

Modélisation Moléculaire

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MM: Programme

1. Forces au Niveau Moléculaire

Propriétés de l'eau et interactions entre atomes

2. Champs de Forces: Charmm; MM3

3. Descriptions Moléculaires:

Formats et Conversions (des SMILES aux XYZ)

4. Techniques de Minimization

5. Dynamique Moléculaire (JPD)

6. Monte-Carlo / Recuit Simulé

8. Propriétés des Drogues

9. Docking: Différentes Approches

10. Criblage Moléculaire Virtuel

Énergie des Liaisons Covalentes

Atoms	e ⁻ pairing	Covalent bond	Bond energy (kJ/mol)
H· + H·	→ H:H	H—H	436
·C· + H·	→ ·C:H	$\begin{array}{c} \\ -C-H \\ \end{array}$	414
·C· + ·C·	→ ·C:C·	$\begin{array}{c} \quad \\ -C-C- \\ \quad \end{array}$	343
·C· + ·N:	→ ·C:N:	$\begin{array}{c} \quad \diagup \\ -C-N \diagdown \\ \end{array}$	292
·C· + ·O:	→ ·C:O:	$\begin{array}{c} \\ -C-O- \\ \end{array}$	351
·C· + ·C·	→ C::C	$\diagdown C=C \diagup$	615
·C· + ·N:	→ C::N:	$\diagdown C=N- \diagup$	615
·C· + ·O:	→ C::O:	$\diagdown C=O \diagup$	686
·O: + ·O:	→ ·O:O:	-O—O-	142
·O: + ·O:	→ O::O:	O=O	402
·N: + ·N:	→ :N::N:	N≡N	946
·N: + H·	→ ·N:H	$\diagdown N-H \diagup$	393
·O: + H·	→ ·O:H	-O—H	460



Liaisons d'Hydrogène

Systemes A—H---B

A/B- atomes électronégatifs

Liaison A—H est polaire laissant le proton du H exposé, ce qui permet aux (paires d') électrons de B d'interagir avec le noyau de H exposé

Magnitude typique: 12 à 30 kJ/mol

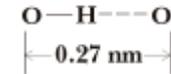
Angle Typique: 180°

Distance H---B beaucoup plus grande que de celle de HB covalent

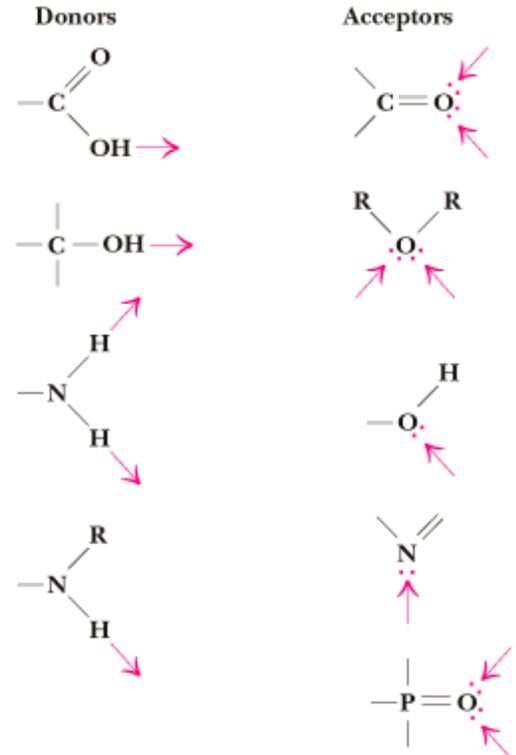
Conséquences importantes et solution.

Bonded atoms	Approximate bond length*
O—H---O	0.27 nm
O—H---O ⁻	0.26 nm
O—H---N	0.29 nm
N—H---O	0.30 nm
N ⁺ —H---O	0.29 nm
N—H---N	0.31 nm

*Lengths given are distances from the atom covalently linked to the H to the atom H-bonded to the hydrogen:

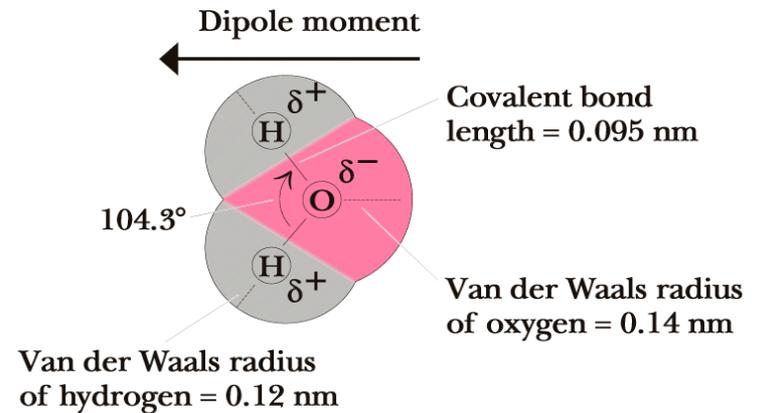


Functional groups which are important H bond donors and acceptors:



Comparaison Eau / Glace

Garrett & Grisham: Biochemistry, 2/e
Figure 2.1



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Liaisons d'Hydrogène et Mouvement

Glace: 4 liaisons de H par molécule d'eau

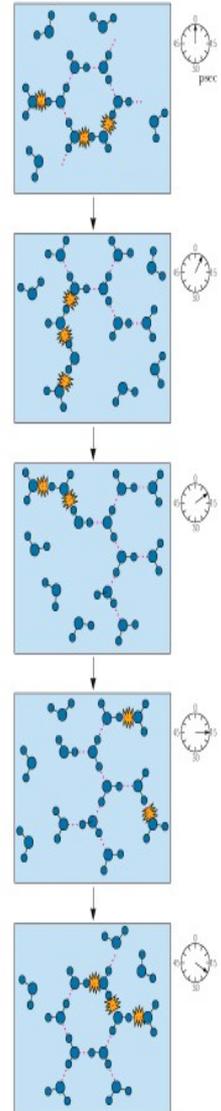
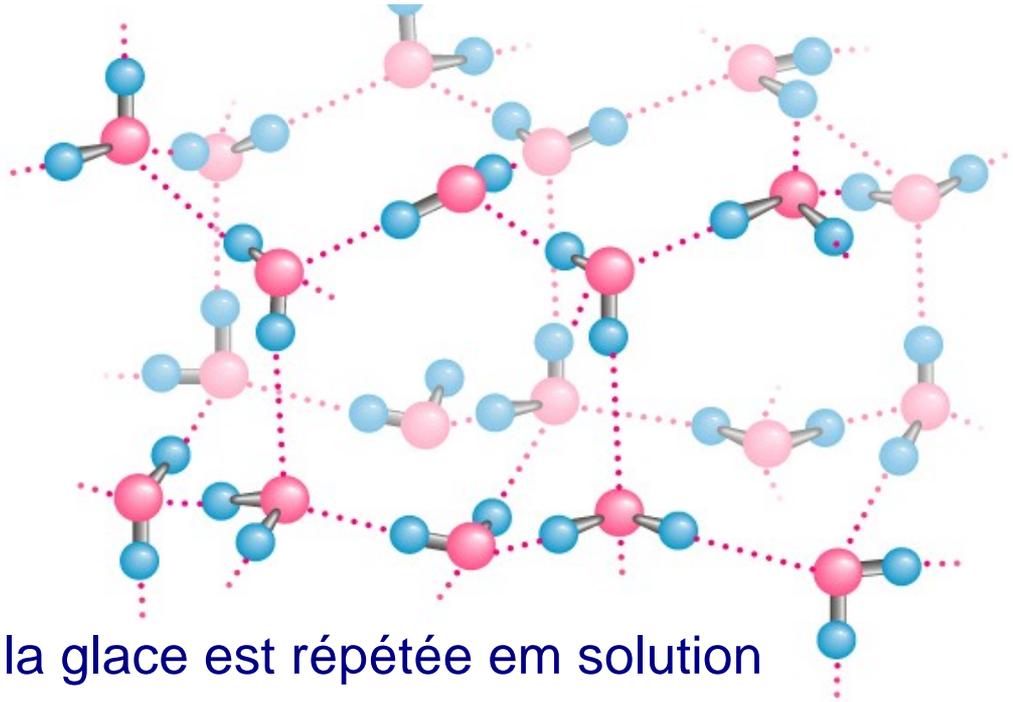
Eau: 2-3 liaisons de H par molécule d'eau

Glace: Temps de vie des Liaisons H $\approx 10 \mu\text{s}$
($1 \mu\text{s} = 10^{-6} \text{ s}$)

Eau: Temps de vie des Liaisons H $\approx 10 \text{ ps}$
($1 \text{ ps} = 10^{-9} \text{ s}$)

