Supplementary Information

S1. Raw Experimental Data Extracted from Hutchinson [1].

Space Velocity / min^{-1}	T / K	p / MPa	y_1, ortho	y_1, para	y_2, ortho	y_2, para	Direction
45.4	76	0.21	0.75	0.25	0.492	0.508	O → P
47.8	76	0.21	0.75	0.25	0.493	0.507	O → P
55.3	76	0.21	0.75	0.25	0.497	0.503	O → P
62.6	76	0.21	0.75	0.25	0.497	0.503	O → P
75.0	76	0.21	0.75	0.25	0.498	0.502	O → P
100.7	76	0.21	0.75	0.25	0.503	0.497	O → P
116.0	76	0.21	0.75	0.25	0.508	0.492	O → P
130.3	76	0.21	0.75	0.25	0.511	0.489	O → P
139.6	76	0.21	0.75	0.25	0.514	0.486	O → P
218.0	76	0.21	0.75	0.25	0.54	0.46	O → P
180.8	76	0.21	0.75	0.25	0.531	0.469	O → P
287.0	76	0.21	0.75	0.25	0.564	0.436	O → P
244.0	76	0.21	0.75	0.25	0.551	0.449	O → P
275.0	76	0.21	0.75	0.25	0.56	0.44	O → P
340.0	76	0.21	0.75	0.25	0.578	0.422	O → P
375.0	76	0.21	0.75	0.25	0.588	0.412	O → P
428.0	76	0.21	0.75	0.25	0.601	0.399	O → P
510.0	76	0.21	0.75	0.25	0.617	0.383	O → P
490.0	76	0.21	0.75	0.25	0.612	0.388	O → P
595.0	76	0.21	0.75	0.25	0.63	0.37	O → P
42.3	76	0.21	0.01	0.99	0.493	0.507	P → O
59.1	76	0.21	0.01	0.99	0.493	0.507	P → O
75.9	76	0.21	0.01	0.99	0.492	0.508	P → O
93.0	76	0.21	0.01	0.99	0.488	0.512	P → O
121.0	76	0.21	0.01	0.99	0.479	0.521	P → O
104.3	76	0.21	0.01	0.99	0.483	0.517	P → O
138.6	76	0.21	0.01	0.99	0.47	0.53	P → O
153.2	76	0.21	0.01	0.99	0.461	0.539	P → O
198.7	76	0.21	0.01	0.99	0.436	0.564	P → O
176.7	76	0.21	0.01	0.99	0.447	0.553	P → O
239.0	76	0.21	0.01	0.99	0.41	0.59	P → O
313.0	76	0.21	0.01	0.99	0.369	0.631	P → O
265.0	76	0.21	0.01	0.99	0.395	0.605	P → O
401.0	76	0.21	0.01	0.99	0.326	0.674	P → O
381.0	76	0.21	0.01	0.99	0.333	0.667	P → O
336.0	76	0.21	0.01	0.99	0.356	0.644	P → O
503.0	76	0.21	0.01	0.99	0.284	0.716	P → O
430.0	76	0.21	0.01	0.99	0.315	0.685	P → O
552.0	76	0.21	0.01	0.99	0.268	0.732	P → O
608.0	76	0.21	0.01	0.99	0.251	0.749	P → O
44.4	76	0.21	0.75	0.25	0.494	0.506	O → P
58.3	76	0.21	0.75	0.25	0.497	0.503	O → P
62.9	76	0.21	0.75	0.25	0.497	0.503	O → P
82.7	76	0.21	0.75	0.25	0.500	0.500	O → P
93.5	76	0.21	0.75	0.25	0.501	0.499	O → P
106.8	76	0.21	0.75	0.25	0.506	0.494	O → P
130.8	76	0.21	0.75	0.25	0.510	0.490	O → P
177.0	76	0.21	0.75	0.25	0.527	0.473	O → P
144.7	76	0.21	0.75	0.25	0.518	0.482	O → P

Space Velocity / min^{-1}	T / K	p / MPa	y_1, ortho	y_1, para	y_2, ortho	y_2, para	Direction
211.0	76	0.21	0.75	0.25	0.542	0.458	O → P
284.0	76	0.21	0.75	0.25	0.568	0.432	O → P
237.0	76	0.21	0.75	0.25	0.551	0.449	O → P
321.0	76	0.21	0.75	0.25	0.579	0.421	O → P
283.0	76	0.21	0.75	0.25	0.568	0.432	O → P
438.0	76	0.21	0.75	0.25	0.610	0.390	O → P
387.0	76	0.21	0.75	0.25	0.600	0.400	O → P
474.0	76	0.21	0.75	0.25	0.616	0.384	O → P
597.0	76	0.21	0.75	0.25	0.638	0.362	O → P
42.1	76	0.21	0.01	0.99	0.494	0.506	P → O
56.9	76	0.21	0.01	0.99	0.494	0.506	P → O
91.5	76	0.21	0.01	0.99	0.490	0.510	P → O
79.9	76	0.21	0.01	0.99	0.492	0.508	P → O
70.8	76	0.21	0.01	0.99	0.493	0.507	P → O
113.1	76	0.21	0.01	0.99	0.485	0.515	P → O
142.4	76	0.21	0.01	0.99	0.472	0.528	P → O
164.9	76	0.21	0.01	0.99	0.462	0.538	P → O
219.0	76	0.21	0.01	0.99	0.434	0.566	P → O
178.4	76	0.21	0.01	0.99	0.454	0.546	P → O
291.0	76	0.21	0.01	0.99	0.396	0.604	P → O
251.0	76	0.21	0.01	0.99	0.417	0.583	P → O
365.0	76	0.21	0.01	0.99	0.359	0.641	P → O
425.0	76	0.21	0.01	0.99	0.330	0.670	P → O
456.0	76	0.21	0.01	0.99	0.319	0.681	P → O
528.0	76	0.21	0.01	0.99	0.291	0.709	P → O
621.0	76	0.21	0.01	0.99	0.263	0.737	P → O
564.0	76	0.21	0.01	0.99	0.280	0.720	P → O
20.0	76	0.42	0.75	0.25	0.490	0.510	O → P
30.0	76	0.42	0.75	0.25	0.491	0.509	O → P
33.3	76	0.42	0.75	0.25	0.491	0.509	O → P
39.7	76	0.42	0.75	0.25	0.492	0.508	O → P
51.0	76	0.42	0.75	0.25	0.495	0.505	O → P
62.6	76	0.42	0.75	0.25	0.500	0.500	O → P
82.7	76	0.42	0.75	0.25	0.510	0.490	O → P
127.1	76	0.42	0.75	0.25	0.537	0.463	O → P
105.7	76	0.42	0.75	0.25	0.523	0.477	O → P
164.3	76	0.42	0.75	0.25	0.558	0.442	O → P
148.3	76	0.42	0.75	0.25	0.550	0.450	O → P
173.4	76	0.42	0.75	0.25	0.561	0.439	O → P
210.0	76	0.42	0.75	0.25	0.580	0.420	O → P
190.5	76	0.42	0.75	0.25	0.572	0.428	O → P
251.0	76	0.42	0.75	0.25	0.597	0.403	O → P
225.0	76	0.42	0.75	0.25	0.587	0.413	O → P
264.0	76	0.42	0.75	0.25	0.601	0.399	O → P
284.0	76	0.42	0.75	0.25	0.608	0.392	O → P
21.1	76	0.42	0.01	0.99	0.492	0.508	P → O
45.3	76	0.42	0.01	0.99	0.489	0.511	P → O
39.2	76	0.42	0.01	0.99	0.491	0.509	P → O
31.5	76	0.42	0.01	0.99	0.491	0.509	P → O
26.7	76	0.42	0.01	0.99	0.492	0.508	P → O
53.4	76	0.42	0.01	0.99	0.486	0.514	P → O
68.8	76	0.42	0.01	0.99	0.475	0.525	P → O
84.2	76	0.42	0.01	0.99	0.463	0.537	P → O
116.7	76	0.42	0.01	0.99	0.434	0.566	P → O

Space Velocity / min^{-1}	T / K	p / MPa	y_1, ortho	y_1, para	y_2, ortho	y_2, para	Direction
99.7	76	0.42	0.01	0.99	0.452	0.548	P → O
123.3	76	0.42	0.01	0.99	0.430	0.570	P → O
137.0	76	0.42	0.01	0.99	0.417	0.583	P → O
149.0	76	0.42	0.01	0.99	0.407	0.593	P → O
215.0	76	0.42	0.01	0.99	0.350	0.650	P → O
179.9	76	0.42	0.01	0.99	0.380	0.620	P → O
232.0	76	0.42	0.01	0.99	0.338	0.662	P → O
306.0	76	0.42	0.01	0.99	0.294	0.706	P → O
270.0	76	0.42	0.01	0.99	0.312	0.688	P → O
8.8	76	0.84	0.75	0.25	0.493	0.507	O → P
11.7	76	0.84	0.75	0.25	0.493	0.507	O → P
16.6	76	0.84	0.75	0.25	0.494	0.506	O → P
20.8	76	0.84	0.75	0.25	0.496	0.504	O → P
29.2	76	0.84	0.75	0.25	0.499	0.501	O → P
33.9	76	0.84	0.75	0.25	0.501	0.499	O → P
43.3	76	0.84	0.75	0.25	0.509	0.491	O → P
49.1	76	0.84	0.75	0.25	0.513	0.487	O → P
67.1	76	0.84	0.75	0.25	0.532	0.468	O → P
58.5	76	0.84	0.75	0.25	0.523	0.477	O → P
89.8	76	0.84	0.75	0.25	0.553	0.447	O → P
82.7	76	0.84	0.75	0.25	0.548	0.452	O → P
69.5	76	0.84	0.75	0.25	0.533	0.467	O → P
118.3	76	0.84	0.75	0.25	0.578	0.422	O → P
103.0	76	0.84	0.75	0.25	0.566	0.434	O → P
135.7	76	0.84	0.75	0.25	0.590	0.410	O → P
146.2	76	0.84	0.75	0.25	0.597	0.403	O → P
158.0	76	0.84	0.75	0.25	0.604	0.396	O → P
9.1	76	0.84	0.01	0.99	0.494	0.506	P → O
12.2	76	0.84	0.01	0.99	0.494	0.506	P → O
18.2	76	0.84	0.01	0.99	0.493	0.507	P → O
23.5	76	0.84	0.01	0.99	0.491	0.509	P → O
27.5	76	0.84	0.01	0.99	0.490	0.510	P → O
30.5	76	0.84	0.01	0.99	0.488	0.512	P → O
51.6	76	0.84	0.01	0.99	0.461	0.539	P → O
34.1	76	0.84	0.01	0.99	0.484	0.516	P → O
44.1	76	0.84	0.01	0.99	0.472	0.528	P → O
55.0	76	0.84	0.01	0.99	0.456	0.544	P → O
67.1	76	0.84	0.01	0.99	0.438	0.562	P → O
81.4	76	0.84	0.01	0.99	0.414	0.586	P → O
104.7	76	0.84	0.01	0.99	0.381	0.619	P → O
97.3	76	0.84	0.01	0.99	0.390	0.610	P → O
117.1	76	0.84	0.01	0.99	0.364	0.636	P → O
128.6	76	0.84	0.01	0.99	0.349	0.651	P → O
143.3	76	0.84	0.01	0.99	0.331	0.669	P → O
157.3	76	0.84	0.01	0.99	0.317	0.683	P → O
4.6	76	1.66	0.75	0.25	0.494	0.506	O → P
6.6	76	1.66	0.75	0.25	0.495	0.505	O → P
8.1	76	1.66	0.75	0.25	0.495	0.505	O → P
10.4	76	1.66	0.75	0.25	0.496	0.504	O → P
13.7	76	1.66	0.75	0.25	0.498	0.502	O → P
16.3	76	1.66	0.75	0.25	0.501	0.499	O → P
21.8	76	1.66	0.75	0.25	0.509	0.491	O → P
24.6	76	1.66	0.75	0.25	0.513	0.487	O → P
35.0	76	1.66	0.75	0.25	0.533	0.467	O → P

