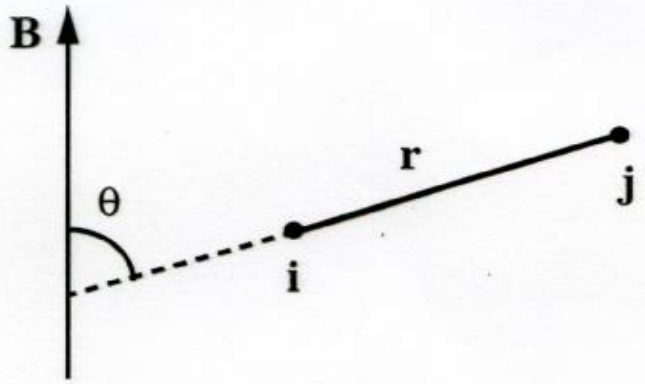
Brønsted acidity=transfer of proton

Solid-OH + ads. Mol. ⇆

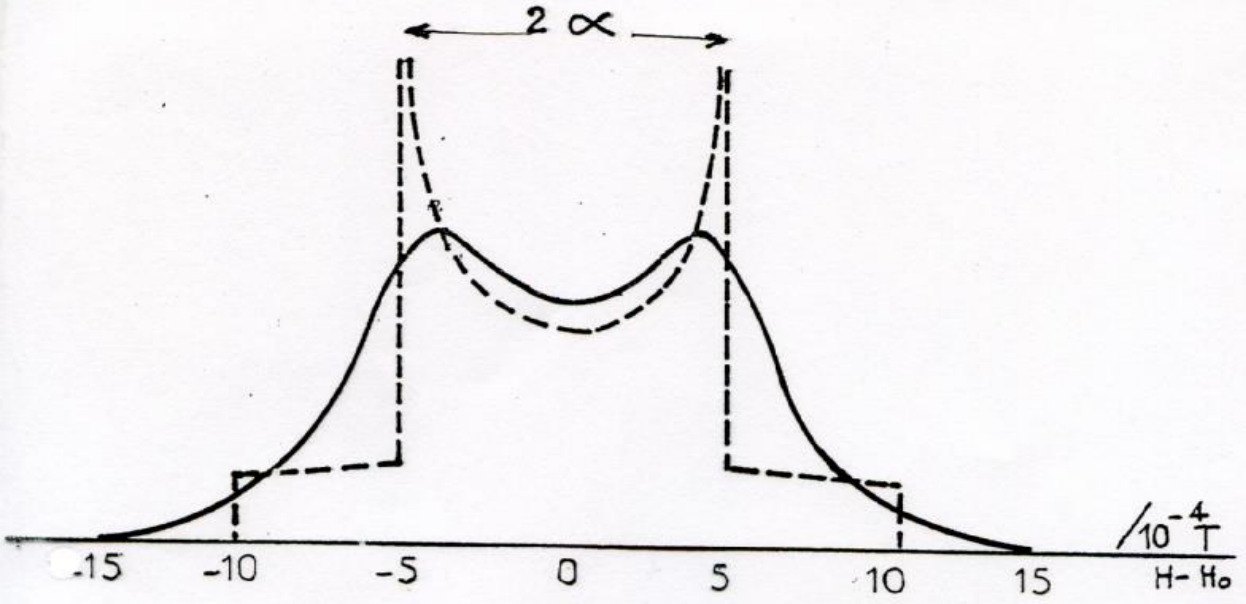
Solid-O^- + (H-ads.mol)+

DIPOLAR MAGNETIC INTERACTION BETWEEN TWO ^{1}H NUCLEI (DMI)

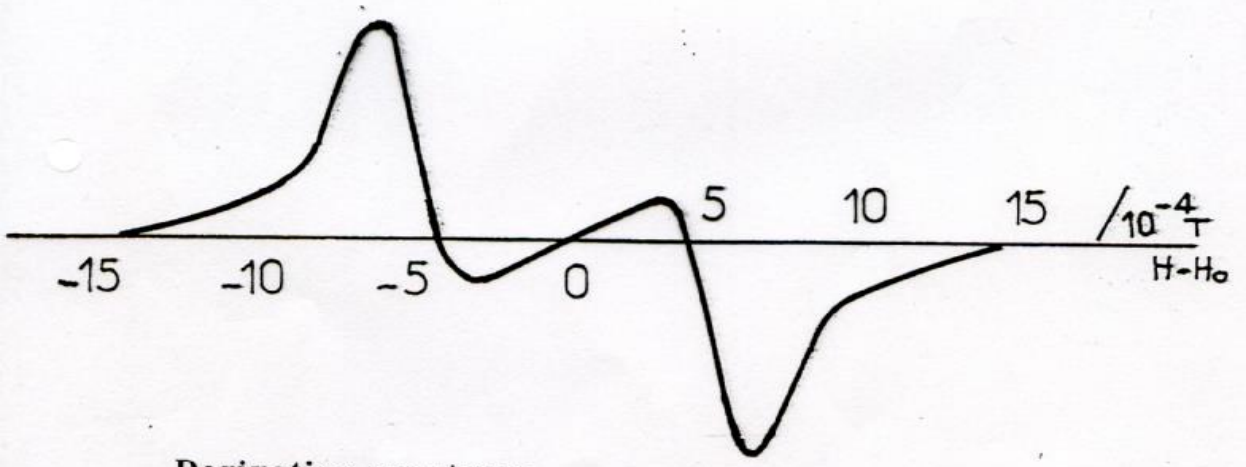
$$DMI = CONSTANT \cdot (1 - 3\ COS^2\ \theta) \cdot r^{-3}$$



For powder samples the interactions must be summer up over all directions.



