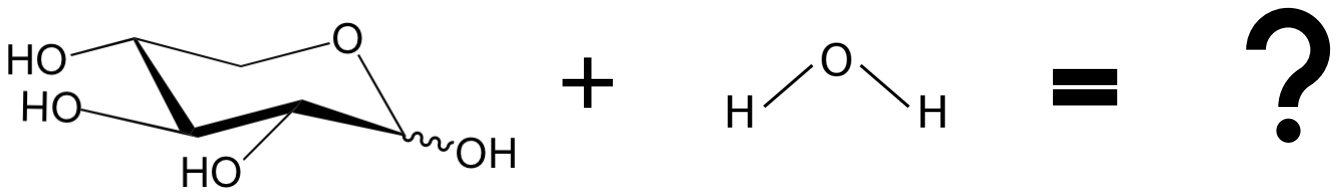
Universidad de Valladolid

76th International Symposium on Molecular Spectroscopy

FIRST MONOSACCHARIDE-WATER COMPLEX CAUGHT BY MICROWAVE SPECTROSCOPY

Elena R. Alonso*[a], Aran Insausti[b], Iker León[a] and Emilio J. Cocinero[b]



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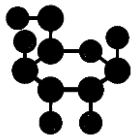
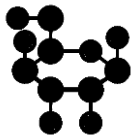
[b] Departamento de Química Física. Universidad del País Vasco (UPV-EHU, Spain).

June 2023

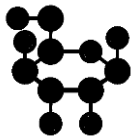
MOTIVATION OF THIS WORK



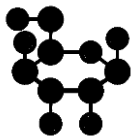
Carbohydrates are one of the major biomolecule playing a key role in many biological systems.



Their molecular structure is essential for an understanding of their function and the molecular basis of their macroscopic properties.



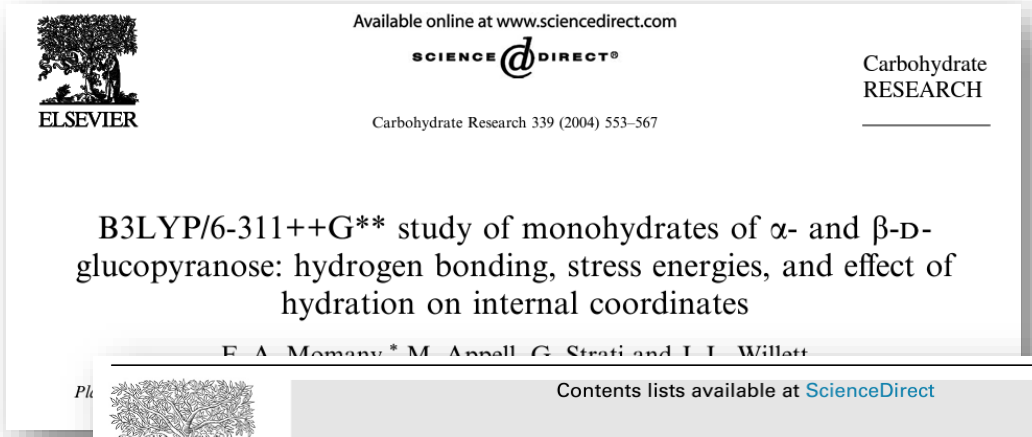
They perform their biological activity in aqueous environments.



Limited microscopic knowledge on how water interacts with monosaccharides.

MOTIVATION OF THIS WORK

A LOT OF COMPUTATIONAL CHEMISTRY RESEARCH ON SUGAR-WATER INTERACTIONS


Available online at www.sciencedirect.com

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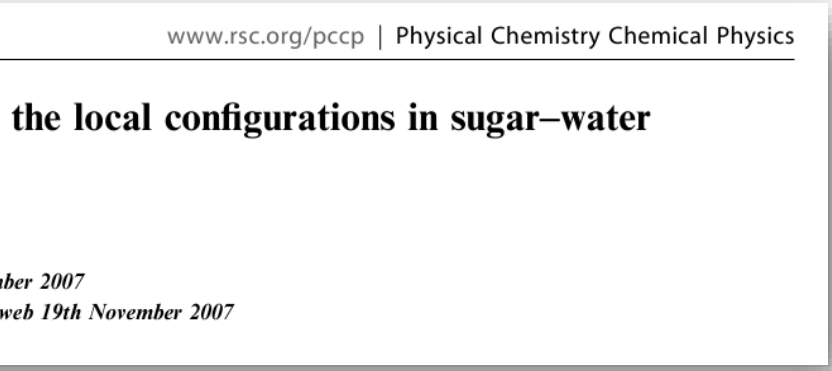
Carbohydrate RESEARCH

Carbohydrate Research 339 (2004) 553–567

ELSEVIER

B3LYP/6-311++G** study of monohydrates of α- and β-D-glucopyranose: hydrogen bonding, stress energies, and effect of hydration on internal coordinates

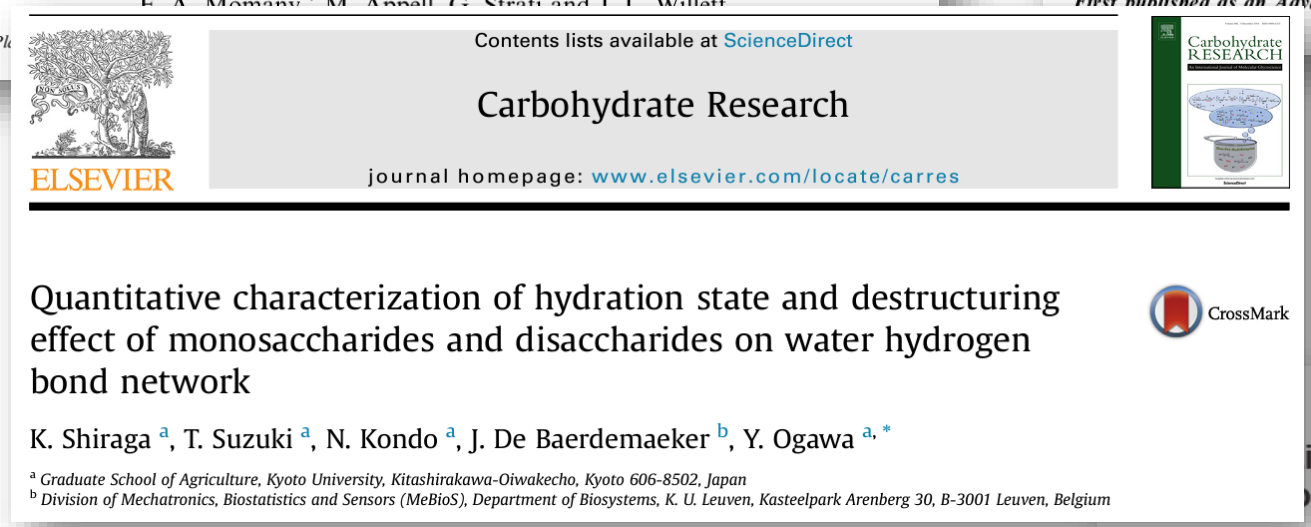

PAPER www.rsc.org/pccp | Physical Chemistry Chemical Physics

The hydration of glucose: the local configurations in sugar–water hydrogen bonds†

Teppei Suzuki*

Received 8th June 2007, Accepted 6th November 2007

First published as an Advance Article on the web 19th November 2007


Contents lists available at ScienceDirect

Carbohydrate Research

journal homepage: www.elsevier.com/locate/carres

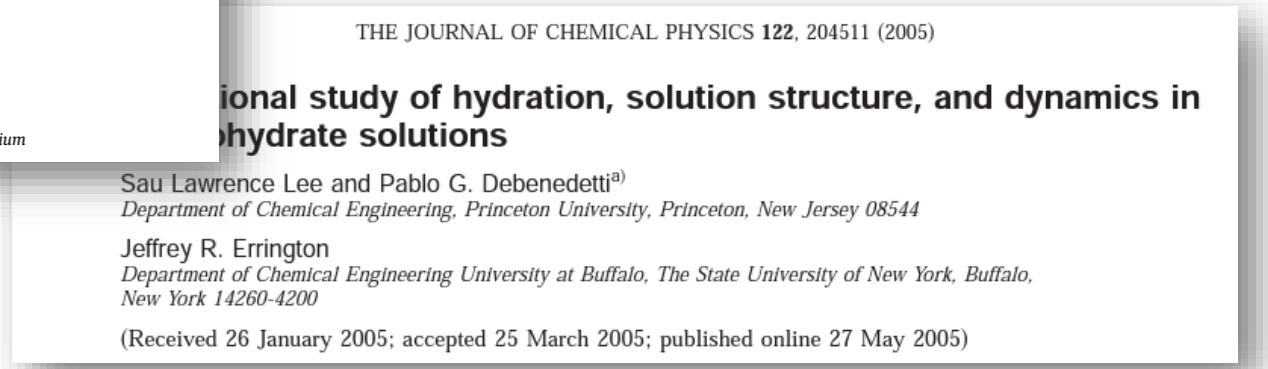
ELSEVIER

Quantitative characterization of hydration state and destructuring effect of monosaccharides and disaccharides on water hydrogen bond network

K. Shiraga [a], T. Suzuki [a], N. Kondo [a], J. De Baerdemaeker [b], Y. Ogawa [a,*]

[a] Graduate School of Agriculture, Kyoto University, Kitashirakawa-Oiwakecho, Kyoto 606-8502, Japan

[b] Division of Mechatronics, Biostatistics and Sensors (MeBioS), Department of Biosystems, K. U. Leuven, Kasteelpark Arenberg 30, B-3001 Leuven, Belgium


THE JOURNAL OF CHEMICAL PHYSICS **122**, 204511 (2005)

…ional study of hydration, solution structure, and dynamics in …hydrate solutions

Sau Lawrence Lee and Pablo G. Debenedetti[a)]

Department of Chemical Engineering, Princeton University, Princeton, New Jersey 08544