Space Velocity / min^{-1}	T / K	p / MPa	y_1, ortho	y_1, para	y_2, ortho	y_2, para	Direction
29.9	76	1.66	0.75	0.25	0.524	0.476	O → P
45.6	76	1.66	0.75	0.25	0.554	0.446	O → P
39.2	76	1.66	0.75	0.25	0.542	0.458	O → P
56.7	76	1.66	0.75	0.25	0.573	0.427	O → P
50.4	76	1.66	0.75	0.25	0.563	0.437	O → P
64.3	76	1.66	0.75	0.25	0.586	0.414	O → P
71.8	76	1.66	0.75	0.25	0.596	0.404	O → P
86.9	76	1.66	0.75	0.25	0.614	0.386	O → P
80.8	76	1.66	0.75	0.25	0.608	0.392	O → P
4.7	76	1.66	0.01	0.99	0.493	0.507	P → O
12.3	76	1.66	0.01	0.99	0.493	0.507	P → O
15.4	76	1.66	0.01	0.99	0.490	0.510	P → O
13.7	76	1.66	0.01	0.99	0.492	0.508	P → O
17.8	76	1.66	0.01	0.99	0.487	0.513	P → O
19.8	76	1.66	0.01	0.99	0.482	0.518	P → O
21.9	76	1.66	0.01	0.99	0.478	0.522	P → O
25.6	76	1.66	0.01	0.99	0.469	0.531	P → O
33.8	76	1.66	0.01	0.99	0.443	0.557	P → O
30.5	76	1.66	0.01	0.99	0.452	0.548	P → O
43.9	76	1.66	0.01	0.99	0.412	0.588	P → O
48.0	76	1.66	0.01	0.99	0.401	0.599	P → O
60.6	76	1.66	0.01	0.99	0.367	0.633	P → O
55.2	76	1.66	0.01	0.99	0.380	0.620	P → O
66.1	76	1.66	0.01	0.99	0.352	0.648	P → O
81.6	76	1.66	0.01	0.99	0.319	0.681	P → O
74.9	76	1.66	0.01	0.99	0.332	0.668	P → O
91.3	76	1.66	0.01	0.99	0.299	0.701	P → O
2.2	76	3.45	0.75	0.25	0.491	0.509	O → P
3.4	76	3.45	0.75	0.25	0.492	0.508	O → P
2.8	76	3.45	0.75	0.25	0.492	0.508	O → P
4.4	76	3.45	0.75	0.25	0.493	0.507	O → P
5.5	76	3.45	0.75	0.25	0.496	0.504	O → P
6.7	76	3.45	0.75	0.25	0.500	0.500	O → P
7.5	76	3.45	0.75	0.25	0.502	0.498	O → P
9.7	76	3.45	0.75	0.25	0.511	0.489	O → P
11.5	76	3.45	0.75	0.25	0.520	0.480	O → P
14.5	76	3.45	0.75	0.25	0.536	0.464	O → P
17.0	76	3.45	0.75	0.25	0.549	0.451	O → P
19.9	76	3.45	0.75	0.25	0.562	0.438	O → P
22.5	76	3.45	0.75	0.25	0.573	0.427	O → P
26.7	76	3.45	0.75	0.25	0.588	0.412	O → P
24.3	76	3.45	0.75	0.25	0.580	0.420	O → P
29.5	76	3.45	0.75	0.25	0.597	0.403	O → P
32.3	76	3.45	0.75	0.25	0.604	0.396	O → P
34.7	76	3.45	0.75	0.25	0.611	0.389	O → P
2.2	76	3.45	0.01	0.99	0.493	0.507	P → O
3.1	76	3.45	0.01	0.99	0.493	0.507	P → O
3.9	76	3.45	0.01	0.99	0.493	0.507	P → O
5.1	76	3.45	0.01	0.99	0.491	0.509	P → O
6.6	76	3.45	0.01	0.99	0.488	0.512	P → O
8.2	76	3.45	0.01	0.99	0.480	0.520	P → O
9.2	76	3.45	0.01	0.99	0.471	0.529	P → O
11.3	76	3.45	0.01	0.99	0.456	0.544	P → O
9.9	76	3.45	0.01	0.99	0.467	0.533	P → O

Space Velocity / min^{-1}	T / K	p / MPa	y_1, ortho	y_1, para	y_2, ortho	y_2, para	Direction
12.8	76	3.45	0.01	0.99	0.444	0.556	P → O
15.3	76	3.45	0.01	0.99	0.425	0.575	P → O
17.7	76	3.45	0.01	0.99	0.407	0.593	P → O
20.3	76	3.45	0.01	0.99	0.386	0.614	P → O
22.9	76	3.45	0.01	0.99	0.369	0.631	P → O
25.1	76	3.45	0.01	0.99	0.353	0.647	P → O
28.2	76	3.45	0.01	0.99	0.335	0.665	P → O
31.5	76	3.45	0.01	0.99	0.316	0.684	P → O
33.5	76	3.45	0.01	0.99	0.307	0.693	P → O
0.9	76	6.96	0.75	0.25	0.492	0.508	O → P
1.5	76	6.96	0.75	0.25	0.492	0.508	O → P
1.8	76	6.96	0.75	0.25	0.492	0.508	O → P
2.5	76	6.96	0.75	0.25	0.496	0.504	O → P
3.1	76	6.96	0.75	0.25	0.499	0.501	O → P
3.7	76	6.96	0.75	0.25	0.502	0.498	O → P
4.3	76	6.96	0.75	0.25	0.508	0.492	O → P
4.8	76	6.96	0.75	0.25	0.513	0.487	O → P
5.8	76	6.96	0.75	0.25	0.523	0.477	O → P
7.0	76	6.96	0.75	0.25	0.537	0.463	O → P
8.4	76	6.96	0.75	0.25	0.550	0.450	O → P
8.9	76	6.96	0.75	0.25	0.558	0.442	O → P
10.6	76	6.96	0.75	0.25	0.570	0.430	O → P
11.3	76	6.96	0.75	0.25	0.577	0.423	O → P
12.6	76	6.96	0.75	0.25	0.587	0.413	O → P
14.0	76	6.96	0.75	0.25	0.597	0.403	O → P
15.4	76	6.96	0.75	0.25	0.604	0.396	O → P
17.1	76	6.96	0.75	0.25	0.614	0.386	O → P
1.0	76	6.96	0.01	0.99	0.499	0.501	P → O
1.7	76	6.96	0.01	0.99	0.499	0.501	P → O
2.4	76	6.96	0.01	0.99	0.498	0.502	P → O
3.1	76	6.96	0.01	0.99	0.492	0.508	P → O
3.8	76	6.96	0.01	0.99	0.487	0.513	P → O
4.3	76	6.96	0.01	0.99	0.481	0.519	P → O
4.7	76	6.96	0.01	0.99	0.474	0.526	P → O
5.4	76	6.96	0.01	0.99	0.463	0.537	P → O
6.2	76	6.96	0.01	0.99	0.450	0.550	P → O
6.7	76	6.96	0.01	0.99	0.440	0.560	P → O
7.5	76	6.96	0.01	0.99	0.428	0.572	P → O
9.1	76	6.96	0.01	0.99	0.401	0.599	P → O
10.0	76	6.96	0.01	0.99	0.390	0.610	P → O
11.0	76	6.96	0.01	0.99	0.375	0.625	P → O
12.9	76	6.96	0.01	0.99	0.350	0.650	P → O
13.5	76	6.96	0.01	0.99	0.342	0.658	P → O
15.9	76	6.96	0.01	0.99	0.316	0.684	P → O
14.4	76	6.96	0.01	0.99	0.333	0.667	P → O

Note: y_1,ortho and y_1,para represent ortho-hydrogen and para-hydrogen mole fractions in hydrogen inlet stream; y_2,ortho and y_2,para represent ortho-hydrogen and para-hydrogen mole fractions in hydrogen outlet stream.

S2. Raw Experimental Data Extracted from Hutchinson et al. [2]

