Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information's

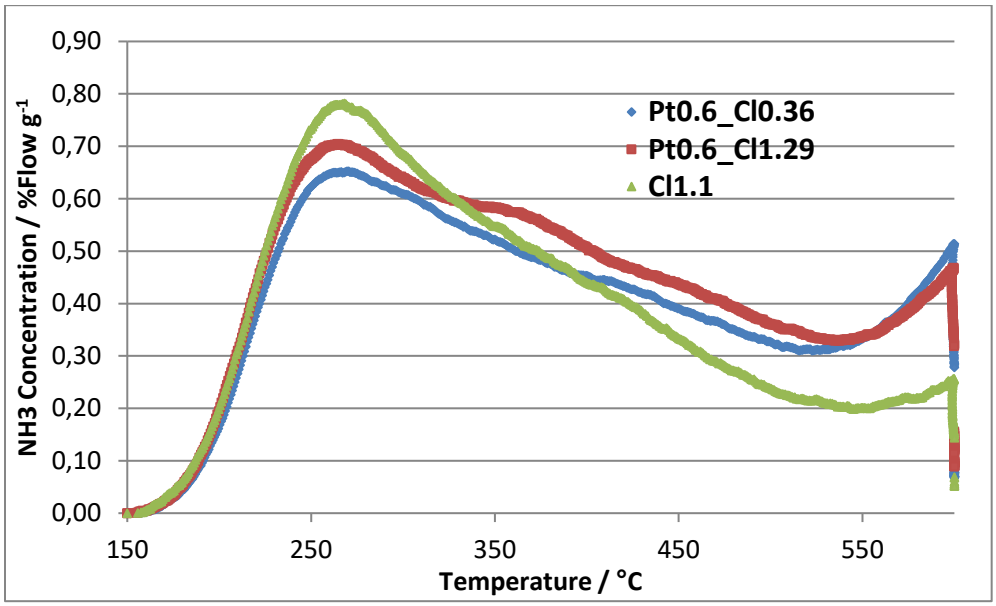
NJC

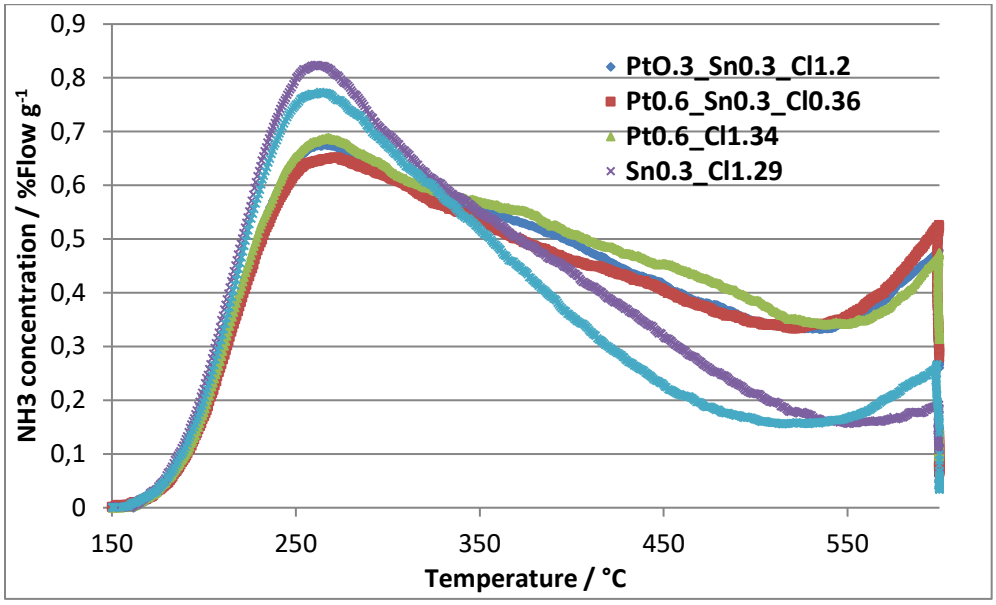
Characterization of the Brønsted acidity of $PtSn/Al_2O_3$ surfaces by adsorption of 2,6-di-tert-butylpyridine

Quentin Rivet, Jordan Meyet, Mickaël Rivallan, Thibaud Nardin, and David Farrusseng

The presented study showed the relevance of using 2,6-di-tert-butylpyridne to probe BAS on alumina catalysts.