Jeffrey R. Errington

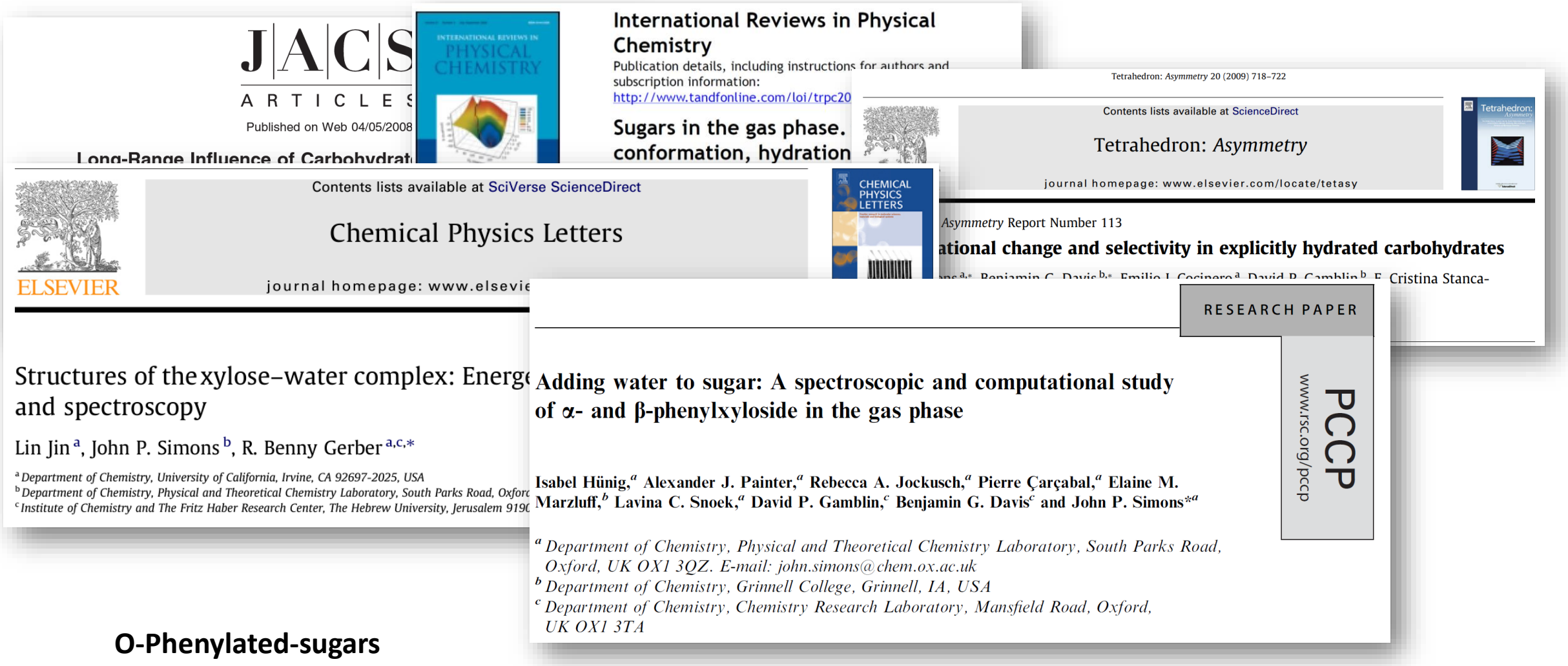
Department of Chemical Engineering University at Buffalo, The State University of New York, Buffalo, New York 14260-4200

(Received 26 January 2005; accepted 25 March 2005; published online 27 May 2005)

many, many more…

MOTIVATION OF THIS WORK

ALSO THERE IS EXPERIMENTAL RESEARCH ON SUGAR-WATER INTERACTIONS

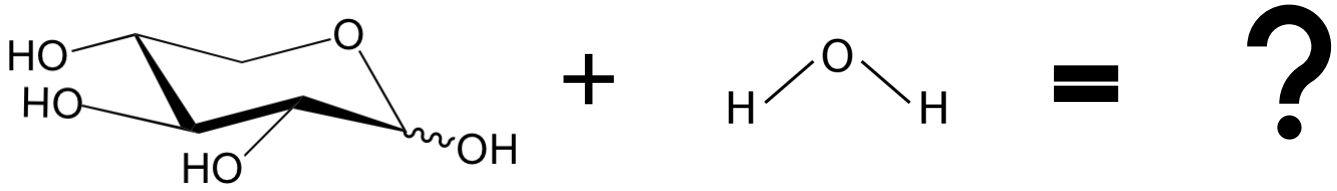


O-Phenylated-sugars

MOTIVATION OF THIS WORK

BUT THERE IS A LACK OF EXPERIMENTAL DATA OF MONOSACCHARIDES-WATER COMPLEXES IN ISOLATION CONDITIONS….

CHARACTERIZE FOR THE FIRST TIME A MONOSACCHARIDE-WATER COMPLEX

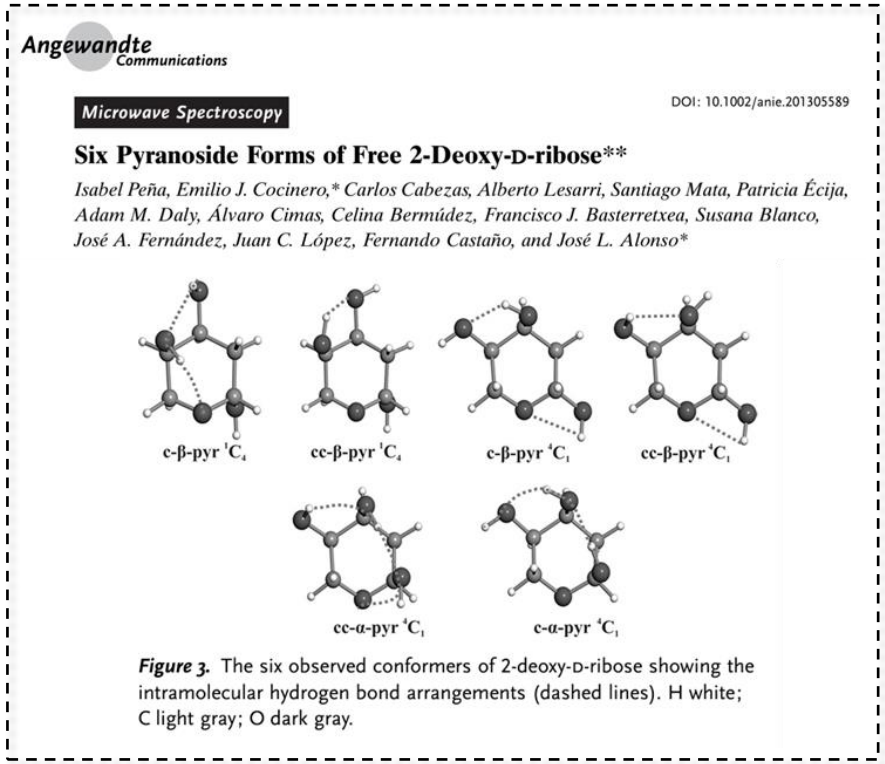


USING HIGH RESOLUTION MICROWAVE SPECTROSCOPY

What system is the best to tackle first?

BACKGROUND

IN OUR GROUP THERE IS PREVIOUS EXPERIENCE IN THE STUDY OF MONOSACCHARIDES



Angewandte Communications

Microwave Spectroscopy

DOI: 10.1002/anie.201305589

Six Pyranoside Forms of Free 2-Deoxy-D-ribose**

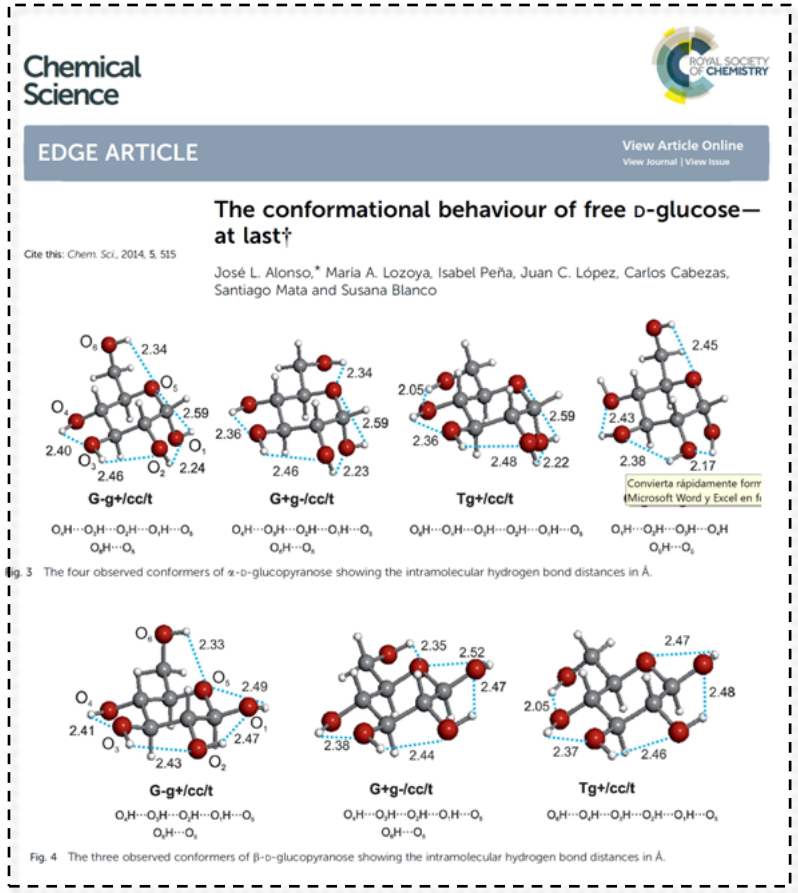
Isabel Peña, Emilio J. Cocinero, Carlos Cabezas, Alberto Lesarri, Santiago Mata, Patricia Écija, Adam M. Daly, Álvaro Cimas, Celina Bermúdez, Francisco J. Basterretxea, Susana Blanco, José A. Fernández, Juan C. López, Fernando Castaño, and José L. Alonso**

c-β-pyr $^1C_4$ cc-β-pyr $^1C_4$ c-β-pyr $^4C_1$ cc-β-pyr $^4C_1$

cc-α-pyr $^4C_1$ c-α-pyr $^4C_1$

Figure 3. The six observed conformers of 2-deoxy-D-ribose showing the intramolecular hydrogen bond arrangements (dashed lines). H white; C light gray; O dark gray.