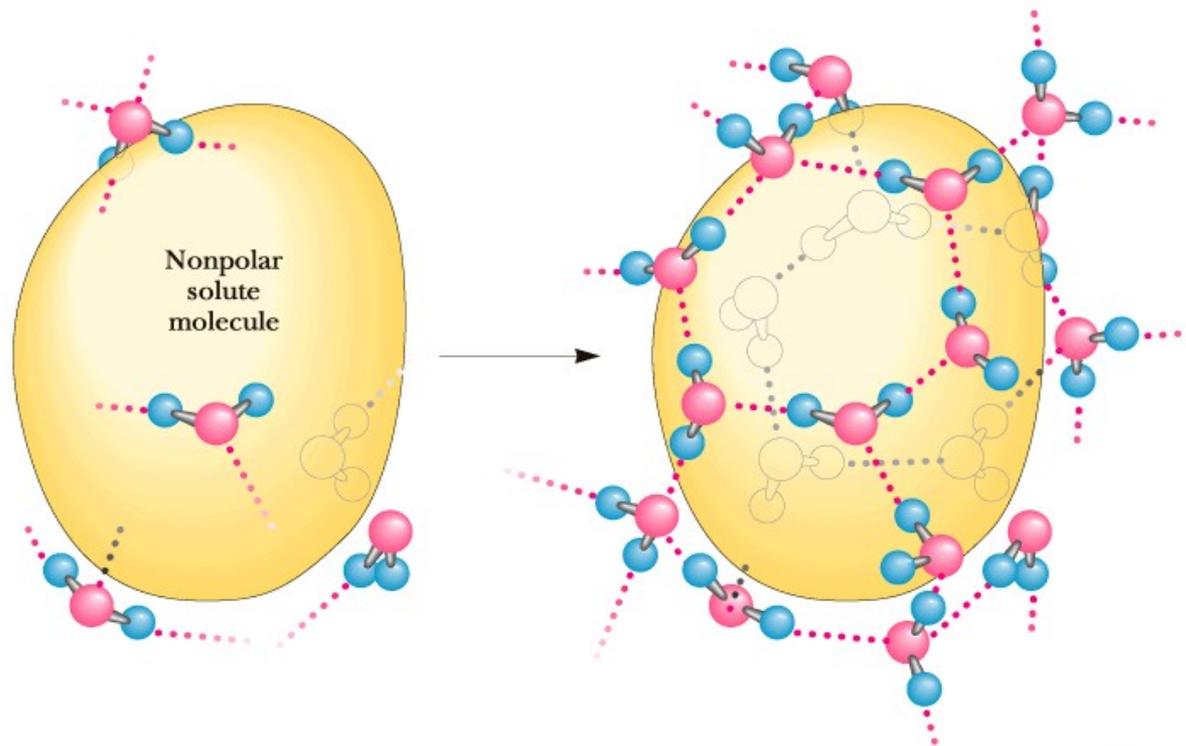
Eau/Glace - Structure Moléculaire Tétraogonale

2.3



- La structure de la glace est répétée em solution
- À 300° K l'énergie de translation et de rotation moyennée est de 7 kJ/mol, soit environ 1/3 de l'énergie nécessaire pour briser une liaison d'hydrogène
- Sous forme liquide, la structure tétraogonale predomine à large échelle mais les liaisons d'hydrogène sont moins stables et se brisent facilement, avec une fréquence telle qui brise l'ordre et rigidité de l'état cristallin

Composants Apolaires em Solution

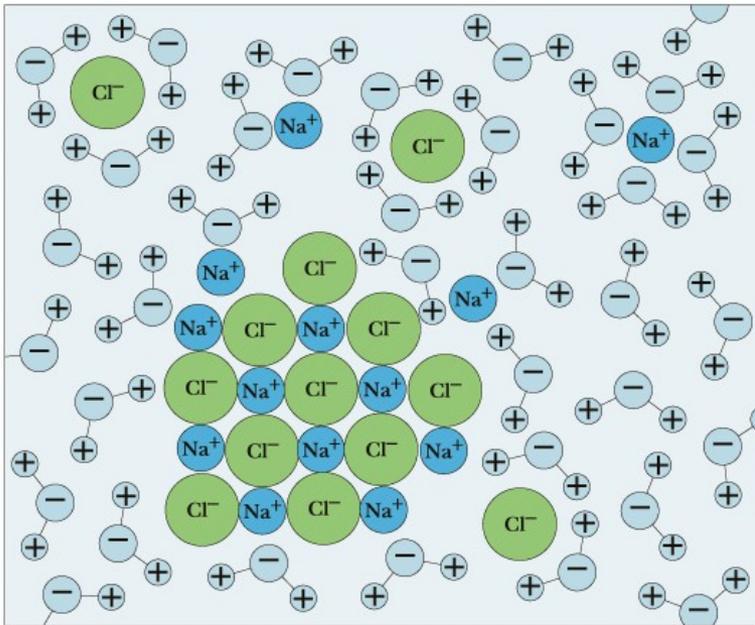


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- L'eau s'organise de façon à minimiser la perte des liaisons d'hydrogène (minimization de l'entropie)
- La première sphère d'hydratation retient la structure tétragonale des liaisons de H
- Les composants apolaires essayent d'éviter l'eau en se groupant

Composants polaires et/ou chargés en solution

Prisham: Biochemistry, 2/e



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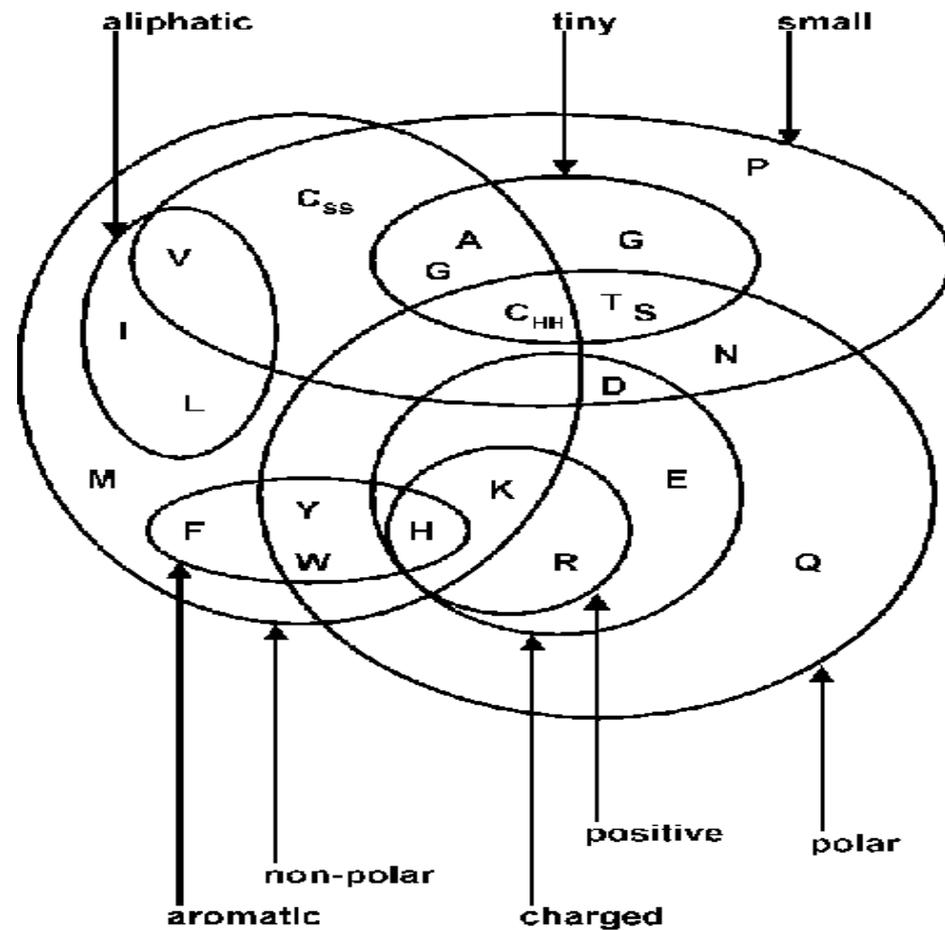
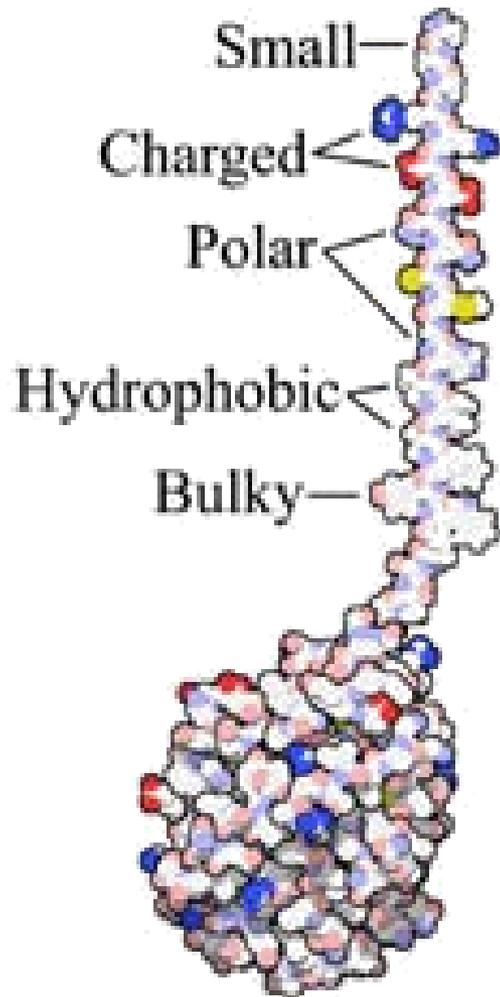
- Plus la densité de charge est forte, plus forte sera la tendance d'interagir avec les molécules d'eau.
- Pour les ions avec la plus grande densité de charge (ex: Na^+ ou des ions avec une charge plus élevée que ± 1), les molécules d'eau seront électrostatiquement ordonnées dans une sphère primaire d'hydratation compacte.
- Quand les ions sont positifs les molécules d'eau auront les hydrogènes pointés vers l'extérieur et quand les ions sont négatifs les hydrogènes de l'eau seront pointés vers l'intérieur (toujours avec une structure tétraogonale)
- Hors la sphère primaire d'hydratation il y aura une région désordonnée où les effets de coordination de l'ion et de la solution sont en compétition.
- Pour des paires d'ions l'effet total sera la combinaison des effets de chacun .