1. Ammonia concentration desorbed during NH3 TPD





2. NH_3 density equation

Equation for the determination of the density of NH_3 measured.

First the thermal desorption profile is deconvoluted arbitrarily giving an amout of ammonia per gram of sample. Then a number of sites per nm^{-2} is calculated:

$$NH_3(site\ nm^{-2}) = \frac{Q_{NH_3} * \mathrm{Na}}{S_{BET}}$$

Q_{NH3} the NH_3 quantity in mol g^{-1}

N_A the Avogadro constant in mol^{-1}

S_{BET} the specific area of the sample in $nm^2\ g^{-1}$

3. Pyridine equation

To obtain a quantification of sites through IR pyridine, equations based on the Beer-Lambert law are used:

- The first equation is the Beer-Lambert law: $A = \varepsilon_\nu \cdot l \cdot C_\nu$

A is the absorbance

ε_ν the molar extinction coefficient in $cm^2\ mol^{-1}$ with ν referring to a specific vibration

L the optical path length in cm

C_ν the concentration of the attenuating specie mol cm^{-3}

- The second and third equation are the derivative means to obtain a quantification of sites either LAS or BAS.

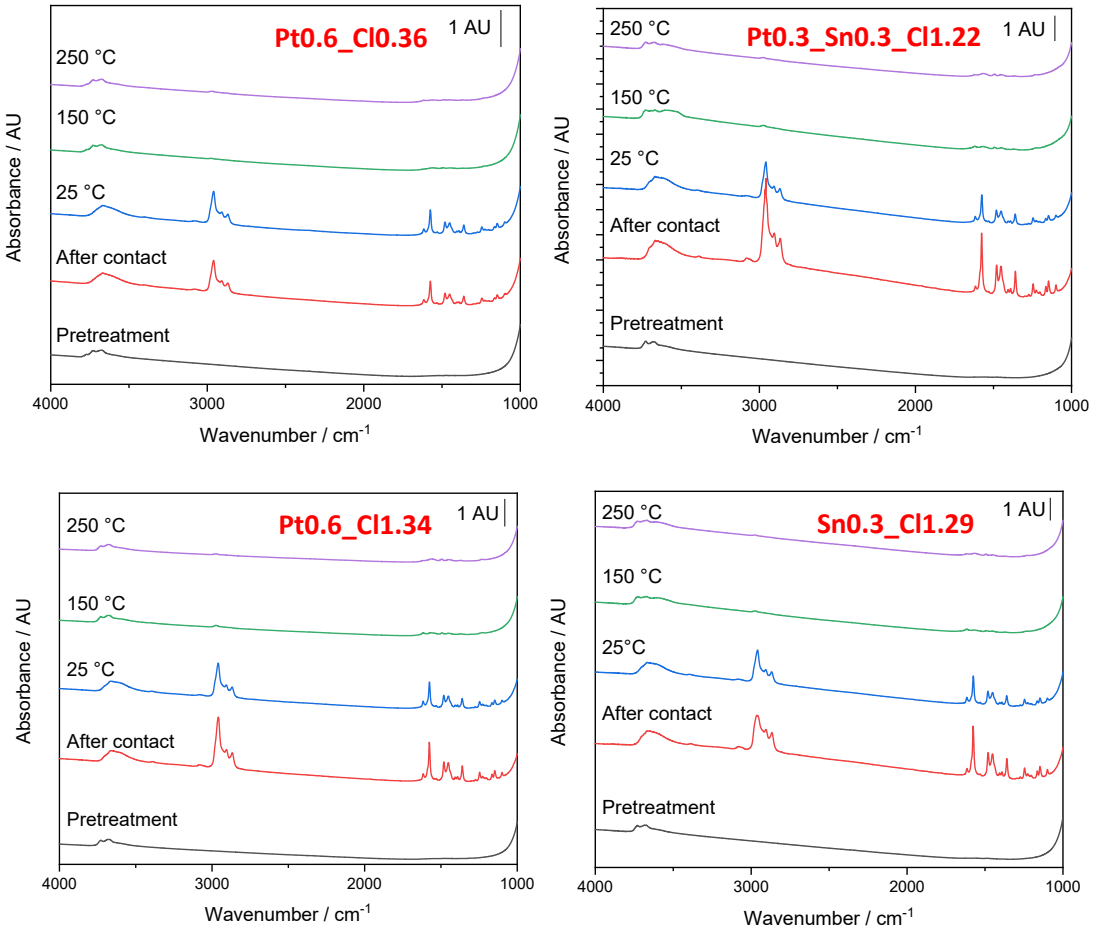
$$l = \frac{m}{S \cdot d} \quad ; \quad BAS\ (mol\ g^{-1}) = \frac{C_\nu}{d} = \frac{A_\nu \cdot S}{\varepsilon_\nu \cdot m}$$