Space Velocity / min^{-1}	T / K	p / MPa	y_1, ortho	y_1, para	y_2, ortho	y_2, para	Direction
30.0	83	0.29	0.002	0.998	0.530	0.470	P → O
37.7	83	0.29	0.002	0.998	0.529	0.471	P → O
57.7	83	0.29	0.002	0.998	0.528	0.472	P → O
86.2	83	0.29	0.002	0.998	0.510	0.490	P → O
96.2	83	0.29	0.002	0.998	0.503	0.497	P → O
117.0	83	0.29	0.002	0.998	0.483	0.517	P → O
176.3	83	0.29	0.002	0.998	0.434	0.566	P → O
190.2	83	0.29	0.002	0.998	0.411	0.589	P → O
209.4	83	0.29	0.002	0.998	0.399	0.601	P → O
260.3	83	0.29	0.002	0.998	0.360	0.640	P → O
296.5	83	0.29	0.002	0.998	0.338	0.662	P → O
299.5	83	0.29	0.002	0.998	0.343	0.657	P → O
353.4	83	0.29	0.002	0.998	0.309	0.691	P → O
373.4	83	0.29	0.002	0.998	0.301	0.699	P → O
388.8	83	0.29	0.002	0.998	0.295	0.705	P → O
440.4	83	0.29	0.002	0.998	0.273	0.727	P → O
26.3	73	0.29	0.002	0.998	0.462	0.538	P → O
53.2	73	0.29	0.002	0.998	0.466	0.534	P → O
90.9	73	0.29	0.002	0.998	0.451	0.549	P → O
133.3	73	0.29	0.002	0.998	0.423	0.577	P → O
191.0	73	0.29	0.002	0.998	0.388	0.612	P → O
228.7	73	0.29	0.002	0.998	0.364	0.636	P → O
293.4	73	0.29	0.002	0.998	0.325	0.675	P → O
346.5	73	0.29	0.002	0.998	0.299	0.701	P → O
390.4	73	0.29	0.002	0.998	0.283	0.717	P → O
439.6	73	0.29	0.002	0.998	0.260	0.740	P → O
445.0	73	0.29	0.002	0.998	0.257	0.743	P → O
535.1	73	0.29	0.002	0.998	0.225	0.775	P → O
542.8	73	0.29	0.002	0.998	0.223	0.777	P → O
616.6	73	0.29	0.002	0.998	0.204	0.796	P → O
787.4	73	0.29	0.002	0.998	0.184	0.816	P → O
807.4	73	0.29	0.002	0.998	0.177	0.823	P → O
21.8	64	0.29	0.002	0.998	0.379	0.621	P → O
40.2	64	0.29	0.002	0.998	0.374	0.626	P → O
64.9	64	0.29	0.002	0.998	0.368	0.632	P → O
128.0	64	0.29	0.002	0.998	0.336	0.664	P → O
158.8	64	0.29	0.002	0.998	0.316	0.684	P → O
180.4	64	0.29	0.002	0.998	0.293	0.707	P → O
227.3	64	0.29	0.002	0.998	0.273	0.727	P → O
271.2	64	0.29	0.002	0.998	0.245	0.755	P → O
320.4	64	0.29	0.002	0.998	0.233	0.767	P → O
328.9	64	0.29	0.002	0.998	0.230	0.770	P → O
363.5	64	0.29	0.002	0.998	0.219	0.781	P → O
418.2	64	0.29	0.002	0.998	0.203	0.797	P → O
444.3	64	0.29	0.002	0.998	0.191	0.809	P → O
479.7	64	0.29	0.002	0.998	0.187	0.813	P → O
545.2	64	0.29	0.002	0.998	0.165	0.835	P → O
643.6	64	0.29	0.002	0.998	0.152	0.848	P → O
18.9	51	0.29	0.002	0.998	0.241	0.759	P → O
73.5	51	0.29	0.002	0.998	0.230	0.770	P → O
90.4	51	0.29	0.002	0.998	0.234	0.766	P → O

Space Velocity / min^{-1}	T / K	p / MPa	y_1, ortho	y_1, para	y_2, ortho	y_2, para	Direction
123.6	51	0.29	0.002	0.998	0.203	0.797	P → O
167.4	51	0.29	0.002	0.998	0.198	0.802	P → O
191.3	51	0.29	0.002	0.998	0.180	0.820	P → O
249.0	51	0.29	0.002	0.998	0.165	0.835	P → O
288.2	51	0.29	0.002	0.998	0.155	0.845	P → O
302.1	51	0.29	0.002	0.998	0.151	0.849	P → O
366.7	51	0.29	0.002	0.998	0.136	0.864	P → O
371.4	51	0.29	0.002	0.998	0.132	0.868	P → O
377.5	51	0.29	0.002	0.998	0.133	0.867	P → O
445.2	51	0.29	0.002	0.998	0.120	0.880	P → O
451.4	51	0.29	0.002	0.998	0.117	0.883	P → O
526.0	51	0.29	0.002	0.998	0.108	0.892	P → O
14.4	41	0.29	0.002	0.998	0.127	0.873	P → O
22.1	41	0.29	0.002	0.998	0.128	0.872	P → O
46.0	41	0.29	0.002	0.998	0.120	0.880	P → O
80.6	41	0.29	0.002	0.998	0.118	0.882	P → O
94.5	41	0.29	0.002	0.998	0.109	0.891	P → O
132.9	41	0.29	0.002	0.998	0.107	0.893	P → O
152.2	41	0.29	0.002	0.998	0.100	0.900	P → O
178.3	41	0.29	0.002	0.998	0.092	0.908	P → O
205.3	41	0.29	0.002	0.998	0.093	0.907	P → O
246.0	41	0.29	0.002	0.998	0.085	0.915	P → O
271.4	41	0.29	0.002	0.998	0.079	0.921	P → O
289.1	41	0.29	0.002	0.998	0.077	0.923	P → O
349.9	41	0.29	0.002	0.998	0.067	0.933	P → O
352.2	41	0.29	0.002	0.998	0.074	0.926	P → O
393.0	41	0.29	0.002	0.998	0.065	0.935	P → O
448.4	41	0.29	0.002	0.998	0.062	0.938	P → O
6.4	80	1.46	0.002	0.998	0.508	0.492	P → O
18.1	80	1.46	0.002	0.998	0.499	0.501	P → O
26.3	80	1.46	0.002	0.998	0.486	0.514	P → O
42.9	80	1.46	0.002	0.998	0.436	0.564	P → O
54.8	80	1.46	0.002	0.998	0.402	0.598	P → O
62.2	80	1.46	0.002	0.998	0.381	0.619	P → O
68.2	80	1.46	0.002	0.998	0.366	0.634	P → O
86.1	80	1.46	0.002	0.998	0.326	0.674	P → O
87.7	80	1.46	0.002	0.998	0.323	0.677	P → O
97.5	80	1.46	0.002	0.998	0.304	0.696	P → O
101.9	80	1.46	0.002	0.998	0.294	0.706	P → O
113.9	80	1.46	0.002	0.998	0.278	0.722	P → O
127.4	80	1.46	0.002	0.998	0.255	0.745	P → O
9.2	76	1.46	0.002	0.998	0.476	0.524	P → O
17.1	76	1.46	0.002	0.998	0.458	0.542	P → O
18.7	76	1.46	0.002	0.998	0.454	0.546	P → O
24.1	76	1.46	0.002	0.998	0.439	0.561	P → O
27.7	76	1.46	0.002	0.998	0.425	0.575	P → O
37.3	76	1.46	0.002	0.998	0.388	0.612	P → O
46.7	76	1.46	0.002	0.998	0.361	0.639	P → O
58.6	76	1.46	0.002	0.998	0.330	0.670	P → O
69.4	76	1.46	0.002	0.998	0.308	0.692	P → O
74.4	76	1.46	0.002	0.998	0.293	0.707	P → O
89.1	76	1.46	0.002	0.998	0.263	0.737	P → O
102.5	76	1.46	0.002	0.998	0.246	0.754	P → O
109.9	76	1.46	0.002	0.998	0.235	0.765	P → O

Space Velocity / min^{-1}	T / K	p / MPa	y_1, ortho	y_1, para	y_2, ortho	y_2, para	Direction
135.0	76	1.46	0.002	0.998	0.210	0.790	P → O
139.6	76	1.46	0.002	0.998	0.198	0.802	P → O
2.6	63	1.46	0.002	0.998	0.369	0.631	P → O
10.2	63	1.46	0.002	0.998	0.368	0.632	P → O
14.8	63	1.46	0.002	0.998	0.359	0.641	P → O
20.9	63	1.46	0.002	0.998	0.348	0.652	P → O
32.1	63	1.46	0.002	0.998	0.310	0.690	P → O
40.1	63	1.46	0.002	0.998	0.297	0.703	P → O
42.5	63	1.46	0.002	0.998	0.292	0.708	P → O
49.3	63	1.46	0.002	0.998	0.264	0.736	P → O
60.4	63	1.46	0.002	0.998	0.244	0.756	P → O
68.2	63	1.46	0.002	0.998	0.235	0.765	P → O
72.2	63	1.46	0.002	0.998	0.225	0.775	P → O
81.2	63	1.46	0.002	0.998	0.216	0.784	P → O
81.4	63	1.46	0.002	0.998	0.219	0.781	P → O
90.1	63	1.46	0.002	0.998	0.203	0.797	P → O
95.3	63	1.46	0.002	0.998	0.202	0.798	P → O
122.2	63	1.46	0.002	0.998	0.175	0.825	P → O
1.4	52	1.46	0.002	0.998	0.248	0.752	P → O
3.2	52	1.46	0.002	0.998	0.251	0.749	P → O
5.2	52	1.46	0.002	0.998	0.244	0.756	P → O
17.7	52	1.46	0.002	0.998	0.221	0.779	P → O
22.5	52	1.46	0.002	0.998	0.213	0.787	P → O
27.9	52	1.46	0.002	0.998	0.204	0.796	P → O
29.3	52	1.46	0.002	0.998	0.204	0.796	P → O
38.9	52	1.46	0.002	0.998	0.177	0.823	P → O
47.3	52	1.46	0.002	0.998	0.163	0.837	P → O
52.0	52	1.46	0.002	0.998	0.160	0.840	P → O
60.4	52	1.46	0.002	0.998	0.142	0.858	P → O
70.2	52	1.46	0.002	0.998	0.144	0.856	P → O
78.2	52	1.46	0.002	0.998	0.127	0.873	P → O
85.7	52	1.46	0.002	0.998	0.114	0.886	P → O
90.3	52	1.46	0.002	0.998	0.110	0.890	P → O
1.2	42	1.46	0.002	0.998	0.134	0.866	P → O
1.8	42	1.46	0.002	0.998	0.130	0.870	P → O
5.2	42	1.46	0.002	0.998	0.130	0.870	P → O
6.2	42	1.46	0.002	0.998	0.127	0.873	P → O
9.0	42	1.46	0.002	0.998	0.128	0.872	P → O
9.6	42	1.46	0.002	0.998	0.121	0.879	P → O
16.4	42	1.46	0.002	0.998	0.114	0.886	P → O
17.9	42	1.46	0.002	0.998	0.112	0.888	P → O
21.9	42	1.46	0.002	0.998	0.107	0.893	P → O
25.5	42	1.46	0.002	0.998	0.102	0.898	P → O
27.7	42	1.46	0.002	0.998	0.098	0.902	P → O
32.9	42	1.46	0.002	0.998	0.092	0.908	P → O
35.1	42	1.46	0.002	0.998	0.092	0.908	P → O
44.3	42	1.46	0.002	0.998	0.079	0.921	P → O
52.4	42	1.46	0.002	0.998	0.072	0.928	P → O
61.6	42	1.46	0.002	0.998	0.069	0.931	P → O
70.6	42	1.46	0.002	0.998	0.057	0.943	P → O
3.2	81	2.90	0.002	0.998	0.511	0.489	P → O
5.0	81	2.90	0.002	0.998	0.518	0.482	P → O
9.0	81	2.90	0.002	0.998	0.508	0.492	P → O
11.2	81	2.90	0.002	0.998	0.498	0.502	P → O

