# GUDRUN/EPSR data analysis of HCl in water (1:17)

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School of neutron scattering F. P. Ricci Santa Margherita di Pula, 2-10-2008 Neutron diffraction on hydrogen chloride (HCI) in water (1:17)

HCI:H<sub>2</sub>O
DCI:D<sub>2</sub>O
HCI:H<sub>2</sub>O / DCI:D<sub>2</sub>O (50/50)

3 measurements  $\rightarrow$  different interaction of neutrons with H or D (isotopic contrast)





Corrections applied to raw data:

- Dead time
- Background scattering
- Attenuation
- Multiple scattering
- Normalizing to the incident beam monitor
- Vanadium calibration
- Inelastic scattering (for samples)

Corrected after EPSR run with reference potential

#### 1) Calibration of the containers thickness

•HCI:H<sub>2</sub>O  $\rightarrow$  nominal thickness 0.1 cm gives 96.1 % of expected level; thickness 0.095 cm gives 100.9 % of expected level.

DCI:D<sub>2</sub>O  $\rightarrow$  the container thickness is very different from the nominal value. We found that the value 0.0875 cm gives 101.8 % of expected level.

•HCI:H<sub>2</sub>O / DCI:D<sub>2</sub>O (50/50)  $\rightarrow$  good agreement with nominal thickness



Flat top-loading TiZr can for the sample changer

#### 2) Working on the samples



Two measures taken at different times gave 96% and 99.7% of expected value  $\rightarrow$  probably due to slight beam instability. We have considered the average of these two runs (98.2% of expected value)

2) Working on the samples



We observe:

1)Large Q level due to incoherent scattering (density)

2)Inelasticity effects at very small Q observed in hydrogenated samples 3)Peaks structure due to coherent scattering 6

#### 3) Incoherent level subtraction



done later.



Fourier transform of the data gave the total g(r) of the three systems. We note that at 0.98 Å the O-H peak is negative and the O-D is positive because the neutron scattering length of D is positive and for H is negative.

#### **Building the EPSR simulation**



We built the simulation box containing 30 H<sup>+</sup>, 30 Cl<sup>-</sup>, 510 H<sub>2</sub>0.

We employed SPC/E model for water molecules and we ran a simulation with this reference potential:

TABLE I.	Lennard-Jones	and	charge	parameters	used	in	the	simulations
described in	this paper.							

Simulation	Atom	ε (kJ/mol)	$\sigma \; (\rm \AA)$	q(e)
All	0,,	0.6500	3.166	-0.8476
	$H_{w}$	0.0000	0.000	+0.4238
	Cl	0.4190	4.380	-0.9000
$H^{+}$	$H^{+}$	0.0075	0.000	+0.9000

#### **Building the EPSR simulation**



Comparison between experimental data and EPSR run with reference potential only

 $HCI:H_2O$  $DCI:D_2O$  $HCI:H_2O / DCI:D_2O$ 

Using GUDRUN inelasticity effects were corrected by means of a stretched exponential function.



# **EPSR simulation: results Fit to experimental data**

Once inelasticity effects were corrected, the potential refinement has been switched on. After thermalization configurations have been accumulated.



#### EPSR simulation: results (1) Water-water RDFs



C:\EPSR17\20080617\_EPSR17\run\HCI\exNAFAVA\solution

# EPSR simulation: results (2) O-O spatial density function (SDF)



2.0-3.3 Å

2.0-4.8 Å

2.0-2.5 Å probable  $H_3^+O-H_2O$  structure

# EPSR simulation: results (3) H<sup>+</sup>-water RDFs



# EPSR simulation: results (4) Cl<sup>-</sup>-water RDFs



#### EPSR simulation: results (5) Ion-ion RDFs



#### Large anion-cation peak

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CI<sup>-</sup> - H<sup>+</sup> RDF and coordination number



Solvent separated ions 16 pairing

#### Conclusions

How does HCI modify the structure of water?

•The double peak structure in the H\*-O RDF and the peak in the O-O RDF at 2.4 Å could be interpreted as:

1) O-H<sup>+</sup>-O structure (delocalized proton)

or as

2) H<sub>3</sub><sup>+</sup>O-H<sub>2</sub>O structure



Presence of solvent separated ions pairing



# **FAIL SAFE**

# Dario Don't touch



#### Amplitude=1; decay constant=1; stretch constant=1



