THE UNIVERSITY *of* TEXAS

HEALTH SCIENCE CENTER AT HOUSTON

SCHOOL *of* HEALTH INFORMATION SCIENCES

Solutions HW 1

For students of HI 6001-100 “Biomolecular Modeling”

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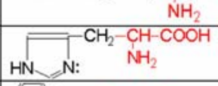
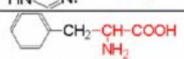
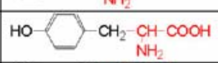
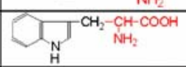
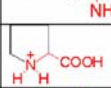
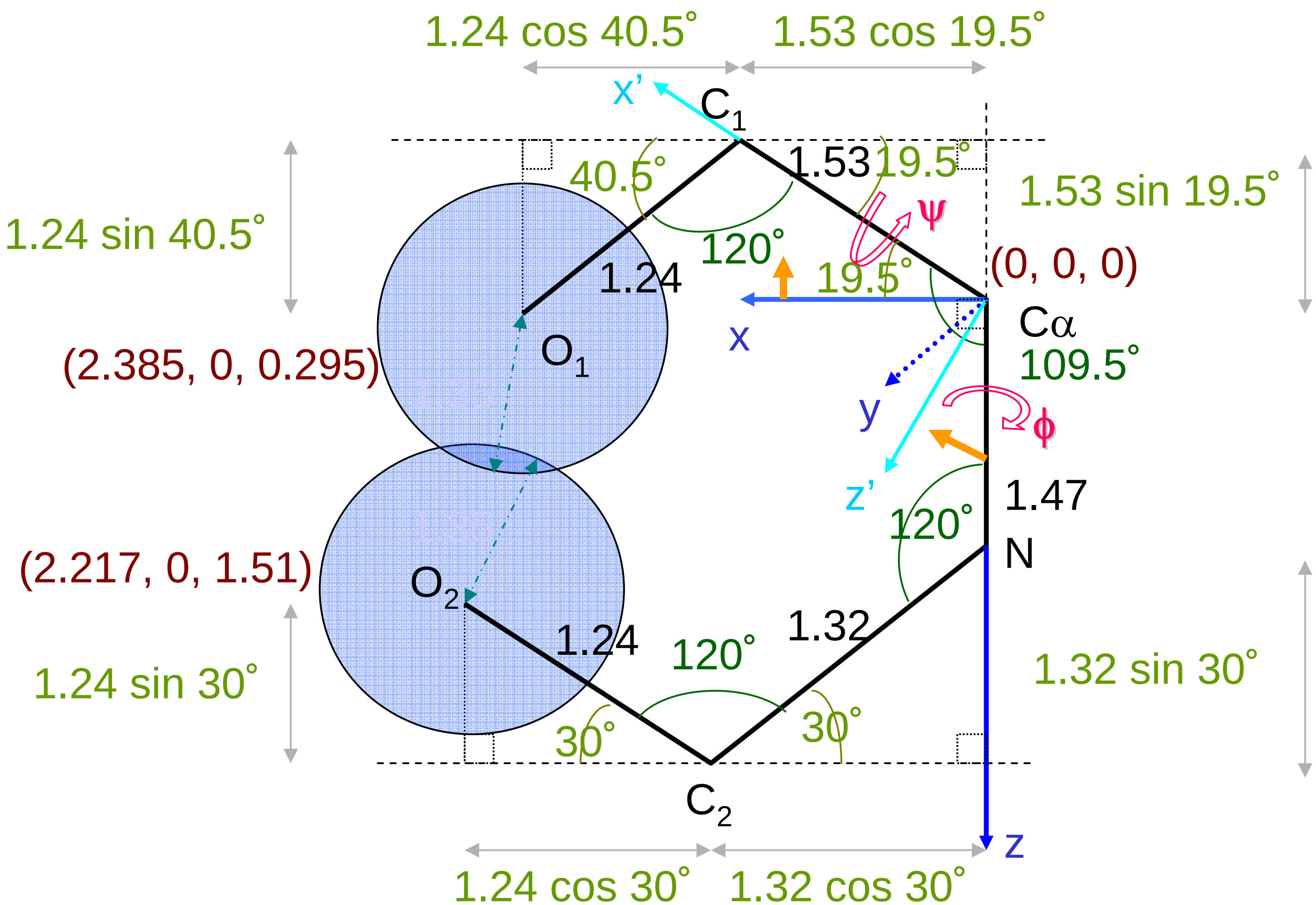
http://biomachina.org/courses/modeling/06.html