Space Velocity / min^{-1}	T / K	p / MPa	y_1, ortho	y_1, para	y_2, ortho	y_2, para	Direction
17.3	81	2.90	0.002	0.998	0.488	0.512	P → O
18.9	81	2.90	0.002	0.998	0.478	0.522	P → O
21.7	81	2.90	0.002	0.998	0.468	0.532	P → O
25.3	81	2.90	0.002	0.998	0.458	0.542	P → O
28.1	81	2.90	0.002	0.998	0.448	0.552	P → O
34.9	81	2.90	0.002	0.998	0.438	0.562	P → O
35.4	81	2.90	0.002	0.998	0.428	0.572	P → O
38.2	81	2.90	0.002	0.998	0.418	0.582	P → O
43.6	81	2.90	0.002	0.998	0.408	0.592	P → O
50.0	81	2.90	0.002	0.998	0.398	0.602	P → O
52.1	81	2.90	0.002	0.998	0.388	0.612	P → O
60.0	81	2.90	0.002	0.998	0.378	0.622	P → O
2.6	75	2.90	0.002	0.998	0.479	0.521	P → O
5.3	75	2.90	0.002	0.998	0.474	0.526	P → O
8.7	75	2.90	0.002	0.998	0.453	0.547	P → O
11.7	75	2.90	0.002	0.998	0.440	0.560	P → O
18.8	75	2.90	0.002	0.998	0.390	0.610	P → O
21.6	75	2.90	0.002	0.998	0.373	0.627	P → O
27.9	75	2.90	0.002	0.998	0.347	0.653	P → O
29.2	75	2.90	0.002	0.998	0.338	0.662	P → O
33.1	75	2.90	0.002	0.998	0.323	0.677	P → O
40.7	75	2.90	0.002	0.998	0.287	0.713	P → O
44.1	75	2.90	0.002	0.998	0.275	0.725	P → O
49.1	75	2.90	0.002	0.998	0.260	0.740	P → O
54.3	75	2.90	0.002	0.998	0.243	0.757	P → O
59.1	75	2.90	0.002	0.998	0.230	0.770	P → O
66.9	75	2.90	0.002	0.998	0.214	0.786	P → O
71.9	75	2.90	0.002	0.998	0.204	0.796	P → O
2.1	64	2.90	0.002	0.998	0.381	0.619	P → O
4.1	64	2.90	0.002	0.998	0.372	0.628	P → O
6.7	64	2.90	0.002	0.998	0.358	0.642	P → O
8.2	64	2.90	0.002	0.998	0.350	0.650	P → O
10.4	64	2.90	0.002	0.998	0.338	0.662	P → O
14.1	64	2.90	0.002	0.998	0.313	0.687	P → O
17.9	64	2.90	0.002	0.998	0.293	0.707	P → O
19.8	64	2.90	0.002	0.998	0.284	0.716	P → O
24.0	64	2.90	0.002	0.998	0.264	0.736	P → O
30.3	64	2.90	0.002	0.998	0.240	0.760	P → O
34.2	64	2.90	0.002	0.998	0.227	0.773	P → O
38.9	64	2.90	0.002	0.998	0.212	0.788	P → O
45.7	64	2.90	0.002	0.998	0.190	0.810	P → O
53.1	64	2.90	0.002	0.998	0.174	0.826	P → O
54.3	64	2.90	0.002	0.998	0.168	0.832	P → O
61.3	64	2.90	0.002	0.998	0.155	0.845	P → O
1.5	53	2.90	0.002	0.998	0.262	0.738	P → O
2.4	53	2.90	0.002	0.998	0.259	0.741	P → O
4.4	53	2.90	0.002	0.998	0.247	0.753	P → O
6.7	53	2.90	0.002	0.998	0.227	0.773	P → O
8.5	53	2.90	0.002	0.998	0.223	0.777	P → O
12.0	53	2.90	0.002	0.998	0.198	0.802	P → O
15.1	53	2.90	0.002	0.998	0.182	0.818	P → O
18.1	53	2.90	0.002	0.998	0.171	0.829	P → O
21.4	53	2.90	0.002	0.998	0.157	0.843	P → O
24.2	53	2.90	0.002	0.998	0.146	0.854	P → O

Space Velocity / min^{-1}	T / K	p / MPa	y_1, ortho	y_1, para	y_2, ortho	y_2, para	Direction
26.0	53	2.90	0.002	0.998	0.142	0.858	P → O
32.0	53	2.90	0.002	0.998	0.123	0.877	P → O
33.5	53	2.90	0.002	0.998	0.122	0.878	P → O
33.9	53	2.90	0.002	0.998	0.122	0.878	P → O
37.7	53	2.90	0.002	0.998	0.119	0.881	P → O
41.3	53	2.90	0.002	0.998	0.111	0.889	P → O
0.8	43	2.90	0.002	0.998	0.130	0.870	P → O
1.6	43	2.90	0.002	0.998	0.124	0.876	P → O
2.3	43	2.90	0.002	0.998	0.123	0.877	P → O
3.7	43	2.90	0.002	0.998	0.121	0.879	P → O
5.2	43	2.90	0.002	0.998	0.114	0.886	P → O
6.1	43	2.90	0.002	0.998	0.110	0.890	P → O
7.1	43	2.90	0.002	0.998	0.105	0.895	P → O
8.8	43	2.90	0.002	0.998	0.098	0.902	P → O
10.0	43	2.90	0.002	0.998	0.093	0.907	P → O
11.9	43	2.90	0.002	0.998	0.089	0.911	P → O
14.3	43	2.90	0.002	0.998	0.078	0.922	P → O
16.0	43	2.90	0.002	0.998	0.074	0.926	P → O
19.1	43	2.90	0.002	0.998	0.068	0.932	P → O
21.5	43	2.90	0.002	0.998	0.062	0.938	P → O
24.4	43	2.90	0.002	0.998	0.058	0.942	P → O
27.9	43	2.90	0.002	0.998	0.056	0.944	P → O
2.0	81	4.22	0.002	0.998	0.519	0.481	P → O
3.2	81	4.22	0.002	0.998	0.514	0.486	P → O
5.1	81	4.22	0.002	0.998	0.504	0.496	P → O
7.2	81	4.22	0.002	0.998	0.494	0.506	P → O
8.3	81	4.22	0.002	0.998	0.484	0.516	P → O
13.2	81	4.22	0.002	0.998	0.474	0.526	P → O
17.1	81	4.22	0.002	0.998	0.464	0.536	P → O
22.1	81	4.22	0.002	0.998	0.454	0.546	P → O
25.2	81	4.22	0.002	0.998	0.444	0.556	P → O
28.5	81	4.22	0.002	0.998	0.434	0.566	P → O
33.0	81	4.22	0.002	0.998	0.424	0.576	P → O
35.6	81	4.22	0.002	0.998	0.414	0.586	P → O
39.7	81	4.22	0.002	0.998	0.404	0.596	P → O
43.6	81	4.22	0.002	0.998	0.394	0.606	P → O
47.9	81	4.22	0.002	0.998	0.384	0.616	P → O
52.6	81	4.22	0.002	0.998	0.374	0.626	P → O
1.6	75	4.22	0.002	0.998	0.476	0.524	P → O
2.7	75	4.22	0.002	0.998	0.468	0.532	P → O
4.6	75	4.22	0.002	0.998	0.464	0.536	P → O
5.9	75	4.22	0.002	0.998	0.452	0.548	P → O
8.7	75	4.22	0.002	0.998	0.429	0.571	P → O
10.1	75	4.22	0.002	0.998	0.415	0.585	P → O
12.8	75	4.22	0.002	0.998	0.391	0.609	P → O
18.3	75	4.22	0.002	0.998	0.347	0.653	P → O
21.6	75	4.22	0.002	0.998	0.326	0.674	P → O
27.8	75	4.22	0.002	0.998	0.296	0.704	P → O
32.2	75	4.22	0.002	0.998	0.269	0.731	P → O
33.9	75	4.22	0.002	0.998	0.259	0.741	P → O
39.1	75	4.22	0.002	0.998	0.238	0.762	P → O
44.8	75	4.22	0.002	0.998	0.219	0.781	P → O
45.7	75	4.22	0.002	0.998	0.218	0.782	P → O
53.7	75	4.22	0.002	0.998	0.197	0.803	P → O

Space Velocity / min^{-1}	T / K	p / MPa	y_1, ortho	y_1, para	y_2, ortho	y_2, para	Direction
1.1	63	4.22	0.002	0.998	0.377	0.623	P → O
2.2	63	4.22	0.002	0.998	0.375	0.625	P → O
2.6	63	4.22	0.002	0.998	0.371	0.629	P → O
4.3	63	4.22	0.002	0.998	0.350	0.650	P → O
5.5	63	4.22	0.002	0.998	0.343	0.657	P → O
7.1	63	4.22	0.002	0.998	0.330	0.670	P → O
11.0	63	4.22	0.002	0.998	0.293	0.707	P → O
13.5	63	4.22	0.002	0.998	0.272	0.728	P → O
16.8	63	4.22	0.002	0.998	0.250	0.750	P → O
21.2	63	4.22	0.002	0.998	0.223	0.777	P → O
19.4	63	4.22	0.002	0.998	0.232	0.768	P → O
23.9	63	4.22	0.002	0.998	0.210	0.790	P → O
27.8	63	4.22	0.002	0.998	0.195	0.805	P → O
30.8	63	4.22	0.002	0.998	0.183	0.817	P → O
36.3	63	4.22	0.002	0.998	0.170	0.830	P → O
37.7	63	4.22	0.002	0.998	0.169	0.831	P → O
0.7	52	4.22	0.002	0.998	0.247	0.753	P → O
1.3	52	4.22	0.002	0.998	0.247	0.753	P → O
2.2	52	4.22	0.002	0.998	0.241	0.759	P → O
3.0	52	4.22	0.002	0.998	0.236	0.764	P → O
4.0	52	4.22	0.002	0.998	0.230	0.770	P → O
4.7	52	4.22	0.002	0.998	0.225	0.775	P → O
6.5	52	4.22	0.002	0.998	0.211	0.789	P → O
8.3	52	4.22	0.002	0.998	0.189	0.811	P → O
8.9	52	4.22	0.002	0.998	0.196	0.804	P → O
10.6	52	4.22	0.002	0.998	0.185	0.815	P → O
11.7	52	4.22	0.002	0.998	0.176	0.824	P → O
13.8	52	4.22	0.002	0.998	0.168	0.832	P → O
14.0	52	4.22	0.002	0.998	0.156	0.844	P → O
17.2	52	4.22	0.002	0.998	0.141	0.859	P → O
20.6	52	4.22	0.002	0.998	0.129	0.871	P → O
21.9	52	4.22	0.002	0.998	0.123	0.877	P → O
24.8	52	4.22	0.002	0.998	0.116	0.884	P → O
28.8	52	4.22	0.002	0.998	0.096	0.904	P → O
0.4	42	4.22	0.002	0.998	0.132	0.868	P → O
0.7	42	4.22	0.002	0.998	0.133	0.867	P → O
1.1	42	4.22	0.002	0.998	0.131	0.869	P → O
1.7	42	4.22	0.002	0.998	0.126	0.874	P → O
3.2	42	4.22	0.002	0.998	0.115	0.885	P → O
4.2	42	4.22	0.002	0.998	0.109	0.891	P → O
5.7	42	4.22	0.002	0.998	0.102	0.898	P → O
6.6	42	4.22	0.002	0.998	0.097	0.903	P → O
8.1	42	4.22	0.002	0.998	0.091	0.909	P → O
8.4	42	4.22	0.002	0.998	0.090	0.910	P → O
9.8	42	4.22	0.002	0.998	0.088	0.912	P → O
10.2	42	4.22	0.002	0.998	0.084	0.916	P → O
11.7	42	4.22	0.002	0.998	0.083	0.917	P → O
1.4	80	5.60	0.002	0.998	0.508	0.492	P → O
1.9	80	5.60	0.002	0.998	0.505	0.495	P → O
2.4	80	5.60	0.002	0.998	0.498	0.502	P → O
3.6	80	5.60	0.002	0.998	0.483	0.517	P → O
5.3	80	5.60	0.002	0.998	0.472	0.528	P → O
7.6	80	5.60	0.002	0.998	0.441	0.559	P → O
9.9	80	5.60	0.002	0.998	0.429	0.571	P → O