6 conformers



Chemical Science

EDGE ARTICLE

View Article Online

The conformational behaviour of free D-glucose—at last†

Cite this: *Chem. Sci.*, 2014, 5, 515

José L. Alonso,* María A. Lozoya, Isabel Peña, Juan C. López, Carlos Cabezas, Santiago Mata and Susana Blanco

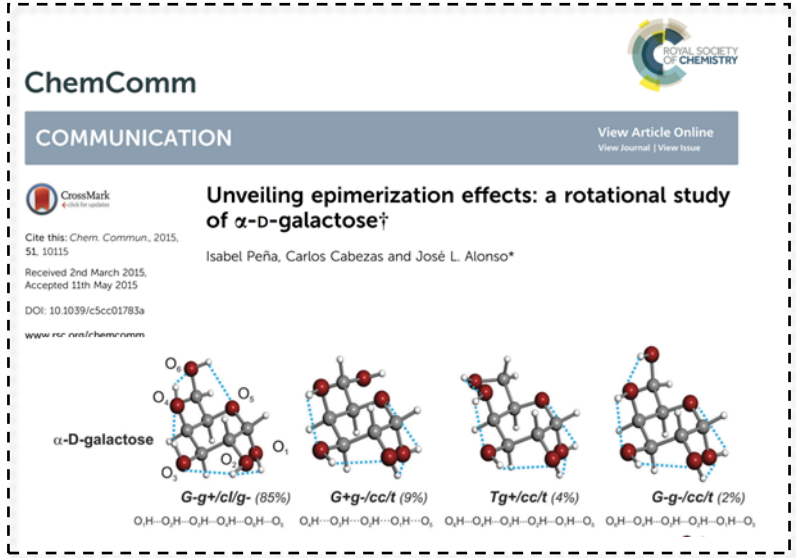
G-g+/cc/t G+g-/cc/t Tg+/cc/t

Fig. 3 The four observed conformers of α-D-glucopyranose showing the intramolecular hydrogen bond distances in Å.

G-g+/cc/t G+g-/cc/t Tg+/cc/t

Fig. 4 The three observed conformers of β-D-glucopyranose showing the intramolecular hydrogen bond distances in Å.

4 conformers of α-anomer
3 conformers of β-anomer



ChemComm

COMMUNICATION

View Article Online

Unveiling epimerization effects: a rotational study of α-D-galactose†

Cite this: *Chem. Commun.*, 2015, 51, 10115

Received 2nd March 2015, Accepted 11th May 2015

DOI: 10.1039/c5cc01783a

Isabel Peña, Carlos Cabezas and José L. Alonso*

α-D-galactose

G-g+/cl/g- (85%) *G+g-/cc/t* (9%) *Tg+/cc/t* (4%) *G-g-/cc/t* (2%)

4 conformers

BACKGROUND

IN OUR GROUP THERE IS PREVIOUS EXPERIENCE IN THE STUDY OF MONOSACCHARIDES

→ **2 conformers**

→ **Intense spectra**

→ **^{13}C characterized**

PCCP RSC Publishing

PAPER View Article Online
View Journal | View Issue

Conformations of D-xylose: the pivotal role of the intramolecular hydrogen-bonding†

Cite this: *Phys. Chem. Chem. Phys.*, 2013, **15**, 18243

Isabel Peña, Santiago Mata, Agustín Martín, Carlos Cabezas, Adam M. Daly and José L. Alonso*

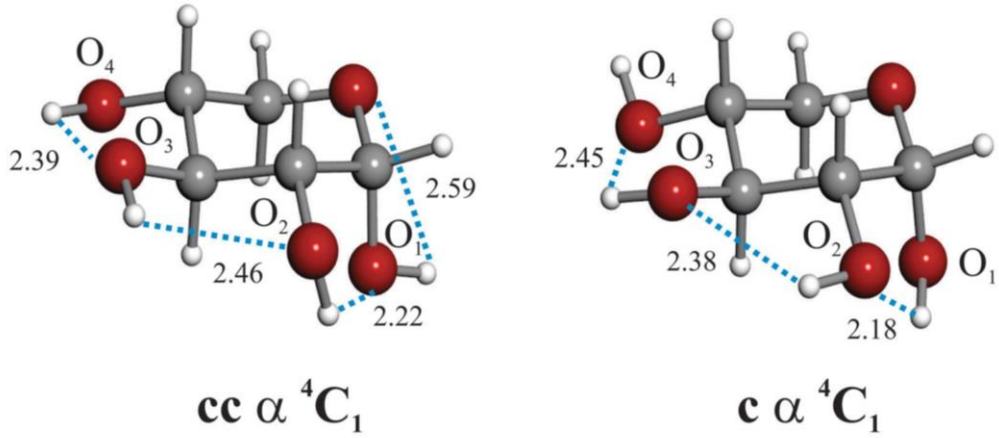


Fig. 4 The three dimensional structures of the two observed conformers of a-D-xylose showing the intramolecular hydrogen bond distances in Å.

EXPERIMENTAL APPROACH

Sugars have high melting points, besides being thermolabile compounds

LASER ABLATION SYSTEM
EKSPLA Nd-YAG picosecond laser

THE JOURNAL OF PHYSICAL CHEMISTRY LETTERS
A JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
pubs.acs.org/JPCL

Shape of Testosterone

Iker León,* Elena R. Alonso, Santiago Mata, and José L. Alonso

Cite This: *J. Phys. Chem. Lett.* 2021, 12, 6983–6987 Read Online

GDCh Communications Angewandte International Edition Chemie
Astrochemistry
How to cite: *Angew. Chem. Int. Ed.* **2021**, *60*, 17410–17414
International Edition: doi.org/10.1002/anie.202105718
German Edition: doi.org/10.1002/ange.202105718

Unveiling Five Naked Structures of Tartaric Acid

*Elena R. Alonso, Iker León, Lucie Kolesniková, Santiago Mata, and Jose Luis Alonso**

Chemistry–A European Journal | Research Article doi.org/10.1002/chem.202203990
Chemistry Europe European Chemical Societies Publishing
www.chemeurj.org

Bringing Machine-Learning Enhanced Quantum Chemistry and Microwave Spectroscopy to Conformational Landscape Exploration: the Paradigmatic Case of 4-Fluoro-Threonine

V. Barone,*[a] M. Fusè,[a] R. Aguado,[b] S. Potenti,[a, c] I. León,[b] E. R. Alonso,[b] S. Mata,[b] F. Lazzari,[a] G. Mancini,[a] L. Spada,[a] A. Gualandi,[c] P. G. Cozzi,[c] C. Puzzarini,*[c] and J. L. Alonso*[b]

Raúl Aguado
TK03

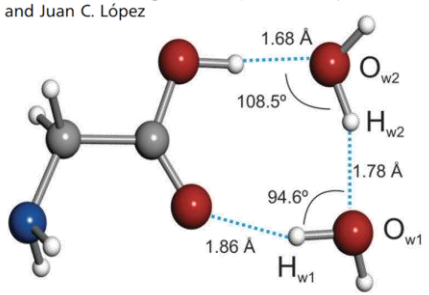
Laser ablation and the formation of water complexes may be adverse processes

ChemComm RSCPublishing
COMMUNICATION View Article Online View Journal | View Issue

Observation of dihydrated glycine†

Cite this: *Chem. Commun.*, 2013, **49**, 3443

José L. Alonso,* Isabel Peña, M. Eugenia Sanz,‡ Vanesa Vaquero, Santiago Mata, Carlos Cabezas and Juan C. López



CHIRAL RECOGNITION OF NEUTRAL ALANINE: A LASER ABLATION ROTATIONAL STUDY

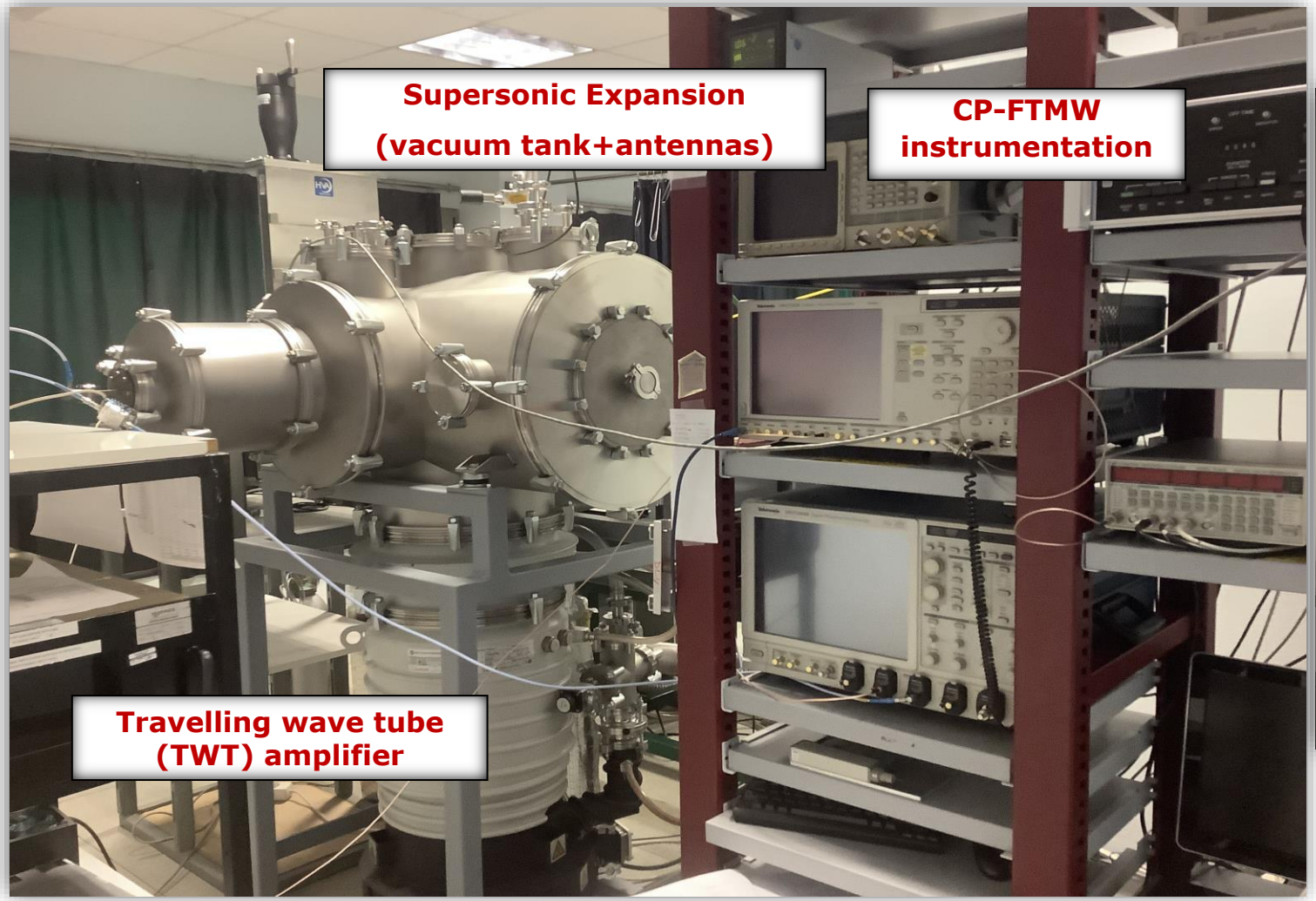
RAÚL AGUADO, SANTIAGO MATA, ELENA R. ALONSO, IKER LEÓN, JOSÉ L. ALONSO, *Grupo de Espectroscopia Molecular, Lab. de Espectroscopia y Bioespectroscopia, Unidad Asociada CSIC, Universidad de Valladolid, Valladolid, Spain.*