Conformational Aspects

Review of Different Macromolecules

- Proteins
 - Backbone
 - Side-chains
- Oligosaccharides
 - Puckering
 - Glycosidic Bonds ("Backbone")
- Nucleotides
 - Backbone
 - Bases

Aminoacides



- Les chaînes latérales confèrent **une fonctionnalité**
- Les chaînes chargées et polaires peuvent former des liaisons d'hydrogène spécifiques à l'origine de la spécificité des **interactions protéine-ligand ou protéine-protéine**
- Les chaînes non-polaires sont importantes dans le support de l'architecture des protéines, le repliement et les **interactions protéine-protéine**

Structure Primaire (1)

La **liaison peptidique** a des caractéristiques particulières:

Configuration *trans* (presque toujours)

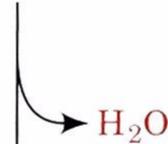
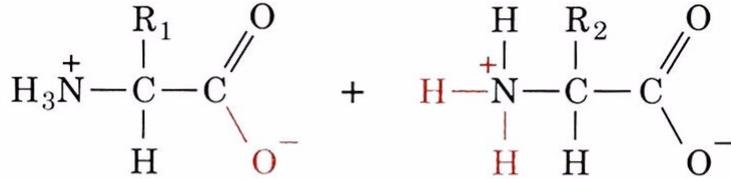
Caractère partiel (40%) de liaison double

Mesure 1,33 Å - plus courte qu'une liaison simple mais plus longue qu'une double

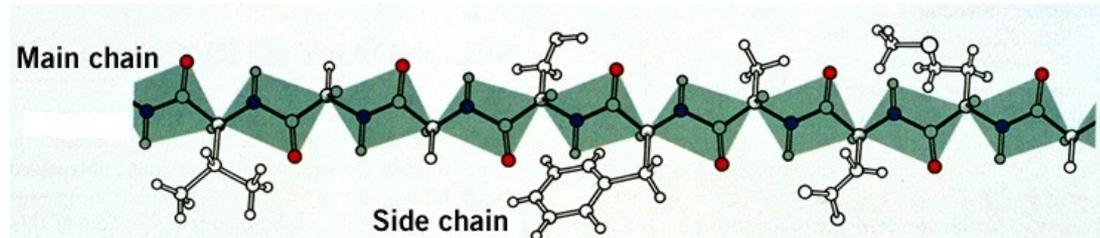
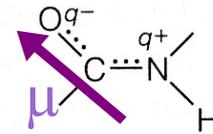
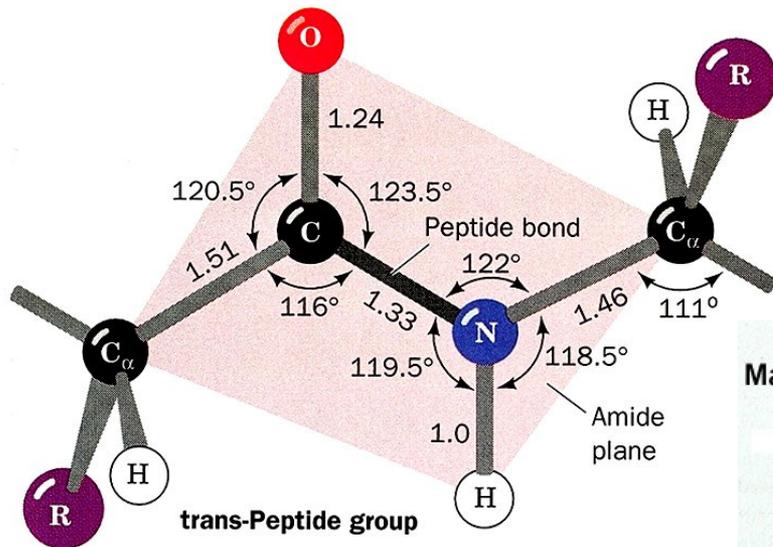
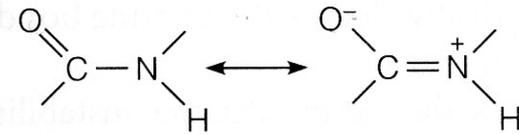
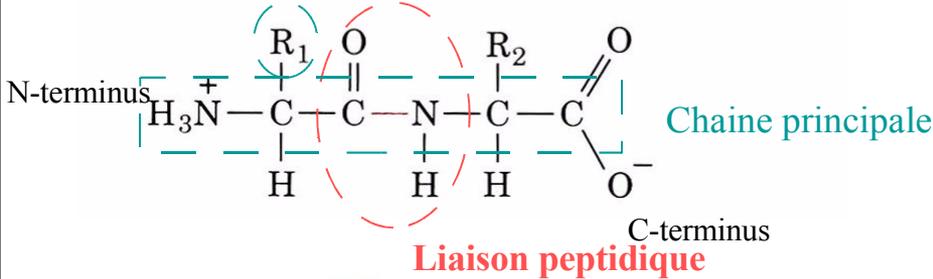
Les six atomes du groupe peptidique sont planaires!

N partiellement positif; O partiellement négatif

Moment dipolaire de 3.5 Debye.



Chaîne laterale



Structure Primaire (2)

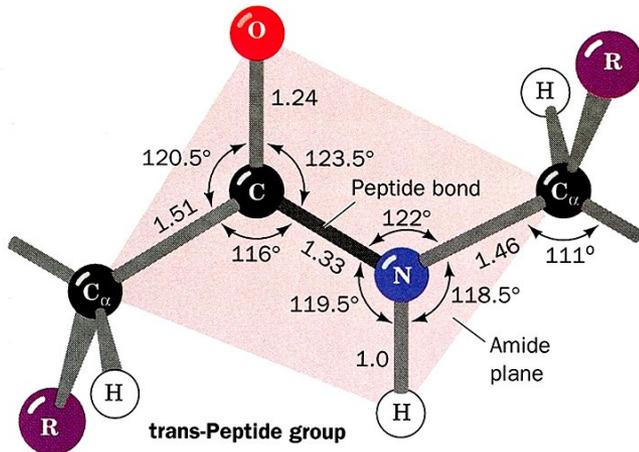
Deux configurations possibles : cis et trans.

Trans est plus favorable sur le plan énergétique. Mais 10 % des prolines dans les protéines sont en configuration cis. Des serines et d'autres aa dans des sites de caractère dynamique se trouvent parfois dans la configuration cis pour "précharger" l'enzyme avec de l'énergie pour la catalyse.

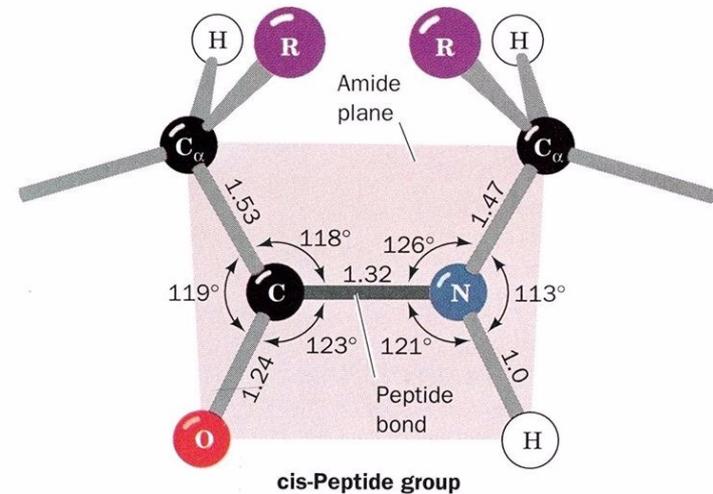
Aspects Configurationnels Trans vs Cis

$$\phi = \text{C}_\alpha\text{-N} \quad \psi = \text{C}_\alpha\text{-C} \quad \omega = \text{C}'\text{-N}$$

• **Trans** ($\phi = \psi = 180^\circ$, $\omega = 180^\circ$)



• **Cis** ($\phi = \psi = 180^\circ$, $\omega = 0^\circ$)



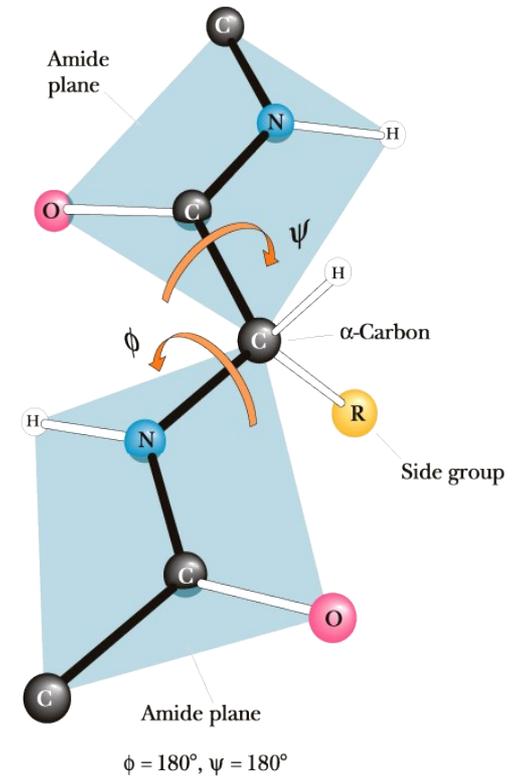
Configuration rare (~10% des Pro)

La chaîne peptidique n'est pas très réactive. Au pH ou elle sera protonnée ou déprotonnée, elle est généralement hydrolysée.

