Ruthenium-Catalyzed Solvent-Free Conversion of Furfural to Furfuryl Alcohol

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Electronic Supplementary Information (ESI)

Chemicals

Furfural, furfuryl alcohol, Ru(III)-acetylacetonate, $RuCl_2(PPh_3)$, 1,2-*bis*(diphenylphoshino)ethane (DPPE), 1,3-*bis*(diphenylphoshino)propane (DPPPr), 1,4-*bis*(diphenylphoshino)butane (DPPB), 1,5-*bis*(diphenylphoshino)pentane (DPPPe), 1,6-*bis*(diphenylphoshino)hexane (DPPH), toluene, and methylene chloride were purchased from Sigma–Aldrich Ltd., Budapest, Hungary.

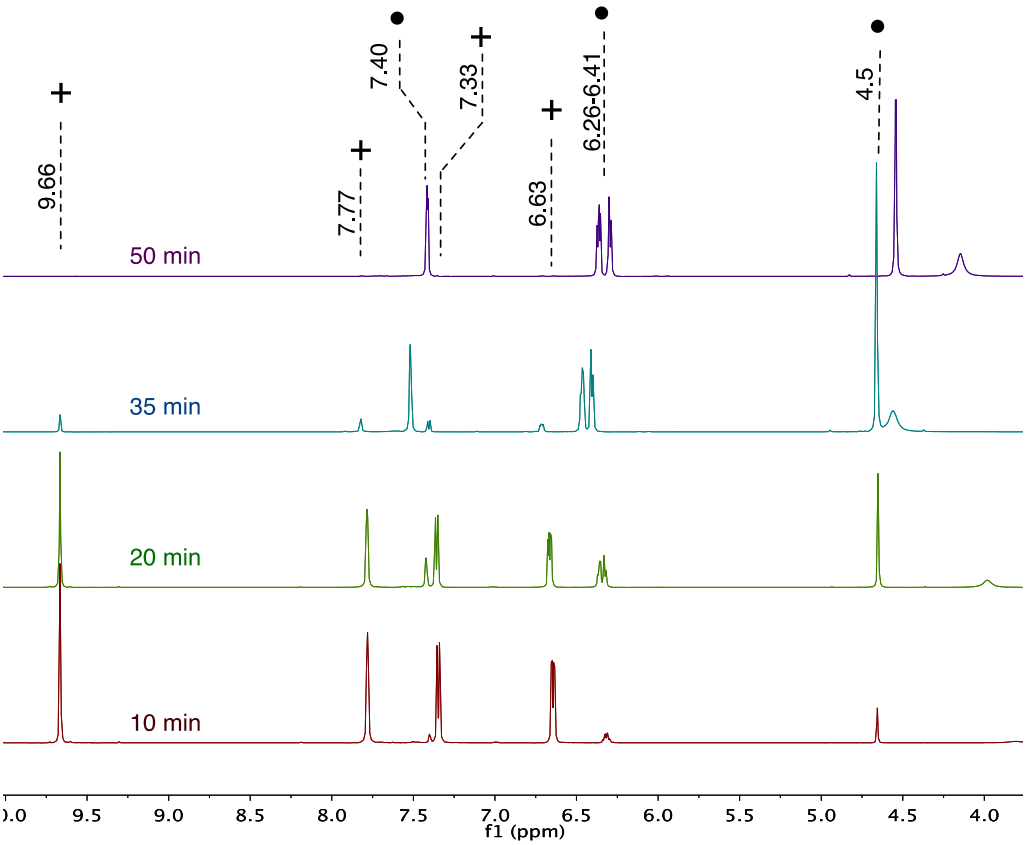

Figure S1: ^{1}H-NMR spectra of the reaction mixtures of solvent-free conversion of furfural to furfuryl alcohol. +: furfural, ●: furfuryl alcohol