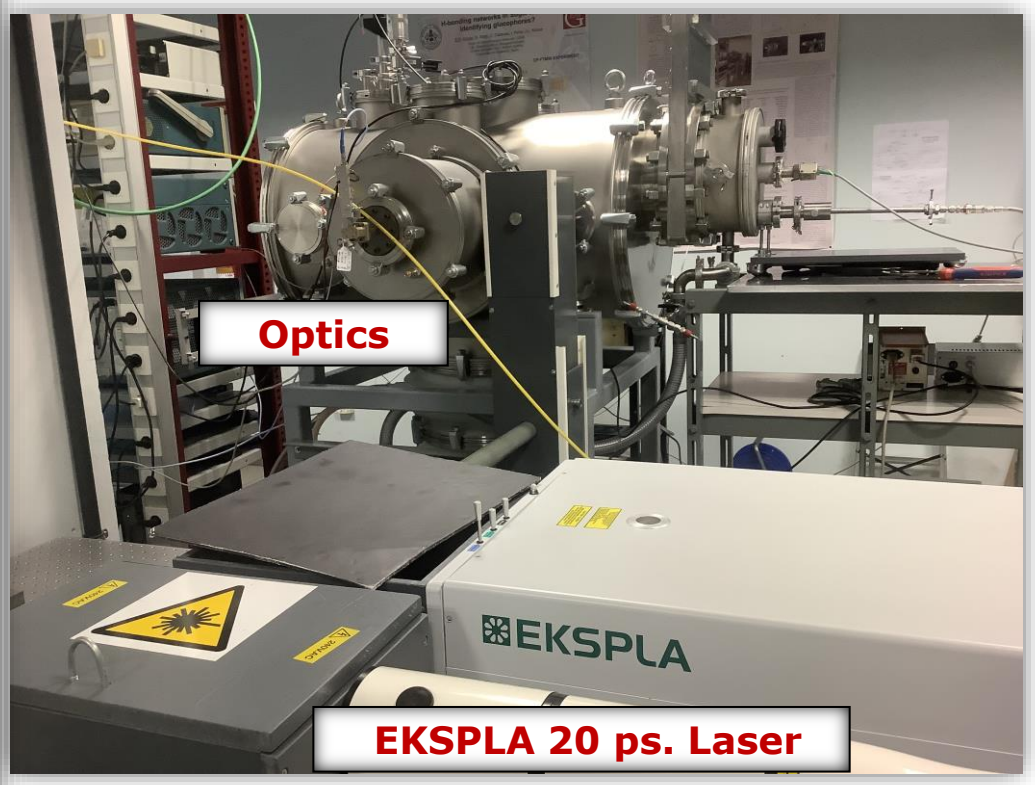
Raúl Aguado
WF06

EXPERIMENTAL METHODOLOGY

Laser Ablation Chirped Pulsed Fourier Transform Microwave (**LA-CP-FTMW)** spectrometer

6.5-18 GHz configuration





EXPERIMENTAL METHODOLOGY

Laser Ablation Chirped Pulsed Fourier Transform Microwave (**LA-CP-FTMW)**

6.5-18 GHz configuration

Variables to consider in the experiment:

Carrier gas

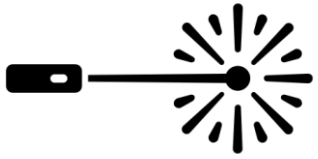
Water ratio

0.01-0.05% water in Neon bottle

Working pressure

15 bar

Laser ablation



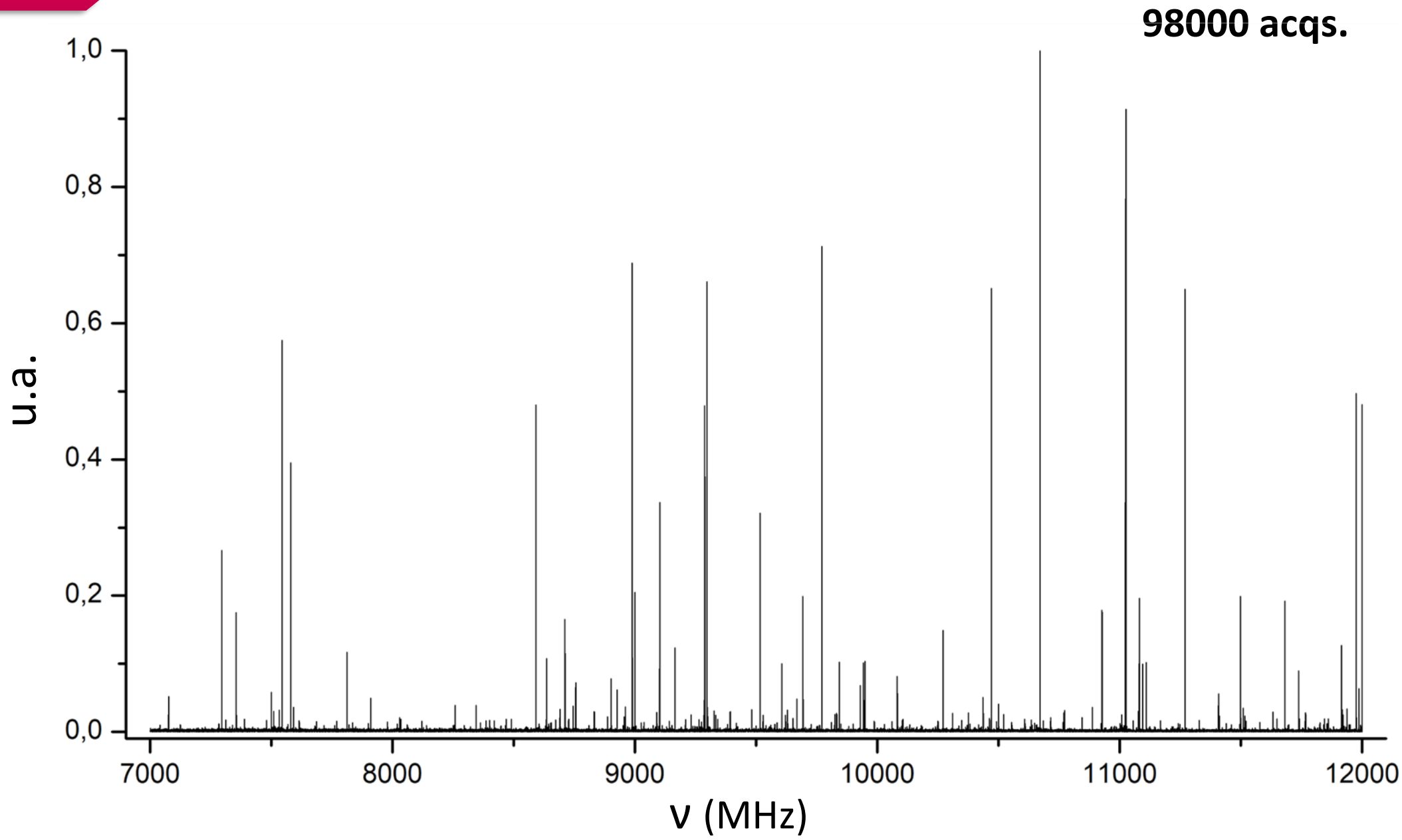
Laser wavelenght

4^{th} Harmonic (266 nm)