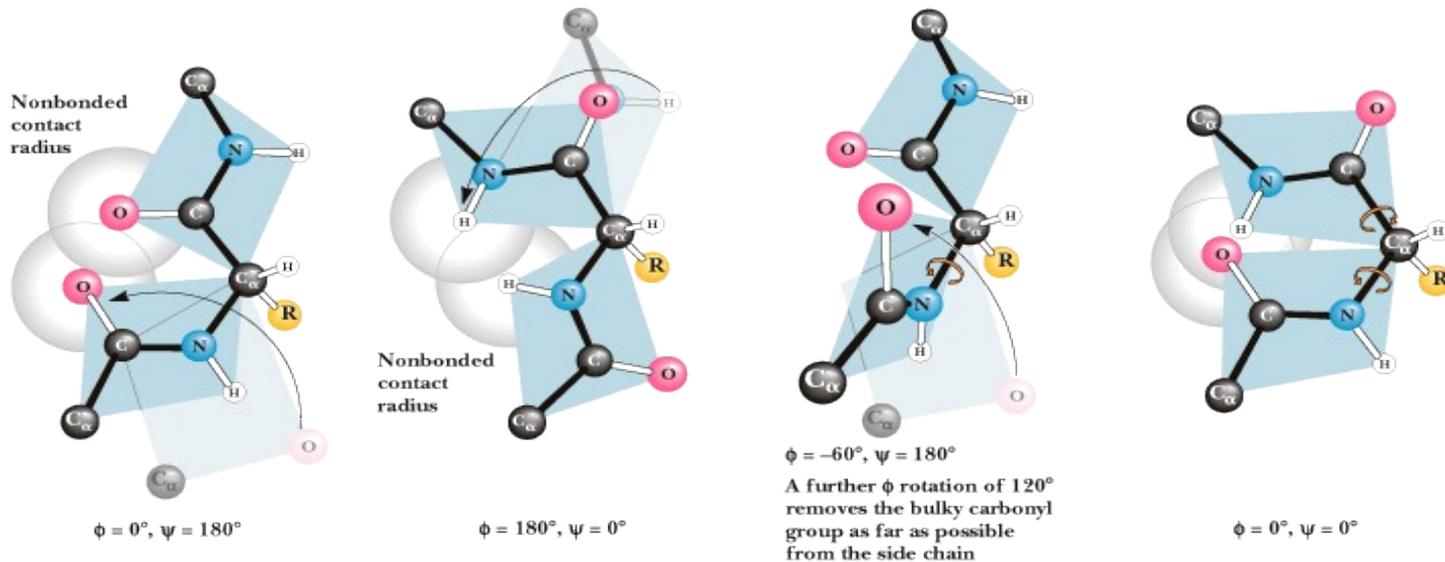
La durée de vie d'une liaison peptidique est ~7 ans (pH neutre, 25°C).

Stéréochimie de la Chaîne Principale

- La conformation locale de la chaîne principale de tous les acides aminés peut être décrite par des valeurs de ϕ / ψ
- Certaines combinaisons de ϕ / ψ sont défavorables du à la superposition d'orbitales



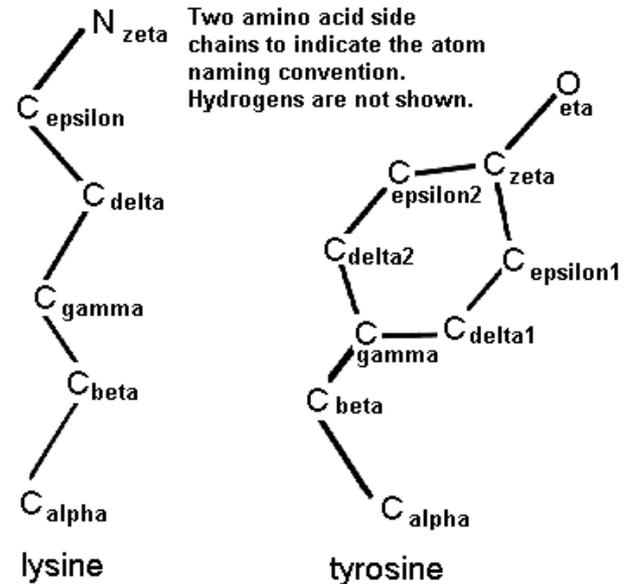
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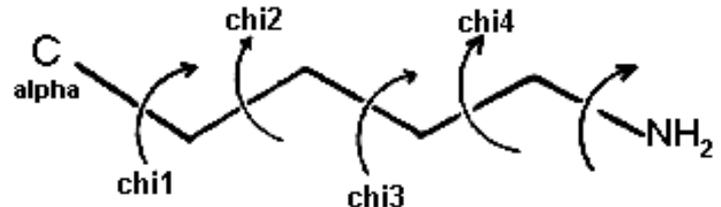
Sidechain Conformation

- Protein sidechains play a key role in molecular recognition and packing of hydrophobic cores of globular proteins
- Protein sidechain conformations tend to exist in a limited number of canonical shapes, usually called rotamers
- Rotamer libraries can be constructed where only 3-50 conformations are taken into account for each side chain

- Side chain atoms of amino acids are named in the Greek alphabet



- Side chain torsion angles are named chi1, chi2, chi3, etc.,



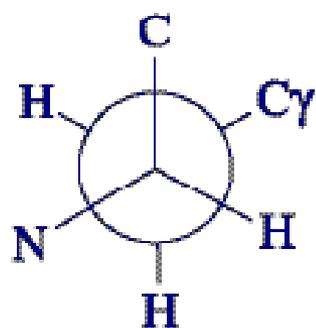
Side chain conformation

- side chains differ in their number of degrees of conformational freedom (some don't have any)
- but side chains of very different size can have the same number of chi angles.

Side-chain angles		χ_1	χ_2	χ_3	χ_4	Atom position fixed by			
Residue	Atom	α	β	γ	δ	ϵ	ζ	η	
Gly		•							Main chain
Ala		•—•							
Pro		•—•—•—•							
Ser		•—•—•—O							χ_1
Cys		•—•—•—S							
Thr		•—•—•—O							
Val		•—•—•—•							
Ile		•—•—•—•—•							χ_1 and χ_2
Leu		•—•—•—•—•							
Asp		•—•—•—•—O							
Asn		•—•—•—•—O—N							
His		•—•—•—•—N—N							
Phe		•—•—•—•—•—•—•—•—•							
Tyr		•—•—•—•—•—•—•—•—•—O							
Trp		•—•—•—•—•—•—•—•—•—N							
Met		•—•—•—•—S—•							χ_1, χ_2 and χ_3
Glu		•—•—•—•—•—O—O							
Gln		•—•—•—•—•—O—N							
Lys		•—•—•—•—•—•—•—•—N							$\chi_1, \chi_2, \chi_3, \chi_4$
Arg		•—•—•—•—•—•—•—N—N—N							

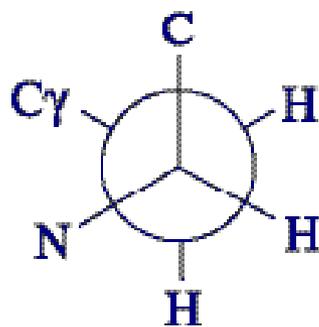
Names of canonical side chain conformations

Newman projection down the C_{α} - C_{β} bond for glutamic acid as an example



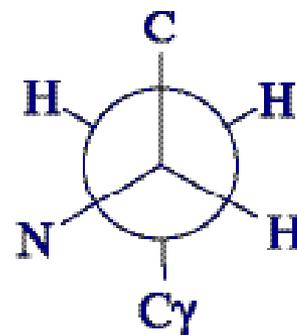
$$\chi_1 = 180^\circ$$

t



$$\chi_1 = +60^\circ$$

g+



$$\chi_1 = -60^\circ$$

g-

t=trans, g=gauche

name of conformation

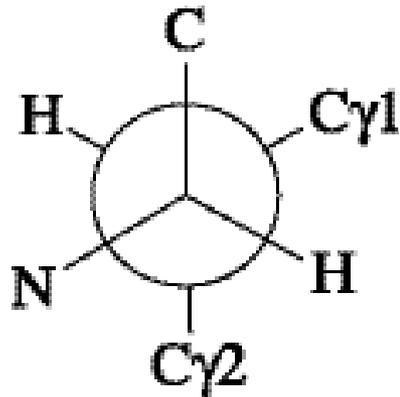
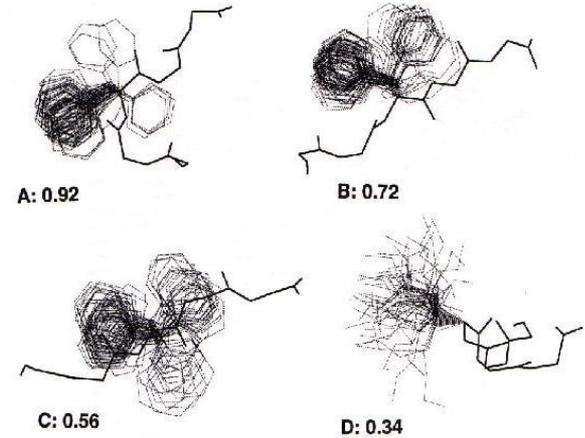
χ_1 is defined by the angle $N-C_{\alpha}-C_{\beta}-C_{\gamma}$

when there is more than one gamma heteroatom the naming follows IUPAC convention.

