Supplementary Information

Role of EFAl species and proximity between Brønsted and metal sites in hydrogenation on bifunctional catalysts

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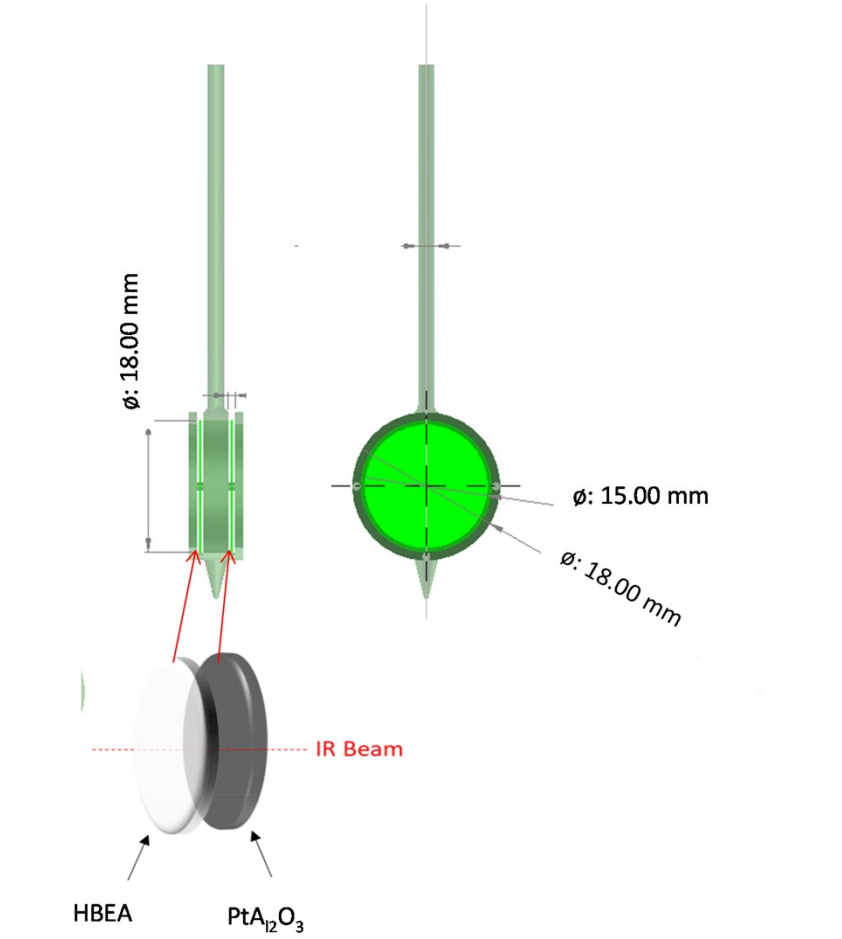

Figure S1. Schematic representation of the PtA|HBEA sample analysis.

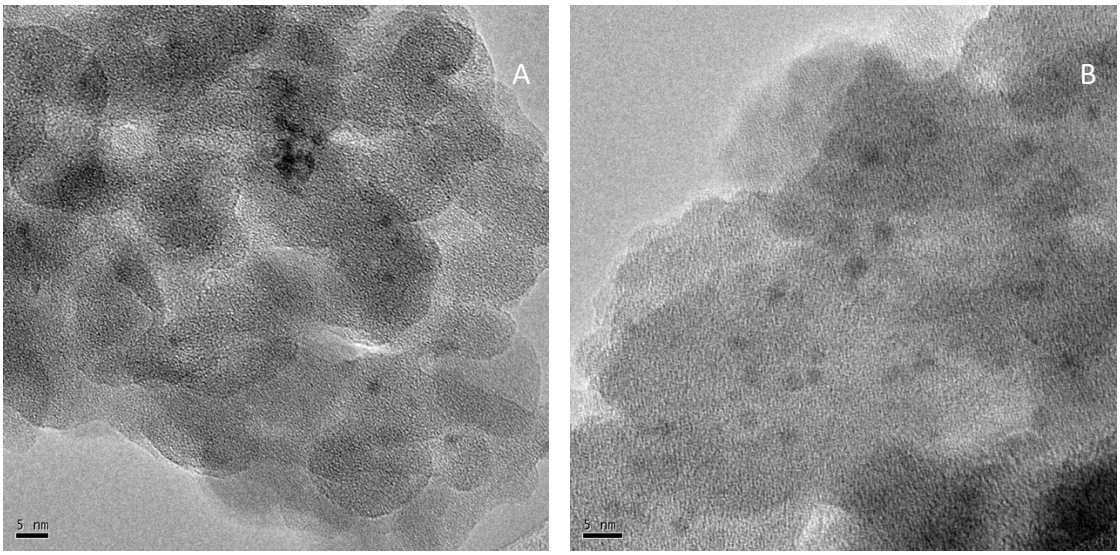

Figure S2. TEM micrographs of 0.5PtHBEA (A) and 1PtHBEA (B) catalysts.

