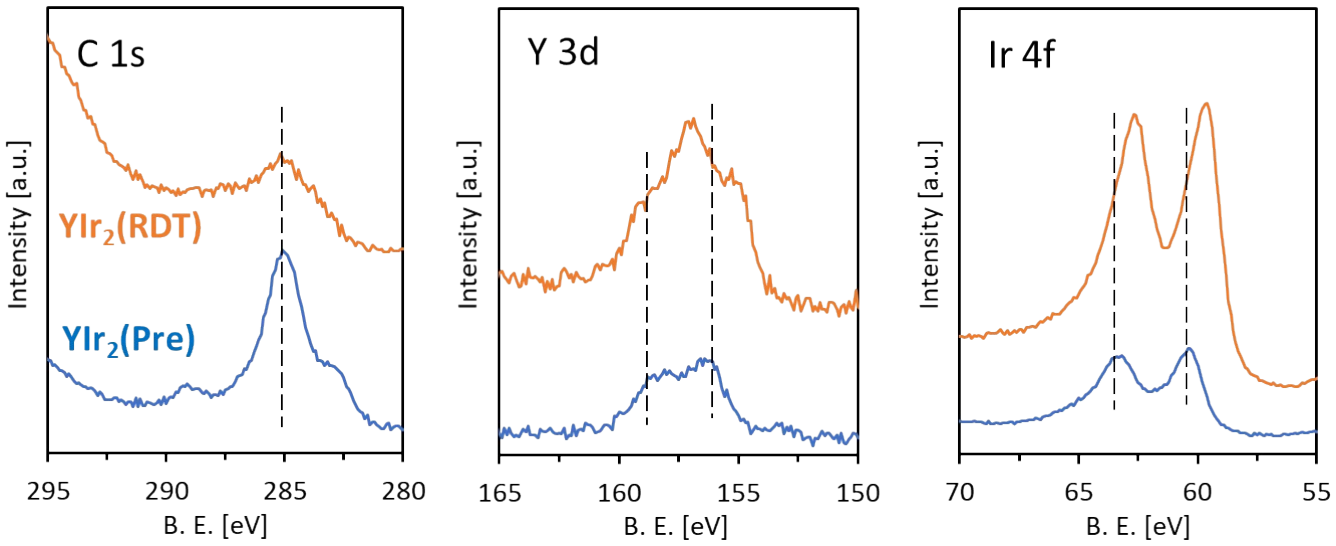


Fig. S16 XPS spectra of YIr_2(Pre) and YIr_2(RDT) for C 1s, Y 3d and Ir 4f. The spectra were calibrated with peaks of C 1s at 285 eV.