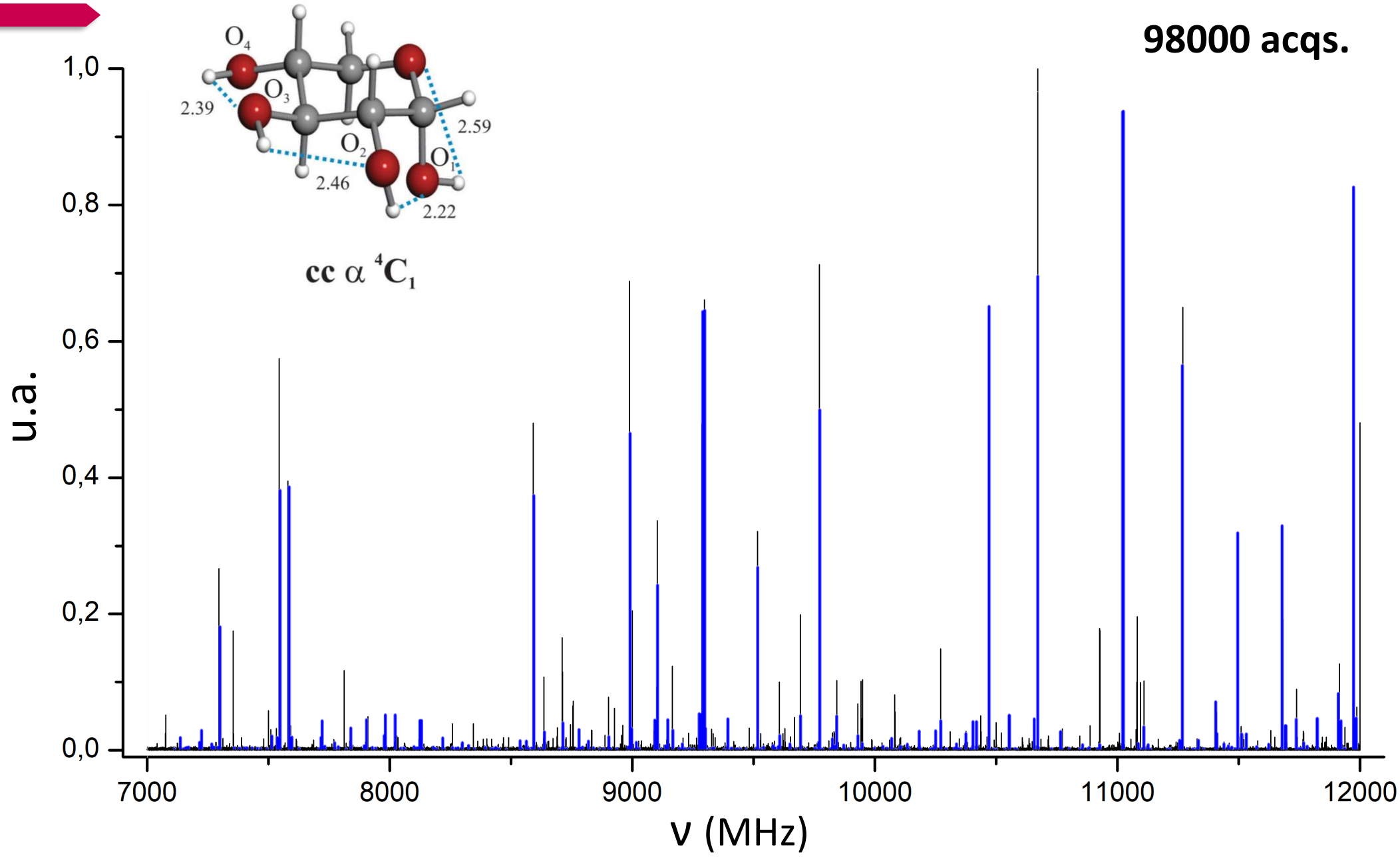
Laser power

10-12mJ/pulse

RESULTS

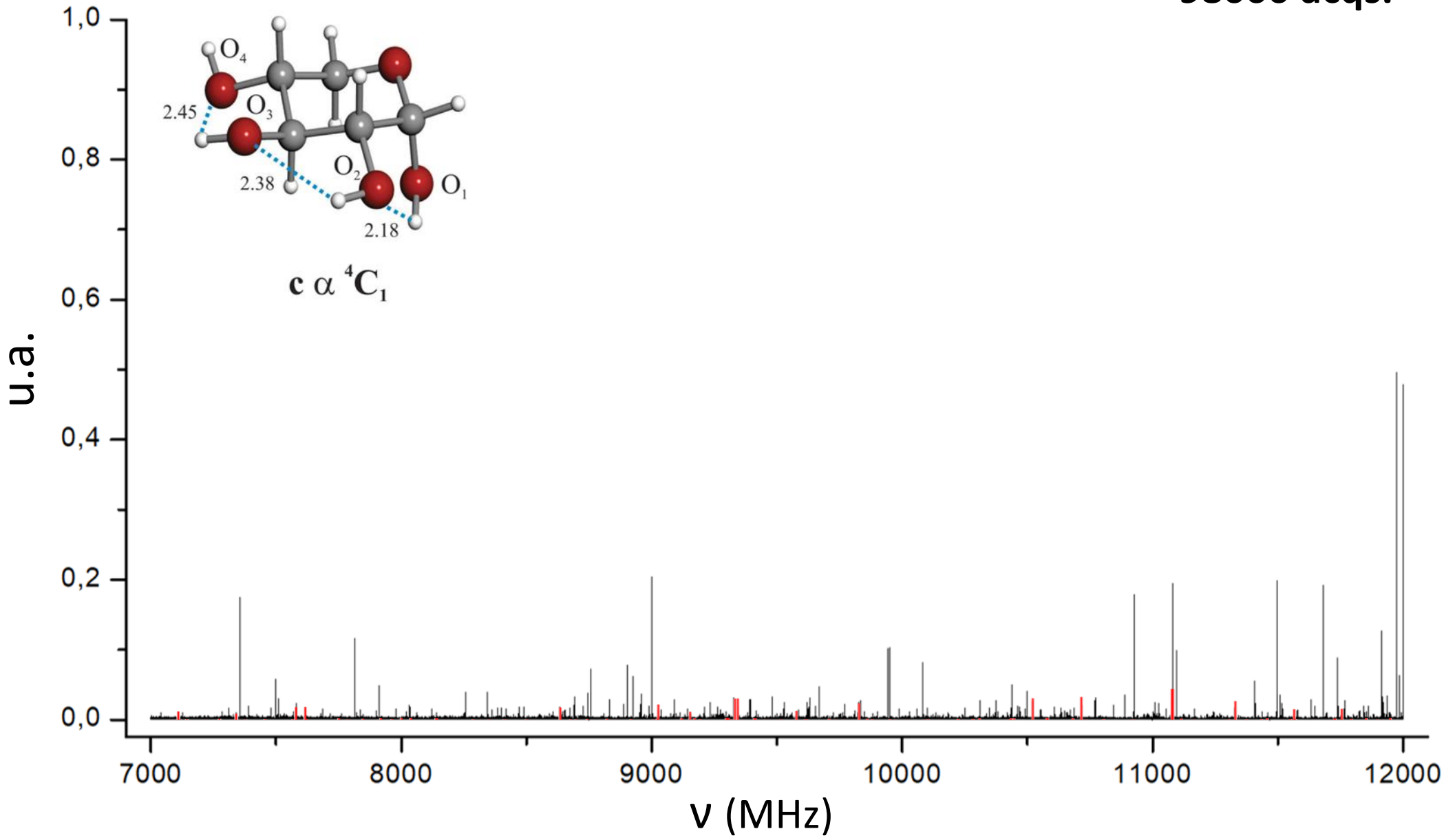

98000 acqs.
1,0
0,8
0,6
0,4
0,2
0,0
u.a.
7000
8000
9000
10000
11000
12000
ν (MHz)

RESULTS

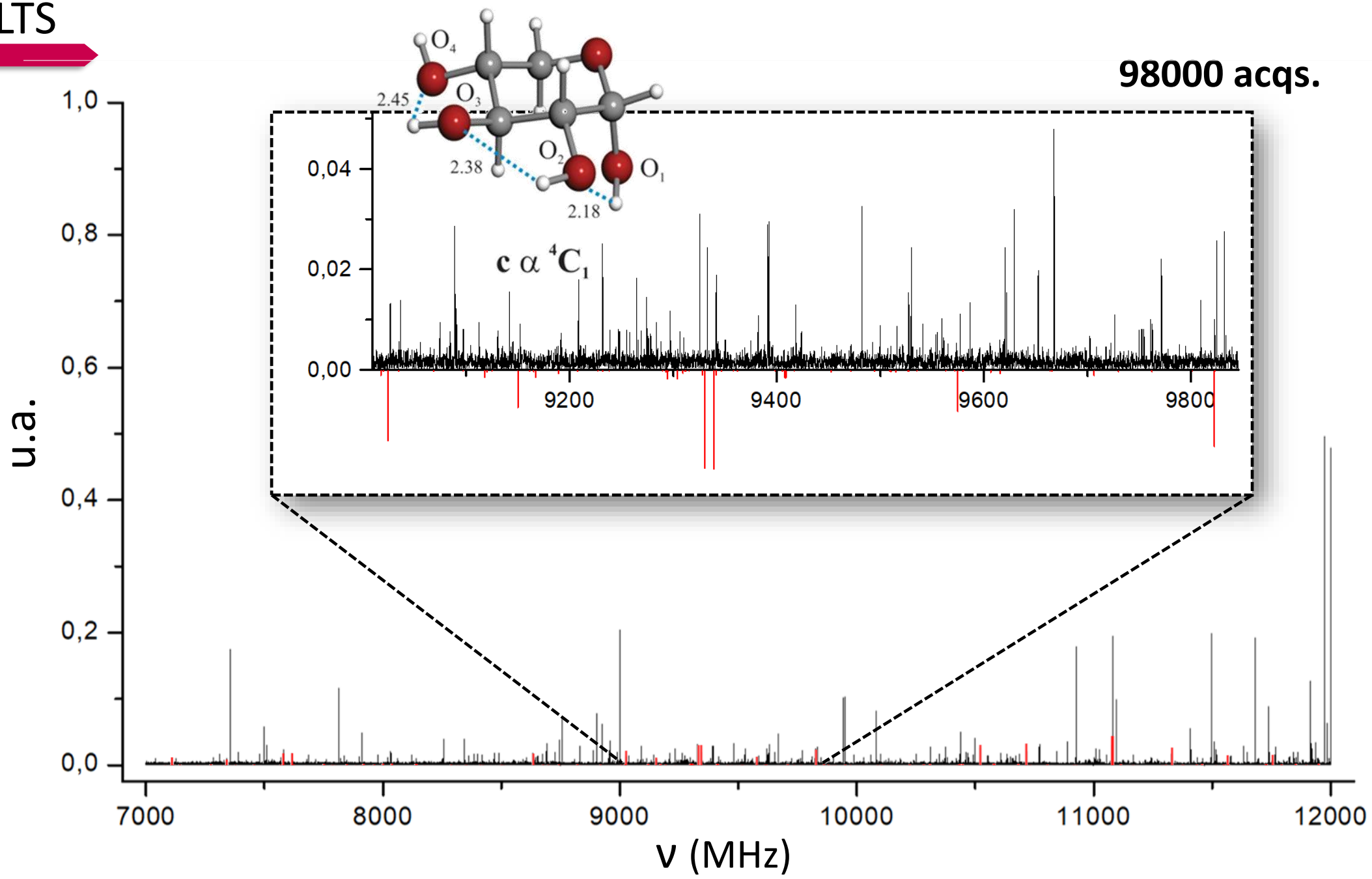

98000 acqs.
O4
O3
O2
O1
2.39
2.59
2.46
2.22
cc α 4C1
u.a.
1,0
0,8
0,6
0,4
0,2
0,0
7000
8000
9000
10000
11000
12000
ν (MHz)

RESULTS

98000 acqs.

