

Supplemental Table S1. Overview of experimental runs

Run No.	T/°C	P/bar	Duration/hrs	Imposed H ₂ pressure/solid buffer assemblage	FSCC used
Set-I Experiments					
HD350-1	350	1	1	1 bar	2 CO ₂ -FSCCs
HD350-2	350	1	2	1 bar	2 CO ₂ -FSCCs
HD350-3	350	1	3	1 bar	2 CO ₂ -FSCCs
HD350-4	350	1	4	1 bar	2 CO ₂ -FSCCs
HD350-5	350	1	5	1 bar	2 CO ₂ -FSCCs
HD300-2	300	1	2	1 bar	2 CO ₂ -FSCCs
HD300-4	300	1	4	1 bar	2 CO ₂ -FSCCs
HD300-6	300	1	6	1 bar	2 CO ₂ -FSCCs
HD300-8	300	1	8	1 bar	2 CO ₂ -FSCCs
HD300-10	300	1	10	1 bar	2 CO ₂ -FSCCs
HD300-12	300	1	12	1 bar	2 CO ₂ -FSCCs
HD250-4	250	1	4	1 bar	2 CO ₂ -FSCCs
HD250-8	250	1	8	1 bar	2 CO ₂ -FSCCs
HD250-12	250	1	12	1 bar	2 CO ₂ -FSCCs
HD250-16	250	1	16	1 bar	2 CO ₂ -FSCCs
HD250-20	250	1	20	1 bar	2 CO ₂ -FSCCs
HD250-24	250	1	24	1 bar	2 CO ₂ -FSCCs
HD200-6	200	1	6	1 bar	2 CO ₂ -FSCCs
HD200-12	200	1	12	1 bar	2 CO ₂ -FSCCs
HD200-18	200	1	18	1 bar	2 CO ₂ -FSCCs
HD200-24	200	1	24	1 bar	2 CO ₂ -FSCCs
HD200-30	200	1	30	1 bar	2 CO ₂ -FSCCs
HD200-36	200	1	36	1 bar	2 CO ₂ -FSCCs
HD200-48	200	1	48	1 bar	2 CO ₂ -FSCCs
HD200-60	200	1	60	1 bar	2 CO ₂ -FSCCs
HD150-12	150	1	12	1 bar	2 CO ₂ -FSCCs
HD150-34	150	1	24	1 bar	2 CO ₂ -FSCCs
HD150-36	150	1	36	1 bar	2 CO ₂ -FSCCs
HD150-48	150	1	48	1 bar	2 CO ₂ -FSCCs
HD150-60	150	1	60	1 bar	2 CO ₂ -FSCCs
HD150-72	150	1	72	1 bar	2 CO ₂ -FSCCs
HD150-96	150	1	96	1 bar	2 CO ₂ -FSCCs
HD150-120	150	1	120	1 bar	2 CO ₂ -FSCCs
HD100-48	100	1	48	1 bar	2 CO ₂ -FSCCs
HD100-72	100	1	72	1 bar	2 CO ₂ -FSCCs
HD100-96	100	1	96	1 bar	2 CO ₂ -FSCCs
HD100-120	100	1	120	1 bar	2 CO ₂ -FSCCs
HD100-168	100	1	168	1 bar	2 CO ₂ -FSCCs
HD100-192	100	1	192	1 bar	2 CO ₂ -FSCCs
HD100-216	100	1	216	1 bar	2 CO ₂ -FSCCs
HD100-264	100	1	264	1 bar	2 CO ₂ -FSCCs
Set-II Experiments					
HM350-3A	350	0.5	3	0.5 bar	3 vacuumed FSCCs
HM350-3B	350	1	3	1 bar	3 vacuumed FSCCs
HM350-3C	350	1.5	3	1.5 bar	3 vacuumed FSCCs
HM350-4A	350	0.5	4	0.5 bar	3 vacuumed FSCCs
HM350-4B	350	1	4	1 bar	3 vacuumed FSCCs
HM350-4C	350	1.5	4	1.5 bar	3 vacuumed FSCCs
HM350-4A	350	0.5	5	0.5 bar	3 vacuumed FSCCs
HM350-4B	350	1	5	1 bar	3 vacuumed FSCCs
HM350-4C	350	1.5	5	1.5 bar	3 vacuumed FSCCs
HM300-8A	300	0.5	8	0.5 bar	3 vacuumed FSCCs
HM300-8B	300	1	8	1 bar	3 vacuumed FSCCs
HM300-8C	300	1.5	8	1.5 bar	3 vacuumed FSCCs
HM300-10A	300	0.5	10	0.5 bar	3 vacuumed FSCCs
HM300-10B	300	1	10	1 bar	3 vacuumed FSCCs
HM300-10C	300	1.5	10	1.5 bar	3 vacuumed FSCCs
HM300-12A	300	0.5	12	0.5 bar	3 vacuumed FSCCs
HM300-12B	300	1	12	1 bar	3 vacuumed FSCCs
HM300-12C	300	1.5	12	1.5 bar	3 vacuumed FSCCs
HM250-16A	250	0.5	16	0.5 bar	3 vacuumed FSCCs
HM250-16B	250	1	16	1 bar	3 vacuumed FSCCs
HM250-16C	250	1.5	16	1.5 bar	3 vacuumed FSCCs
HM250-20A	250	0.5	20	0.5 bar	3 vacuumed FSCCs

