Structure of ice surface : evidence for the existence of amorphous and non microporous ice

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Problem

- Measurement of high specific surface area (A)
- Measurement of low heat of adsorption (ΔQ): anomalously low if there is a pore confinement effect
- Does large specific surface prove microporosity ?

➢ Re-investigation of adsorption isotherm studies:

- Comparison of amorphous (Ia) and crystalline (Ic) ices
- Comparison of various adsorbates
- Use of infrared co-measurements to check modifications in ice structure

Experimental conditions

Ice formation

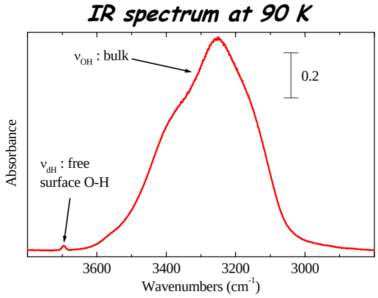
- H_2O:Ar (1:30) gas mixture sprayed into the cell at 40 K.
- Sample slowly annealed (0.2 $K.min^{-1}$) to 90 K at which ice is expected to be amorphous.

Adsorbates

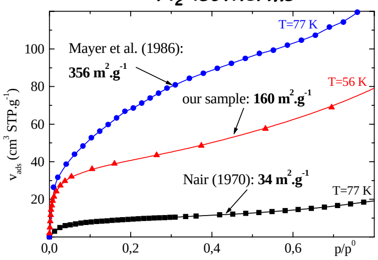
	N_2	CO	CH_4	Ar
Size (Å)	3-4.1	3.7-4.2	4.2	3.8

Ice sample characterization

IR spectrum at 90 K



N_2 isotherms

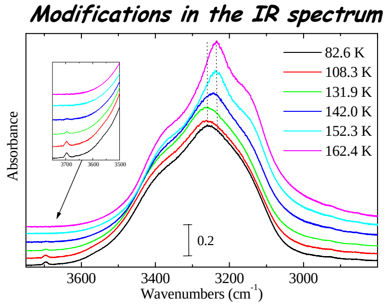


- IR spectrum typical of that of amorphous ice
- Type II isotherms in agreement with other studies
  - ➢ Similar values of A : 100-300 $m^2.g^{-1}$
  - ➢ Similar values of ΔQ : 2.5 $kJ.mol^{-1}$

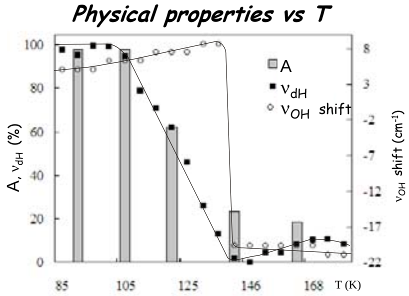
➢ **Analogous physical properties for our samples and for those obtained directly by water vapor deposition**

Ice sample annealing

Modifications in the IR spectrum



Physical properties vs T



- T>110 K : decrease in A and ν_{dH}

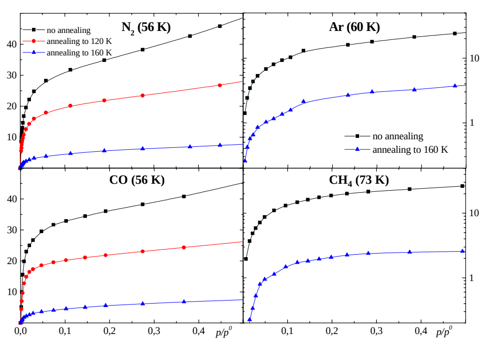
➢ **Surface re-arrangement before crystallization**

- T>150 K : A(Ic) = 15 % A(Ia)
  no more ν_{dH} signal

➢ **Less dH bonds for Ic than for Ia**

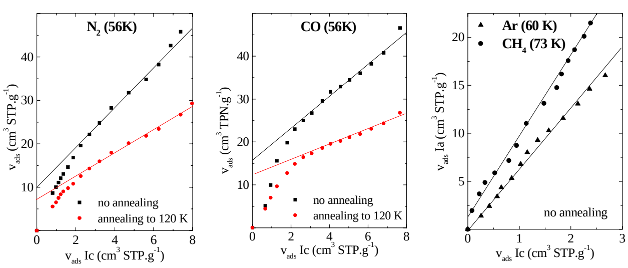
Microporosity analysis

Isotherms on Ia and Ic



- Crystalline ice is taken as reference of non porous material

α-plot



- Deviation from linearity observed only for CO and N_2

➢ **Specific N_2-, CO-dH interactions rather than confinement effet**

Conclusions

- N_2 is not suitable to probe porosity
- Evidence for the existence of amorphous and non microporous ice

➢ Model of grain assembly (size < 65nm) ?

- Open surface favours molecular mobility, diffusion and reactions

➢ Importance for the understanding of interstellar reaction mechanisms ?