Problem 1

Amino Acid		Structure	pKa	H+ on	H+ off	pH 2.0	pH 7.3	pH13.0
Alanine	A	H3N+ $CH_3-CH(NH_2)-COOH$	8.0	+1	0	+1	+1	0
Alanine	A	$CH_3-CH(NH_2)-COOH$						
Valine	V	$(H_3C)_2CH-CH(NH_2)-COOH$						
Leucine	L	$(H_3C)_2CH-CH_2-CH(NH_2)-COOH$						
Isoleucine	I	$H_3C-CH_2-CH(CH_3)-CH(NH_2)-COOH$						
Threonine	T	$H_3C-CH(OH)-CH(NH_2)-COOH$						
Serine	S	$HO-CH_2-CH(NH_2)-COOH$						
Glutamine	Q	$H_2N-C(=O)-CH_2-CH_2-CH(NH_2)-COOH$						
Asparagine	N	$H_2N-C(=O)-CH_2-CH(NH_2)-COOH$						
Lysine	K	$H_2N-(CH_2)_4-CH(NH_2)-COOH$	10.0	+1	0	+1	+1	0
Arginine	R	$H_2N-C(=NH)-NH-CH_2-CH_2-CH_2-CH(NH_2)-COOH$	12.0	+1	0	+1	+1	0
Aspartate	D	$HOOC-CH_2-CH(NH_2)-COOH$	4.4	0	-1	0	-1	-1
Glutamate	E	$HOOC-CH_2-CH_2-CH(NH_2)-COOH$	4.4	0	-1	0	-1	-1
Histidine	H		6.5	+1	0	+1	0	0
Phenylalanine	F							
Tyrosine	Y		10.0	0	-1	0	0	-1
Tryptophan	W							
Methionine	M	$H_3C-S-(CH_2)_2-CH(NH_2)-COOH$						
Cysteine	C	$HS-CH_2-CH(NH_2)-COOH$	8.5	0	-1	0	0	-1
Proline	P							
Glycine	G	$H-CH(NH_2)-COOH$						
Alanine	A	$CH_3-CH(NH_2)-COOH$						
Alanine	A	$CH_3-CH(NH_2)-COOH$ COO -	3.1	0	-1	0	-1	-1
Net charge				pH<pKa	pH>pKa	+4	0	-5

Problem 2



All length units are in Å (0.1nm)

Rotating O_2 by ϕ about Cα-N (z axis):

$$O_2' = Rz(\phi) \bullet \begin{bmatrix} 2.217 \\ 0 \\ 1.51 \end{bmatrix} = \begin{bmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2.217 \\ 0 \\ 1.51 \end{bmatrix}$$

$$= \begin{bmatrix} 2.217\cos\phi + 0 + 0 \\ 2.217\sin\phi + 0 + 0 \\ 0 + 0 + 1.51 \end{bmatrix}$$

$$= \begin{bmatrix} 2.217\cos\phi \\ 2.217\sin\phi \\ 1.51 \end{bmatrix}$$

Double-check:
Based on dihedral angle definition, rotation by small positive Φ means O_2 moves into the plane (positive y value)

Before rotating O_1 about Cα-C_1, rotate the frame by19.5°about y:

$$Ry(19.5°) \bullet \begin{bmatrix} 2.385 \\ 0 \\ 0.295 \end{bmatrix} = \begin{bmatrix} \cos 19.5° & 0 & -\sin 19.5° \\ 0 & 1 & 0 \\ \sin 19.5° & 0 & \cos 19.5° \end{bmatrix} \begin{bmatrix} 2.385 \\ 0 \\ 0.295 \end{bmatrix}$$

$$= \begin{bmatrix} 2.248 + 0 - 0.098 \\ 0 + 0 + 0 \\ 0.796 + 0 + 0.278 \end{bmatrix}$$

$$= \begin{bmatrix} 2.15 \\ 0 \\ 1.074 \end{bmatrix}$$

Double-check:
In the new coordinate system, the z component must be much larger whereas x remains similar

