Adsorption of small molecules on amorphous ice: Volumetric and FT-IR isotherm co-measurements
I. Different probe molecules

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Aims of the study:

- Control the adsorbed amount step by step from submonolayer to solid condensation
- Obtain quantitative information and comparison for various gases

Volumetric and FT-IR co-measurements

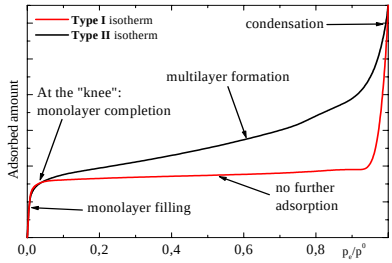
Volumetry allows us to :
- control the adsorbed amount
- determine specific surface area, net heat of adsorption, type of wetting …

Copper isothermal cell (20-300 K)

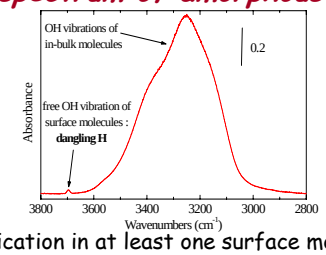
FT-IR spectroscopy allows us to :
- determine surface modes of ice by measuring modifications in its IR signal during adsorption
- measure modifications in the signal of the adsorbate

How to interpret a volumetric isotherm ?

- **type I** ⇔ monolayer
- **type II** ⇔ monolayer + multilayer
- Position of the knee ⇔ adsorbate-surface interaction
- Height of the plateau ⇔ specific surface area



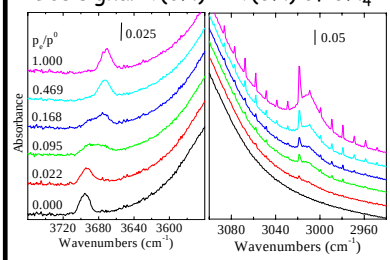
IR spectrum of amorphous ice



- modification in at least one surface mode can be measured during adsorption
- high surface area (with CH_4): **100-200 m²/g**

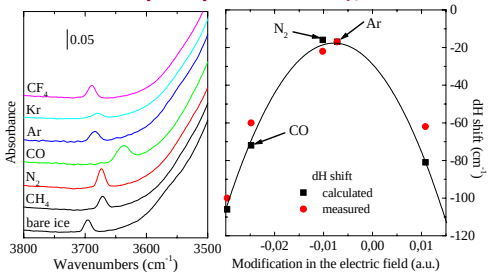
Modifications in IR spectrum

Ice signal: ν(dH) ν(CH) of CH_4



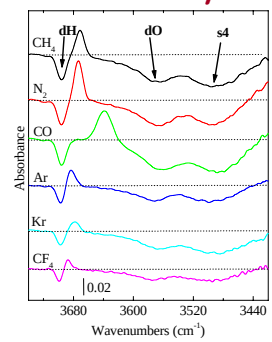
Measurement of integrated absorbance at each step of the isotherm ⇒ « **IR isotherm** »(1)

Shift of the dH mode

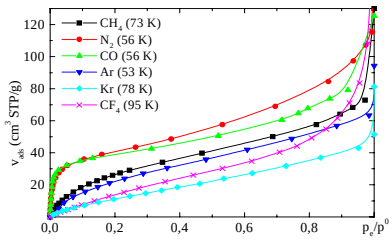


Calculations using **CRYSTAL98** ⇒ quadratic dependency of the shift in the modification in the electric field above dH during adsorption: **vibrational Stark effect**(2)

IR difference spectra

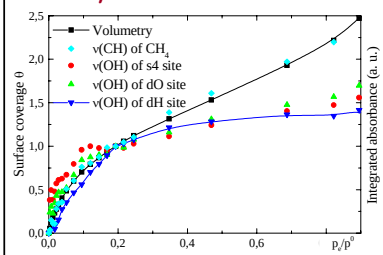


Volumetric isotherms



- CO, N_2 : «strong» interaction with ice, good wetting
- CH_4, Ar, Kr : weaker interaction with ice
- CF_4 : very weak interaction with ice, no wetting

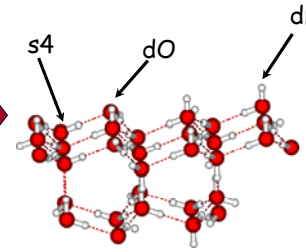
CH_4/Ice IR isotherms



- **Type I (ice)** ⇔ surface phenomenon
- **Type II (CH_4)** ⇔ surface + multilayer

Three surface sites

Using Devlin's notation*



A model of ice surface

* J.P. Devlin et al, *J. Phys. Chem.*, 99 (1995), 16534

References

(1) C. Manca, C. Martin, P. Roubin, *Chem. Phys. Lett.*, 330 (2000), 21
(2) C. Manca, A. Allouche, *J. Chem. Phys.*, 114 (2001), 4226

Conclusions :

- **Different types of wetting**
- **Three adsorption sites on amorphous ice**
- **Surface electric field modification**