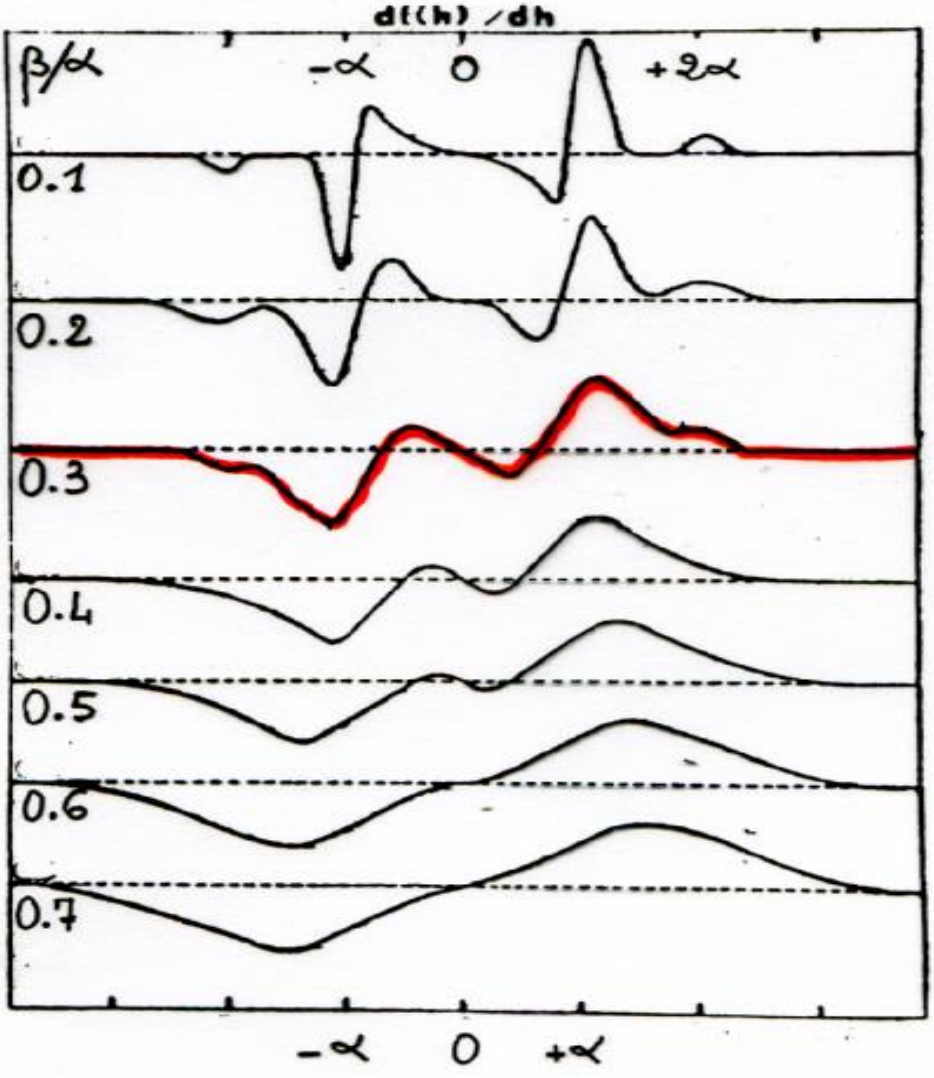
Isolated, isotropically oriented spin 1/2 pairs ----
Real adsorption spectrum ——

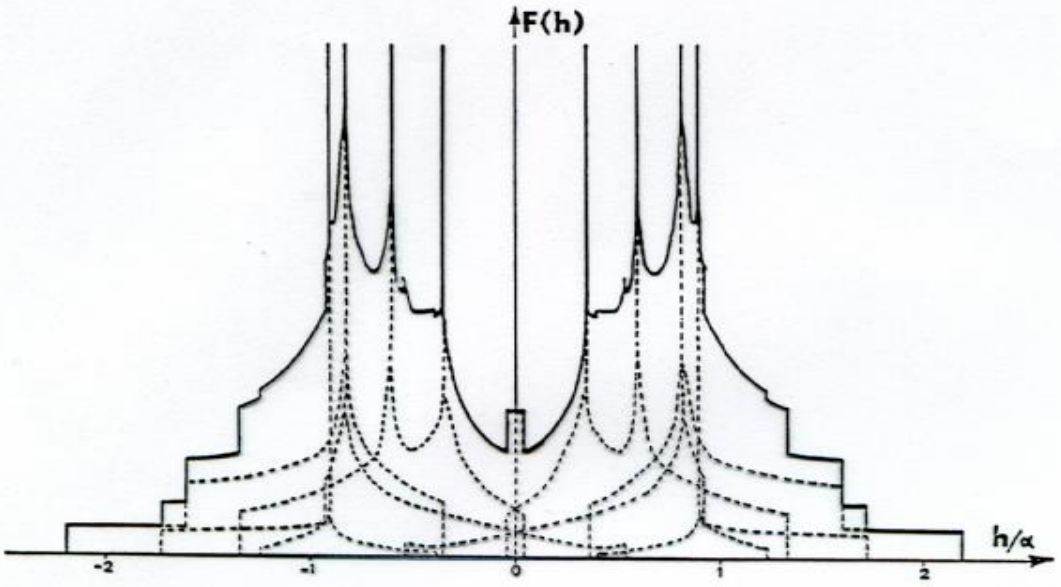


Derivative spectrum

$\alpha = \frac{3}{2}\mu r^{-3}$ $\beta = \frac{3}{2}\mu x^{-3}$ μ = magnetic moment

