Supplementary Materials for

High-throughput screening of multimetallic catalysts for three-way catalysis

Son Dinh Le[a], Nhan Nu Thanh Ton[a], Kalaivani Seenivasan[a], Patchanee Chammingkwan[a], Supareak Praserthdam[b], Toshiaki Taniike[a,⋆]

[a]*Graduate School of Advanced Science and Technology, Japan Advanced Institute of Science and Technology (JAIST), 1-1 Asahidai, Nomi, Ishikawa 923-1292, Japan*

[b]*High-Performance Computing Unit (CECC-HCU), Center of Excellence on Catalysis and Catalytic Reaction Engineering (CECC), Chulalongkorn University, Bangkok, 10330, Thailand*

⋆Corresponding author. Email: taniike@jaist.ac.jp

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Table S1: List of chemicals used in the present research

Chemical	**Formula**	**Supplier**	M (g mol^{-1})	Purity
Iridium(III) acetylacetonate	$Ir(C_5H_7O_2)_3$	Sigma Aldrich	489.54	97
Palladium(II) acetylacetonate	$Pd(C_5H_7O_2)_2$	Sigma Aldrich	304.64	99
Bis(acetylacetonato)platinum(II)	$Pt(C_5H_7O_2)_2$	Wako Chemical	393.3	98
Rhodium(III) acetylacetonate	$Rh(C_5H_7O_2)_3$	Sigma Aldrich	400.23	97
Silver acetylacetonate	$Ag(C_5H_7O_2)$	Sigma Aldrich	206.98	98
Cobalt(II) acetylacetonate	$Co(C_5H_7O_2)_2$	Sigma Aldrich	257.15	97
Nickel(II) acetylacetonate	$Ni(C_5H_7O_2)_2$	Sigma Aldrich	256.91	95
Iron(III) acetylacetonate	$Fe(C_5H_7O_2)_3$	Sigma Aldrich	353.17	97
Indium(III) acetylacetonate	$In(C_5H_7O_2)_3$	Sigma Aldrich	412.14	99.99
Chromium(III) acetylacetonate	$Cr(C_5H_7O_2)_3$	Sigma Aldrich	349.32	99.99
Manganese(II) acetylacetonate	$Mn(C_5H_7O_2)_2$	Sigma Aldrich	253.15	100
Ruthenium(III) acetylacetonate	$Ru(C_5H_7O_2)_3$	Sigma Aldrich	398.39	97
Copper(III) acetylacetonate	$Cu(C_5H_7O_2)_2$	Sigma Aldrich	261.76	99.9
Poly(vinylpyrrolidone) K30	$(C_6H_9NO)_n$	Wako Chemical	40,000	
1-methyl-2-pyrrolidone, anhydrous	C_5H_9NO	Sigma Aldrich	99.13	99.5
Triethylene glycol	$C_6H_{14}O_4$	Alfa Aesar	150.17	99
Lithium triethylborohydride	$Li(C_2H_5)_3BH$	Sigma Aldrich	105.95	
Methanol	CH_3OH	Kanto Chemical	32.04	99.8
Hexane	$CH_3(CH_2)_4CH_3$	Kanto Chemical	86.18	96.0

Table S2: Elemental composition acquired by XRF and average particle size acquired by TEM for all synthesized MNPs samples

No.	Combination	Atomic composition	Average size (nm)
1	PdRh	47:53	3.5 ± 0.6
2	PtRh	54:46	2.0 ± 0.4
3	RhCu	83:17	3.0 ± 0.5
4	PdRu	70:30	3.9 ± 0.6
5	PdCu	73:27	2.8 ± 0.4
6	PdRhCu	42:40:18	3.0 ± 0.5
7	PdRhRu	45:38:17	2.5 ± 0.5
8	PdRhNi	42:31:27	3.0 ± 0.7
9	PdRhFe	39:33:28	3.1 ± 0.4
10	PtRhCu	43:39:18	2.4 ± 0.9
11	PdRhCo	37:35:28	3.4 ± 0.5
12	PtRhNi	44:33:23	2.6 ± 0.6
13	PtRhCo	37:34:29	2.3 ± 0.3
14	PtRhFe	42:31:27	1.7 ± 0.3
15	PtRhRu	49:37:14	1.7 ± 0.4
16	PdPtRh	34:37:29	3.4 ± 0.4
17	PdRuFe	51:17:32	3.3 ± 0.7
18	PdRuCo	47:21:32	2.7 ± 0.5
19	PdPtCo	35:41:24	3.5 ± 0.5
20	PdPtCu	37:49:14	3.1 ± 0.5
21	PdRuNi	50:19:31	3.0 ± 0.6
22	PdPtFe	31:42:27	3.5 ± 0.5
23	PtRuCo	52:18:30	2.5 ± 0.5
24	PdPtRhFe	29:30:25:16	3.5 ± 0.4
25	CrCuRhPd	19:21:27:33	2.9 ± 0.5
26	PdPtRhCu	30:31:25:14	3.8 ± 0.5
27	PdRhCoFe	33:30:19:18	4.1 ± 0.7
28	PdRhCuFe	32:27:18:23	2.9 ± 0.5
29	PdRhCuCo	30:30:15:25	3.1 ± 0.5
30	MnFeRuRh	20:23:20:37	3.0 ± 0.4
31	CrMnPdIr	18:19:35:27	3.6 ± 0.7