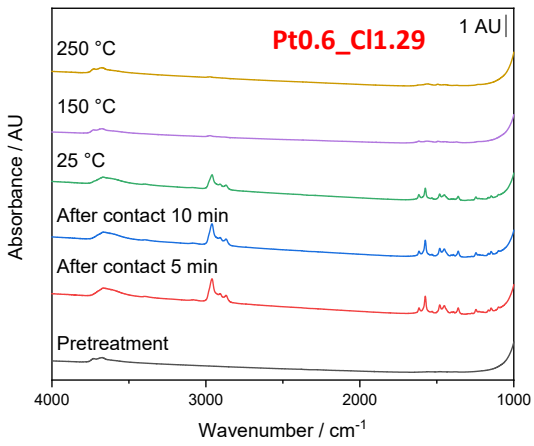
m the mass of the sample in g ; S the surface area of the sample in cm^2 ; d the density of the sample in g cm^{-3}

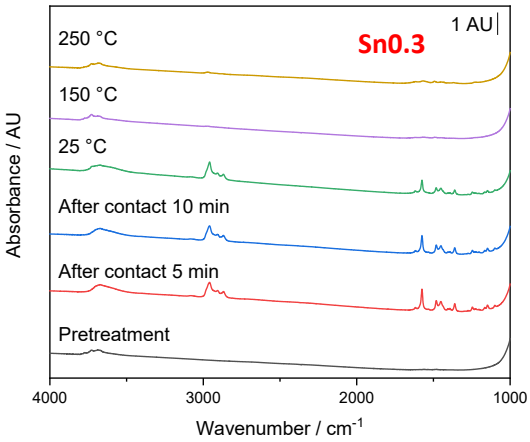
BAS the number of Brønsted acid site in mol g^{-1} ; A_ν the integrated absorbance in cm-1 ; ε_ν the apparent molar extinction coefficient in cm mol^{-1}.

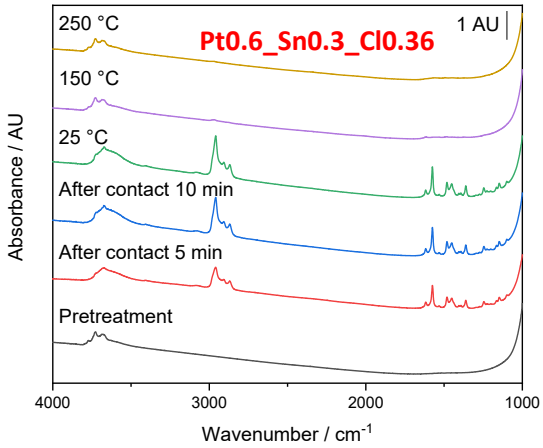
Same calculations as in section 2 are deployed to acquire density of SAB in site nm^{-2}