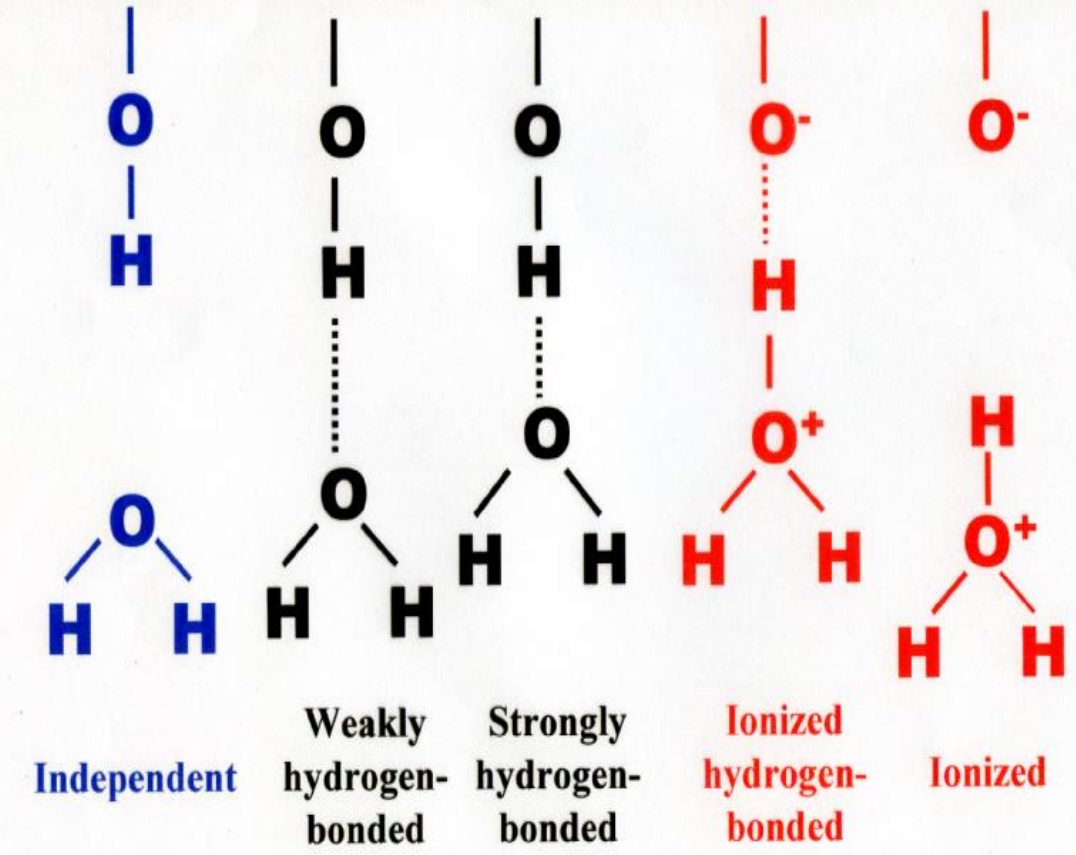
r = distance between the two ^1H

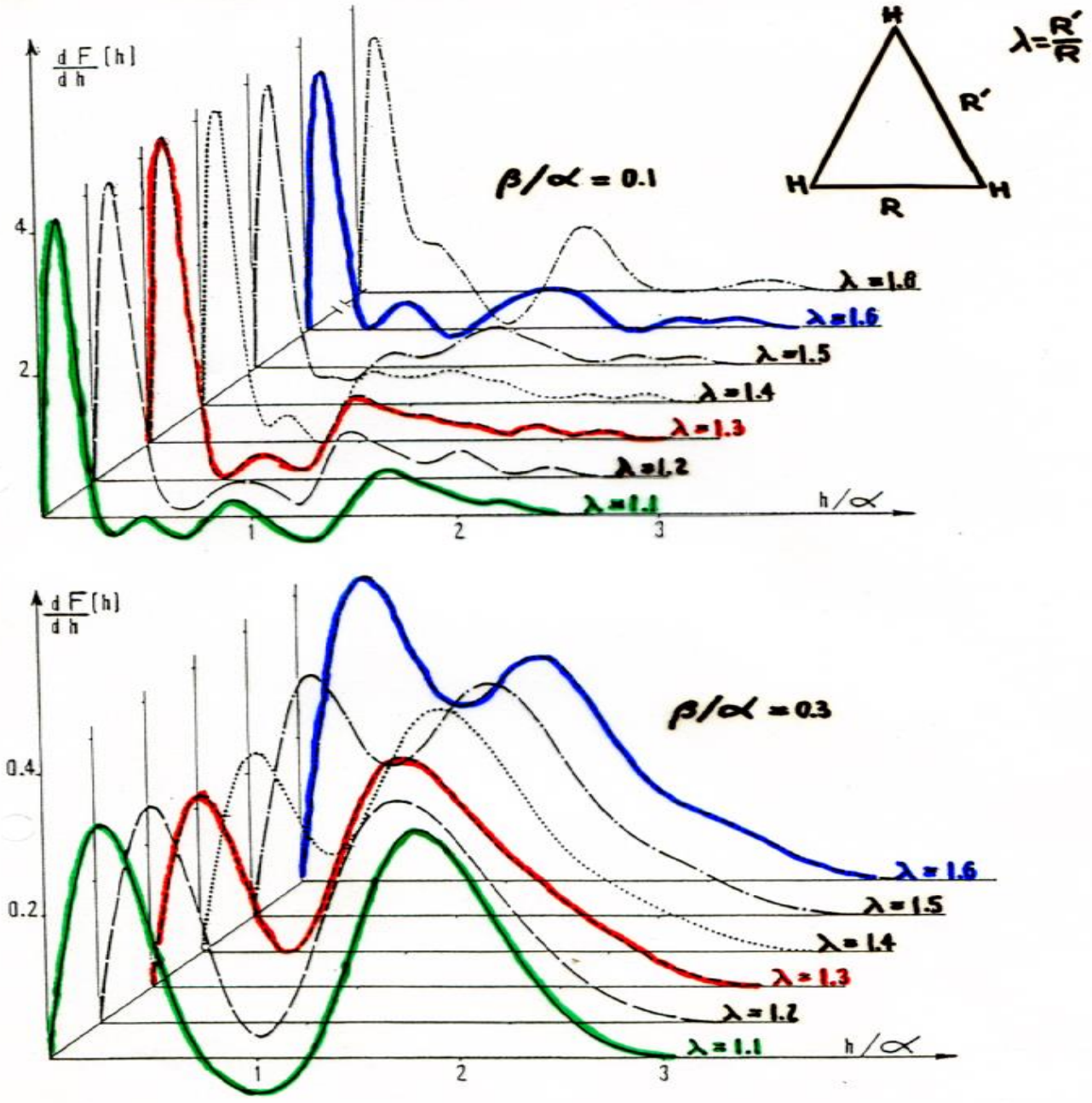

d((h) /dh
β/α
-α
0
+2α
0.1
0.2
0.3
0.4
0.5
0.6
0.7
-α
0
+α



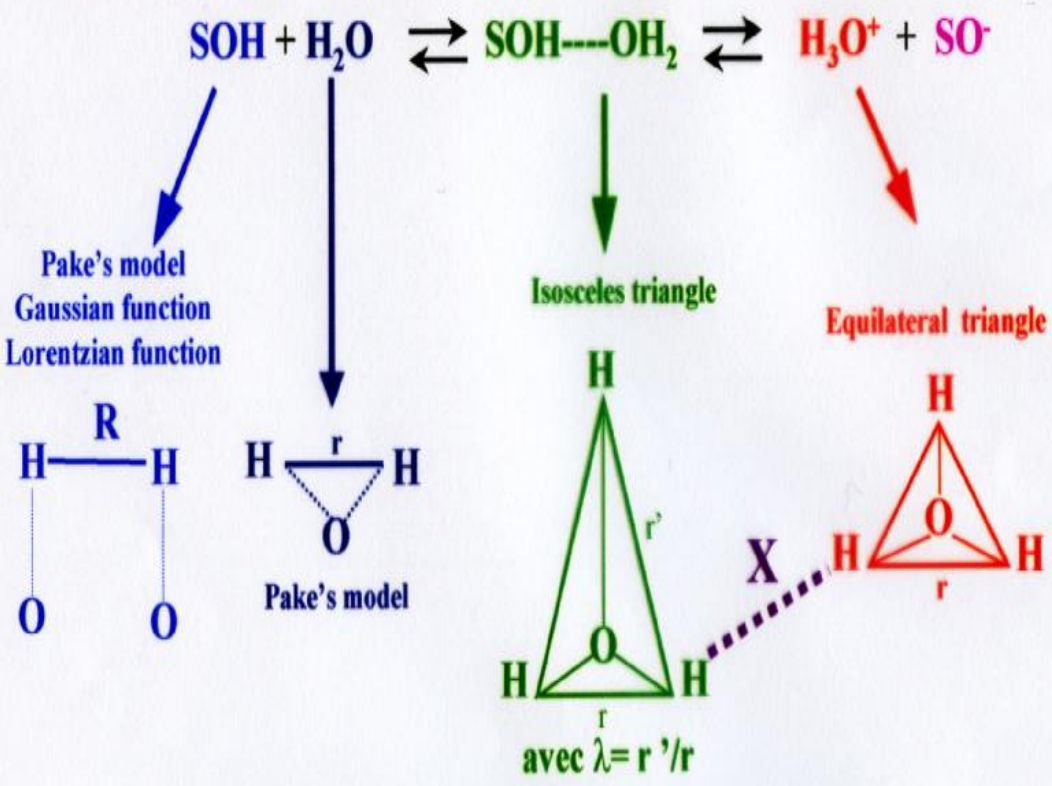
Shapes of the individual lines (----) and of the total absorption (——) for isolated isosceles triangular magnetic configurations of spins 1/2 isotropically orientated in the space; the ratio λ of one of the equal sides to the base of the triangle is 1.30.

Interactions between a water molecule and an OH group




$\frac{dF[h]}{dh}$
$\beta/\alpha = 0.1$
H
R'
H
H
R
$\lambda = \frac{R'}{R}$
4
2
$\lambda = 1.6$
$\lambda = 1.5$
$\lambda = 1.4$