Space Velocity / min^{-1}	T / K	p / MPa	y_1, ortho	y_1, para	y_2, ortho	y_2, para	Direction
12.6	80	5.60	0.002	0.998	0.400	0.600	P → O
14.6	80	5.60	0.002	0.998	0.383	0.617	P → O
17.0	80	5.60	0.002	0.998	0.369	0.631	P → O
18.7	80	5.60	0.002	0.998	0.349	0.651	P → O
21.3	80	5.60	0.002	0.998	0.332	0.668	P → O
24.5	80	5.60	0.002	0.998	0.310	0.690	P → O
26.5	80	5.60	0.002	0.998	0.302	0.698	P → O
30.9	80	5.60	0.002	0.998	0.280	0.720	P → O
35.3	80	5.60	0.002	0.998	0.261	0.739	P → O
1.2	73	5.60	0.002	0.998	0.463	0.537	P → O
1.5	73	5.60	0.002	0.998	0.462	0.538	P → O
3.1	73	5.60	0.002	0.998	0.446	0.554	P → O
4.2	73	5.60	0.002	0.998	0.429	0.571	P → O
5.5	73	5.60	0.002	0.998	0.414	0.586	P → O
7.8	73	5.60	0.002	0.998	0.389	0.611	P → O
9.9	73	5.60	0.002	0.998	0.365	0.635	P → O
11.2	73	5.60	0.002	0.998	0.353	0.647	P → O
16.7	73	5.60	0.002	0.998	0.304	0.696	P → O
18.3	73	5.60	0.002	0.998	0.294	0.706	P → O
20.3	73	5.60	0.002	0.998	0.280	0.720	P → O
22.5	73	5.60	0.002	0.998	0.263	0.737	P → O
26.1	73	5.60	0.002	0.998	0.244	0.756	P → O
28.6	73	5.60	0.002	0.998	0.233	0.767	P → O
31.7	73	5.60	0.002	0.998	0.219	0.781	P → O
34.7	73	5.60	0.002	0.998	0.208	0.792	P → O
39.0	73	5.60	0.002	0.998	0.190	0.810	P → O
0.8	61	5.60	0.002	0.998	0.358	0.642	P → O
1.5	61	5.60	0.002	0.998	0.357	0.643	P → O
1.9	61	5.60	0.002	0.998	0.349	0.651	P → O
2.8	61	5.60	0.002	0.998	0.339	0.661	P → O
3.2	61	5.60	0.002	0.998	0.333	0.667	P → O
5.1	61	5.60	0.002	0.998	0.306	0.694	P → O
7.0	61	5.60	0.002	0.998	0.292	0.708	P → O
8.7	61	5.60	0.002	0.998	0.279	0.721	P → O
10.2	61	5.60	0.002	0.998	0.261	0.739	P → O
12.7	61	5.60	0.002	0.998	0.242	0.758	P → O
14.2	61	5.60	0.002	0.998	0.232	0.768	P → O
16.8	61	5.60	0.002	0.998	0.213	0.787	P → O
19.5	61	5.60	0.002	0.998	0.199	0.801	P → O
21.2	61	5.60	0.002	0.998	0.187	0.813	P → O
26.3	61	5.60	0.002	0.998	0.167	0.833	P → O
31.3	61	5.60	0.002	0.998	0.150	0.850	P → O
0.7	51	5.60	0.002	0.998	0.245	0.755	P → O
1.1	51	5.60	0.002	0.998	0.240	0.760	P → O
1.4	51	5.60	0.002	0.998	0.235	0.765	P → O
1.8	51	5.60	0.002	0.998	0.235	0.765	P → O
2.5	51	5.60	0.002	0.998	0.227	0.773	P → O
3.2	51	5.60	0.002	0.998	0.223	0.777	P → O
4.4	51	5.60	0.002	0.998	0.211	0.789	P → O
5.9	51	5.60	0.002	0.998	0.194	0.806	P → O
8.4	51	5.60	0.002	0.998	0.178	0.822	P → O
10.5	51	5.60	0.002	0.998	0.160	0.840	P → O
11.6	51	5.60	0.002	0.998	0.155	0.845	P → O
13.3	51	5.60	0.002	0.998	0.144	0.856	P → O

Space Velocity / min^{-1}	T / K	p / MPa	y_1, ortho	y_1, para	y_2, ortho	y_2, para	Direction
13.9	51	5.60	0.002	0.998	0.141	0.859	P → O
16.6	51	5.60	0.002	0.998	0.130	0.870	P → O
19.0	51	5.60	0.002	0.998	0.119	0.881	P → O
21.4	51	5.60	0.002	0.998	0.114	0.886	P → O
0.5	41	5.60	0.002	0.998	0.126	0.874	P → O
0.9	41	5.60	0.002	0.998	0.123	0.877	P → O
1.6	41	5.60	0.002	0.998	0.122	0.878	P → O
2.3	41	5.60	0.002	0.998	0.118	0.882	P → O
3.3	41	5.60	0.002	0.998	0.117	0.883	P → O
4.1	41	5.60	0.002	0.998	0.107	0.893	P → O
5.1	41	5.60	0.002	0.998	0.101	0.899	P → O
5.8	41	5.60	0.002	0.998	0.096	0.904	P → O
7.2	41	5.60	0.002	0.998	0.087	0.913	P → O
7.4	41	5.60	0.002	0.998	0.090	0.910	P → O
8.5	41	5.60	0.002	0.998	0.084	0.916	P → O
10.1	41	5.60	0.002	0.998	0.079	0.921	P → O
11.5	41	5.60	0.002	0.998	0.072	0.928	P → O
13.0	41	5.60	0.002	0.998	0.066	0.934	P → O
15.1	41	5.60	0.002	0.998	0.059	0.941	P → O
1.1	79	6.98	0.002	0.998	0.505	0.495	P → O
1.8	79	6.98	0.002	0.998	0.498	0.502	P → O
2.4	79	6.98	0.002	0.998	0.494	0.506	P → O
2.7	79	6.98	0.002	0.998	0.490	0.510	P → O
3.6	79	6.98	0.002	0.998	0.481	0.519	P → O
5.4	79	6.98	0.002	0.998	0.456	0.544	P → O
7.8	79	6.98	0.002	0.998	0.428	0.572	P → O
9.6	79	6.98	0.002	0.998	0.407	0.593	P → O
10.5	79	6.98	0.002	0.998	0.399	0.601	P → O
12.8	79	6.98	0.002	0.998	0.374	0.626	P → O
14.8	79	6.98	0.002	0.998	0.355	0.645	P → O
19.0	79	6.98	0.002	0.998	0.321	0.679	P → O
20.1	79	6.98	0.002	0.998	0.315	0.685	P → O
22.3	79	6.98	0.002	0.998	0.299	0.701	P → O
25.3	79	6.98	0.002	0.998	0.282	0.718	P → O
28.2	79	6.98	0.002	0.998	0.266	0.734	P → O
1.1	72	6.98	0.002	0.998	0.456	0.544	P → O
1.9	72	6.98	0.002	0.998	0.455	0.545	P → O
2.5	72	6.98	0.002	0.998	0.448	0.552	P → O
3.2	72	6.98	0.002	0.998	0.435	0.565	P → O
4.8	72	6.98	0.002	0.998	0.412	0.588	P → O
6.7	72	6.98	0.002	0.998	0.387	0.613	P → O
8.7	72	6.98	0.002	0.998	0.364	0.636	P → O
10.5	72	6.98	0.002	0.998	0.346	0.654	P → O
13.8	72	6.98	0.002	0.998	0.311	0.689	P → O
16.8	72	6.98	0.002	0.998	0.297	0.703	P → O
18.6	72	6.98	0.002	0.998	0.276	0.724	P → O
23.1	72	6.98	0.002	0.998	0.243	0.757	P → O
25.7	72	6.98	0.002	0.998	0.231	0.769	P → O
27.9	72	6.98	0.002	0.998	0.219	0.781	P → O
29.4	72	6.98	0.002	0.998	0.212	0.788	P → O
31.0	72	6.98	0.002	0.998	0.204	0.796	P → O
0.9	63	6.98	0.002	0.998	0.364	0.636	P → O
1.5	63	6.98	0.002	0.998	0.354	0.646	P → O
1.9	63	6.98	0.002	0.998	0.346	0.654	P → O

Space Velocity / min^{-1}	T / K	p / MPa	y_1, ortho	y_1, para	y_2, ortho	y_2, para	Direction
2.4	63	6.98	0.002	0.998	0.339	0.661	P → O
3.2	63	6.98	0.002	0.998	0.329	0.671	P → O
5.0	63	6.98	0.002	0.998	0.304	0.696	P → O
6.3	63	6.98	0.002	0.998	0.287	0.713	P → O
8.7	63	6.98	0.002	0.998	0.256	0.744	P → O
10.7	63	6.98	0.002	0.998	0.238	0.762	P → O
13.2	63	6.98	0.002	0.998	0.216	0.784	P → O
14.9	63	6.98	0.002	0.998	0.204	0.796	P → O
16.5	63	6.98	0.002	0.998	0.193	0.807	P → O
18.3	63	6.98	0.002	0.998	0.181	0.819	P → O
20.3	63	6.98	0.002	0.998	0.170	0.830	P → O
23.5	63	6.98	0.002	0.998	0.156	0.844	P → O
24.7	63	6.98	0.002	0.998	0.150	0.850	P → O
0.6	51	6.98	0.002	0.998	0.240	0.760	P → O
1.1	51	6.98	0.002	0.998	0.236	0.764	P → O
1.6	51	6.98	0.002	0.998	0.230	0.770	P → O
1.9	51	6.98	0.002	0.998	0.227	0.773	P → O
3.1	51	6.98	0.002	0.998	0.209	0.791	P → O
3.9	51	6.98	0.002	0.998	0.199	0.801	P → O
4.7	51	6.98	0.002	0.998	0.190	0.810	P → O
6.0	51	6.98	0.002	0.998	0.176	0.824	P → O
8.1	51	6.98	0.002	0.998	0.156	0.844	P → O
9.1	51	6.98	0.002	0.998	0.149	0.851	P → O
10.6	51	6.98	0.002	0.998	0.137	0.863	P → O
12.5	51	6.98	0.002	0.998	0.127	0.873	P → O
13.3	51	6.98	0.002	0.998	0.120	0.880	P → O
14.9	51	6.98	0.002	0.998	0.111	0.889	P → O
15.3	51	6.98	0.002	0.998	0.110	0.890	P → O
18.2	51	6.98	0.002	0.998	0.100	0.900	P → O
0.5	41	6.98	0.002	0.998	0.121	0.879	P → O
0.8	41	6.98	0.002	0.998	0.124	0.876	P → O
1.1	41	6.98	0.002	0.998	0.122	0.878	P → O
1.4	41	6.98	0.002	0.998	0.121	0.879	P → O
2.0	41	6.98	0.002	0.998	0.115	0.885	P → O
2.7	41	6.98	0.002	0.998	0.111	0.889	P → O
3.7	41	6.98	0.002	0.998	0.101	0.899	P → O
4.2	41	6.98	0.002	0.998	0.101	0.899	P → O
5.3	41	6.98	0.002	0.998	0.090	0.910	P → O
6.8	41	6.98	0.002	0.998	0.083	0.917	P → O
8.2	41	6.98	0.002	0.998	0.075	0.925	P → O
9.2	41	6.98	0.002	0.998	0.071	0.929	P → O
10.5	41	6.98	0.002	0.998	0.068	0.932	P → O
11.7	41	6.98	0.002	0.998	0.060	0.940	P → O
12.7	41	6.98	0.002	0.998	0.059	0.941	P → O
13.6	41	6.98	0.002	0.998	0.053	0.947	P → O