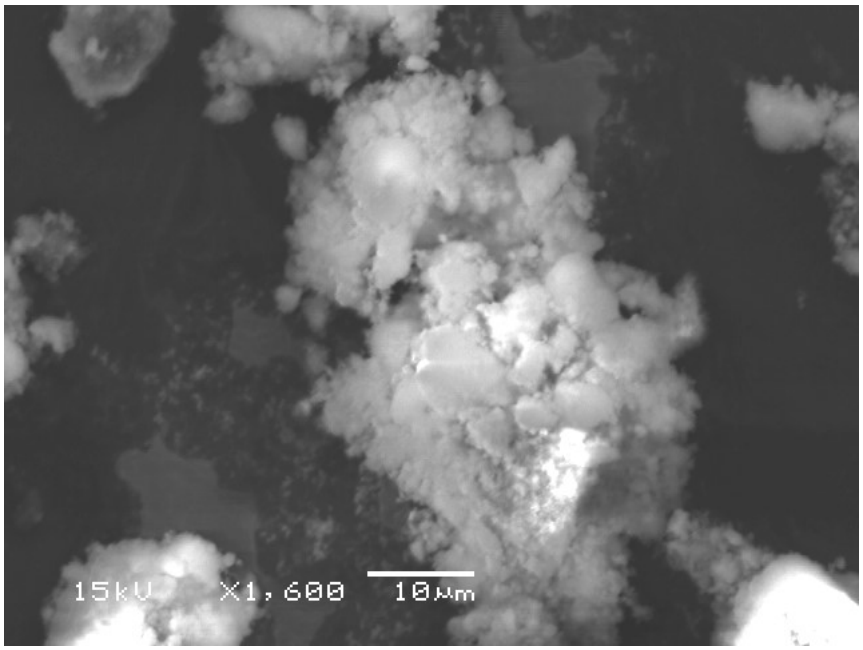

Figure S3. SEM micrographs of HBEA.

Table S1. Impact of the mixture between γ-Al_2O_3 and HBEA on acid properties of PtA+HBEA samples.

	Brønsted acidity – [PyH^+] [a] ($\mu mol.g^{-1}$)	Lewis acidity – [PyL] [b] ($\mu mol.g^{-1}$)
HBEA (CP-814E - Zeolyst)[c]	448	208
Al_2O_3[d]	-	172
Al_2O_3 + HBEA (50-50)	169 (224)[e]	145 (190)[e]

[a] number of protonic sites able to retain pyridine [PyH^+] at 220 °C.

[b] Lewis sites able to retain pyridine [PyL] at 220 °C.

[c] BEA zeolite from Zeolyst (ref: CP-814E) was used as a replacement for the sample used in the main manuscript due to unavailability of the original HBEA zeolite.

[d] The Al_2O_3 sample presented in this table is a new batch made from the same boehmite material as the one presented in the main manuscript.

[e] Values in brackets correspond to theoretical site density based on the relative proportions of Al_2O_3 and HBEA in the sample.