$\lambda = 1.3$
$\lambda = 1.2$
$\lambda = 1.1$
h/α
1
2
3
$\frac{dF[h]}{dh}$
$\beta/\alpha = 0.3$
0.4
0.2
$\lambda = 1.6$
$\lambda = 1.5$
$\lambda = 1.4$
$\lambda = 1.3$
$\lambda = 1.2$
$\lambda = 1.1$
h/α
1
2
3

Equilibria between OH groups and water molecules
Magnetic configurations of the species are shown

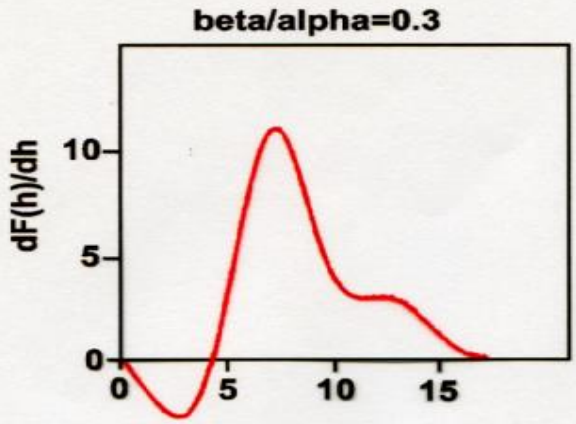


Internal parameters : $r, R \leftrightarrow \alpha \approx \frac{1}{r^3}, \frac{1}{R^3}$

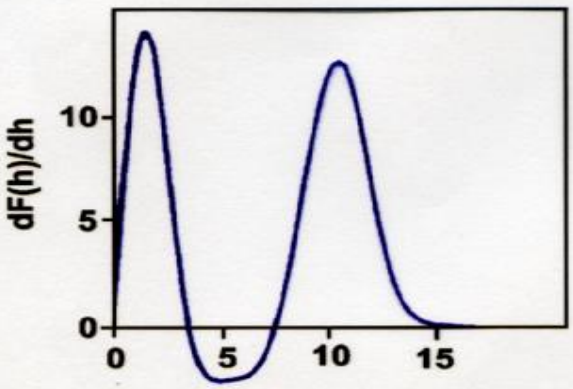
Gaussian function : $X \leftrightarrow \beta \approx \frac{1}{X^3}$

External parameters

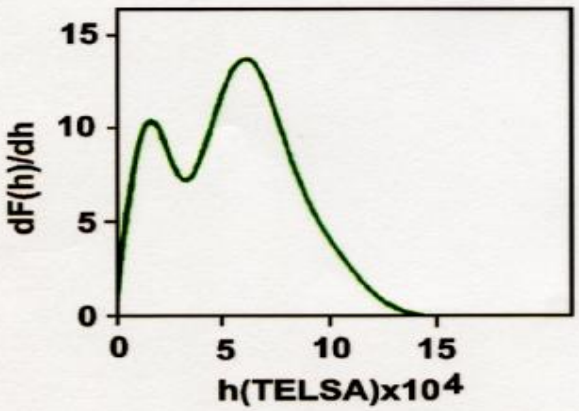
Evolution des spectres 2 spins et 3 spins