HM250-20B	250	1	20	1 bar	3 vacuumed FSCCs
HM250-20C	250	1.5	20	1.5 bar	3 vacuumed FSCCs
HM250-24A	250	0.5	24	0.5 bar	3 vacuumed FSCCs
HM250-24B	250	1	24	1 bar	3 vacuumed FSCCs
HM250-24C	250	1.5	24	1.5 bar	3 vacuumed FSCCs
HM200-36A	200	0.5	36	0.5 bar	3 vacuumed FSCCs
HM200-36B	200	1	36	1 bar	3 vacuumed FSCCs
HM200-36C	200	1.5	36	1.5 bar	3 vacuumed FSCCs
HM200-48A	200	0.5	48	0.5 bar	3 vacuumed FSCCs
HM200-48B	200	1	48	1 bar	3 vacuumed FSCCs
HM200-48C	200	1.5	48	1.5 bar	3 vacuumed FSCCs
HM200-60A	200	0.5	60	0.5 bar	3 vacuumed FSCCs
HM200-60B	200	1	60	1 bar	3 vacuumed FSCCs
HM200-60C	200	1.5	60	1.5 bar	3 vacuumed FSCCs

Set-III Experiments

NNO400-6	400	1000	6	Ni-NiO-H ₂ O	4 vacuumed FSCCs
NNO400-12	400	1000	12	Ni-NiO-H ₂ O	4 vacuumed FSCCs
NNO400-36	400	1000	36	Ni-H ₂ O	4 vacuumed FSCCs
NNO400-48	400	1000	48	Ni-NiO-H ₂ O	4 vacuumed FSCCs
NNO350-6	350	1000	6	Ni-NiO-H ₂ O	4 vacuumed FSCCs
NNO350-12	350	1000	12	Ni-NiO-H ₂ O	4 vacuumed FSCCs
NNO350-36	350	1000	36	Ni-H ₂ O	4 vacuumed FSCCs
NNO350-48	350	1000	48	Ni-NiO-H ₂ O	4 vacuumed FSCCs
NNO350-96	350	1000	96	Ni-NiO-H ₂ O	4 vacuumed FSCCs
NNO300-6	300	1000	6	Ni-NiO-H ₂ O	3 vacuumed FSCCs
NNO300-12	300	1000	12	Ni-NiO-H ₂ O	4 vacuumed FSCCs
NNO300-24	300	1000	24	Ni-NiO-H ₂ O	4 vacuumed FSCCs
NNO300-48	300	1000	48	Ni-H ₂ O	4 vacuumed FSCCs
NNO300-72	300	1000	72	Ni-NiO-H ₂ O	4 vacuumed FSCCs
NNO300-96	300	1000	96	Ni-NiO-H ₂ O	4 vacuumed FSCCs
NNO250-24	250	1000	24	Ni-NiO-H ₂ O	4 vacuumed FSCCs
NNO250-72	250	1000	72	Ni-NiO-H ₂ O	4 vacuumed FSCCs
NNO250-120	250	1000	120	Ni-H ₂ O	4 vacuumed FSCCs
NNO250-168	250	1000	168	Ni-NiO-H ₂ O	4 vacuumed FSCCs
CCO400-6	400	1000	6	Co-CoO-H ₂ O	4 vacuumed FSCCs
CCO400-12	400	1000	12	Co-CoO-H ₂ O	4 vacuumed FSCCs
CCO400-24	400	1000	24	Co-H ₂ O	4 vacuumed FSCCs
CCO400-36	400	1000	36	Co-H ₂ O	4 vacuumed FSCCs
CCO400-48	400	1000	48	Co-CoO-H ₂ O	4 vacuumed FSCCs
CCO350-6	350	1000	6	Co-CoO-H ₂ O	4 vacuumed FSCCs
CCO350-12	350	1000	12	Co-CoO-H ₂ O	4 vacuumed FSCCs
CCO350-24	350	1000	24	Co-H ₂ O	3 vacuumed FSCCs
CCO350-48	350	1000	48	Co-CoO-H ₂ O	3 vacuumed FSCCs
CCO350-72	350	1000	72	Co-CoO-H ₂ O	3 vacuumed FSCCs
CCO300-6	300	1000	6	Co-CoO-H ₂ O	4 vacuumed FSCCs
CCO300-12	300	1000	12	Co-CoO-H ₂ O	4 vacuumed FSCCs
CCO300-24	300	1000	24	Co-CoO-H ₂ O	4 vacuumed FSCCs
CCO300-48	300	1000	48	Co-H ₂ O	4 vacuumed FSCCs
CCO300-72	300	1000	72	Co-CoO-H ₂ O	4 vacuumed FSCCs
CCO250-24	250	1000	24	Co-CoO-H ₂ O	4 vacuumed FSCCs
CCO250-72	250	1000	72	Co-CoO-H ₂ O	4 vacuumed FSCCs
CCO250-120	250	1000	120	Co-H ₂ O	4 vacuumed FSCCs
CCO250-168	250	1000	168	Co-CoO-H ₂ O	4 vacuumed FSCCs