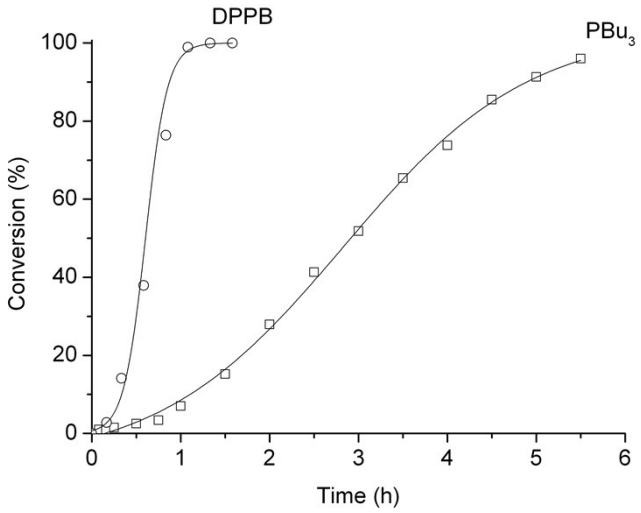

Figure S2. Conversion of furfural to furfuryl alcohol in the presence of DPPB and Pbu3 modified ru-catalysts

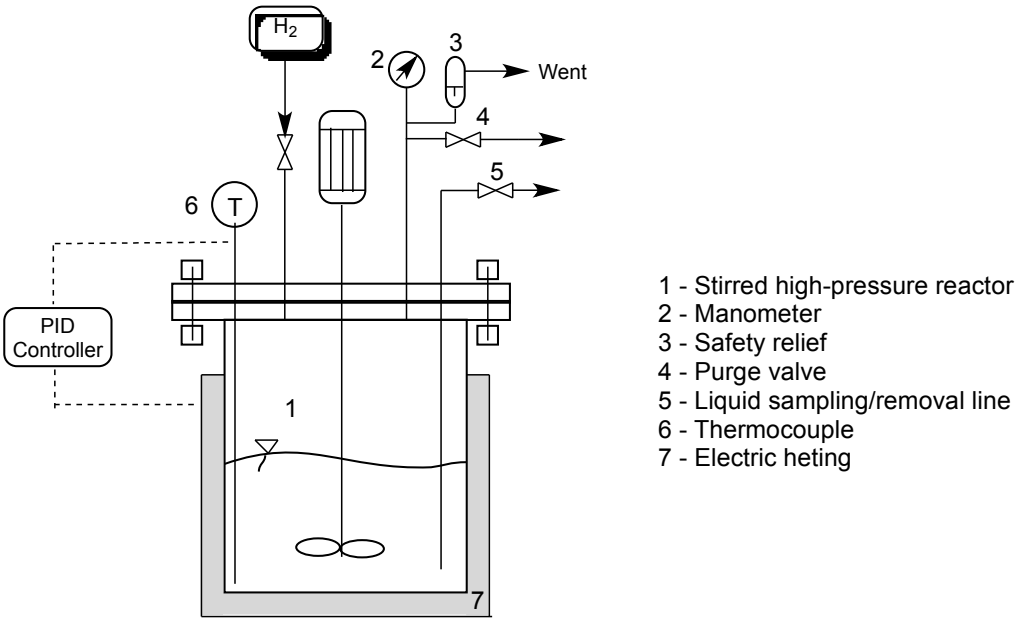

Figure S3. Configuration of Parr High-pressure stirred reactor

ESI-Table S1. Data for catalyst recycling

Cycle	Catalyst +Ligand +Residue	m (FAL) (g)	n (FAL) (mmol)	Conversion after 0.5 h (%)	Conversion after 1.3 h (%)	m (Distillate) (g)	m (Residue) (g)	TON	Sum of TON
1	0.8727*	34.6	360.04	71.2	>99.9	30.11	3.342	1885	1885
2	3.342	34.8	362.12	98.7	>99.9	31.57	5.48	1896	3781
3	5.48	34.3	356.92	99.4	>99.9	32.73	5.95	1869	5650
4	5.95	34.5	359.00	98.8	>99.9	32.09	6.48	1880	7529
5	6.48	34.2	355.88	79.5	>99.9	31.17	9.52	1863	9392
6	9.52	34.9	363.16	89.1	>99.9	31.2	9.51	1901	11294
7	9.51	34.1	354.84	80.6	>99.9	32.89	9.13	1858	13152
8	9.13	34.5	359.00	75.2	>99.9	32.02	9.37	1880	15031
9	9.37	34.7	361.08	68	>99.9	32.43	9.84	1890	16922
10	9.84	34.3	356.92	73.9	>99.9	34.22	10.02	1869	18790
11	10.02	34.4	357.96	73.9	>99.9	30.05	11.24	1874	20665
12	11.24	34.2	355.88	75	>99.9	31.12	11.2	1863	22528
Some of FAL loaded		413.5			Sum of Distillates	381.6			
					Sum of Distillates (Mass balance)	92.3%			

*: Only catalyst precursor + ligand