2 spins H_2O
r = 150 pm



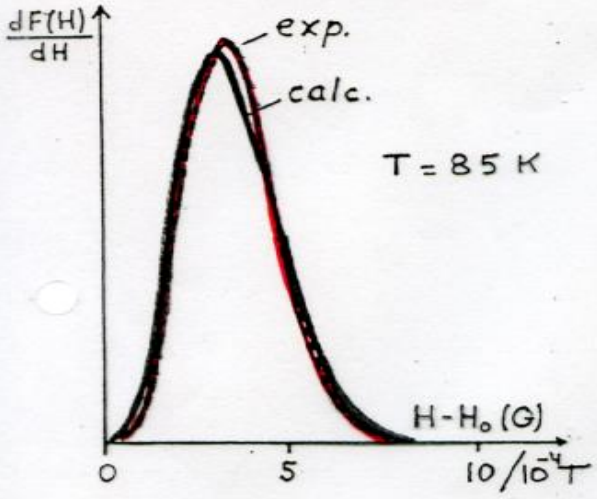
3 spins (triangle équilatéral)
r = 165 pm

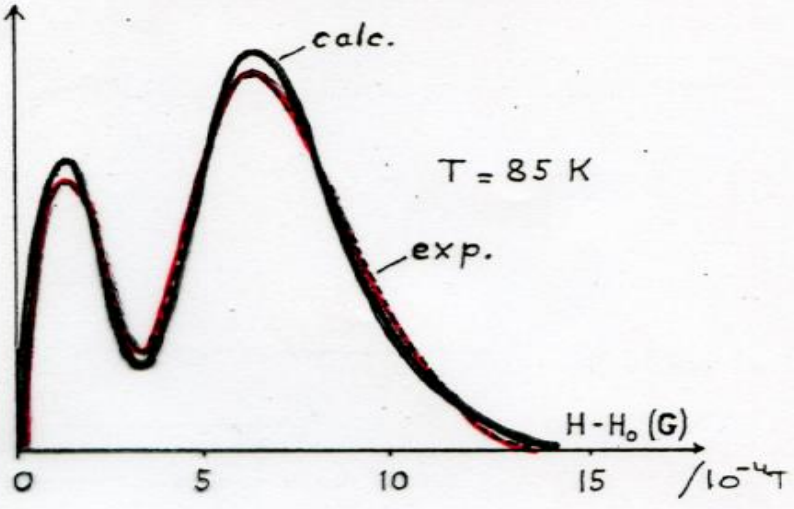


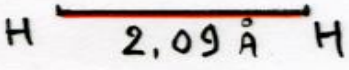
3 spins (triangle isocèle)
r = 160 pm ; r' = 224 pm

$AlH_6P_3O_{12}$

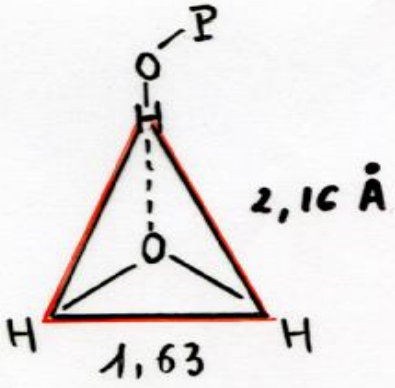
$Al(H_2PO_4)_3$ | $H_2(AlP_3O_{10}).2H_2O$