<http://www.chem.qmw.ac.uk/iupac/misc/biop.html>

Rotamers

- a particular combination of angles χ_1, χ_2 , etc. for a particular residue is known as a *rotamer*.
- for example, for aspartate, if one considers only the *canonical staggered forms*, there are nine (3^2) possible rotamers: $g^+g, g^+g^-, gg^+, gg^-, tg^+, g^+t, tg^-, gt^-, tt$
- not all rotamers are equally likely.
- for example, valine prefers its *t* rotamer.

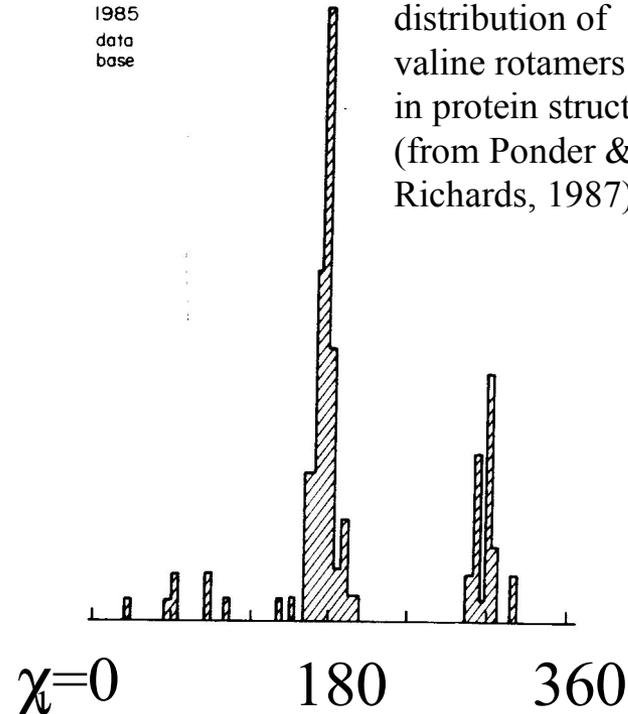


$$\chi_1 = 180^\circ$$

t

1985
data
base

distribution of
valine rotamers
in protein structures
(from Ponder &
Richards, 1987)



Rotamers (2)

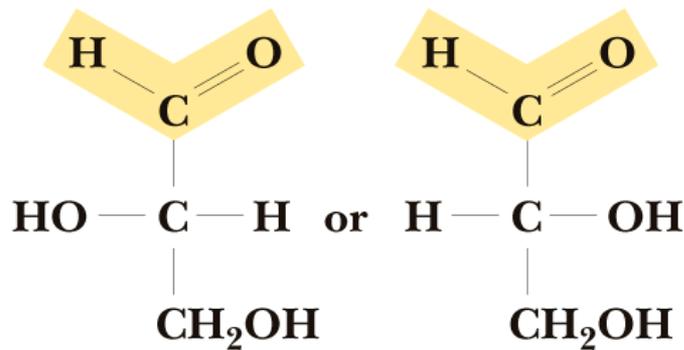
	Pept	Num	NChi	Natm	Chi1	Chi2	Chi3	Chi4	Chi5
1)	ALA	1	1	4	180				
2)	CYS	1	2	5	-65	180			
	CYS	2			-178	180			
	CYS	3			64	180			
3)	ASP	1	2	6	-70	-32			
	ASP	2			-171	-171			
	ASP	3			62	4			
4)	GLU	1	3	9	-66	178	174		
	GLU	2			-69	180	-15		
	GLU	3			-64	-65	-45		
	GLU	4			-174	176	-173		
	GLU	5			179	175	8		
	GLU	6			-175	70	57		
	GLU	7			-65	79	8		
	GLU	8			72	178	41		
	GLU	9			50	-87	-161		
	GLU	10			65	176	-120		
5)	PHE	1	2	14	-69	93			
	PHE	2			178	73			
	PHE	3			65	89			
	PHE	4			-70	-20			
6)	GLY	1	0	1					

	Pept	Num	NChi	Natm	Chi1	Chi2	Chi3	Chi4	Chi5
7)	HIS	1	2	11	-62	-84			
	HIS	2			-177	68			
	HIS	3			-67	97			
	HIS	4			-168	-108			
	HIS	5			64	-95			
	HIS	6			68	81			
8)	ILE	1	4	13	-62	163	180	180	
	ILE	2			63	164	180	180	
	ILE	3			-57	-59	180	180	
	ILE	4			-168	161	180	180	
	ILE	5			-156	72	180	180	
9)	LYS	1	5	16	-70	-179	180	180	180
	LYS	2			-172	180	180	180	180
	LYS	3			-61	-71	-178	180	180
	LYS	4			-173	-174	77	180	180
	LYS	5			-174	70	-174	180	180
	LYS	6			70	-172	179	180	180
	LYS	7			-69	178	79	180	180
	LYS	8			-71	-172	-72	180	180
	LYS	9			-170	-176	-74	180	180
	LYS	10			-71	90	-168	180	180
	LYS	11			-70	-83	-80	180	180
	LYS	12			69	-156	-75	180	180
	LYS	13			-160	82	75	180	180
	LYS	14			70	175	67	180	180
	LYS	15			-73	-99	69	180	180
	LYS	16			-64	89	77	180	180
10)	LEU	1	4	13	-62	170	180	180	
	LEU	2			-176	66	180	180	
	LEU	3			-99	25	180	180	
	LEU	4			-168	-161	180	180	
	LEU	5			-83	-80	180	180	
	LEU	6			61	85	180	180	

Rotamers (3)

	Pept	Num	NChi	Natm	Chi1	Chi2	Chi3	Chi4	Chi5	Pept	Num	NChi	Natm	Chi1	Chi2	Chi3	Chi4	Chi5	
										15)	ARG	1	5	18	-176	156	-175	180	180
											ARG	2			-67	-176	-76	180	180
											ARG	3			-178	171	62	180	180
											ARG	4			-72	166	72	180	180
11)	MET	1	4	11	-66	-67	-67	180			ARG	5			-60	-60	171	180	180
	MET	2			-68	180	74	180			ARG	6			78	171	172	180	180
	MET	3			-72	179	180	180			ARG	7			-172	-170	-66	180	180
	MET	4			179	178	77	180			ARG	8			-69	175	180	180	180
	MET	5			-169	-169	-101	180			ARG	9			-59	-74	-75	180	180
	MET	6			-61	-67	131	180			ARG	10			66	158	74	180	180
	MET	7			-170	65	76	180			ARG	11			74	-169	-80	180	180
	MET	8			80	-172	180	180											
	MET	9			-74	-173	-82	180		16)	SER	1	2	5	65	180			
	MET	10			-66	-67	140	180			SER	2			-63	180			
											SER	3			-178	180			
12)	ASN	1	2	8	-72	-44				17)	THR	1	3	8	-61	180	180		
	ASN	2			-171	12					THR	2			65	180	180		
	ASN	3			-69	131					THR	3			-160	180	180		
	ASN	4			66	12													
13)	PRO	1	5	9	26.9	-29.4	22.8	-5.5	-14.2	18)	VAL	1	3	10	173	180	180		
	PRO	2			-21.8	31.2	-30.9	17.3	3.3		VAL	2			-62	180	180		
	PRO	3			0.3	-0.8	1.3	-1.1	0.5		VAL	3			72	180	180		
14)	GLN	1	3	11	-63	178	-3			19)	TRP	1	2	18	-178	82			
	GLN	2			-68	-179	-176				TRP	2			-67	85			
	GLN	3			-68	-64	-42				TRP	3			-174	-101			
	GLN	4			-173	180	1				TRP	4			64	93			
	GLN	5			-172	68	32				TRP	5			57	-86			
	GLN	6			-66	-70	140				TRP	6			-74	-86			
	GLN	7			-174	-177	179				TRP	7			-73	4			
	GLN	8			-170	68	-124			20)	TYR	1	3	15	-64	102	180		
	GLN	9			69	-173	-10				TYR	2			-66	-87	180		
	GLN	10			64	-169	116				TYR	3			-178	74	180		
											TYR	4			-177	-103	180		
											TYR	5			65	-96	180		
											TYR	6			62	89	180		