Supplemental Table S2. Raman peak height ratios between H₂ and CO₂ (*HR*) measured in two quenched CO₂-FSCCs (A and B) after being exposed to 1 bar of H₂ in a cold-sealed pressure vessel for various experimental durations at a fixed *T* between 350 and 100 °C.

350 °C					300 °C					250 °C				
Duration/hour	CO ₂ -FSCC-A		CO ₂ -FSCC-B		Duration/hour	CO ₂ -FSCC-A		CO ₂ -FSCC-B		Duration/hour	CO ₂ -FSCC-A		CO ₂ -FSCC-B	
	<i>HR</i>	1σ	<i>HR</i>	1σ		<i>HR</i>	1σ	<i>HR</i>	1σ		<i>HR</i>	1σ	<i>HR</i>	1σ
1	0.82	0.04	2.09	0.09	2	0.90	0.01	1.51	0.02	4	0.42	0.04	1.21	0.03
2	1.02	0.05	2.47	0.23	4	1.20	0.06	2.08	0.10	8	0.79	0.02	2.16	0.06
3	1.17	0.03	2.83	0.08	6	1.23	0.06	2.09	0.07	12	1.02	0.03	2.72	0.14
4	1.20	0.03	2.83	0.11	8	1.37	0.03	2.28	0.12	16	1.13	0.04	2.85	0.04
5	1.16	0.04	2.91	0.15	10	1.36	0.05	2.27	0.06	20	1.14	0.02	2.81	0.11
					12	1.35	0.04	2.24	0.05	24	1.11	0.03	2.80	0.04
200 °C					150 °C					100 °C				
Duration/hour	CO ₂ -FSCC-A		CO ₂ -FSCC-B		Duration/hour	CO ₂ -FSCC-A		CO ₂ -FSCC-B		Duration/hour	CO ₂ -FSCC-A		CO ₂ -FSCC-B	
	<i>HR</i>	1σ	<i>HR</i>	1σ		<i>HR</i>	1σ	<i>HR</i>	1σ		<i>HR</i>	1σ	<i>HR</i>	1σ
6	0.3	0.01	0.82	0.04	12	0.41	0.03	0.63	0.04	48	0.45	0.02	0.78	0.07
12	0.48	0.00	1.20	0.03	24	0.55	0.01	0.99	0.06	72	0.60	0.05	1.07	0.02
18	0.64	0.02	1.56	0.11	36	0.76	0.01	1.29	0.03	96	0.65	0.01	1.17	0.06
24	0.69	0.03	1.80	0.04	48	0.91	0.02	1.61	0.02	120	0.71	0.07	1.30	0.04
30	0.74	0.03	1.87	0.09	60	0.96	0.03	1.77	0.03	168	0.82	0.06	1.50	0.05
36	0.82	0.02	2.08	0.04	72	1.15	0.06	1.95	0.08	192	0.96	0.05	1.68	0.04
48	0.82	0.01	2.16	0.05	96	1.31	0.05	2.26	0.02	216	1.11	0.03	2.09	0.05
60	0.83	0.04	2.10	0.07	120	1.32	0.08	2.28	0.03	264	1.17	0.07	2.08	0.07