Note: y_1,ortho and y_1,para represent ortho-hydrogen and para-hydrogen mole fractions in hydrogen inlet stream; y_2,ortho and y_2,para represent ortho-hydrogen and para-hydrogen mole fractions in hydrogen outlet stream.

S3. Raw Experimental Data Extracted from Weitzel et al. [3]

Space Velocity (STP) / min^{-1}	T / K	p / MPa	y_1, ortho	y_1, para	y_2, ortho	y_2, para	Direction
355.4	86	0.24	0.75	0.25	0.553	0.447	O → P
545.0	86	0.24	0.75	0.25	0.568	0.432	O → P
739.9	86	0.24	0.75	0.25	0.580	0.420	O → P
842.7	86	0.24	0.75	0.25	0.580	0.420	O → P
1037.7	86	0.24	0.75	0.25	0.594	0.406	O → P
1140.5	86	0.24	0.75	0.25	0.597	0.403	O → P
1281.3	86	0.24	0.75	0.25	0.607	0.393	O → P
1386.9	86	0.24	0.75	0.25	0.613	0.387	O → P
1557.4	86	0.24	0.75	0.25	0.619	0.381	O → P
259.8	76	0.24	0.75	0.25	0.487	0.513	O → P
544.3	76	0.24	0.75	0.25	0.499	0.501	O → P
807.8	76	0.24	0.75	0.25	0.516	0.484	O → P
965.9	76	0.24	0.75	0.25	0.526	0.474	O → P
1345.2	76	0.24	0.75	0.25	0.547	0.453	O → P
1682.5	76	0.24	0.75	0.25	0.567	0.433	O → P
1956.4	76	0.24	0.75	0.25	0.578	0.422	O → P
2362.1	76	0.24	0.75	0.25	0.595	0.405	O → P
303.4	63	0.24	0.75	0.25	0.381	0.619	O → P
456.2	63	0.24	0.75	0.25	0.391	0.609	O → P
609.1	63	0.24	0.75	0.25	0.406	0.594	O → P
701.3	63	0.24	0.75	0.25	0.411	0.589	O → P
725.0	63	0.24	0.75	0.25	0.417	0.583	O → P
785.6	63	0.24	0.75	0.25	0.422	0.578	O → P
925.3	63	0.24	0.75	0.25	0.435	0.565	O → P
1078.2	63	0.24	0.75	0.25	0.452	0.548	O → P
1186.3	63	0.24	0.75	0.25	0.461	0.539	O → P
163.3	59	0.24	0.75	0.25	0.338	0.662	O → P
181.7	59	0.24	0.75	0.25	0.336	0.664	O → P
374.1	59	0.24	0.75	0.25	0.352	0.648	O → P
521.7	59	0.24	0.75	0.25	0.364	0.636	O → P
724.6	59	0.24	0.75	0.25	0.376	0.624	O → P
985.6	59	0.24	0.75	0.25	0.408	0.592	O → P
1415.1	59	0.24	0.75	0.25	0.442	0.558	O → P
1744.4	59	0.24	0.75	0.25	0.455	0.545	O → P
2000.1	59	0.24	0.75	0.25	0.488	0.512	O → P
183.8	55	0.24	0.75	0.25	0.286	0.714	O → P
373.6	55	0.24	0.75	0.25	0.306	0.694	O → P
529.1	55	0.24	0.75	0.25	0.325	0.675	O → P
729.4	55	0.24	0.75	0.25	0.337	0.663	O → P
1420.0	55	0.24	0.75	0.25	0.409	0.591	O → P
1707.1	55	0.24	0.75	0.25	0.420	0.580	O → P
2012.9	55	0.24	0.75	0.25	0.453	0.547	O → P
165.0	52	0.24	0.75	0.25	0.254	0.746	O → P
196.5	52	0.24	0.75	0.25	0.250	0.750	O → P
373.2	52	0.24	0.75	0.25	0.274	0.726	O → P
723.8	52	0.24	0.75	0.25	0.309	0.691	O → P
1013.8	52	0.24	0.75	0.25	0.344	0.656	O → P
1422.4	52	0.24	0.75	0.25	0.387	0.613	O → P
1627.7	52	0.24	0.75	0.25	0.388	0.612	O → P
2007.4	52	0.24	0.75	0.25	0.431	0.569	O → P
185.5	48	0.24	0.75	0.25	0.209	0.791	O → P

Space Velocity (STP) / min^{-1}	T / K	p / MPa	y_1, ortho	y_1, para	y_2, ortho	y_2, para	Direction
375.4	48	0.24	0.75	0.25	0.235	0.765	O → P
536.2	48	0.24	0.75	0.25	0.257	0.743	O → P
736.6	48	0.24	0.75	0.25	0.277	0.723	O → P
1422.0	48	0.24	0.75	0.25	0.359	0.641	O → P
1500.9	48	0.24	0.75	0.25	0.350	0.650	O → P
2004.4	48	0.24	0.75	0.25	0.405	0.595	O → P
2444.6	48	0.24	0.75	0.25	0.443	0.557	O → P
171.9	45	0.24	0.75	0.25	0.171	0.829	O → P
382.8	45	0.24	0.75	0.25	0.195	0.805	O → P
744.1	45	0.24	0.75	0.25	0.242	0.758	O → P
1044.8	45	0.24	0.75	0.25	0.290	0.710	O → P
1218.6	45	0.24	0.75	0.25	0.299	0.701	O → P
1421.7	45	0.24	0.75	0.25	0.329	0.671	O → P
1738.1	45	0.24	0.75	0.25	0.369	0.631	O → P
2006.8	45	0.24	0.75	0.25	0.382	0.618	O → P
182.0	41	0.24	0.75	0.25	0.134	0.866	O → P
379.7	41	0.24	0.75	0.25	0.154	0.846	O → P
532.7	41	0.24	0.75	0.25	0.181	0.819	O → P
746.3	41	0.24	0.75	0.25	0.206	0.794	O → P
1263.1	41	0.24	0.75	0.25	0.273	0.727	O → P
1423.9	41	0.24	0.75	0.25	0.296	0.704	O → P
1761.2	41	0.24	0.75	0.25	0.317	0.683	O → P
2009.1	41	0.24	0.75	0.25	0.352	0.648	O → P
2441.4	41	0.24	0.75	0.25	0.396	0.604	O → P
178.9	37	0.24	0.75	0.25	0.091	0.909	O → P
194.7	37	0.24	0.75	0.25	0.093	0.907	O → P
387.1	37	0.24	0.75	0.25	0.110	0.890	O → P
532.2	37	0.24	0.75	0.25	0.136	0.864	O → P
751.1	37	0.24	0.75	0.25	0.164	0.836	O → P
1043.9	37	0.24	0.75	0.25	0.218	0.782	O → P
1178.2	37	0.24	0.75	0.25	0.221	0.779	O → P
1423.6	37	0.24	0.75	0.25	0.262	0.738	O → P
1705.4	37	0.24	0.75	0.25	0.277	0.723	O → P
2008.7	37	0.24	0.75	0.25	0.322	0.678	O → P
165.3	33	0.24	0.75	0.25	0.055	0.945	O → P
183.8	33	0.24	0.75	0.25	0.058	0.942	O → P
389.3	33	0.24	0.75	0.25	0.073	0.927	O → P
531.7	33	0.24	0.75	0.25	0.095	0.905	O → P
747.9	33	0.24	0.75	0.25	0.118	0.882	O → P
1230.4	33	0.24	0.75	0.25	0.181	0.819	O → P
1346.5	33	0.24	0.75	0.25	0.200	0.800	O → P
1425.7	33	0.24	0.75	0.25	0.217	0.783	O → P
1702.3	33	0.24	0.75	0.25	0.233	0.767	O → P
2011.0	33	0.24	0.75	0.25	0.288	0.712	O → P
2461.7	33	0.24	0.75	0.25	0.335	0.665	O → P
172.8	28	0.24	0.75	0.25	0.022	0.978	O → P
193.9	28	0.24	0.75	0.25	0.026	0.974	O → P
391.6	28	0.24	0.75	0.25	0.040	0.960	O → P
586.6	28	0.24	0.75	0.25	0.059	0.941	O → P
750.1	28	0.24	0.75	0.25	0.079	0.921	O → P
1048.2	28	0.24	0.75	0.25	0.131	0.869	O → P
1356.5	28	0.24	0.75	0.25	0.152	0.848	O → P
1433.1	28	0.24	0.75	0.25	0.180	0.820	O → P
1535.9	28	0.24	0.75	0.25	0.188	0.812	O → P