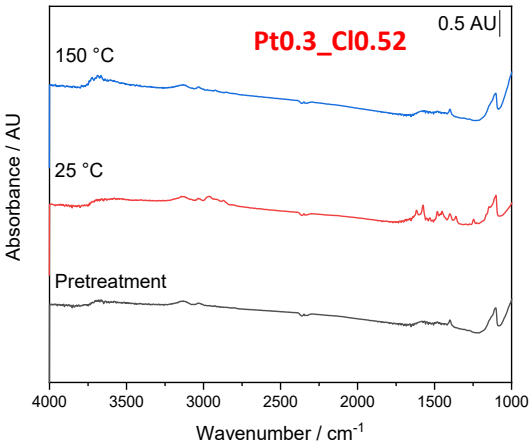
4. IR spectra obtained with the 2,6DTBPyr probe molecule

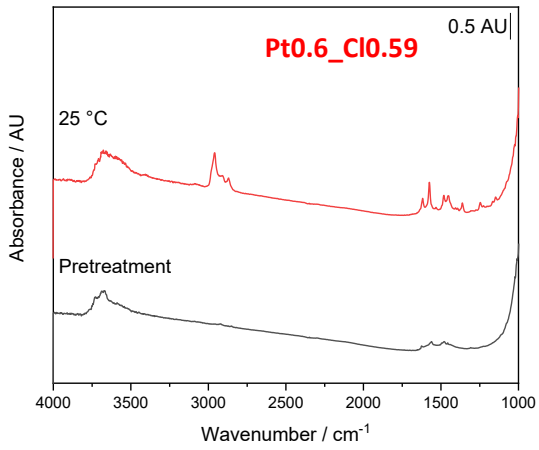



Pt0.6_Cl1.29
1 AU
250 °C
150 °C
25 °C
After contact 10 min
After contact 5 min
Pretreatment
Absorbance / AU
4000
3000
2000
1000
Wavenumber / cm-1


Sn0.3
1 AU
250 °C
150 °C
25 °C
After contact 10 min
After contact 5 min
Pretreatment
Absorbance / AU
4000
3000
2000
1000
Wavenumber / cm-1

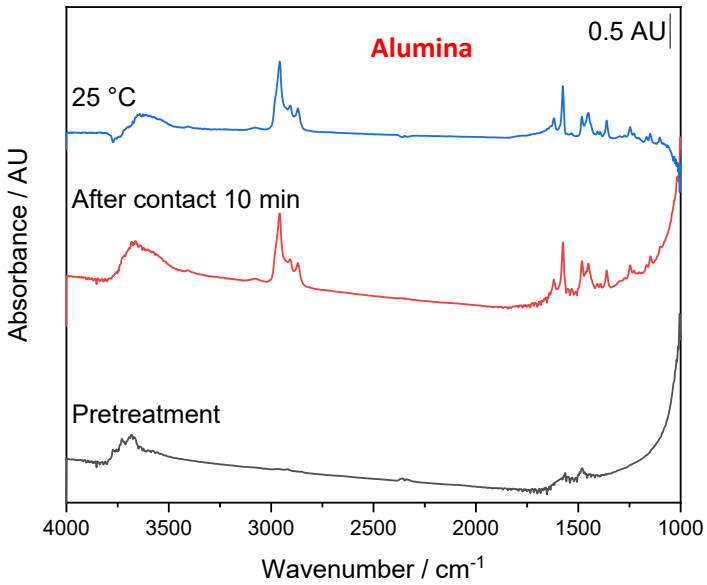

Pt0.6_Sn0.3_Cl0.36
1 AU
250 °C
150 °C
25 °C
After contact 10 min
After contact 5 min
Pretreatment
Absorbance / AU
4000
3000
2000
1000
Wavenumber / cm-1