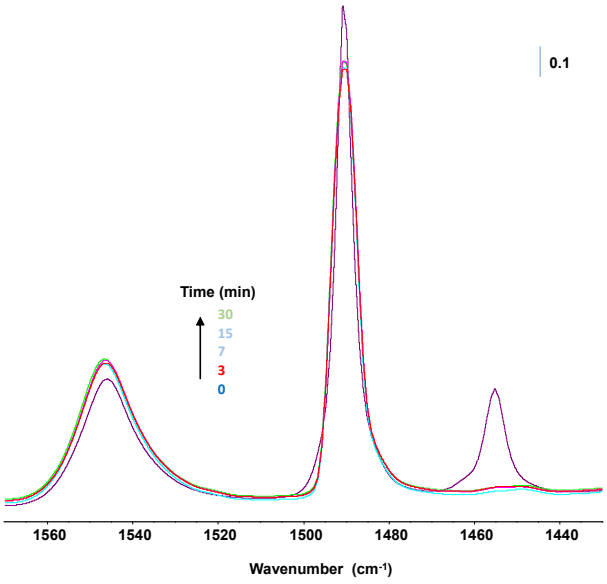

Figure S4. Pyridinium (PyH^+ - 1545 cm^{-1}) and pyridine coordinated on Lewis sites (PyL – 1455 cm^{-1}) bands evolution time with a hydrogen pressure of 6 mbar in the infrared cell for 1PtHBEA saturated with pyridine at 220 °C

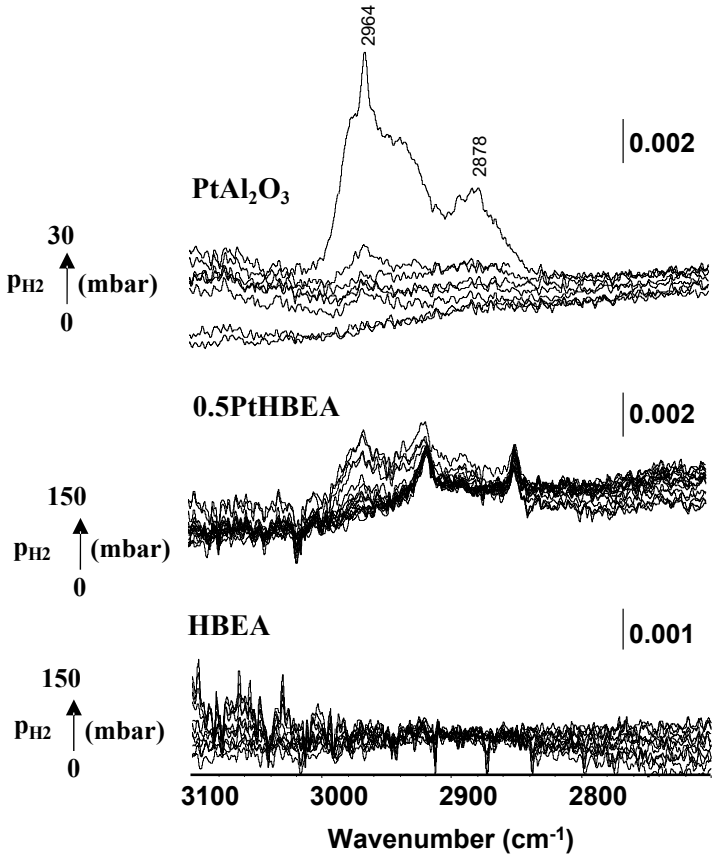

Figure S5. C-H characteristic bands (3100 – 2700 cm^{-1}) of the gas phase as function of hydrogen pressure during the hydrogenation of adsorbed pyridine at 220°C .

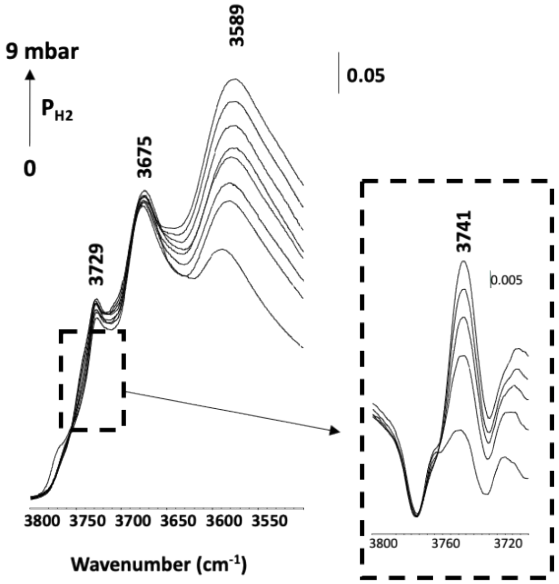

Figure S6. Hydroxyl characteristic bands (3500 – 3850 cm^{-1}) of $PtAl_2O_3$ catalyst as function of hydrogen pressure during the hydrogenation of adsorbed pyridine at 220°C . In the square is highlighted the variation of the band at 3471 cm-1 relative to the reference spectrum at P(H_2) = 0 mbar.