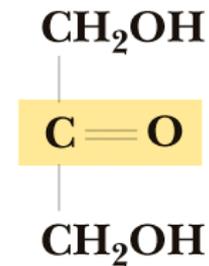
Aldoses / Cetoses



L-isomer

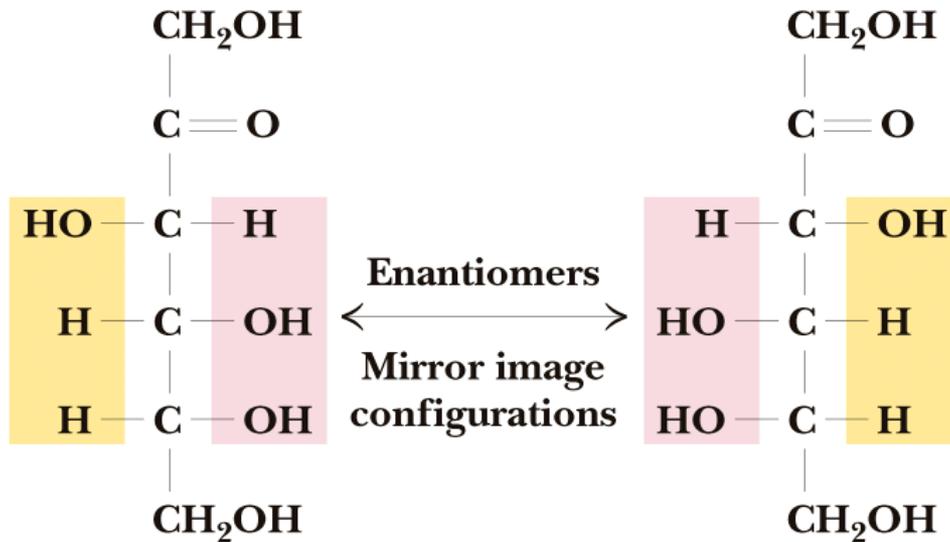
D-isomer

Glyceraldehyde



Dihydroxy-
acetone

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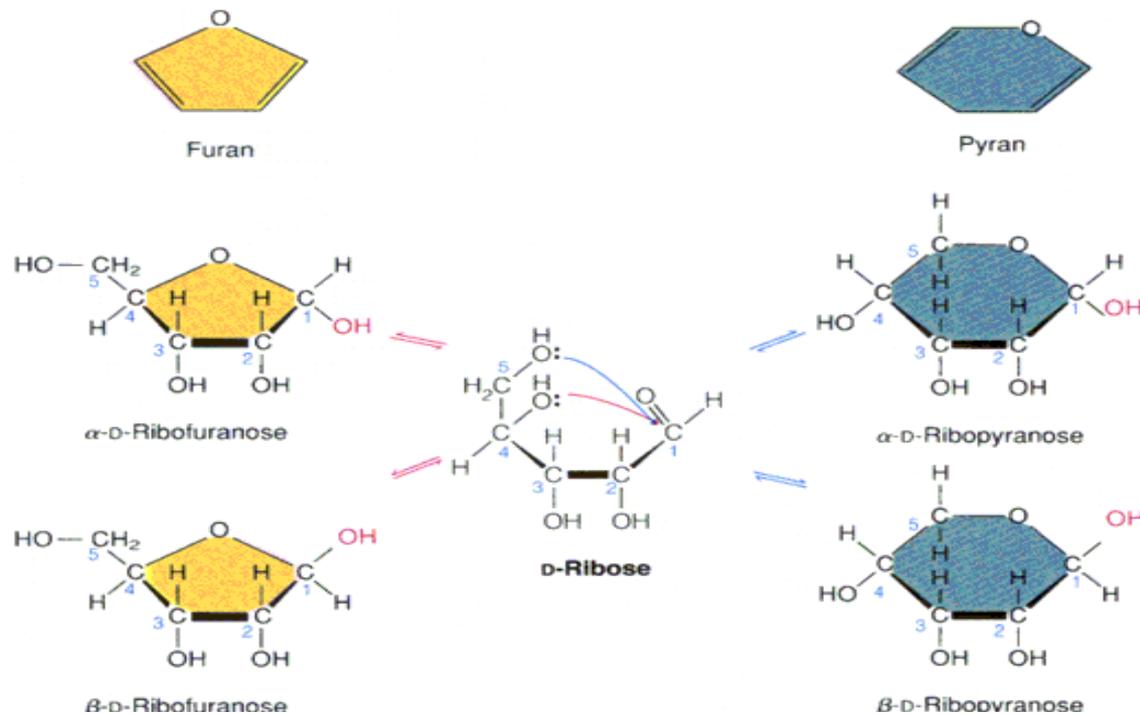


D-Fructose

L-Fructose

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Rings (5,6) – Four Possible Forms



Composition of Aqueous Solutions of D-Aldoses at Equilibrium

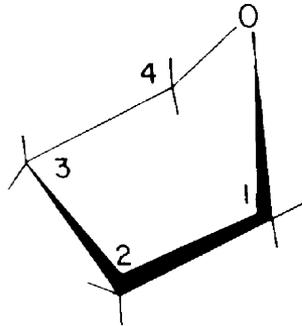
Aldose	% Pyranose			% Furanose ^a		
	α	β	Total	α	β	Total
Allose	16	71	87	(3.5)	5	(8.5)
Altrose	27	40	67	20	13	33
Glucose	38	62	100	0.1	<0.2	
Mannose	65.5	34.5	100	—	—	—
Gulose	<0.1	78	78	<0.1	22	22
Idose	39	36	75	11	14	25
Galactose	29	64	93	3	4	7
Talose	40	29	69	20	11	31
Ribose	21	59	80	6	14	20
Arabinose	63	34	97	(2.5)	2	(4.5)
Xylose	36.5	63	99.5			0.5
Lyxose	70	28	98	1.5	0.5	2

^a Figures in parentheses were obtained by different authors, and totals therefore do not add up to 100%.

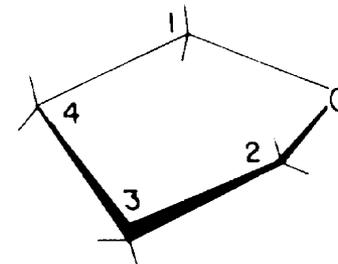
Conformation des Oses (1)

- Furanoses - Envelopes (E) vs Twist (T)

Envelope forms



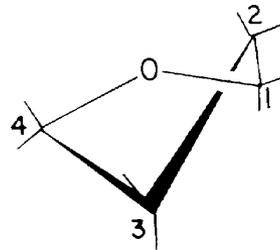
0E



E_0

Possible envelope forms (10): ${}^1E; E_1; {}^2E; E_2; {}^3E; E_3; {}^4E; E_4; {}^0E; E_0$