Space Velocity (STP) / min^{-1}	T / K	p / MPa	y_1, ortho	y_1, para	y_2, ortho	y_2, para	Direction
1699.2	28	0.24	0.75	0.25	0.191	0.809	O → P
2018.3	28	0.24	0.75	0.25	0.242	0.758	O → P
2469.2	28	0.24	0.75	0.25	0.295	0.705	O → P
291.1	23	0.24	0.75	0.25	0.005	0.995	O → P
388.6	23	0.24	0.75	0.25	0.014	0.986	O → P
528.3	23	0.24	0.75	0.25	0.026	0.974	O → P
583.6	23	0.24	0.75	0.25	0.028	0.972	O → P
749.6	23	0.24	0.75	0.25	0.040	0.960	O → P
1029.1	23	0.24	0.75	0.25	0.074	0.926	O → P
1060.8	23	0.24	0.75	0.25	0.086	0.914	O → P
1316.5	23	0.24	0.75	0.25	0.115	0.885	O → P
1353.4	23	0.24	0.75	0.25	0.113	0.887	O → P
1427.3	23	0.24	0.75	0.25	0.131	0.869	O → P
1564.4	23	0.24	0.75	0.25	0.149	0.851	O → P
1664.4	23	0.24	0.75	0.25	0.144	0.856	O → P
2002.0	23	0.24	0.75	0.25	0.196	0.804	O → P
2479.2	23	0.24	0.75	0.25	0.249	0.751	O → P
370.6	60	0.24	0.49	0.52	0.338	0.662	O → P
512.9	60	0.24	0.49	0.52	0.341	0.659	O → P
688.4	60	0.24	0.49	0.52	0.353	0.647	O → P
773.3	60	0.24	0.49	0.52	0.347	0.653	O → P
982.1	60	0.24	0.49	0.52	0.358	0.642	O → P
1183.5	60	0.24	0.49	0.52	0.367	0.633	O → P
1732.3	60	0.24	0.49	0.52	0.385	0.615	O → P
1756.2	60	0.24	0.49	0.52	0.379	0.621	O → P
2181.0	60	0.24	0.49	0.52	0.385	0.615	O → P
2413.8	60	0.24	0.49	0.52	0.395	0.605	O → P
397.6	55	0.24	0.49	0.52	0.293	0.707	O → P
554.7	55	0.25	0.49	0.52	0.300	0.700	O → P
772.7	55	0.26	0.49	0.52	0.304	0.696	O → P
942.9	55	0.27	0.49	0.52	0.327	0.673	O → P
987.1	55	0.27	0.49	0.52	0.317	0.683	O → P
1166.3	55	0.28	0.49	0.52	0.327	0.673	O → P
1739.0	55	0.29	0.49	0.52	0.343	0.657	O → P
2193.3	55	0.29	0.49	0.52	0.348	0.652	O → P
2413.3	55	0.30	0.49	0.52	0.361	0.639	O → P
258.5	51	0.32	0.49	0.52	0.250	0.750	O → P
398.9	51	0.33	0.49	0.52	0.254	0.746	O → P
445.1	51	0.33	0.49	0.52	0.252	0.748	O → P
557.9	51	0.34	0.49	0.52	0.263	0.737	O → P
772.2	51	0.35	0.49	0.52	0.275	0.725	O → P
1001.4	51	0.36	0.49	0.52	0.289	0.711	O → P
1178.8	51	0.36	0.49	0.52	0.298	0.702	O → P
1526.1	51	0.37	0.49	0.52	0.308	0.692	O → P
1731.3	51	0.38	0.49	0.52	0.319	0.681	O → P
2013.9	51	0.38	0.49	0.52	0.327	0.673	O → P
2191.2	51	0.39	0.49	0.52	0.326	0.674	O → P
2427.7	51	0.40	0.49	0.52	0.338	0.662	O → P
235.6	48	0.42	0.49	0.52	0.200	0.800	O → P
256.0	48	0.42	0.49	0.52	0.205	0.795	O → P
389.2	48	0.43	0.49	0.52	0.221	0.779	O → P
444.5	48	0.44	0.49	0.52	0.215	0.785	O → P
463.1	48	0.44	0.49	0.52	0.222	0.778	O → P
557.3	48	0.45	0.49	0.52	0.228	0.772	O → P

Space Velocity (STP) / min^{-1}	T / K	p / MPa	y_1, ortho	y_1, para	y_2, ortho	y_2, para	Direction
773.6	48	0.46	0.49	0.52	0.241	0.759	O → P
997.1	48	0.47	0.49	0.52	0.247	0.753	O → P
1028.6	48	0.47	0.49	0.52	0.251	0.749	O → P
1169.0	48	0.48	0.49	0.52	0.255	0.745	O → P
1187.6	48	0.49	0.49	0.52	0.264	0.736	O → P
1520.1	48	0.49	0.49	0.52	0.274	0.726	O → P
1741.9	48	0.50	0.49	0.52	0.289	0.711	O → P
2019.1	48	0.51	0.49	0.52	0.302	0.698	O → P
2211.1	48	0.51	0.49	0.52	0.300	0.700	O → P
2432.9	48	0.52	0.49	0.52	0.314	0.686	O → P
251.5	42	0.54	0.49	0.52	0.147	0.853	O → P
253.4	42	0.55	0.49	0.52	0.154	0.846	O → P
273.5	42	0.56	0.49	0.52	0.139	0.861	O → P
393.9	42	0.56	0.49	0.52	0.164	0.836	O → P
451.1	42	0.57	0.49	0.52	0.160	0.840	O → P
565.8	42	0.58	0.49	0.52	0.173	0.827	O → P
684.0	42	0.58	0.49	0.52	0.179	0.821	O → P
774.7	42	0.59	0.49	0.52	0.189	0.811	O → P
987.2	42	0.60	0.49	0.52	0.199	0.801	O → P
1170.3	42	0.60	0.49	0.52	0.217	0.783	O → P
1530.5	42	0.61	0.49	0.52	0.228	0.772	O → P
1735.8	42	0.62	0.49	0.52	0.250	0.750	O → P
2022.1	42	0.62	0.49	0.52	0.258	0.742	O → P
2217.9	42	0.63	0.49	0.52	0.263	0.737	O → P
2449.0	42	0.64	0.49	0.52	0.278	0.722	O → P
256.3	37	0.66	0.49	0.52	0.097	0.903	O → P
258.1	37	0.67	0.49	0.52	0.094	0.906	O → P
395.0	37	0.67	0.49	0.52	0.114	0.886	O → P
450.3	37	0.68	0.49	0.52	0.109	0.891	O → P
566.8	37	0.69	0.49	0.52	0.121	0.879	O → P
687.2	37	0.69	0.49	0.52	0.141	0.859	O → P
770.3	37	0.70	0.49	0.52	0.140	0.860	O → P
988.3	37	0.71	0.49	0.52	0.151	0.849	O → P
1180.7	37	0.71	0.49	0.52	0.172	0.828	O → P
1302.6	37	0.72	0.49	0.52	0.176	0.824	O → P
1533.6	37	0.73	0.49	0.52	0.186	0.814	O → P
1746.2	37	0.73	0.49	0.52	0.208	0.792	O → P
2049.3	37	0.74	0.49	0.52	0.220	0.780	O → P
2093.6	37	0.75	0.49	0.52	0.223	0.777	O → P
2213.7	37	0.75	0.49	0.52	0.223	0.777	O → P
2439.1	37	0.76	0.49	0.52	0.233	0.767	O → P
257.5	32	0.78	0.49	0.52	0.058	0.942	O → P
265.0	32	0.79	0.49	0.52	0.061	0.939	O → P
399.7	32	0.80	0.49	0.52	0.059	0.941	O → P
398.1	32	0.80	0.49	0.52	0.073	0.927	O → P
446.0	32	0.81	0.49	0.52	0.068	0.932	O → P
566.3	32	0.82	0.49	0.52	0.082	0.918	O → P
690.0	32	0.82	0.49	0.52	0.081	0.919	O → P
777.1	32	0.83	0.49	0.52	0.106	0.894	O → P
985.9	32	0.84	0.49	0.52	0.111	0.889	O → P
1183.8	32	0.84	0.49	0.52	0.131	0.869	O → P
1309.4	32	0.85	0.49	0.52	0.133	0.867	O → P
1531.1	32	0.86	0.49	0.52	0.146	0.854	O → P
1747.5	32	0.87	0.49	0.52	0.167	0.833	O → P

Space Velocity (STP) / min^{-1}	T / K	p / MPa	y_1, ortho	y_1, para	y_2, ortho	y_2, para	Direction
2021.0	32	0.87	0.49	0.52	0.179	0.821	O → P
2065.2	32	0.88	0.49	0.52	0.170	0.830	O → P
2218.6	32	0.89	0.49	0.52	0.181	0.819	O → P
2440.4	32	0.89	0.49	0.52	0.200	0.800	O → P
255.4	30	0.91	0.49	0.52	0.039	0.961	O → P
353.3	30	0.92	0.49	0.52	0.040	0.960	O → P
397.7	30	0.93	0.49	0.52	0.048	0.952	O → P
445.8	30	0.93	0.49	0.52	0.052	0.948	O → P
569.7	30	0.94	0.49	0.52	0.064	0.936	O → P
778.6	30	0.95	0.49	0.52	0.080	0.920	O → P
889.5	30	0.95	0.49	0.52	0.085	0.915	O → P
989.2	30	0.96	0.49	0.52	0.089	0.911	O → P
1187.1	30	0.97	0.49	0.52	0.110	0.890	O → P
1288.7	30	0.98	0.49	0.52	0.111	0.889	O → P
1532.6	30	0.98	0.49	0.52	0.123	0.877	O → P
1747.2	30	0.99	0.49	0.52	0.147	0.853	O → P
2009.5	30	1.00	0.49	0.52	0.154	0.846	O → P
2026.2	30	1.00	0.49	0.52	0.158	0.842	O → P
2223.9	30	1.01	0.49	0.52	0.164	0.836	O → P
2436.5	30	1.02	0.49	0.52	0.181	0.819	O → P
257.0	27	1.04	0.49	0.52	0.021	0.979	O → P
345.6	27	1.04	0.49	0.52	0.020	0.980	O → P
404.8	27	1.05	0.49	0.52	0.025	0.975	O → P
449.1	27	1.06	0.49	0.52	0.028	0.972	O → P
567.4	27	1.07	0.49	0.52	0.036	0.964	O → P
900.1	27	1.07	0.49	0.52	0.057	0.943	O → P
1001.7	27	1.08	0.49	0.52	0.055	0.945	O → P
1192.2	27	1.09	0.49	0.52	0.081	0.919	O → P
1197.7	27	1.09	0.49	0.52	0.077	0.923	O → P
1304.9	27	1.10	0.49	0.52	0.083	0.917	O → P
1534.0	27	1.11	0.49	0.52	0.091	0.909	O → P
1739.3	27	1.11	0.49	0.52	0.113	0.887	O → P
2023.8	27	1.12	0.49	0.52	0.122	0.878	O → P
2229.0	27	1.13	0.49	0.52	0.133	0.867	O → P
2449.0	27	1.13	0.49	0.52	0.152	0.848	O → P
266.0	24	1.15	0.49	0.52	0.005	0.995	O → P
338.0	24	1.16	0.49	0.52	0.005	0.995	O → P
400.8	24	1.17	0.49	0.52	0.008	0.992	O → P
454.5	24	1.18	0.49	0.52	0.014	0.986	O → P
570.9	24	1.18	0.49	0.52	0.018	0.982	O → P
894.2	24	1.19	0.49	0.52	0.032	0.968	O → P
1019.8	24	1.20	0.49	0.52	0.031	0.969	O → P
1184.4	24	1.20	0.49	0.52	0.047	0.953	O → P
1308.1	24	1.21	0.49	0.52	0.049	0.951	O → P
1500.3	24	1.22	0.49	0.52	0.058	0.942	O → P
1746.2	24	1.22	0.49	0.52	0.081	0.919	O → P
2025.2	24	1.23	0.49	0.52	0.089	0.911	O → P
2235.9	24	1.24	0.49	0.52	0.100	0.900	O → P
2437.3	24	1.24	0.49	0.52	0.113	0.887	O → P