Note: In the calculations, the peak heights of the S₀(1) rotational band (near 588 cm⁻¹) of H₂ and the upper band of the CO₂ Fermi diad (near 1388 cm⁻¹) were used; σ is the standard deviation.

Supplemental Table S3. Experimental results of hydrogen pressure measurements in vacuumed FSCCs at room T , $(P_{H_2})_{RT}$, after equilibrium at a fixed T (350, 300, 250, and 200 °C) under a fixed external H_2 pressure (1.5, 1.0, and 0.5 bar) in CSPVs, $(P_{H_2})_{CSPV}$, and calculated H_2 pressures of vacuumed FSCCs at experimental T , $(P_{H_2})_T$, based on the ideal gas law (Eq. (1)).

$T = 350\text{ °C}$										
Duration/hour	Vacuumed FSCC	$(P_{H_2})_{CSPV} = 1.5\text{ bar}$			$(P_{H_2})_{CSPV} = 1.0\text{ bar}$			$(P_{H_2})_{CSPV} = 0.5\text{ bar}$		
		$(P_{H_2})_{RT}$	$(P_{H_2})_T$	ΔP_{H_2}	$(P_{H_2})_{RT}$	$(P_{H_2})_T$	ΔP_{H_2}	$(P_{H_2})_{RT}$	$(P_{H_2})_T$	ΔP_{H_2}
3	A	0.73	1.53	0.03	0.47	0.98	-0.02	0.23	0.48	-0.02
	B	0.75	1.56	0.06	0.46	0.96	-0.04	0.24	0.50	0.00
	C	0.72	1.50	0.00	0.48	1.00	0.00	0.24	0.50	0.00
4	A	0.70	1.46	-0.04	0.44	0.91	-0.09	0.23	0.48	-0.02
	B	0.72	1.51	0.01	0.47	0.98	-0.02	0.23	0.48	-0.02
	C	0.72	1.50	0.00	0.45	0.94	-0.06	0.23	0.48	-0.02
5	A	0.70	1.46	-0.04	0.44	0.92	-0.08	0.23	0.49	-0.01
	B	0.71	1.49	-0.01	0.44	0.92	-0.08	0.23	0.47	-0.03
	C	0.72	1.50	0.00	0.44	0.92	-0.08	0.23	0.48	-0.02
$T = 300\text{ °C}$										
Duration/hour	Vacuumed FSCC	$(P_{H_2})_{CSPV} = 1.5\text{ bar}$			$(P_{H_2})_{CSPV} = 1.0\text{ bar}$			$(P_{H_2})_{CSPV} = 0.5\text{ bar}$		
		$(P_{H_2})_{RT}$	$(P_{H_2})_T$	ΔP_{H_2}	$(P_{H_2})_{RT}$	$(P_{H_2})_T$	ΔP_{H_2}	$(P_{H_2})_{RT}$	$(P_{H_2})_T$	ΔP_{H_2}
8	A	0.76	1.46	-0.04	0.48	0.93	-0.07	0.28	0.53	0.03
	B	0.78	1.49	-0.01	0.47	0.91	-0.09	0.27	0.51	0.01
	C	0.77	1.48	-0.02	0.48	0.92	-0.08	0.27	0.51	0.01
10	A	0.78	1.50	0.00	0.48	0.92	-0.08	0.26	0.50	0.01
	B	0.74	1.43	-0.07	0.48	0.92	-0.08	0.26	0.50	0.00
	C	0.78	1.51	0.01	0.49	0.94	-0.06	0.27	0.52	0.02
12	A	0.74	1.43	-0.07	0.48	0.93	-0.07	0.27	0.51	0.01