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No.	Combination	Atomic composition	Average size (nm)
32	CrNiPdAg	20:20:35:25	3.8 ± 0.7
33	AgCoPdPtRh	18:17:20:25:20	2.8 ± 0.4
34	CoNiRuRhPd	18:17:15:26:24	3.1 ± 0.4
35	NiCoPdPtRh	16:18:20:24:22	4.5 ± 0.7
36	AgIrPdPtRh	14:19:21:23:23	3.0 ± 0.3
37	FeCoRuRhIr	21:21:18:26:14	3.2 ± 0.3
38	NiCoFePtPd	17:19:20:22:22	3.4 ± 0.4
39	CrMnCuRhAg	12:12:20:28:28	3.7 ± 0.3
40	NiInPdPtRh	17:13:20:25:25	5.1 ± 0.6
41	CrRuPdPtRh	10:15:20:30:25	2.6 ± 0.4
42	NiFePdPtRh	16:17:17:27:23	3.3 ± 0.5
43	MnRuPdPtRh	16:18:20:26:20	2.4 ± 0.4
44	RuAgPdPtRh	15:12:20:26:27	3.2 ± 0.4
45	CrMnCuPdPt	18:15:17:27:23	3.0 ± 0.4
46	CoFePdPtRh	14:19:21:23:23	3.0 ± 0.5
47	MnCuRuPdPt	10:20:19:22:28	3.0 ± 0.4
48	CoNiRuPtAg	17:22:10:31:20	3.1 ± 0.4
49	NiCuRhIrIn	20:15:24:25:16	3.1 ± 0.5
50	CrNiRuPdAg	10:18:12:35:25	3.5 ± 0.4
51	FeNiIrPtAg	18:15:17:27:23	4.8 ± 0.5

