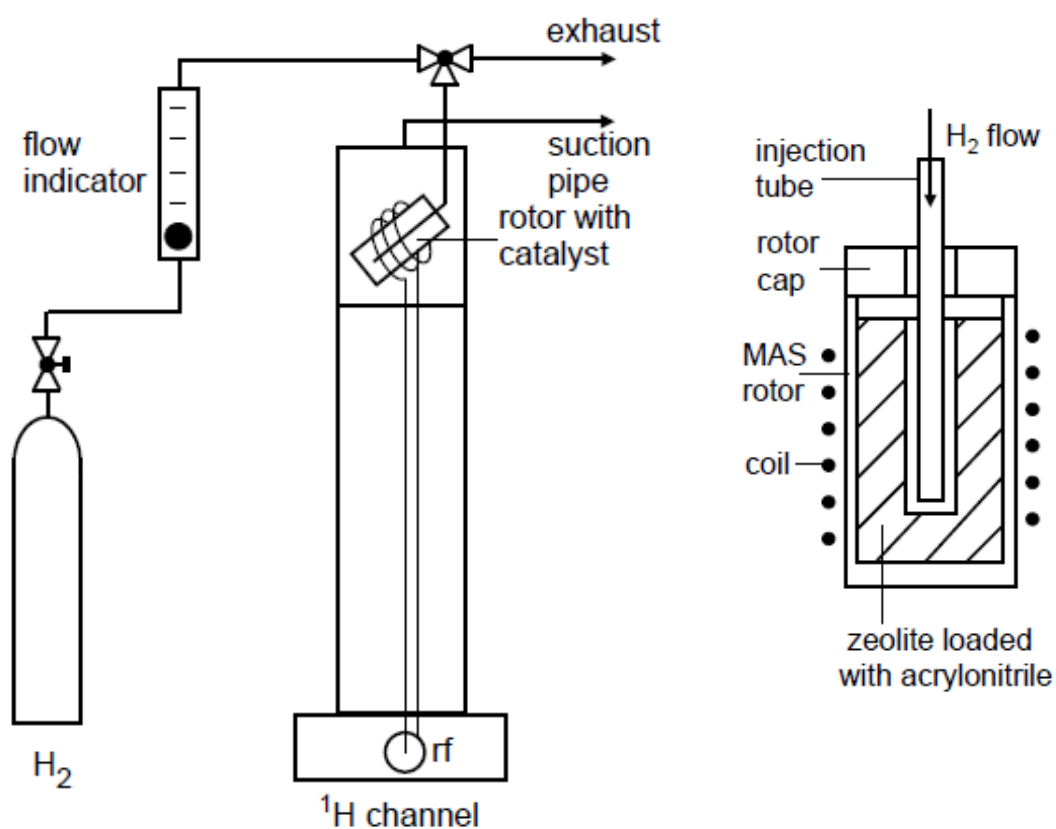


Supporting Information

Relationships between the Hydrogenation and Dehydrogenation Properties of Rh-, Ir-, Pd-, and Pt-Containing Zeolites Y Studied by In Situ MAS NMR Spectroscopy and Conventional Heterogeneous Catalysis

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Scheme S1. Scheme of the in situ flow MAS NMR probe (left) and the reactant injection system for the in situ MAS NMR rotor (right). For further details, see references 1 to 4.

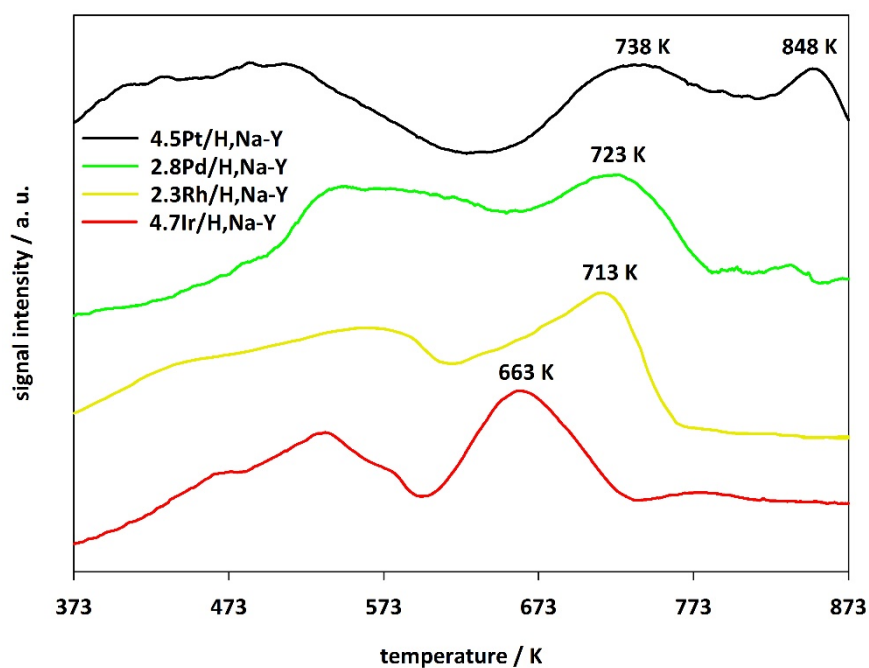


Figure S1. Temperature-programmed desorption of hydrogen (H_2 -TPD) from the noble metal-containing zeolites Y with high metal contents. The high temperature (HT) peaks are marked with their temperature values.