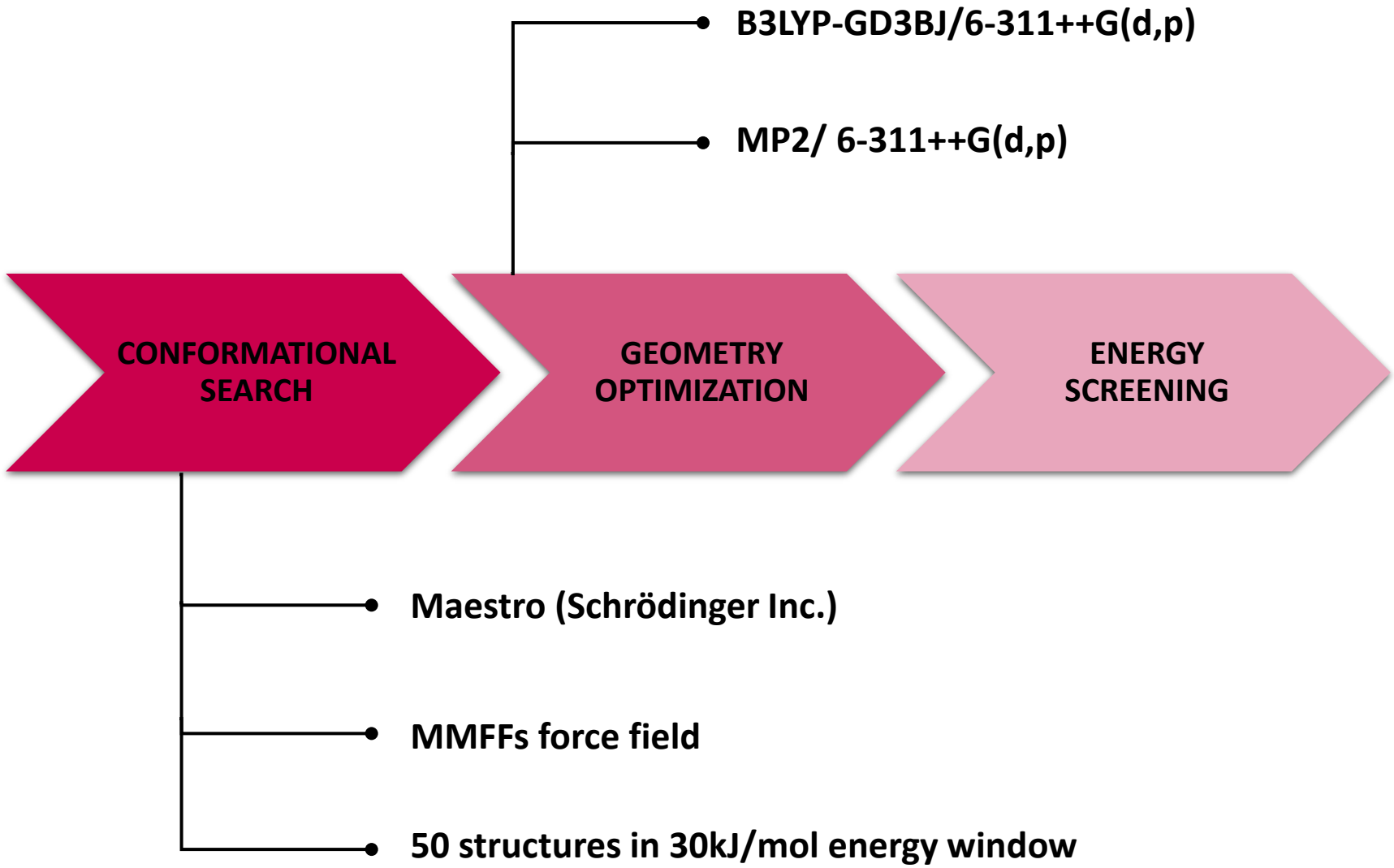


RESULTS


98000 acqs.
O4
O3
O2
O1
2.45
2.38
2.18
c α 4C1
0,04
0,02
0,00
9200
9400
9600
9800
1,0
0,8
0,6
0,4
0,2
0,0
u.a.
7000
8000
9000
10000
11000
12000
ν (MHz)

RESULTS

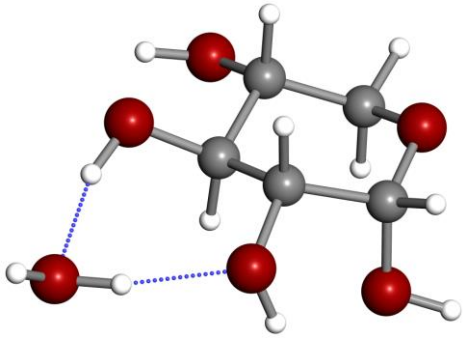
Computational support



RESULTS

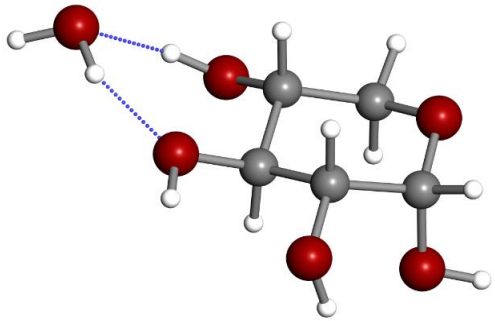
cc-α-$^1C_4$ configuration

cc-O_3H-w-O_2H



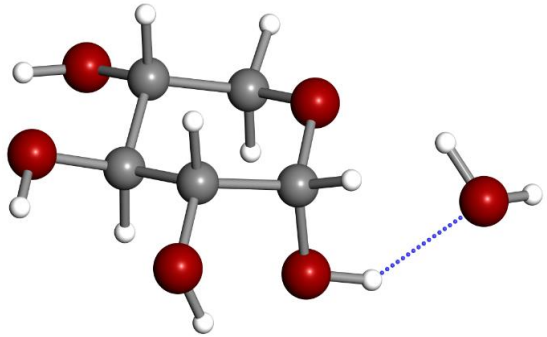
$E_{ZPE}(cm^{-1})$ 0/189

cc-O_4H-w-O_3H



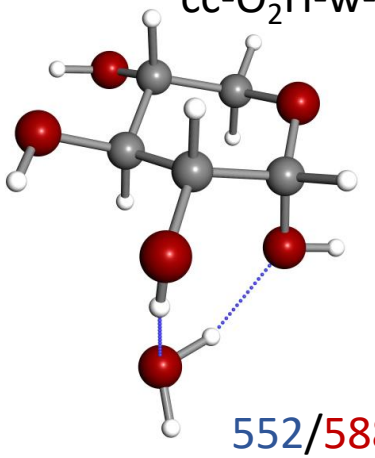
38/168

cc-O_R-w-O_1H



100/0

cc-O_2H-w-O_1H



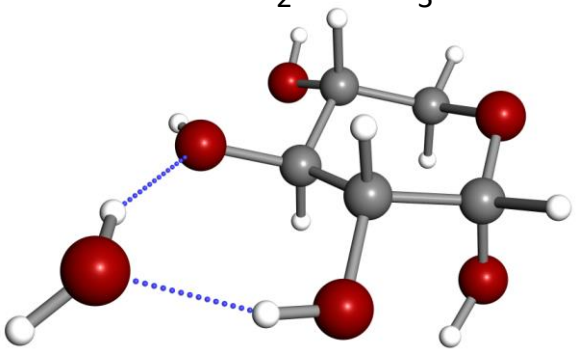
552/588

$E_{ZPE}(cm^{-1})$ **B3LYP-GD3BJ/6-311++G(d,p)**

MP2/ 6-311++G(d,p)

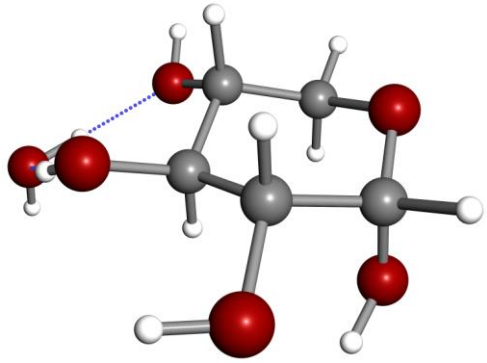
c-α-$^1C_4$ configuration

c-O_2H-w-O_3H



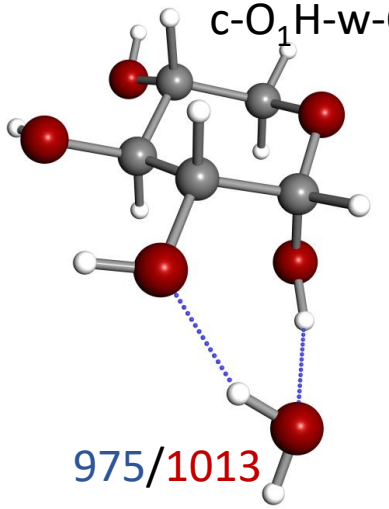
590/705

c-O_3H-w-O_4H



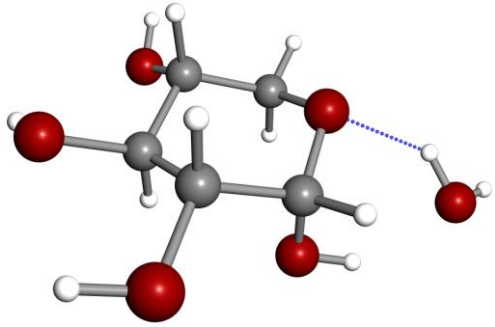
685/762

c-O_1H-w-O_2H



975/1013

c-O_1H-w-O_R

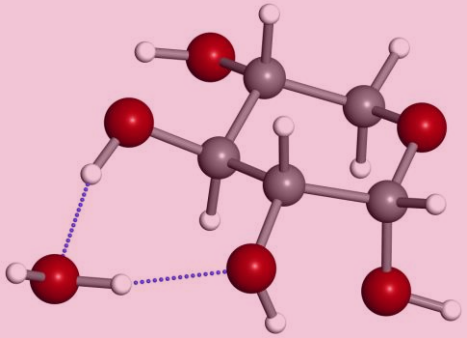


1569/1412

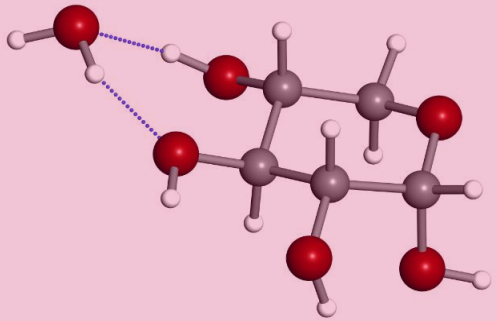
RESULTS

cc-α-$^1C_4$ configuration

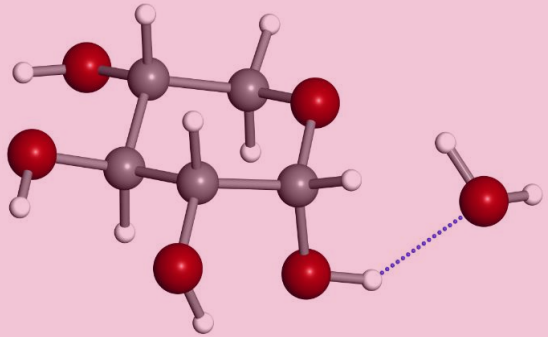
cc-OH_3-OH_2



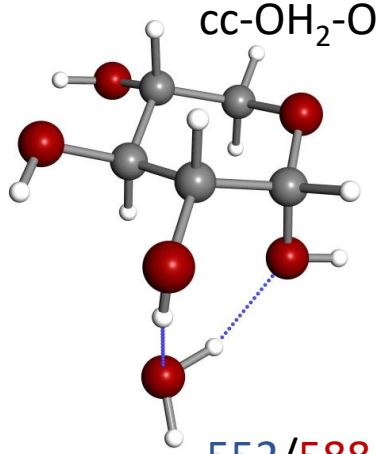
cc-OH_4-OH_3



cc-O_R-OH_1



cc-OH_2-OH_1



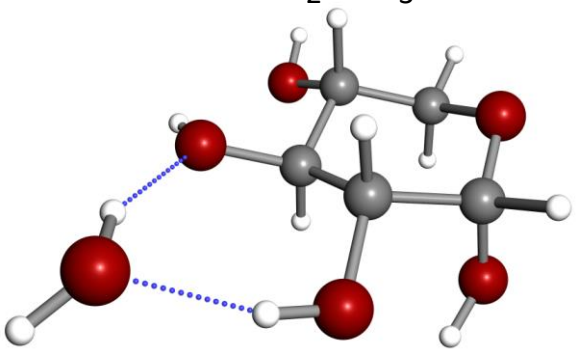
$E_{ZPE}(cm^{-1})$ 0/189 38/168 100/0 552/588

