Supporting Information

Solvent effects on heterogeneous catalysis in selective hydrogenation of cinnamaldehyde over a conventional Pd/C catalyst

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Table S1. Solvatochromic parameters and H_2 solubility of various solvents.

No.	Solvents	π* (-)[a]	α (-)[b]	β (-)[c]	X_{H_2} x 10^4 (-)[d]
1	1-Butanol	0.47	0.79	0.88	2.63[2]
2	2-Propanol	0.48	0.76	0.95	4.61[2]
3	*N,N*'-Dimethylformamide	0.88	0	0.69	1.47[2]
4	Diethyl ether	0.27	0	0.47	3.46[2]
5	Triethylamine	0.14	0	0.71	1.45[e]
6	Tetrahydrofuran	0.58	0	0.55	2.74[3]
7	Furan	--	0	0.14	2.79[e]
8	4-Methylpyridine	0.84	0	0.67	1.25[e]
9	Pyridine	0.87	0	0.64	1.62[4]
10	Toluene	0.54	0	0.11	3.15[2]
11	*n*-Hexane	0.04	0	0	6.63[2]
12	Benzene	0.59	0	0.1	2.76[4]

[a] Polarity/polarizability index according to Ref. [1].

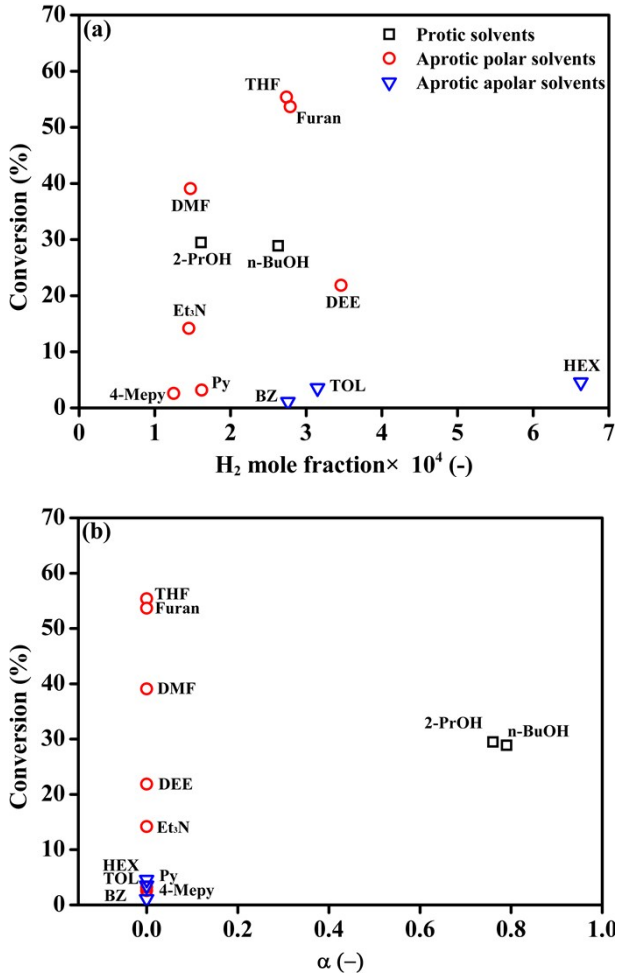
[b] Hydrogen-bond-donation ability according to Ref. [1].

[c] Hydrogen-bond-acceptance ability according to Ref. [1].

[d] H_2 solubility in solvent mole fraction at 298 K and 1 atm according to Ref. [2-4].

[e] The value was measured according to references [5, 6]. In a typical experiment for the measurement of solubility of H_2, a known volume of solvent was introduced into the autoclave and heated to 298 K. After the thermal equilibrium was attained, the

reactor was flushed with H_2 and pressurized to 1 MPa. The solvent then was stirred for about 20 min to equilibrate the liquid phase with H_2. The change in the pressure in the autoclave was recorded till it became unchanged. The solubility was calculated in mole fraction as $\chi_A = (P_i - P_A)\, V_g / RTV_L \rho_s$, where χ_A represents the mole fraction of H_2 in the liquid phase, P_i and P_A are the initial and final pressure readings in the autoclave, V_g and V_L are the volumes of the gas and liquid phases, respectively, R is the gas constant, T is the temperature, and ρ_s is the molar density of the liquid.



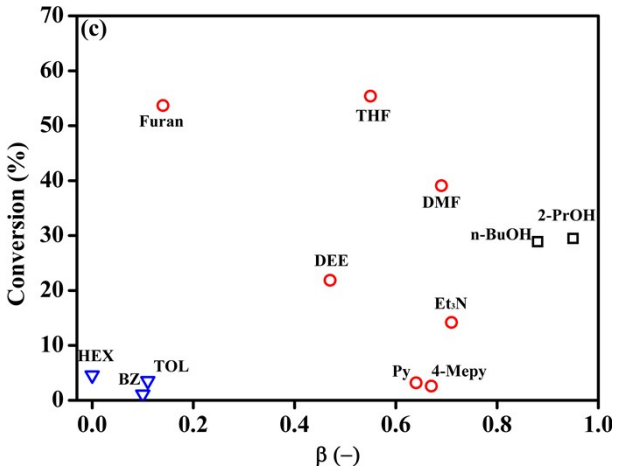


Figure S1. Plot of the total conversion observed in CAL hydrogenation over 5% Pd/C vs. (a) the mole fraction of H_2 in solvents, (b) the α and (c) the β value of the solvents (Table S1). Numbers given correspond to the different solvents in Figure 1(a).