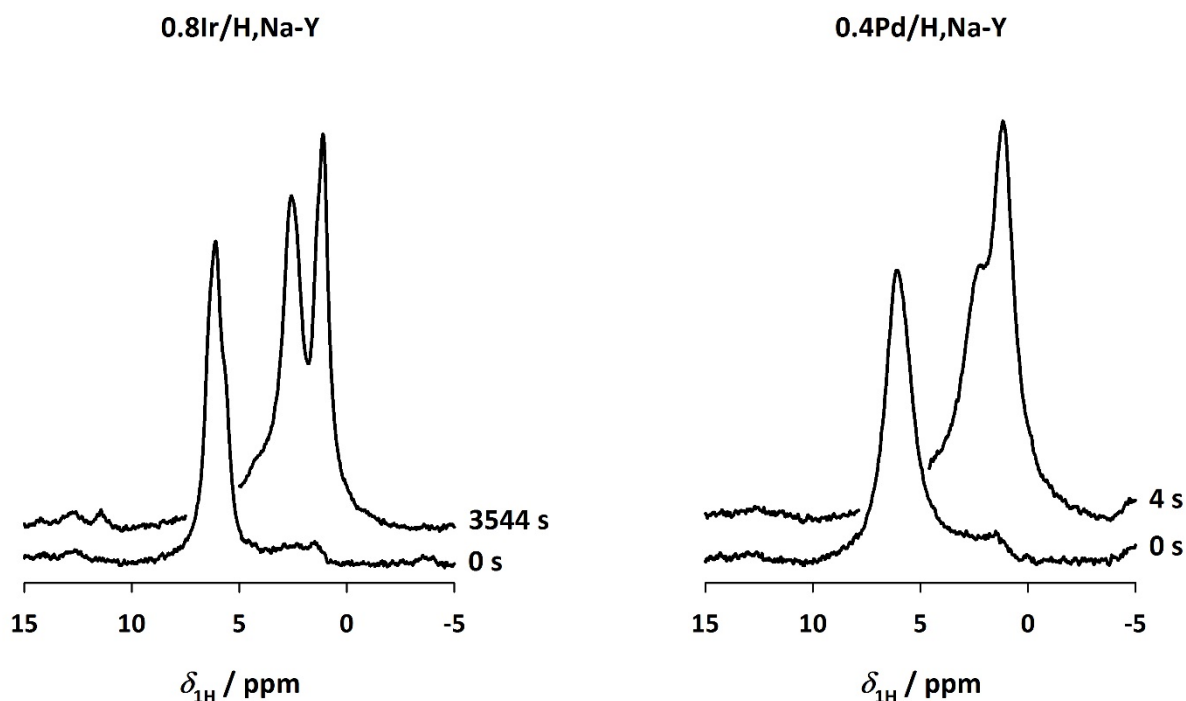


Figure S2. In situ 1H MAS NMR spectra recorded during the hydrogenation of acrylonitrile on the zeolites 0.8Ir/H,Na-Y and 0.4Pd/H,Na-Y at reaction times of 0 s (bottom) and at reaction times of 3544 s and 4 s (top), respectively, under semibatch conditions at 298 K.

Table S1. Sample Designations, Noble Metal (NM) Contents in wt.% and per Unit Cell (u.c.⁻¹), Noble Metal Dispersions, *D*, and Densities of Acidic OH Groups (acOH), Taken from Ref. 5.

samples	NM content ^{a)}	NM content ^{a)}	<i>D</i> ^{b)}	densities of
	/ wt.%	/ u.c. ⁻¹	/ %	acOH ^{c)} / u.c. ⁻¹
0.4Rh/H,Na-Y	0.4	0.4	54	0.15
2.3Rh/H,Na-Y	2.3	2.9	80	3.14
0.8Ir/H,Na-Y	0.8	0.6	121	0.27
4.7Ir/H,Na-Y	4.7	3.3	130	4.24
0.4Pd/H,Na-Y	0.4	0.5	19	0.12
2.8Pd/H,Na-Y	2.8	3.4	43	2.10
0.8Pt/H,Na-Y	0.8	0.5	73	0.20
4.5Pt/H,Na-Y	4.5	3.1	92	2.54

^{a)} Determined by chemical analysis using ICP-OES with an accuracy of $\pm 10\%$.

^{b)} Dispersion, *D*, determined by H₂ chemisorption assuming a stoichiometry of 1 H atom per Rh, Ir, Pd, and Pt atom with an accuracy of $\pm 5\%$.

^{c)} Determined by quantitative ¹H MAS NMR spectroscopy of ammonia-loaded samples with an accuracy of $\pm 10\%$.

Table S2. Selectivities to Propene, *S*_{C3=}, Methane, *S*_{C1}, Ethene, *S*_{C2=}, and Ethane, *S*_{C2}, in the Dehydrogenation of Propane on the Noble Metal-Containing Zeolites Y under Study, Determined under Atmospheric Pressure, at 828 K, and after TOS = 35 and 140 min.

samples	<i>S</i> _{C3=} ^{a)} / %		<i>S</i> _{C1} ^{a)} / %		<i>S</i> _{C2=} ^{a)} / %		<i>S</i> _{C2} ^{a)} / %	
TOS / min	35	140	35	140	35	140	35	140
0.4Rh/H,Na-Y	74	84	4	5	3	4	< 1	< 1
2.3Rh/H,Na-Y	80	84	6	5	4	5	< 1	< 1
0.8Ir/H,Na-Y	63	74	25	19	5	5	2	1
4.7Ir/H,Na-Y	57	74	29	21	3	2	1	< 1
0.4Pd/H,Na-Y	49	46	25	24	27	30	< 1	< 1
2.8Pd/H,Na-Y	62	64	24	18	12	17	1	< 1
0.8Pt/H,Na-Y	69	76	23	18	3	5	4	2
4.5Pt/H,Na-Y	51	68	37	28	2	2	7	2

^{a)} Determined by gas chromatography with an accuracy of $\pm 2\%$.

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