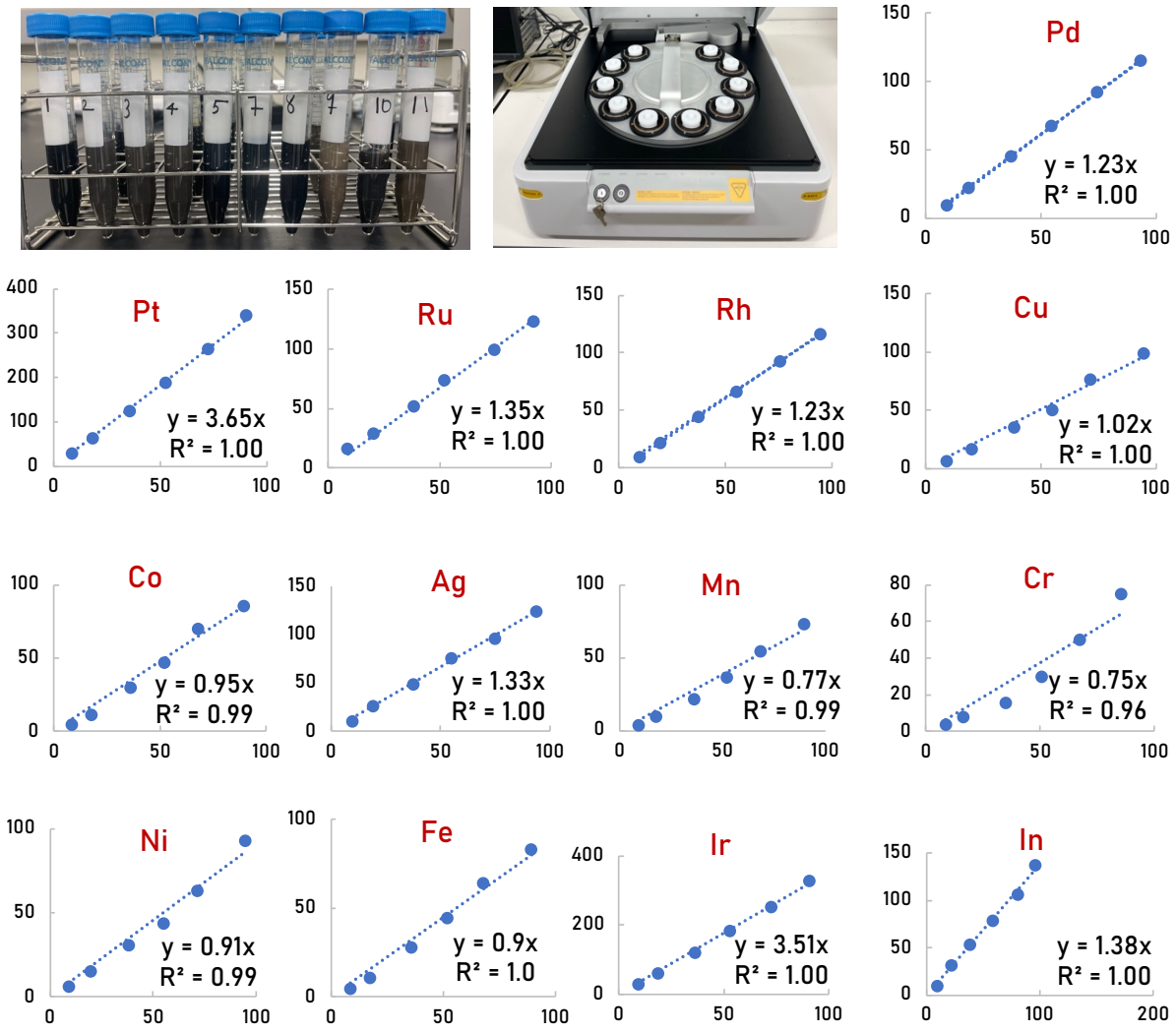

Figure S1: Demonstration of XRF measurements and calibration curves for 13 metals used in the present research