$E_{ZPE}(cm^{-1})$ **B3LYP-GD3BJ/6-311++G(d,p)**

MP2/ 6-311++G(d,p)

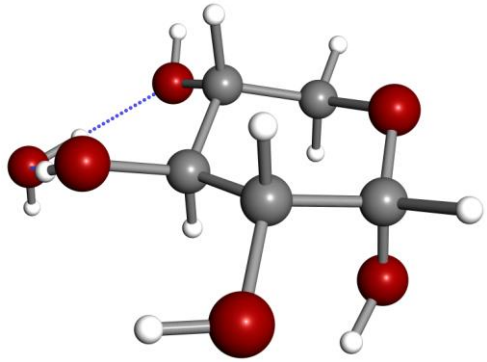
c-α-$^1C_4$ configuration

c-OH_2-OH_3



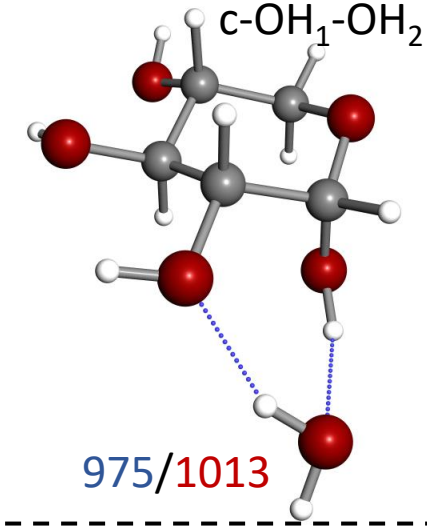
590/705

c-OH_3-OH_4



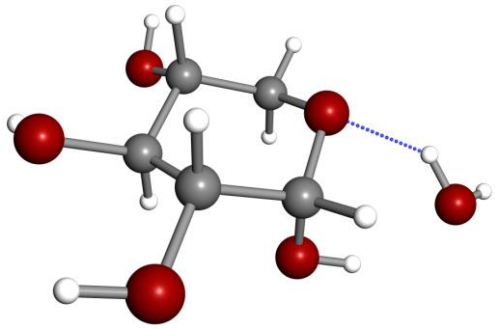
685/762

c-OH_1-OH_2



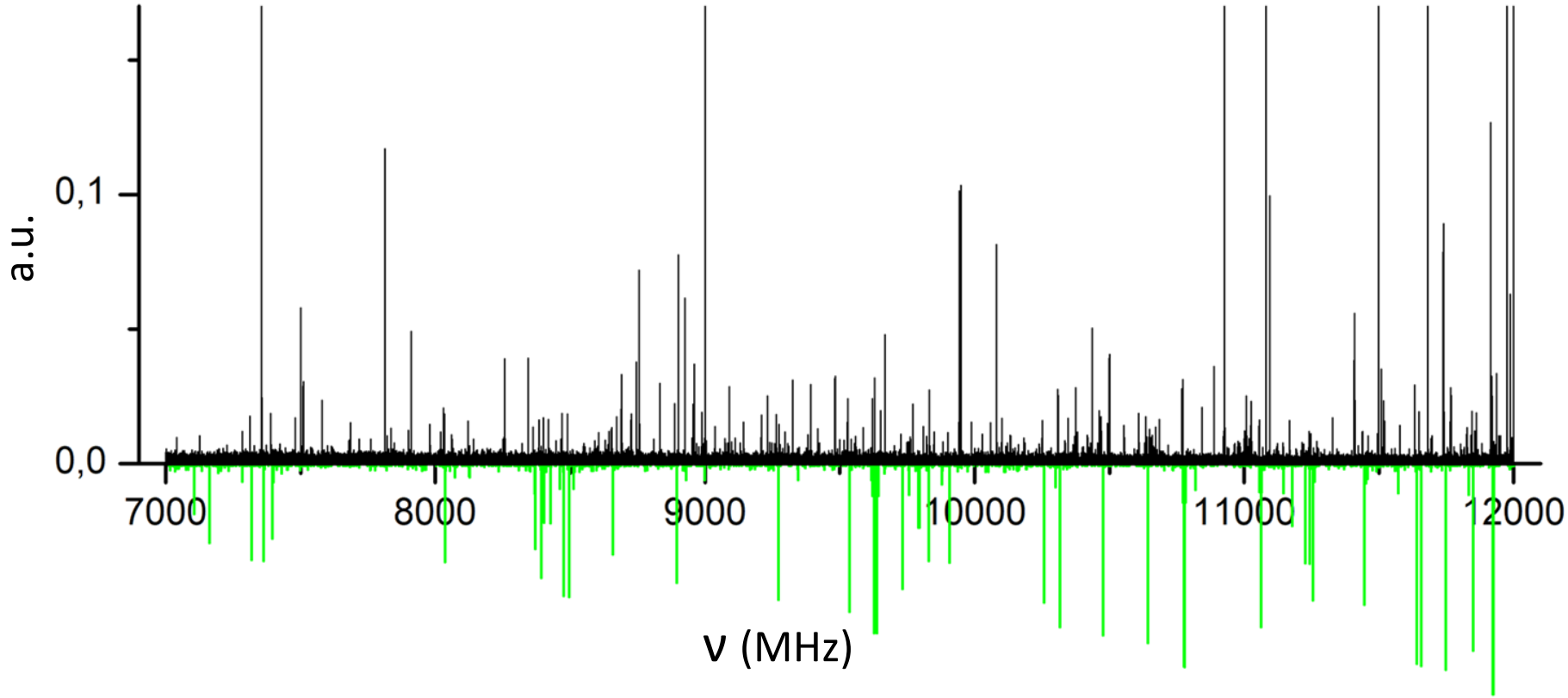
975/1013

c-OH_1-O_R



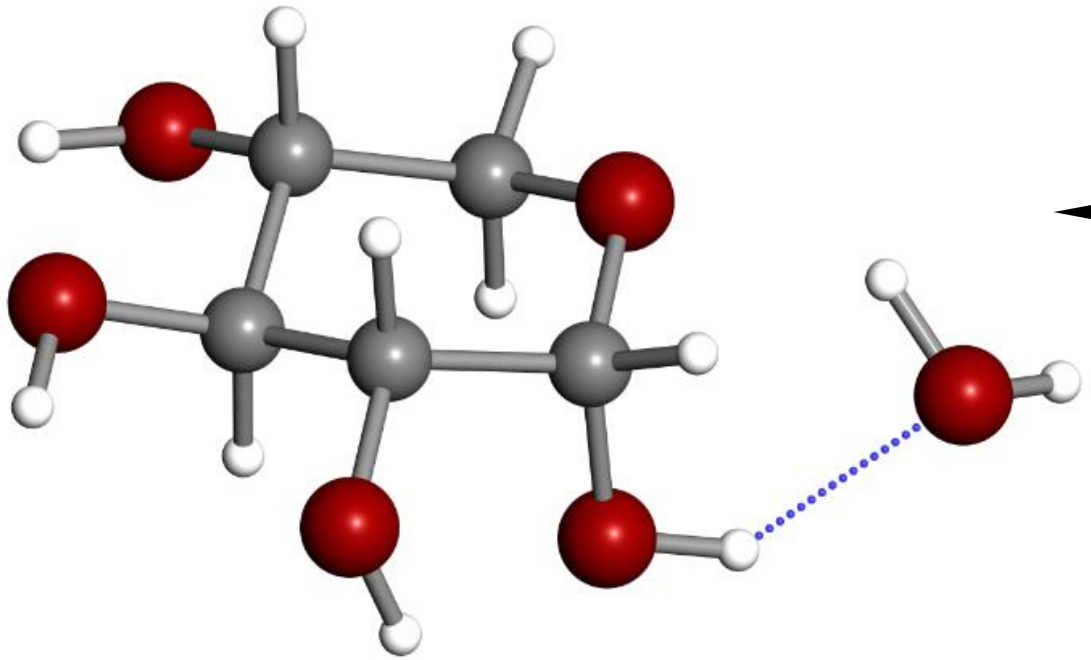
1569/1412

RESULTS



DISCUSSION

$cc\text{-}O_R\text{-}w\text{-}O_1H$



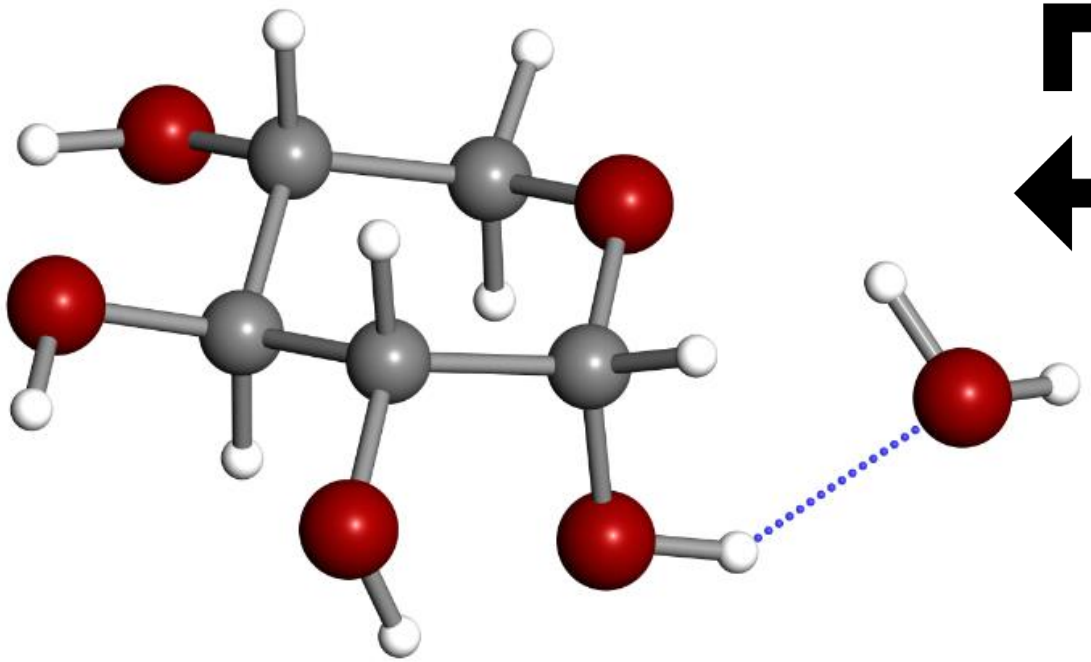
The structure of the monosaccharide in the complex remains the same as the structure already determined in the gas phase for α-xylopyranose.