	B	0.74	1.43	-0.07	0.48	0.92	-0.08	0.25	0.49	-0.01
	C	0.73	1.41	-0.09	0.48	0.93	-0.07	0.26	0.50	0.01
$T = 250\text{ °C}$										
Duration/hour	Vacuumed FSCC	$(P_{H_2})_{CSPV} = 1.5\text{ bar}$			$(P_{H_2})_{CSPV} = 1.0\text{ bar}$			$(P_{H_2})_{CSPV} = 0.5\text{ bar}$		
		$(P_{H_2})_{RT}$	$(P_{H_2})_T$	ΔP_{H_2}	$(P_{H_2})_{RT}$	$(P_{H_2})_T$	ΔP_{H_2}	$(P_{H_2})_{RT}$	$(P_{H_2})_T$	ΔP_{H_2}
16	A	0.86	1.50	0.00	0.55	0.96	-0.04	0.27	0.47	-0.03
	B	0.88	1.55	0.05	0.57	1.00	0.00	0.27	0.47	-0.03
	C	0.84	1.48	-0.02	0.55	0.97	-0.03	0.27	0.47	-0.03
20	A	0.89	1.57	0.07	0.56	0.98	-0.02	0.26	0.46	-0.04
	B	0.90	1.57	0.07	0.58	1.02	0.02	0.26	0.46	-0.04
	C	0.89	1.57	0.07	0.58	1.02	0.02	0.26	0.46	-0.04
24	A	0.89	1.57	0.07	0.55	0.96	-0.04	0.27	0.47	-0.03
	B	0.91	1.59	0.09	0.57	1.00	0.00	0.27	0.47	-0.03
	C	0.89	1.56	0.06	0.59	1.03	0.03	0.26	0.46	-0.04
$T = 200\text{ °C}$										
Duration/hour	Vacuumed FSCC	$(P_{H_2})_{CSPV} = 1.5\text{ bar}$			$(P_{H_2})_{CSPV} = 1.0\text{ bar}$			$(P_{H_2})_{CSPV} = 0.5\text{ bar}$		
		$(P_{H_2})_{RT}$	$(P_{H_2})_T$	ΔP_{H_2}	$(P_{H_2})_{RT}$	$(P_{H_2})_T$	ΔP_{H_2}	$(P_{H_2})_{RT}$	$(P_{H_2})_T$	ΔP_{H_2}
36	A	0.93	1.48	-0.02	0.61	0.97	-0.03	0.32	0.51	0.01
	B	0.92	1.46	-0.04	0.60	0.95	-0.05	0.32	0.5	0.00
	C	0.91	1.45	-0.05	0.63	0.99	-0.01	0.32	0.51	0.01
42	A	0.91	1.44	-0.05	0.62	0.98	-0.02	0.32	0.5	0.00
	B	0.91	1.44	-0.06	0.64	1.02	0.02	0.31	0.49	-0.01
	C	0.94	1.49	-0.01	0.63	0.99	-0.01	0.31	0.49	-0.01
48	A	0.89	1.41	-0.09	0.62	0.98	-0.02	0.31	0.49	-0.02
	B	0.91	1.44	-0.06	0.63	1.00	0.00	0.31	0.49	-0.01
	C	0.90	1.43	-0.07	0.62	0.98	-0.02	0.31	0.49	0.00

Note: $\Delta P_{H_2} = (P_{H_2})_T - (P_{H_2})_{CSPV}$, and the unit of the $(P_{H_2})_{RT}$, $(P_{H_2})_T$ and ΔP_{H_2} data is in bar.

Supplemental Table S4. Measured H_2 pressures at room temperature, $(P_{H_2})_{RT}$, in quenched vacuumed FSCCs that were equilibrated for various durations with Ni-NiO buffer at 1000 bar and a fixed T (250, 300, 350 and 400 °C) and the calculated $\log (f_{O_2})_{1,T}$.