Pt0.3_Cl0.52
0.5 AU
150 °C
25 °C
Pretreatment
Absorbance / AU
4000
3500
3000
2500
2000
1500
1000
Wavenumber / cm-1


Pt0.6_Cl0.59
0.5 AU
25 °C
Pretreatment
Absorbance / AU
4000
3500
3000
2500
2000
1500
1000
Wavenumber / cm-1

5. Alumina support IR characterization

Catalyst	BAS Site nm^{-2}	BAS $\mu mol\ g^{-1}$	D_{Cl} Cl nm^{-2}
Alumina	0.042	11.67	0



6. Article figure with %Cl and µmol g^{-1} units

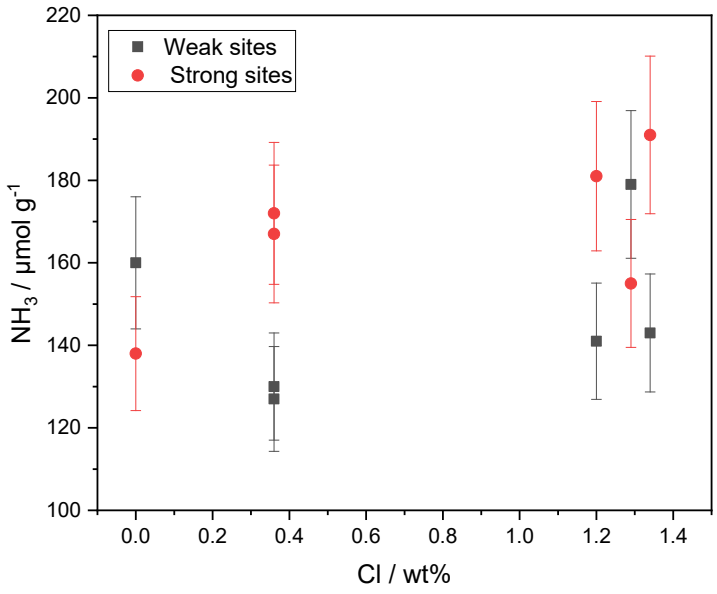


Fig. 1 Concentration of NH3 desorbed in regard to the chlorine loading of catalyst

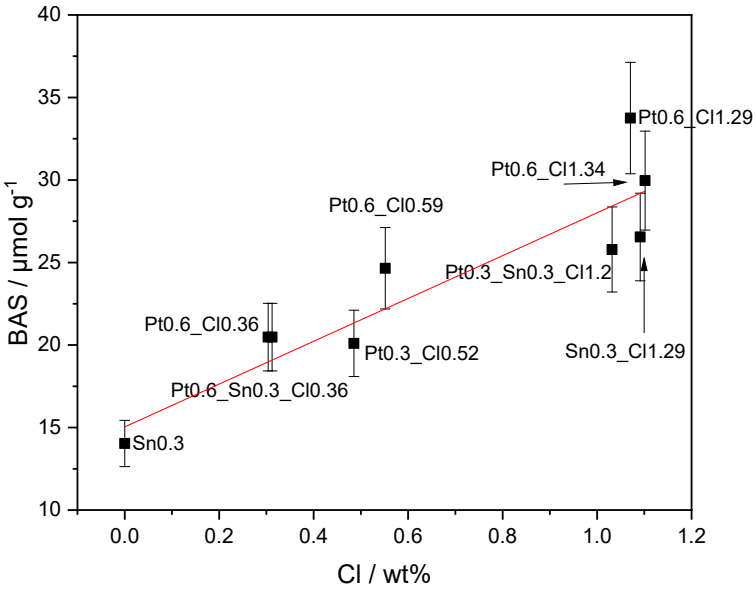


Fig. 4 Concentration of Brønsted acid sites in regard to the chlorine loading of catalyst