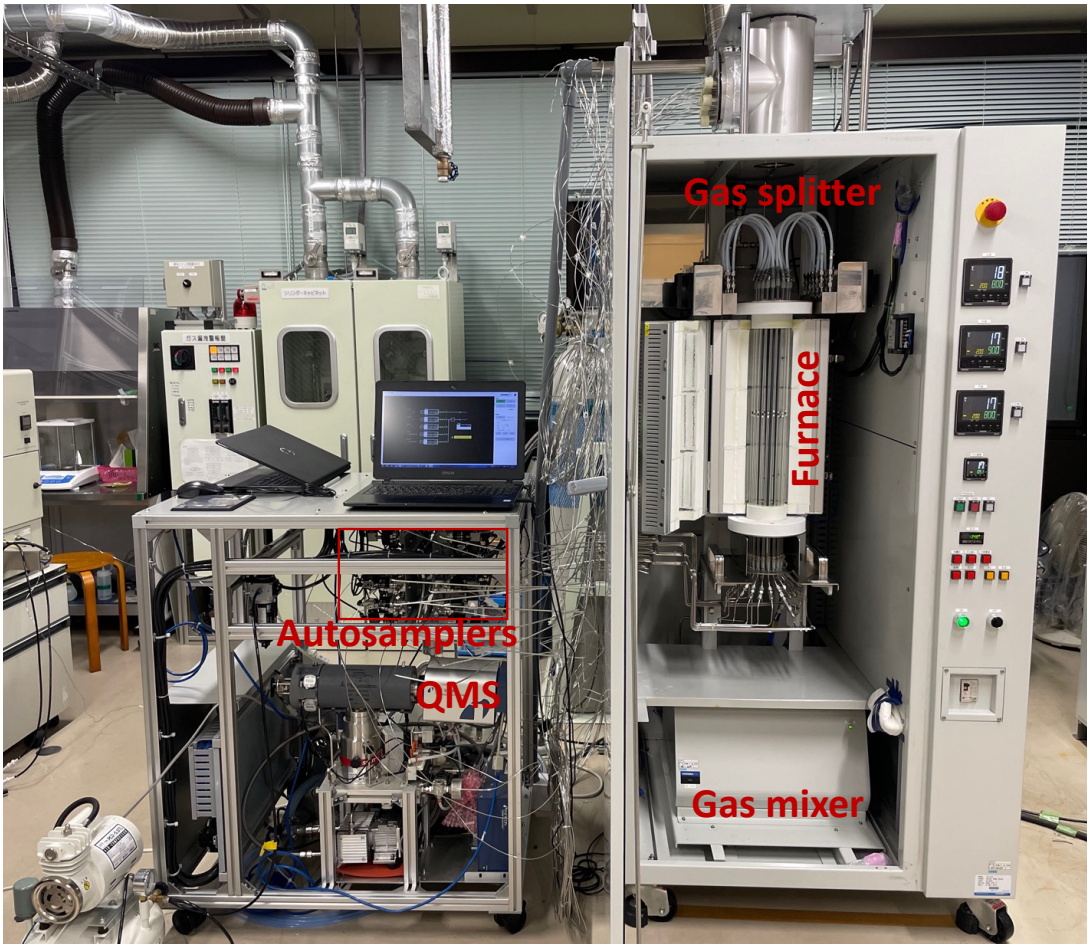

Figure S2: High-throughput screening instrument used for catalyst evaluation

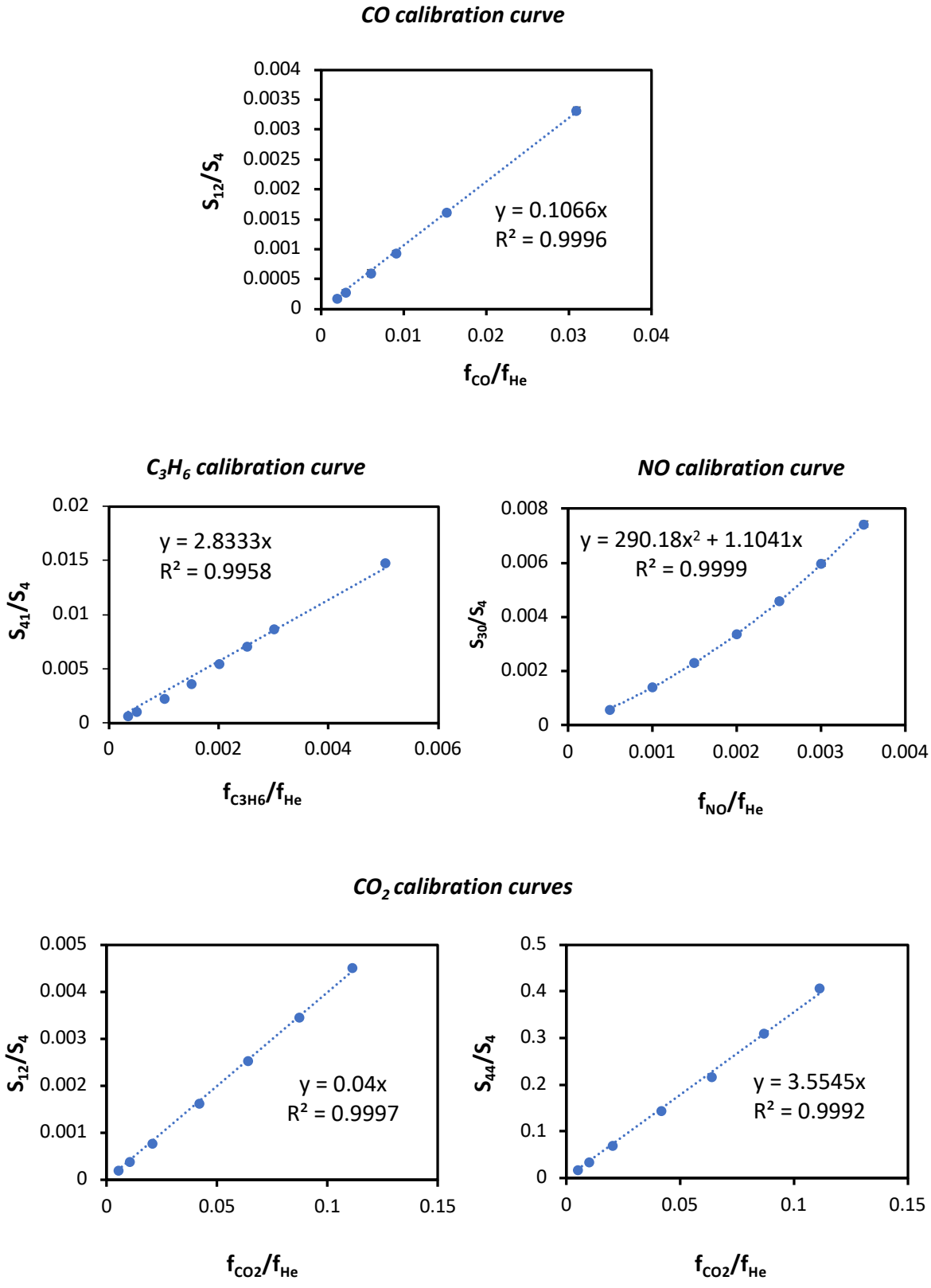

Figure S3: Calibration curves used for calculating the relative pressure of individual gas species

Table S3: Abundance values of all the used elements and its log to the base 10

Element	Abundance (ppm)	log(A)
Cr	102	2.0
Mn	950	3.0
Fe	56300	4.8
Co	25	1.4
Ni	84	1.9
Cu	60	1.8
Ru	0.001	−3.0
Rh	0.001	−3.0
Pd	0.015	−1.8
Ag	0.075	−1.1
In	0.25	−0.6
Ir	0.001	−3.0
Pt	0.005	−2.3