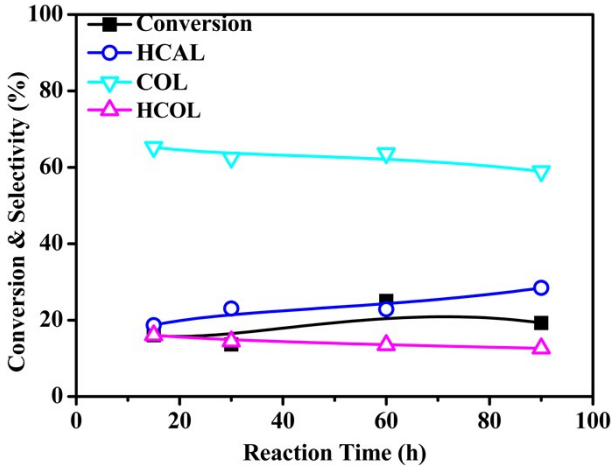


Figure S2. Conversion and selectivity obtained in pyridine over Pd/C as a function of reaction time. Reaction conditions: CAL, 5 mmol; 5% Pd/C, 5 mg; pyridine, 5 mL; H_2, 4 MPa; 80 °C.

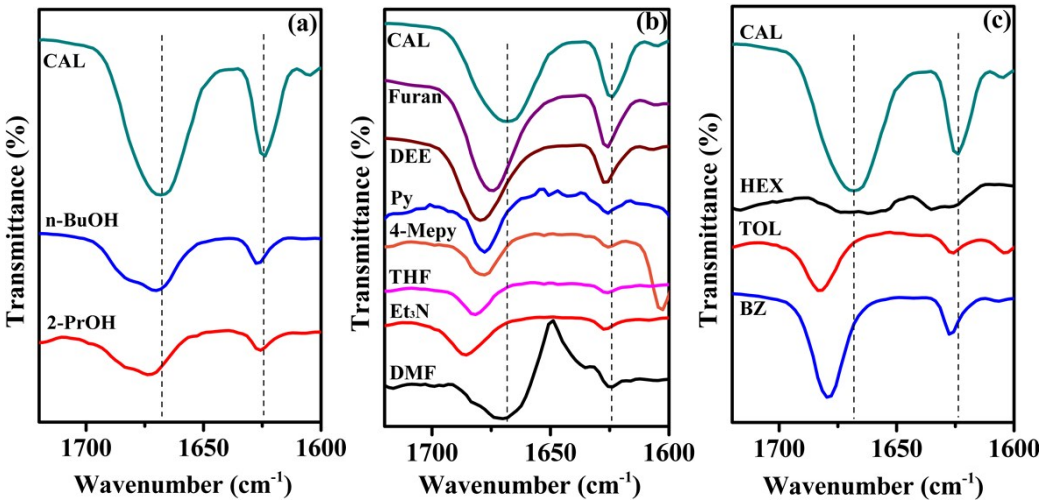


Figure S3. ATR-FTIR spectra of CAL in different solvents measured at 50 °C. CAL, 5 mmol; solvent, 5 mL. (a) protic solvents, (b) aprotic polar solvents, (c) aprotic apolar solvents.

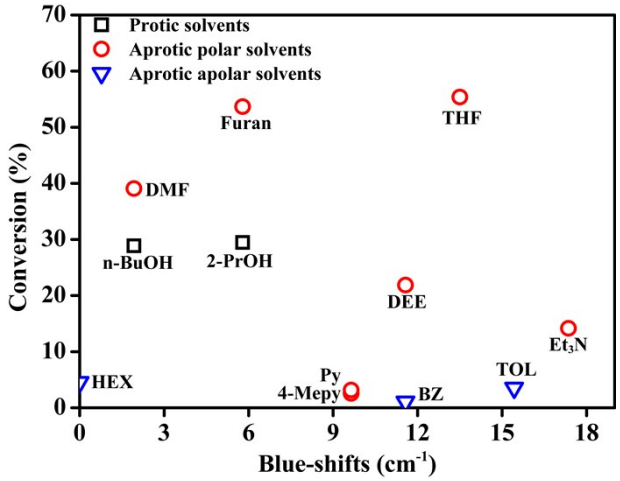


Figure S4. Plot of total conversion in CAL hydrogenation (Fig. 1(a)) vs. the extent of blue-shift of ν(C=O) absorption band in various solvents (Fig. S3†). Conditions: CAL 5 mmol, solvent 5 mL, 50 °C. For solvent abbreviations, see Fig. 1's caption.

References

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