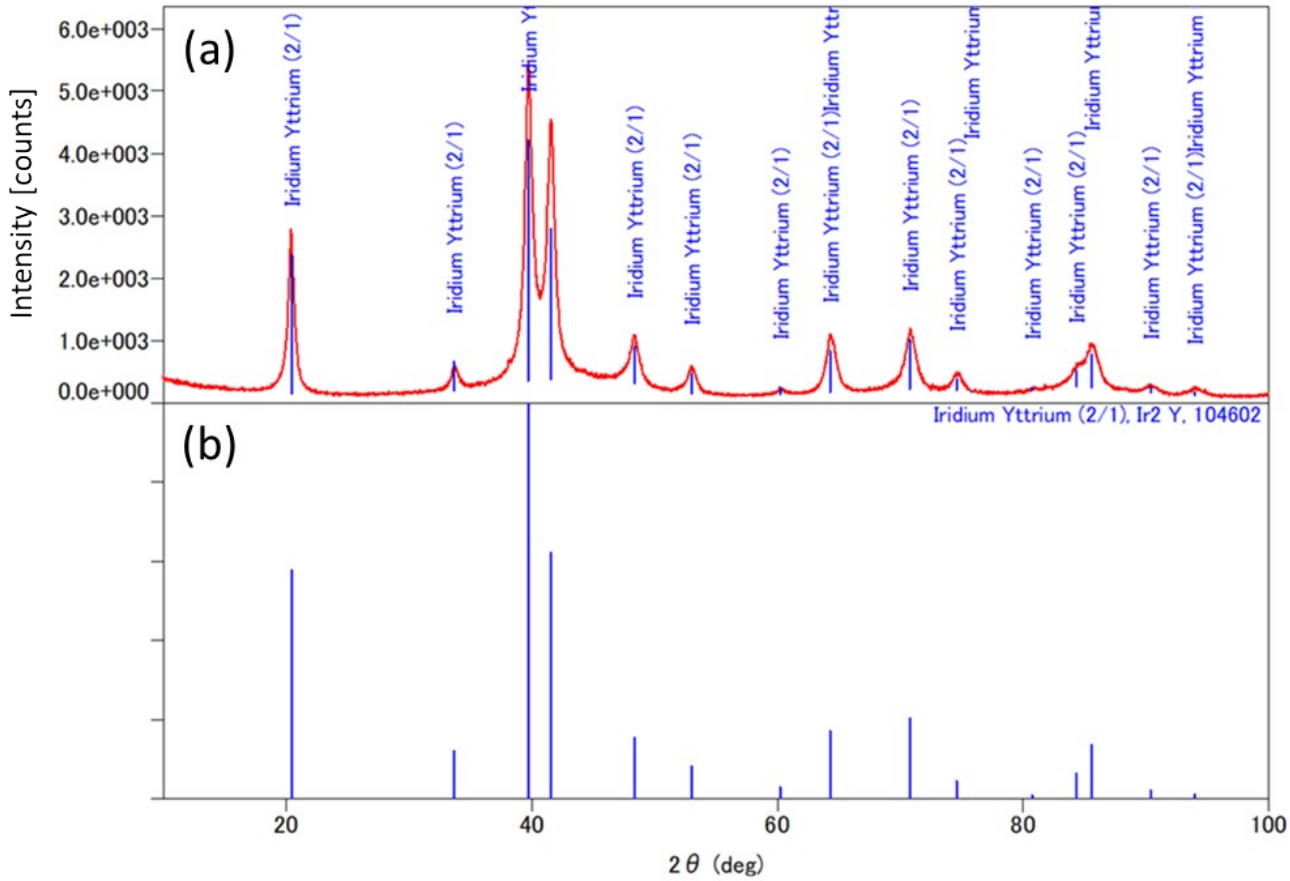


Fig. S17 (a) XRD patterns of spent YIr_2(RDT) and (b) reference peaks for YIr_2. The measurement and analysis were conducted by using a XRD apparatus of SmartLab (Rigaku Corporation) with CuKα radiation at 40 kV and 45 mA

Table S3 Comparison of catalytic performance in C=O bond hydrogenation to alcohols.

Catalyst	Substrate	Reductant	Temperature [°C]	Time [h]	Yield of alcohol [%]	ref.
3wt%Pt/C	cyclohexanone	H_2 (0.1 MPa)	room temperature	16	27	This work
YIr_2(RDT)	cyclohexanone	H_2 (0.1 MPa)	room temperature	16	10	
Pre-reduced YIr_2(RDT)	cyclohexanone	H_2 (0.1 MPa)	room temperature	16	4	
1wt%Ir/Y_2O_3	cyclohexanone	H_2 (0.1 MPa)	room temperature	16	<0.05	
1wt%Ir/SiO_2	cyclohexanone	H_2 (0.1 MPa)	room temperature	16	0	
YRh(RDT)	cyclohexanone	H_2 (0.1 MPa)	room temperature	16	0	
Ir/C	4-methyl benzaldehyde	H_2 balloon (0.1 MPa)	100	10	3	[1]
Ir@CN	4-methyl benzaldehyde	H_2 balloon (0.1 MPa)	100	10	4	
Pd/C	4-methyl benzaldehyde	H_2 balloon (0.1 MPa)	100	10	40	

Reference

[1] Zhi Wang, Lei Huang, Longfei Geng, Rizhi Chen, Weihong Xing, Yong Wang and Jun Huang, *Catal. Lett.* 2015, **145**, 1008.