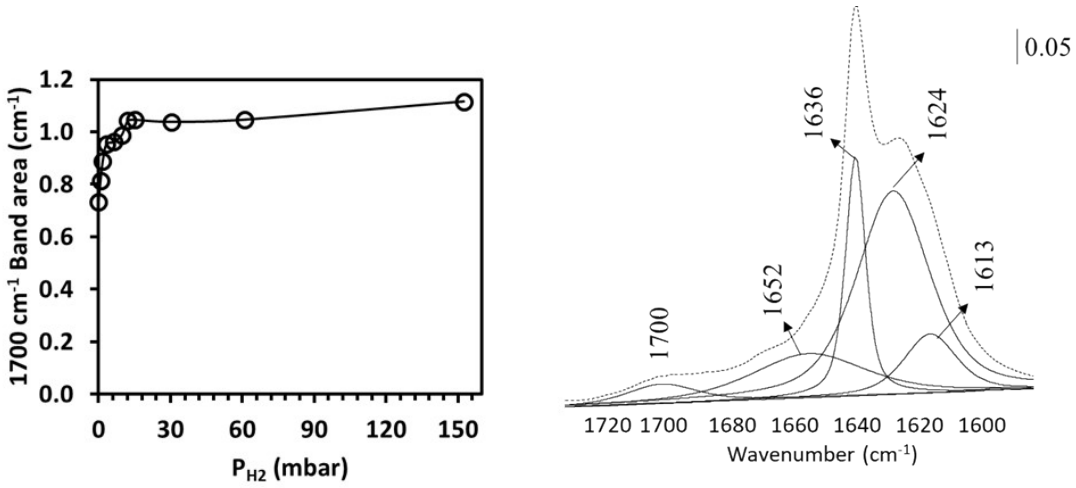

Figure S7. Left) Evolution of the 1700 cm^{-1} band characteristic of Al-H bond. Right) Deconvolution of the IR spectrum of HBEA adsorbed with pyridine under 9 mbar of H_2.

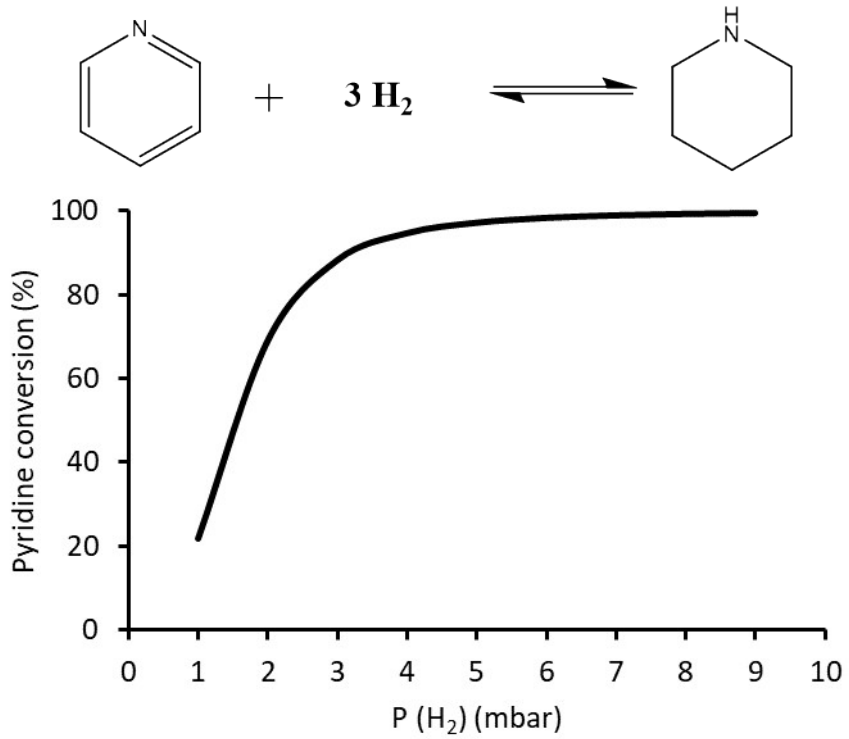

Figure S8. Equilibrium conversion the hydrogenation of pyridine adsorbed on 0.5PtHBEA (Py=9.6 µmol) as a function of hydrogen pressure. The reaction was considered to occur in the gas phase at 220 °C, and system volume, i.e., IR cell volume is 544.4 mL.