The water binds to the oxigen of the ring and the anomeric hydroxyl group (O_1H)

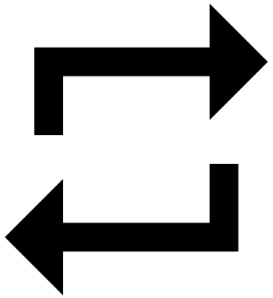
COULD THIS BE CONSIDERED THE FIRST STEP IN THE MUTARROTATION PROCESS?

DISCUSSION

cc-O_R-w-O_1H



CONTRAST RESULTS



RESEARCH PAPER

PCCP

www.rsc.org/pccp

Adding water to sugar: A spectroscopic and computational study of α- and β-phenylxyloside in the gas phase

Isabel Hünig,[a] Alexander J. Painter,[a] Rebecca A. Jockusch,[a] Pierre Çarçabal,[a] Elaine M. Marzluff,[b] Lavina C. Snoek,[a] David P. Gamblin,[c] Benjamin G. Davis[c] and John P. Simons*[a]

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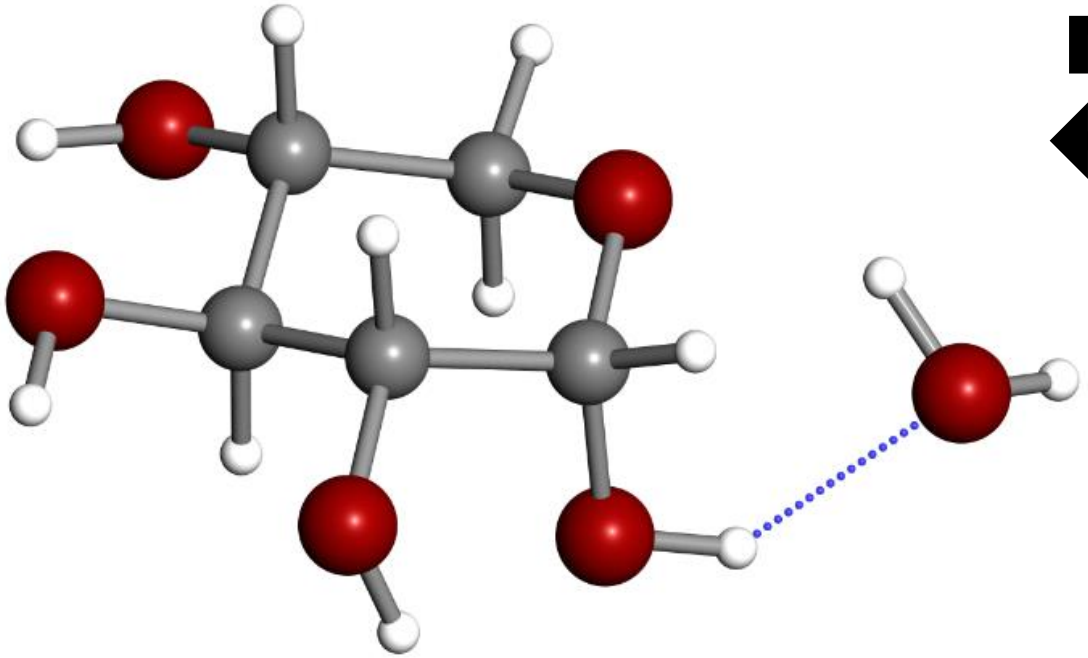
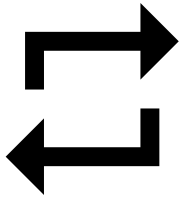
DISCUSSION

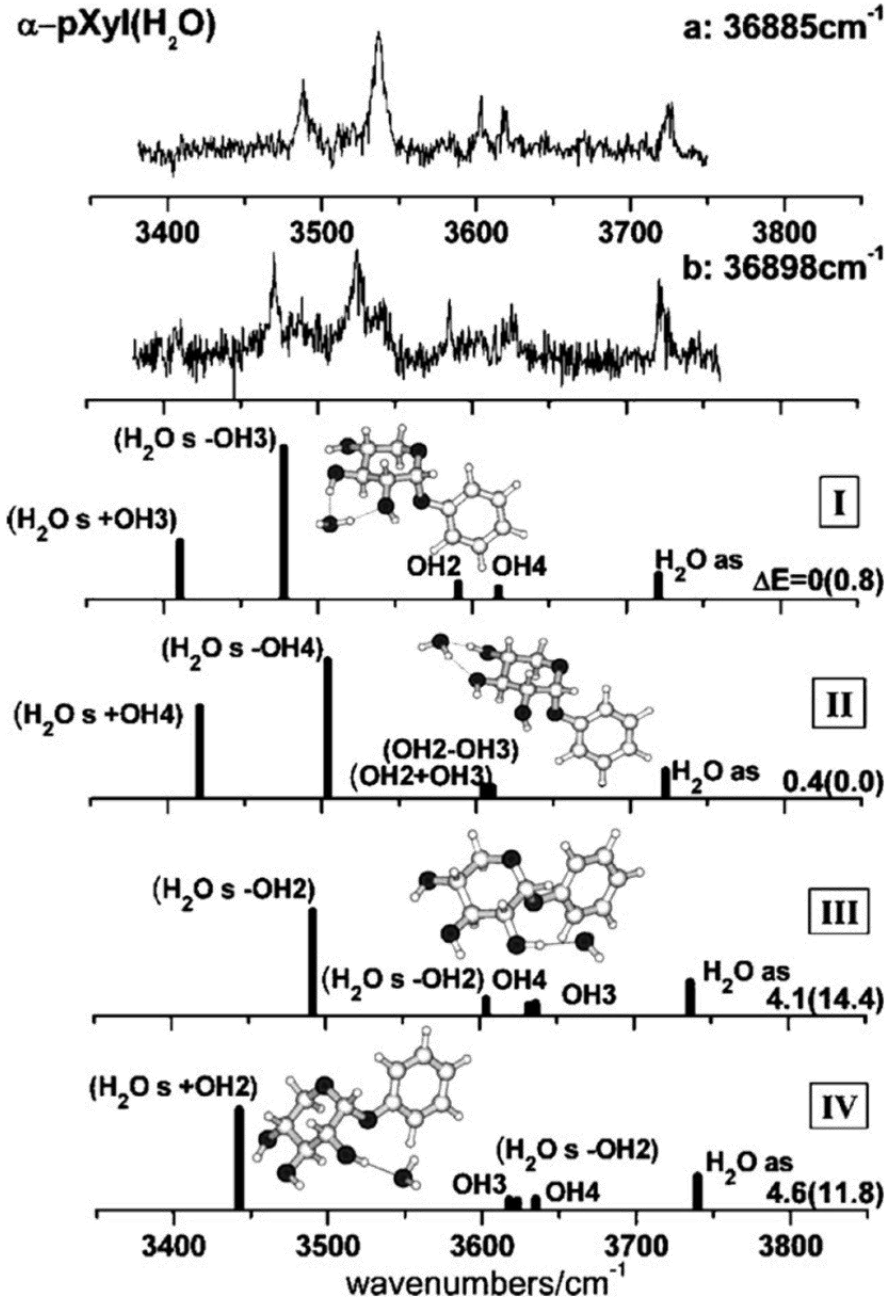
cc-O_R-w-O_1H



CONTRAST RESULTS



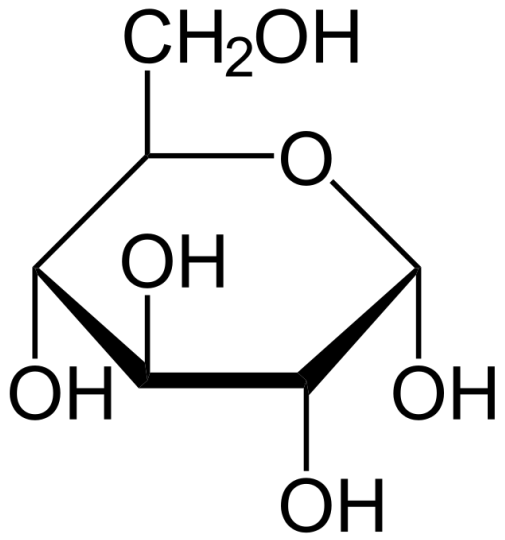
Phys. Chem. Chem. Phys., 2005,**7**, 2474-2480



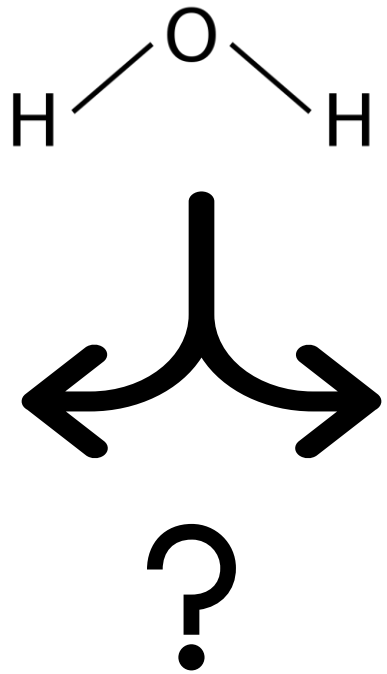
THE CHROMOPHORE DISTURBS THE PREFERENCES IN THE BINDING OF THE WATER MOLECULE TO THE MONOSACCHARIDE

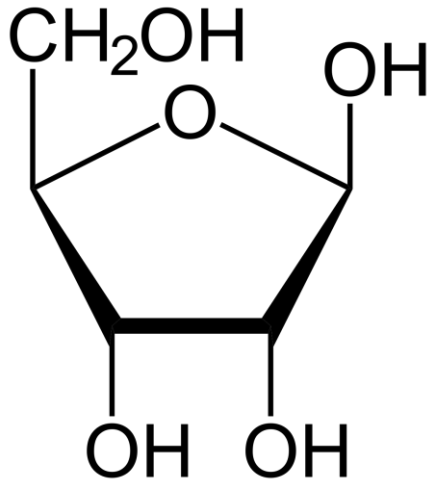
FUTURE PERSPECTIVES

EXTEND THESE STUDIES TO OTHER MONOSACCHARIDES TO BETTER UNDERSTAND THE BINDING SITE PREFERENCES OF THE WATER MOLECULE



ALDOHEXOSES





ALDOPENTOSES

ACKNOWLEDGMENTS

http://www.gem.uva.es/

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