T °C	P bar	Time hour	Starting material	$(P_{H_2})_{RT}^a$ bar	$(f_{H_2})_{P,T}^b$	$\log (f_{H_2})_{P,T}$	$\log K_w^c$	$\log (f_{H_2O})_{P,T}^d$	$\log (f_{O_2})_{P,T}^e$	$\log (f_{O_2})_{1,T}^f$
400	1000	6	Ni-NiO-H ₂ O	0.75 (± 0.03)	1.70	0.23	16.34	2.42	-28.30	-28.37 (± 0.03)
		12	Ni-NiO-H ₂ O	0.36 (± 0.02)	0.81	-0.09	16.34	2.42	-27.67	-27.74 (± 0.05)
		36	Ni-H ₂ O	0.36 (± 0.02)	0.81	-0.09	16.34	2.42	-27.66	-27.73 (± 0.05)
		48	Ni-NiO-H ₂ O	0.38 (± 0.02)	0.86	-0.07	16.34	2.42	-27.71	-27.78 (± 0.05)
350	1000	6	Ni-NiO-H ₂ O	0.50 (± 0.03)	1.05	0.02	17.84	2.24	-31.24	-31.31 (± 0.04)
		12	Ni-NiO-H ₂ O	0.26 (± 0.02)	0.55	-0.26	17.84	2.24	-30.68	-30.75 (± 0.07)
		36	Ni-H ₂ O	0.28 (± 0.02)	0.58	-0.23	17.84	2.24	-30.73	-30.80 (± 0.07)
		48	Ni-NiO-H ₂ O	0.30 (± 0.02)	0.63	-0.20	17.84	2.24	-30.80	-30.87 (± 0.06)
		96	Ni-NiO-H ₂ O	0.30 (± 0.02)	0.63	-0.20	17.84	2.24	-30.80	-30.87 (± 0.06)
300	1000	6	Ni-NiO-H ₂ O	0.41 (± 0.02)	0.78	-0.11	19.63	2.02	-35.01	-35.09 (± 0.05)
		12	Ni-NiO-H ₂ O	0.15 (± 0.02)	0.29	-0.54	19.63	2.02	-34.14	-34.22 (± 0.12)
		24	Ni-NiO-H ₂ O	0.13 (± 0.02)	0.25	-0.60	19.63	2.02	-34.02	-34.10 (± 0.13)
		48	Ni-H ₂ O	0.13 (± 0.02)	0.25	-0.60	19.63	2.02	-34.03	-34.11 (± 0.13)
		72	Ni-NiO-H ₂ O	0.15 (± 0.02)	0.29	-0.54	19.63	2.02	-34.14	-34.22 (± 0.12)
		96	Ni-NiO-H ₂ O	0.13 (± 0.02)	0.25	-0.60	19.63	2.02	-34.02	-34.10 (± 0.13)
250	1000	24	Ni-NiO-H ₂ O	0.08 (± 0.02)	0.14	-0.86	21.75	1.74	-38.30	-38.39 (± 0.22)
		72	Ni-NiO-H ₂ O	0.07 (± 0.02)	0.12	-0.90	21.75	1.74	-38.20	-38.29 (± 0.25)
		120	Ni-H ₂ O	0.07 (± 0.02)	0.12	-0.90	21.75	1.74	-38.20	-38.29 (± 0.25)
		168	Ni-NiO-H ₂ O	0.07 (± 0.02)	0.12	-0.90	21.75	1.74	-38.20	-38.29 (± 0.25)

^a Measured through the Raman quantitative method described in Appendix A; uncertainty of $(P_{H_2})_{RT}$ is shown in parentheses and was calculated based on method describe in Appendix C.

^b f_{H_2} values at 1000 bar and T calculated through Eqs. (1) and (2) in the main text.

^c Data from Robie and Hemingway (1995).

^d Data from Burnham et al. (1969).

^e Calculated from Eq. (4).

^f The oxygen fugacity at 1 bar and experimental T ($(f_{O_2})_{1,T}$) was calculated based on Eq. (5) using molar volume data from Robie and Hemingway (1995); uncertainty of $(f_{O_2})_{1,T}$ is shown in parentheses and was calculated based on method described in Appendix C; equilibrated $(f_{O_2})_{1,T}$ values are shown in bold font.

Supplemental Table S5. Measured H_2 pressures at room temperature, $(P_{H_2})_{RT}$, in quenched vacuumed FSCCs that were equilibrated for various durations with Co-CoO buffer at 1000 bar and a fixed T (250, 300, 350, and 400 °C) and the calculated $\log (f_{O_2})_{1,T}$.