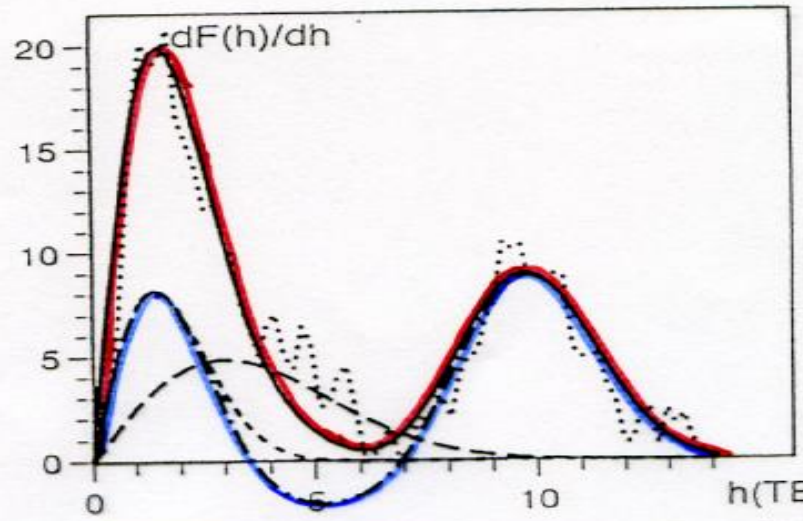




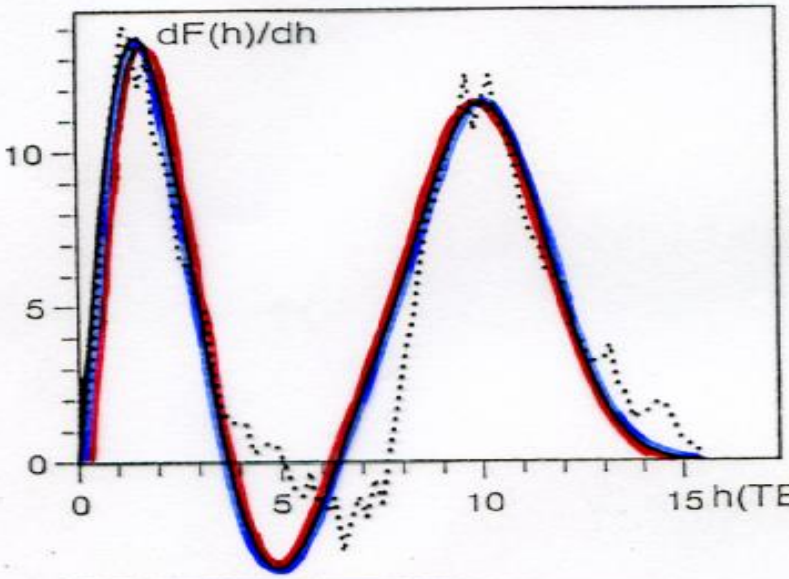
X = 2,51 Å



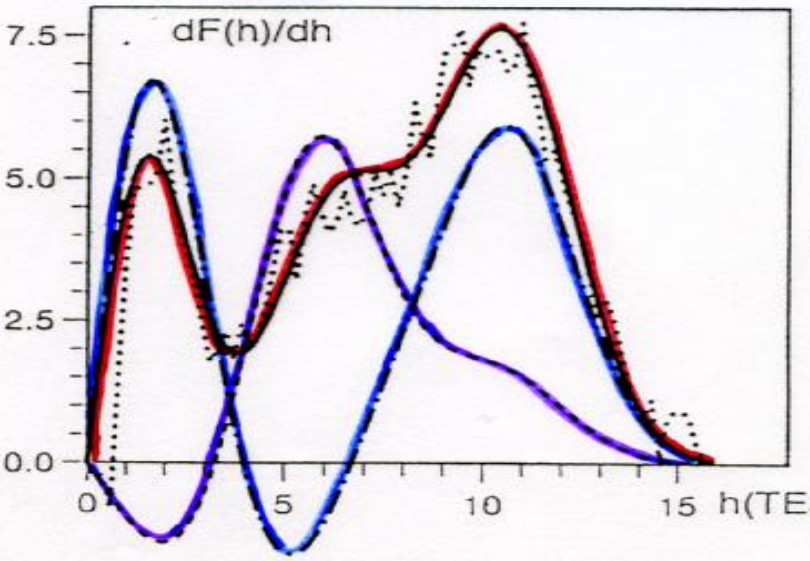
X = 2,40 Å



NAFION-H.0.51H_2O



NAFION-H.1.0H_2O

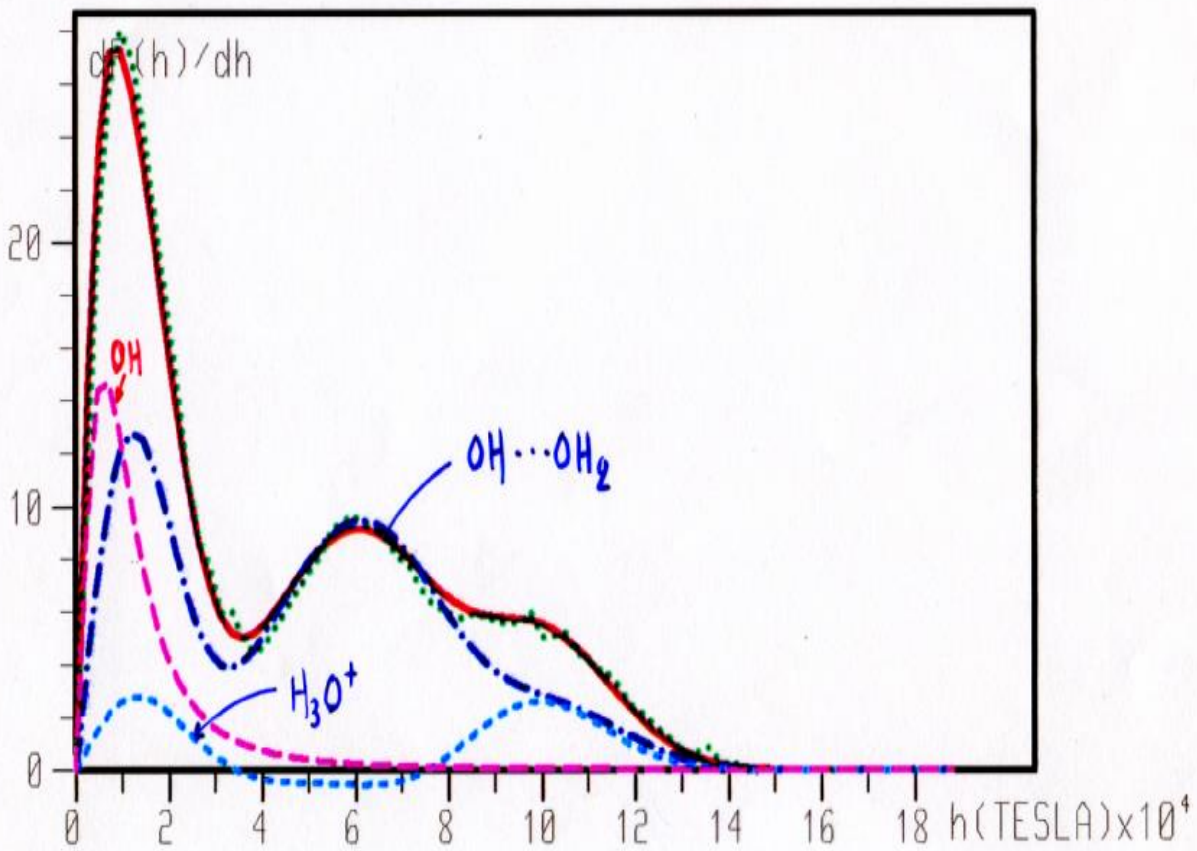


NAFION-H.2.1H_2O

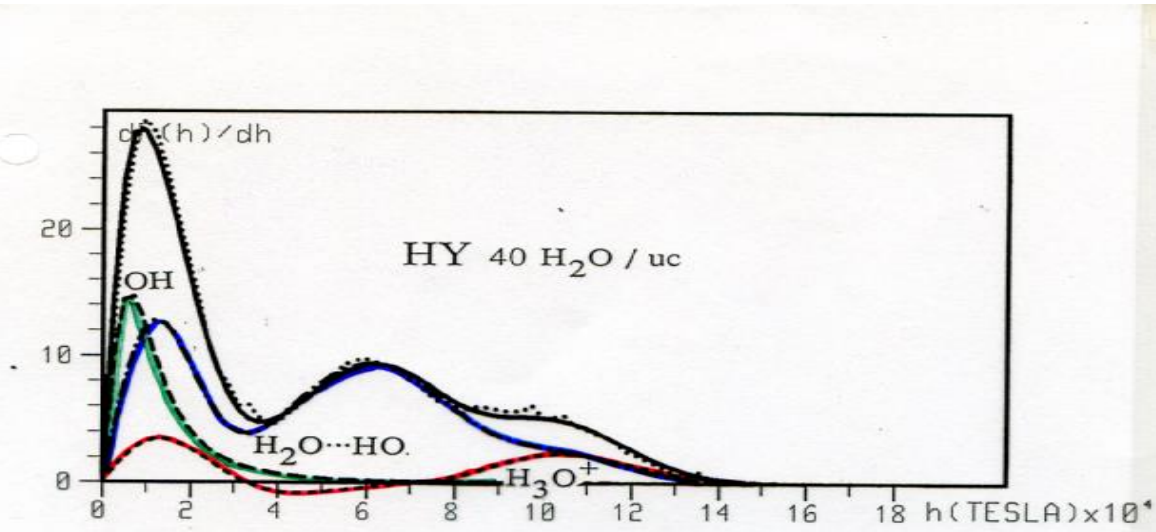
HY,48 OH/uc, +40 H_2O

cd:38

s848Y64,40-33s085
EPSIL=0.0001 NOMBRE DE GAUSS PAR PAS= 0.238000
COURBE CALCULEE
COURBE EXPERIMENTALE
T. ISOCELE OMEGA=0.7300 R=1.600A. X=2.530A. ALP=5.164G. BETA=1.306G. GAM=0.253 LAM=1.460 R'=2.336A. CD= 0.000G.
T. EQUILATERAL OMEGA=0.1900 R=1.660A. X=2.480A. ALP=4.624G. BETA=1.387G. GAM=0.300 LAM=0.000 R'=0.000A. CD= 0.000G.
F. LORENTZIENNE OMEGA=0.0800 R=0.000A. X=0.000A. ALP=0.000G. BETA=0.000G. GAM=0.000 LAM=0.000 R'=0.000A. CD= 1.050G.