Twist forms



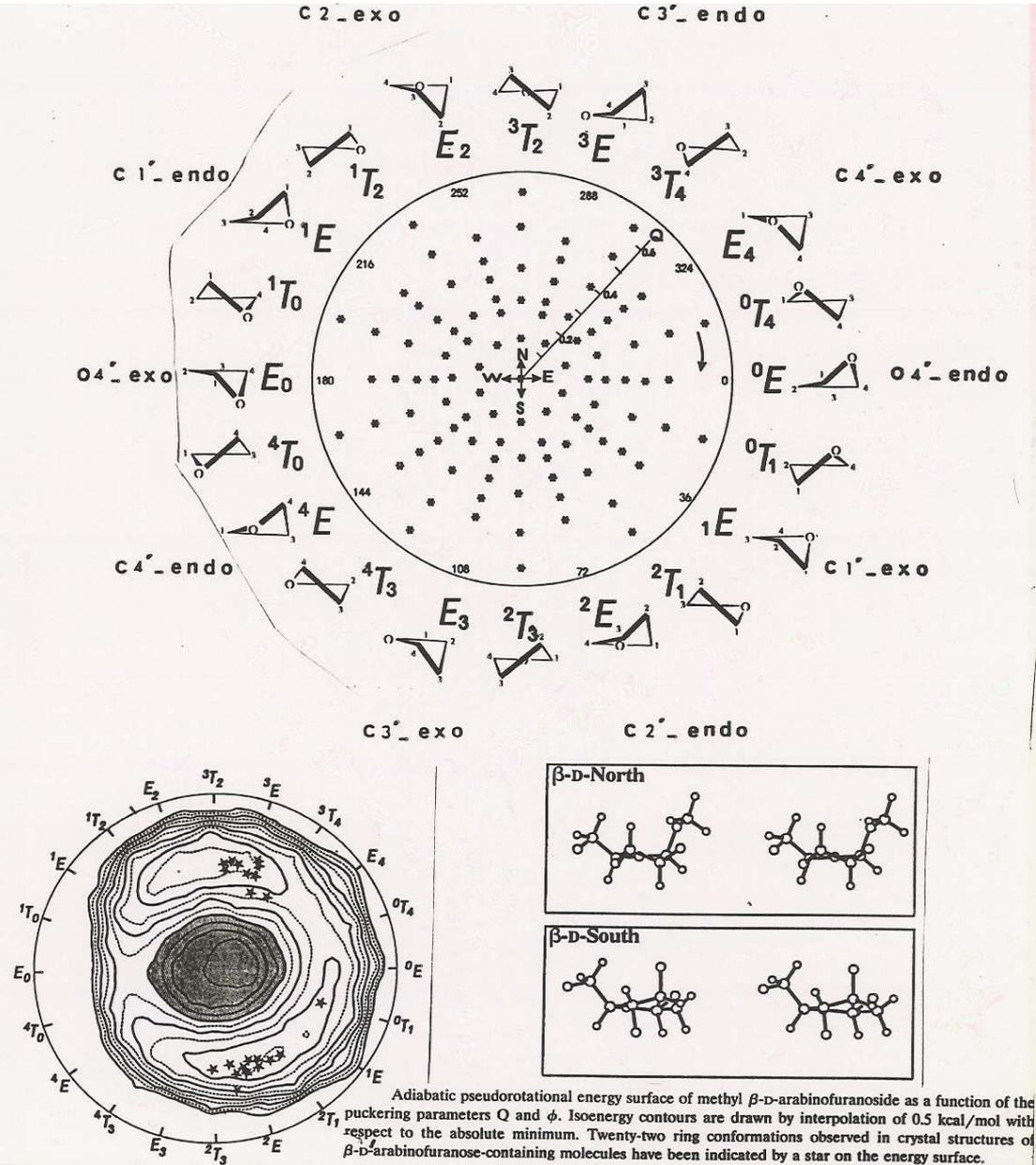
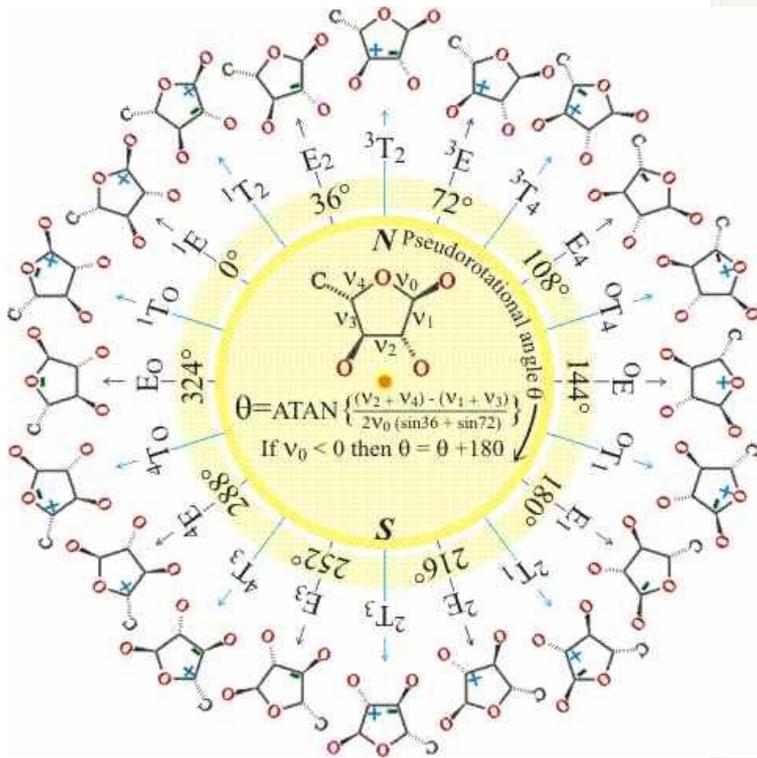
2T_3

Possible twist forms (10): ${}^0T_1; {}^1T_0; {}^1T_2; {}^2T_1; {}^2T_3; {}^3T_2; {}^3T_4; {}^4T_3; {}^0T_4; {}^4T_0$

Conformation des Oses (2)

- Puckering des Furanoses:

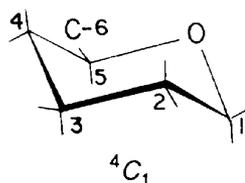
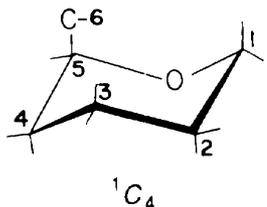
$\alpha\beta$ -L-Arabinofuranose



Conformation des Oses (3)

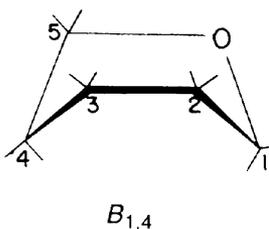
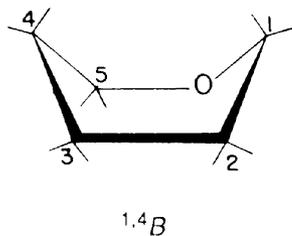
- Pyranoses - Chaise (C) ;
Bateau (B) ; Autres

Chair forms



Possible chair forms (2): 1C_4 and 4C_1

Boat forms

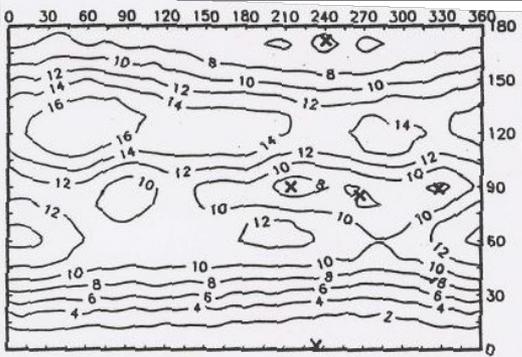


Possible boat forms (6): ${}^{1,4}B$; $B_{1,4}$; ${}^{2,5}B$; $B_{2,5}$; ${}^{0,3}B$; $B_{0,3}$

Conformation of D-Aldopyranoses in Aqueous Solutions

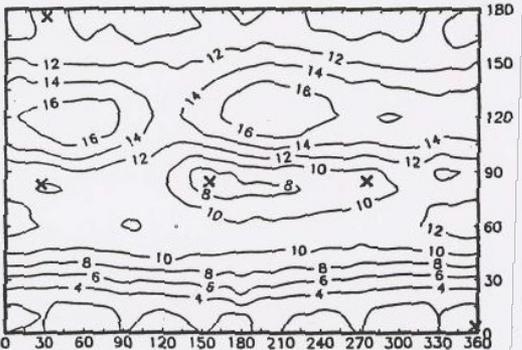
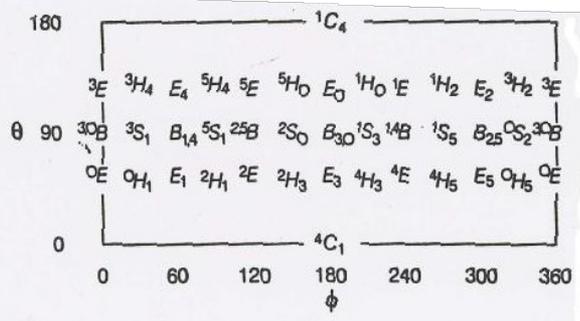
	Found by NMR	Found by thermodynamic calculation	Interaction energies (kJ/mole)	
			4C_1	1C_4
Aldohexoses				
α -D-Allose	4C_1	4C_1	16.33	22.40
β -D-Allose	4C_1	4C_1	12.35	25.33
α -D-Altrose	${}^4C_1, {}^1C_4$	${}^4C_1, {}^1C_4$	15.28	16.12
β -D-Altrose	4C_1	4C_1	14.03	22.40
α -D-Galactose	4C_1	4C_1	11.93	26.38
β -D-Galactose	4C_1	4C_1	10.47	32.45
α -D-Glucose	4C_1	4C_1	10.05	27.84
β -D-Glucose	4C_1	4C_1	8.58	33.49
α -D-Gulose	4C_1	4C_1	16.75	19.89
β -D-Gulose	4C_1	4C_1	12.77	22.82
α -D-Idose	${}^4C_1, {}^1C_4$	${}^4C_1, {}^1C_4$	18.21	16.12
β -D-Idose	4C_1	4C_1	16.96	22.40
α -D-Mannose	4C_1	4C_1	10.47	23.24
β -D-Mannose	4C_1	4C_1	12.35	32.03
α -D-Talose	4C_1	4C_1	14.86	24.70
β -D-Talose	4C_1	4C_1	16.75	33.49
Aldopentoses				
α -D-Arabinose	1C_4	1C_4	13.40	8.58
β -D-Arabinose	${}^4C_1, {}^1C_4$	${}^4C_1, {}^1C_4$	12.14	10.05
α -D-Lyxose	${}^4C_1, {}^1C_4$	${}^4C_1, {}^1C_4$	8.58	10.89
β -D-Lyxose	4C_1	4C_1	10.47	14.86
α -D-Ribose	${}^4C_1, {}^1C_4$	${}^4C_1, {}^1C_4$	14.44	14.86
β -D-Ribose	${}^4C_1, {}^1C_4$	${}^4C_1, {}^1C_4$	10.47	12.98
α -D-Xylose	4C_1	4C_1	8.16	15.07
β -D-Xylose	4C_1	4C_1	6.70	16.33

Conformation des Oses (4)



α -D-Glucopyranose

Locations of characteristic conformers on the surface representing the Cremer-Pople puckering space.