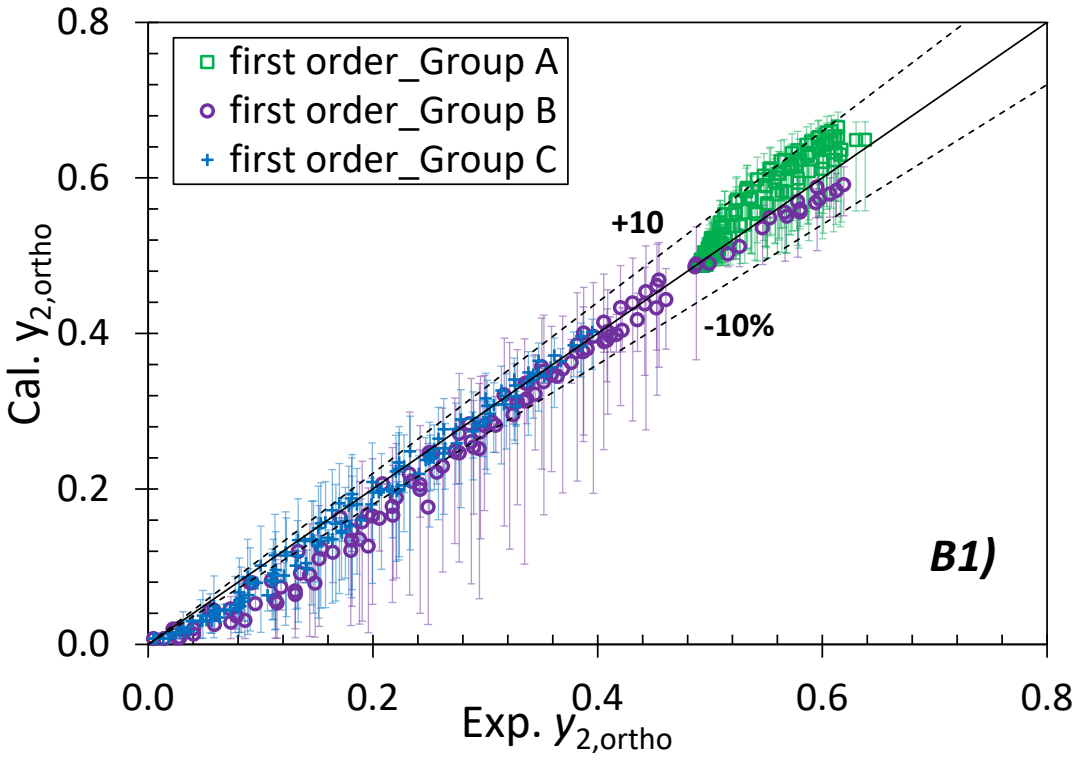
Note: y_1,ortho and y_1,para represent ortho-hydrogen and para-hydrogen mole fractions in hydrogen inlet stream; y_2,ortho and y_2,para represent ortho-hydrogen and para-hydrogen mole fractions in hydrogen outlet stream

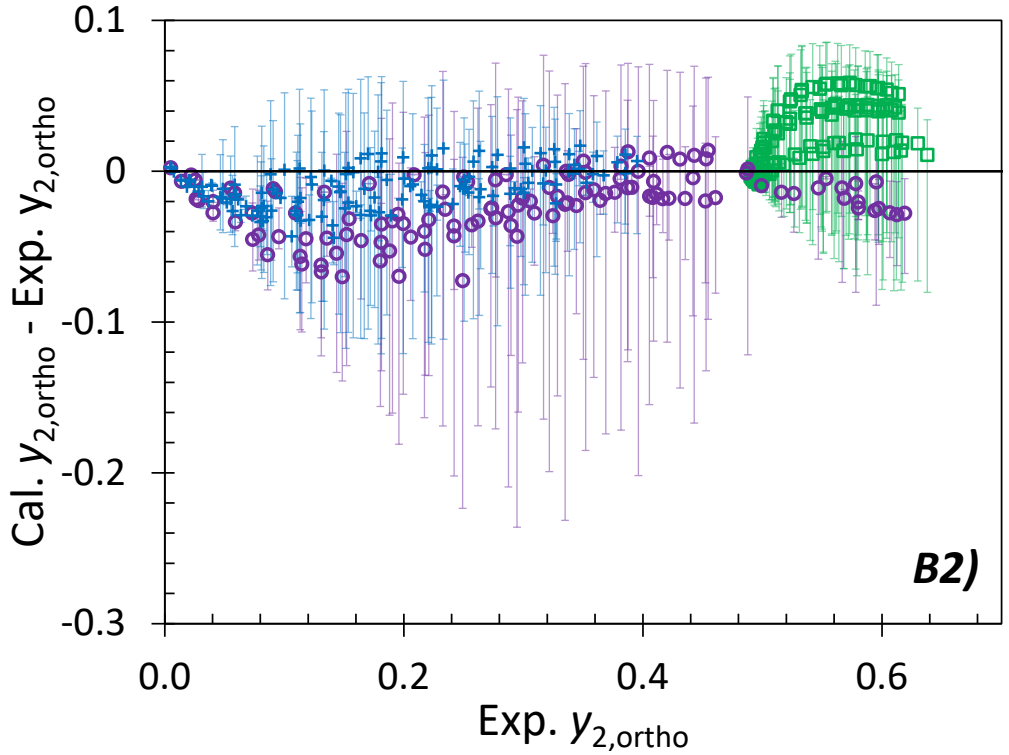
S4. Non-HFO Catalysts along with Pre-treatment Methods [4, 5]

Table S4. Non-HFO catalysts along with pre-treatment methods.

Catalysts	Pre-heating Fluid	Pre-heating Duration / hrs	Pre-cooling Fluid
19% Cr_2O_3 + Al_2O_3	Hydrogen	5	Hydrogen
0.5% CuO +Al_2O_3	Air	2	Air / Helium
0.5% NiO + Al_2O_3	Air	2	Air / Helium
0.5% Cu + Al_2O_3	Hydrogen	4	Hydrogen
0.5% Ni(A) + Al_2O_3	Hydrogen	12	Hydrogen
0.5% Ni(B) + Al_2O_3	Hydrogen	12	Helium
0.5% Mn_2O_3 + Al_2O_3	Hydrogen	4	Hydrogen
0.5% Tb_2O_3 + Al_2O_3	Hydrogen	4	Hydrogen
0.5 % Pd + Al_2O_3	Hydrogen	4	Hydrogen
0.5% Ni(I) + Al_2O_3	Hydrogen	12	Hydrogen
0.5% Ni(X) + Al_2O_3	Hydrogen	12	Hydrogen
0.5% TbO_2 + ZrO_2	Air	2	Air / Helium

S5. First-Order Kinetics Plots with Error Bars





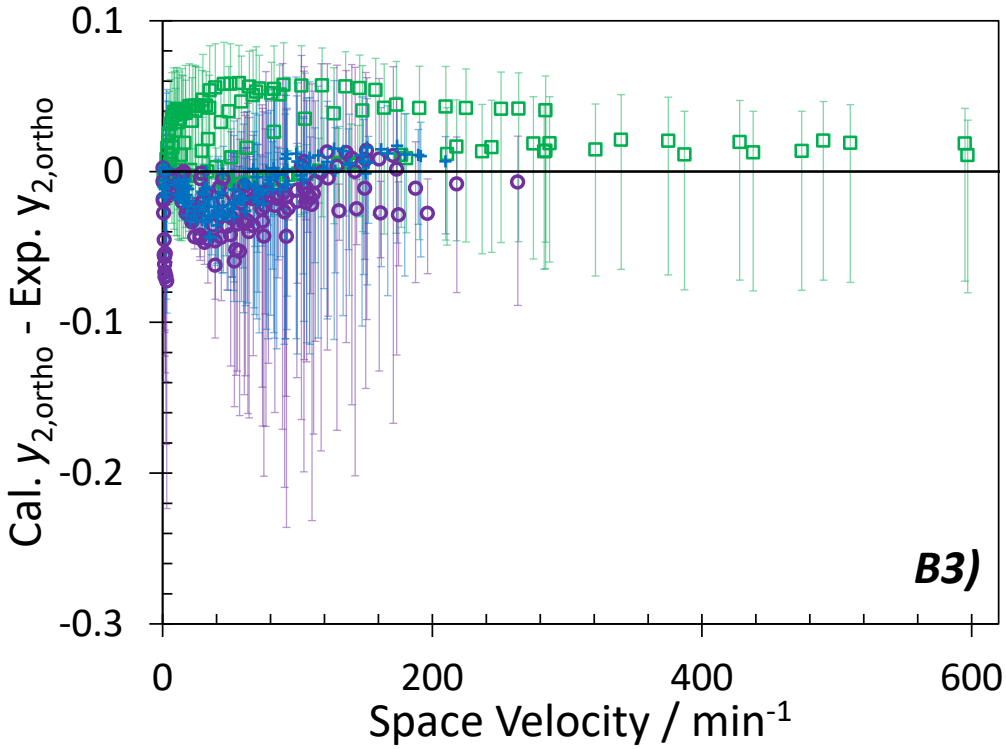


Figure S5 Parity plots (*B1*) and absolute deviation plots (*B2, B3*) of fitted first-order kinetic using coefficients reported by Donaubauer et al. [6] on the ortho-para conversion literature datasets of Hutchinson (forward reactions only) (Group A) [1] and Weitzel et al. [3] (Group B - inlet para hydrogen mole fraction = 25%; Group C - inlet para hydrogen mole fraction = 51.5%). The x-axes in (*B1, B2*) represent the experimental effluent ortho-hydrogen fraction and the x-axes in (B*3*) represent the experimental space velocity; The y-axes in (*B1*) represent the calculated effluent ortho-hydrogen fraction and the y-axes in (*B2, B3*) represent the absolute deviation between the calculated and experimental ortho-hydrogen fraction; The positive and negative error bars represent the calculated ortho-hydrogen fractions employing the corrected minimum or maximum values of E_{a,k_1}, a_1 and b_1 as tabulated in **Table 6**. The solid line is $y = x$ and the dashed lines are $y = (1 \pm 0.1)x$. Data shown for hydrous ferric oxide catalysts only.

Reference

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5. N. Wakao, P. W. Selwood and J. M. Smith, *AIChE Journal*, 1962, **8**, 478-481.
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