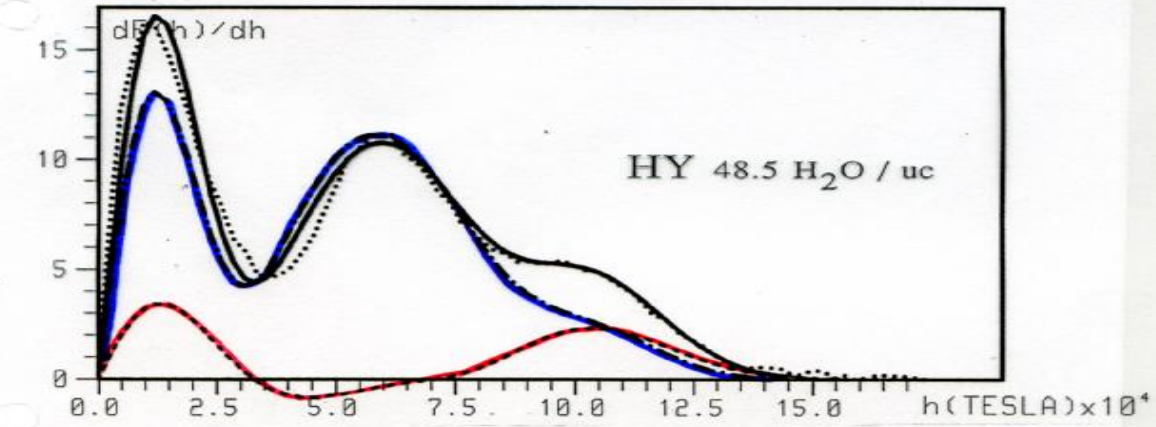


HY, 48 OH/uc, + H_2O

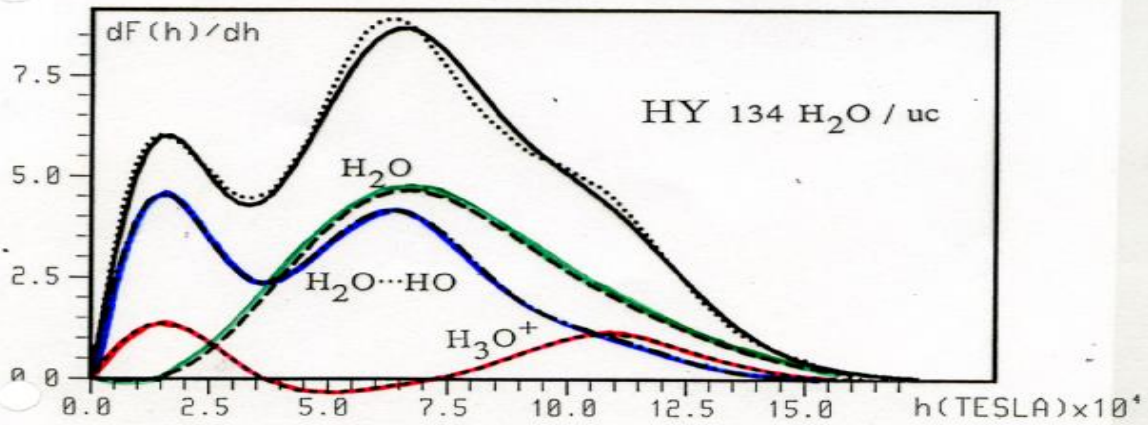


48 OH

40 H_2O

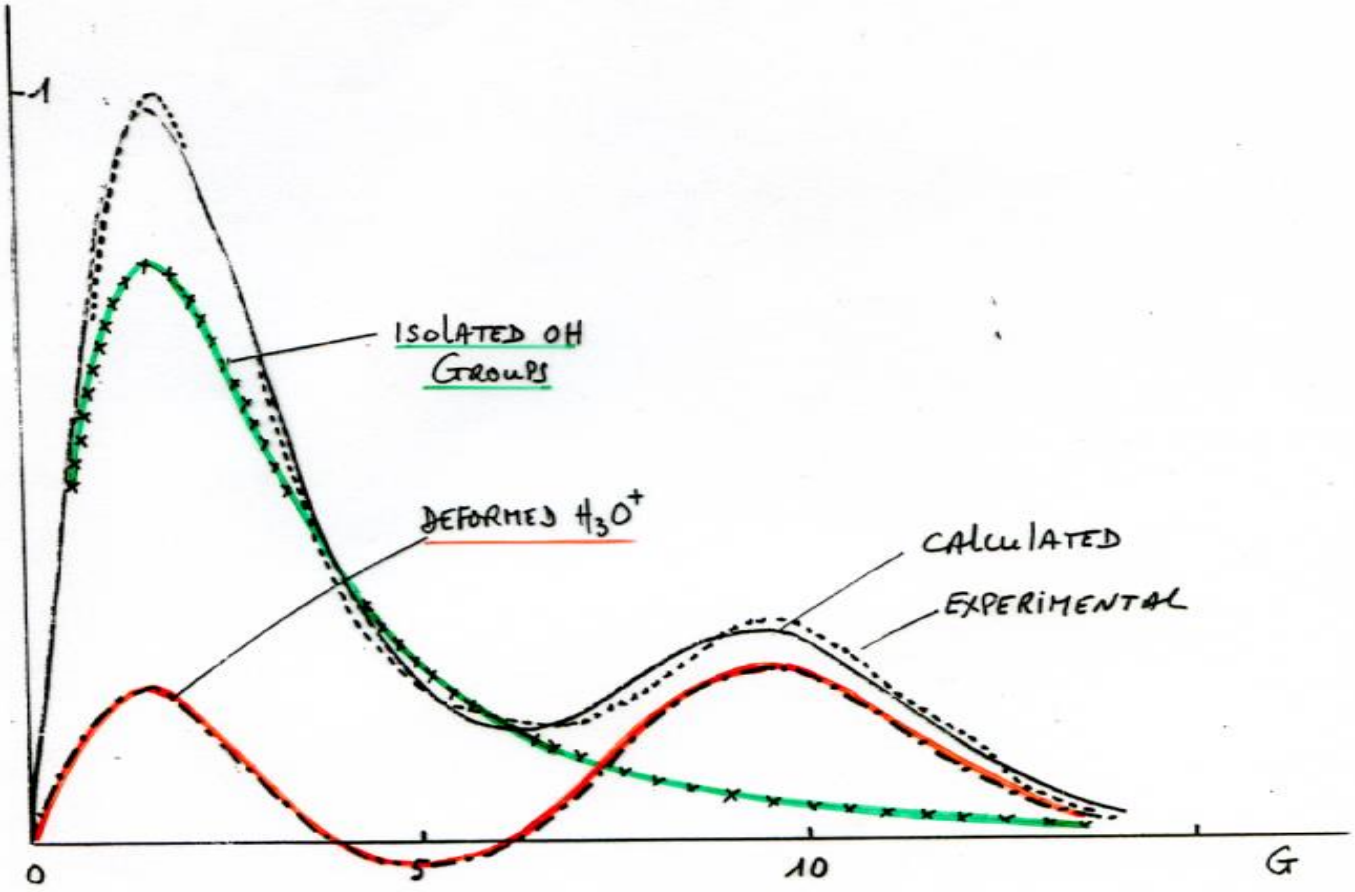


48.5 H_2O

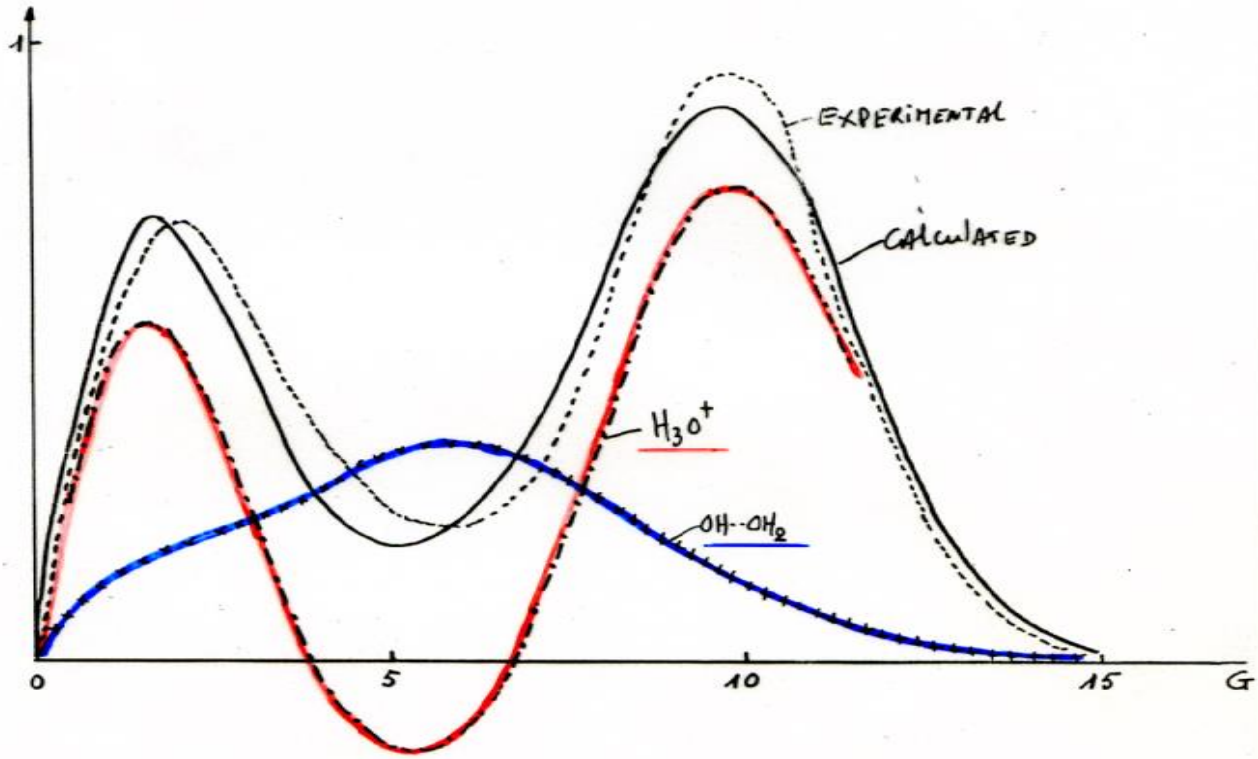


134 H_2O

- **Protonic conductors**



$$H(H_2O)_{0.2}SbO_3 \longrightarrow (H_3O)_{0.2}\ H_{0.8}SbO_3$$



$$H(H_2O)SbO_3 \longrightarrow (H_3O)_{0.7}\ \underline{H_{0.3}\cdots(H_2O)_{0.3}}\ SbO_3$$