T °C	P bar	Time hours	Starting material	$(P_{H_2})_{RT}^a$ bar	$(f_{H_2})_{P,T}^b$	$\log (f_{H_2})_{P,T}$	$\log K_w^c$	$\log (f_{H_2O})_{P,T}^d$	$\log (f_{O_2})_{P,T}^e$	$\log (f_{O_2})_{1,T}^f$
400	1000	6	Co-CoO-H ₂ O	1.22 (± 0.04)	2.75	0.44	16.34	2.42	-28.72	-28.80 (± 0.03)
		12	Co-CoO-H ₂ O	1.13 (± 0.04)	2.56	0.41	16.34	2.42	-28.66	-28.73 (± 0.03)
		24	Co-H ₂ O	1.09 (± 0.04)	2.46	0.39	16.34	2.42	-28.62	-28.70 (± 0.03)
		36	Co-H ₂ O	1.11 (± 0.04)	2.50	0.40	16.34	2.42	-28.64	-28.71 (± 0.03)
		48	Co-CoO-H ₂ O	1.06 (± 0.04)	2.39	0.38	16.34	2.42	-28.60	-28.68 (± 0.03)
350	1000	6	Co-CoO-H ₂ O	0.72 (± 0.03)	1.50	0.18	17.84	2.24	-31.55	-31.63 (± 0.04)
		12	Co-CoO-H ₂ O	0.92 (± 0.03)	1.93	0.29	17.84	2.24	-31.77	-31.85 (± 0.03)
		24	Co-H ₂ O	0.93 (± 0.03)	1.95	0.29	17.84	2.24	-31.78	-31.86 (± 0.03)
		48	Co-CoO-H ₂ O	0.99 (± 0.04)	2.06	0.31	17.84	2.24	-31.83	-31.91 (± 0.03)
		72	Co-CoO-H ₂ O	0.99 (± 0.04)	2.06	0.31	17.84	2.24	-31.83	-31.91 (± 0.03)
300	1000	6	Co-CoO-H ₂ O	0.13 (± 0.02)	0.25	-0.60	19.63	2.02	-34.02	-34.11 (± 0.14)
		12	Co-CoO-H ₂ O	0.45 (± 0.02)	0.87	-0.06	19.63	2.02	-35.09	-35.19 (± 0.05)
		24	Co-CoO-H ₂ O	0.45 (± 0.02)	0.87	-0.06	19.63	2.02	-35.09	-35.19 (± 0.05)
		48	Co-H ₂ O	0.49 (± 0.02)	0.94	-0.03	19.63	2.02	-35.17	-35.26 (± 0.04)
		72	Co-CoO-H ₂ O	0.46 (± 0.02)	0.88	-0.05	19.63	2.02	-35.11	-35.20 (± 0.04)
250	1000	24	Co-CoO-H ₂ O	0.20 (± 0.02)	0.35	-0.45	21.75	1.74	-39.10	-39.20 (± 0.09)
		72	Co-CoO-H ₂ O	0.18 (± 0.02)	0.31	-0.51	21.75	1.74	-39.00	-39.10 (± 0.10)
		120	Co-H ₂ O	0.18 (± 0.02)	0.31	-0.51	21.75	1.74	-39.00	-39.10 (± 0.10)
		168	Co-CoO-H ₂ O	0.20 (± 0.02)	0.35	-0.46	21.75	1.74	-39.10	-39.20 (± 0.10)

^a Measured through the Raman quantitative method described in Appendix A; uncertainty of $(P_{H_2})_{RT}$ is shown in parentheses and was calculated based on the method describe in Appendix C.

^b Calculated through Eqs. (1) and (2) in the main text.

^c Data from Robie and Hemingway (1995).

^d Data from Burnham et al. (1969).

^e Calculated from Eq. (4).

^f The oxygen fugacity at 1 bar and experimental T ($(f_{O_2})_{1,T}$) was calculated based on Eq. (5) using molar volume data from Robie and Hemingway (1995); uncertainty of $(f_{O_2})_{1,T}$ was is shown in parentheses and was calculated based on method describe in Appendix C; equilibrated $(f_{O_2})_{1,T}$ values are shown in bold font.

Supplemental reference:

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