β -D-Glucopyranose

Puckering des Pyranoses

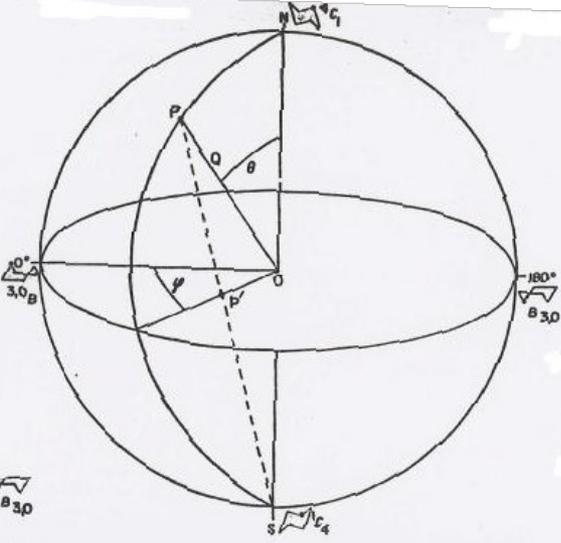
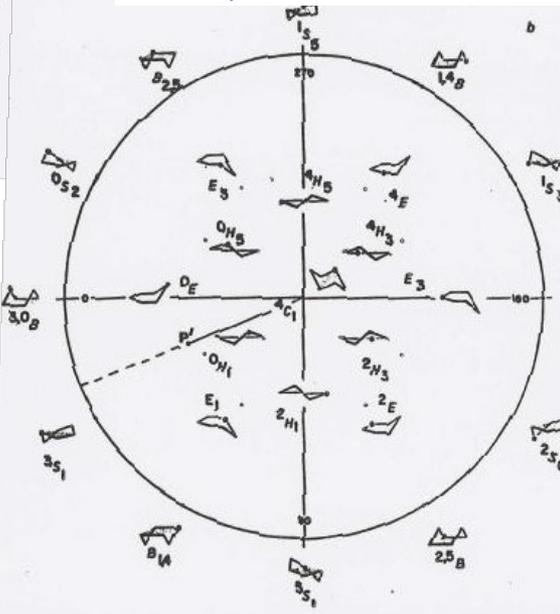


Fig. 1(a) The spherical-coordinate system of the Cremer and Pople puckering parameters for six-membered rings.

Fig. 1(b) Stereogram of the puckering parameters for a pyranoid ring. The *E* and *H* conformations are those of the upper hemisphere of Fig. 1a, namely, distorted 4C_1 conformations. Those of the lower hemisphere, namely, distorted 1C_4 , are related by symmetry at the center of the circle. That is, 0E becomes 3E , and 0H_1 becomes 3H_4 for 1C_4 distortions.

Table 1
Cremer-Pople puckering values and energies for the local minima for the aldopyranoses and analogues from MM3(92) with $\epsilon = 3.0$

	q (Å)	Φ (degrees)	Θ (degrees)	Approximate characteristic form	Steric energy (kcal/mol)	Relative energy (kcal/mol)
Cyclohexane	0.569	157.6	0.0	C	8.04	0.00
	0.756	150.0	90.0	S	13.80	5.76
Tetrahydropyran	0.573	300.0	3.8	C	8.46	0.00
	0.755	147.5	88.4	1S_3	13.92	5.54
2-Hydroxytetrahydropyran	0.749	270.0	90.0	1S_3	14.66	6.20
	0.552	201.4	3.2	4C_1	7.47	0.00
	0.582	136.8	175.5	1C_4	7.80	0.33
	0.729	322.9	88.6	0S_2	11.44	2.97
	0.756	94.3	90.6	3S_1	12.42	3.95
α -D-Allopyranose	0.768	210.2	92.8	1S_3	14.66	6.19
	0.560	179.4	2.6	4C_1	13.09	0.00
	0.547	284.8	175.3	1C_4	14.50	1.41
	0.760	336.4	92.4	0S_2	17.56	4.47
β -D-Allopyranose	0.762	213.6	90.3	1S_3	20.22	7.13
	0.590	1.4	4.1	4C_1	11.65	0.00
	0.501	12.3	171.8	1C_4	15.56	3.91
	0.766	24.0	87.2	3S_1	17.34	5.69
α -D-Altropyranose	0.760	338.8	88.1	${}^0S_2/{}^3O_B$	17.74	6.09
	0.702	155.6	84.4	2S_0	18.56	6.91
	0.552	289.6	174.8	1C_4	13.28	0.00
	0.539	259.7	5.2	4C_1	13.64	0.36
	0.772	334.6	90.8	0S_2	14.78	1.50
β -D-Altropyranose	0.574	351.3	5.7	4C_1	12.55	0.00
	0.519	348.6	170.5	1C_4	15.02	2.47
	0.773	24.7	87.5	3S_1	15.44	2.89
	0.754	274.3	87.5	1S_3	17.53	4.98
α -D-Galactopyranose	0.554	242.0	2.7	4C_1	11.30	0.00
	0.538	225.2	177.0	1C_4	16.95	5.65
	0.761	211.8	90.1	1S_3	17.11	5.81
	0.744	331.0	90.0	0S_2	18.24	6.94
	0.586	21.5	3.7	4C_1	10.40	0.00
β -D-Galactopyranose	0.693	211.4	82.2	1S_3	17.20	6.80
	0.752	336.7	88.2	0S_2	19.01	8.66
	0.758	23.0	85.8	3S_1	19.16	8.76
	0.497	354.0	172.5	1C_4	19.24	8.84
	0.565	234.4	2.7	4C_1	10.75	0.00
α -D-Glucopyranosé	0.525	241.6	172.1	1C_4	15.95	5.20
	0.774	215.0	90.3	1S_3	17.26	6.51
	0.750	267.3	85.6	1S_3	18.00	7.25
	0.739	328.0	89.0	0S_2	18.08	7.33
	0.598	358.0	3.7	4C_1	9.76	0.00
β -D-Glucopyranose	0.715	155.1	84.6	2S_0	16.27	6.51
	0.472	31.3	175.6	1C_4	18.34	8.58
	0.723	274.0	84.6	1S_3	18.42	8.66
	0.730	27.2	82.9	3S_1	18.94	9.18

	q (Å)	Φ (degrees)	Θ (degrees)	Approximate characteristic form	Steric energy (kcal/mol)	Relative energy (kcal/mol)
α -D-Gulopyranose	0.548	21.6	0.2	4C_1	14.01	0.00
	0.556	240.8	177.8	1C_4	14.85	0.84
	0.752	329.3	89.8	0S_2	15.26	1.25
β -D-Gulopyranose	0.576	20.9	5.1	4C_1	12.01	0.00
	0.520	35.7	169.2	1C_4	15.61	3.60
	0.767	337.0	88.2	0S_2	15.69	3.68
	0.655	168.8	81.7	${}^2S_0/B_{3,0}$	20.44	8.43
α -D-Idopyranose	0.777	328.6	89.8	0S_2	13.06	0.00
	0.569	266.8	177.4	1C_4	13.24	0.18
	0.531	287.8	4.3	4C_1	13.61	0.55
β -D-Idopyranose	0.568	6.2	7.9	4C_1	12.62	0.00
	0.536	15.2	171.4	1C_4	14.87	2.25
	0.738	282.9	90.2	${}^1S_3/B_{2,5}$	15.72	3.10
	0.785	22.6	87.6	3S_1	17.16	4.50
α -D-Mannopyranose	0.664	209.7	83.0	1S_3	22.74	10.12
	0.550	257.1	6.2	4C_1	11.18	0.00
	0.761	322.6	87.9	0S_2	15.42	4.24
	0.537	258.5	171.0	1C_4	15.56	4.38
β -D-Mannopyranose	0.714	171.4	87.1	${}^2S_0/B_{3,0}$	17.99	6.81
	0.582	355.6	3.6	4C_1	11.28	0.00
	0.760	282.3	89.2	${}^1S_3/B_{2,5}$	18.14	6.86
	0.491	314.5	173.0	1C_4	18.42	7.16
α -D-Talopyranose	0.686	163.8	83.8	${}^2S_0/B_{3,0}$	18.79	7.51
	0.752	22.6	86.0	3S_1	19.21	7.91
	0.550	254.8	6.4	4C_1	11.79	0.00
	0.768	328.6	89.1	0S_2	15.48	3.69
β -D-Talopyranose	0.552	258.6	175.3	1C_4	16.32	4.52
	0.758	211.3	90.2	1S_3	19.04	7.25
	0.584	7.1	3.8	4C_1	11.59	0.00
	0.523	323.2	168.9	1C_4	18.96	7.37
	0.764	326.9	89.5	0S_2	19.54	7.95
	0.729	279.0	88.6	${}^1S_3/B_{2,5}$	19.67	8.08
	0.686	203.5	80.5	1S_3	21.48	9.89

^a Corresponds to axial form.

^b Corresponds to equatorial form.

Carbohydrate Research 264 (1994) 1-19

Modeling of aldopyranosyl ring puckering with MM3(92)

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Conformation des Oses (5)