Now rotate about x' ($C\alpha$-C_1) by ψ:

$$Rx(\psi)\bullet\begin{bmatrix}2.15\\0\\1.074\end{bmatrix}=\begin{bmatrix}1 & 0 & 0\\0 & \cos\psi & -\sin\psi\\0 & \sin\psi & \cos\psi\end{bmatrix}\begin{bmatrix}2.15\\0\\1.074\end{bmatrix}$$

$$=\begin{bmatrix}2.15+0+0\\0+0-1.074\sin\psi\\0+0+1.074\cos\psi\end{bmatrix}$$

$$=\begin{bmatrix}2.15\\-1.074\sin\psi\\1.074\cos\psi\end{bmatrix}$$

Double-check:
Based on dihedral angle definition, rotation by small positive Ψ *means* O_1 *moves out of the plane (negative y value)*

Rotate the reference frame back by -19.5° about y to match the original coordinate system:

$$O_1' = Ry(-19.5°) \bullet \begin{bmatrix} 2.15 \\ -1.074\sin\psi \\ 1.074\cos\psi \end{bmatrix} = \begin{bmatrix} \cos(-19.5°) & 0 & -\sin(-19.5°) \\ 0 & 1 & 0 \\ \sin(-19.5°) & 0 & \cos(-19.5°) \end{bmatrix} \begin{bmatrix} 2.15 \\ -1.074\sin\psi \\ 1.074\cos\psi \end{bmatrix}$$

$$= \begin{bmatrix} 2.027 + 0 + 0.359\cos\psi \\ 0 - 1.074\sin\psi + 0 \\ -0.718 + 0 + 1.012\cos\psi \end{bmatrix}$$

$$= \begin{bmatrix} 2.027 + 0.359\cos\psi \\ -1.074\sin\psi \\ -0.718 + 1.012\cos\psi \end{bmatrix}$$

To solve for unknown ϕ and ψ, use the distance between O_1 and O_2

When $\phi = \psi$:

$$(2.217\cos\phi - 2.027 - 0.359\cos\phi)^2 + (2.217\sin\phi + 1.074\sin\phi)^2 + (1.51 + 0.718 - 1.012\cos\phi)^2 = 2.7^2$$

$$(1.858\cos\phi - 2.027)^2 + (3.291\sin\phi)^2 + (2.228 - 1.012\cos\phi)^2 = 7.29$$

$$3.452\cos^2\phi - 7.532\cos\phi + 4.1087 + 10.831\sin^2\phi + 4.964 - 4.509\cos\phi + 1.024\cos^2\phi - 7.29 = 0$$

$$\sin^2 + \cos^2 = 1 \Rightarrow$$

$$3.452\cos^2\phi - 7.532\cos\phi + 4.1087 + 10.831 - 10.831\cos^2\phi + 4.964 - 4.509\cos\phi + 1.024\cos^2\phi - 7.29 = 0$$

$$-6.355\cos^2\phi - 12.041\cos\phi + 12.6137 = 0$$

$$6.355\cos^2\phi + 12.041\cos\phi - 12.6137 = 0$$

$$\cos\phi = \frac{-12.041 \pm \sqrt{12.041^2 - 4(6.355)(-12.6137)}}{2(6.355)}$$

$$= \frac{-12.041 \pm \sqrt{144.986 - 320.64}}{12.71} = \frac{-12.041 \pm 21.578}{12.71}$$

$$= 0.750 \text{ or } -2.645 \text{ (ignored)}$$

invert cosine:

$\phi = 41.4°$ $\quad \phi = -41.4°$

$\psi = 41.4°$ $\quad \psi = -41.4°$

Likewise, when ϕ=-ψ

$\phi = -73.975°$ $\quad \phi = 73.975°$

$\psi = 73.975°$ $\quad \psi = -73.975°$

Problem 3

```
proc torus {} {

          set step 0.03
          set a 3
          set c 8

          for {set u 0} { $u < 6.2831853 } { set u [expr $u + $step]} {

                    for {set v 0} { $v < 6.2831853 } { set v [expr $v + $step]} {

                              set u1 [expr $step + $u]
                              set v1 [expr $step + $v]

                              set x0 [expr  ($c+$a*cos($v))*cos($u)]
                              set y0 [expr  ($c+$a*cos($v))*sin($u)]
                              set z0 [expr  $a*sin($v)]

                              set x1 [expr  ($c+$a*cos($v))*cos($u1)]
                              set y1 [expr  ($c+$a*cos($v))*sin($u1)]
                              set z1 [expr  $a*sin($v)]

                              set x2 [expr  ($c+$a*cos($v1))*cos($u)]
                              set y2 [expr  ($c+$a*cos($v1))*sin($u)]
                              set z2 [expr  $a*sin($v1)]

                              set x3 [expr  ($c+$a*cos($v1))*cos($u1)]
                              set y3 [expr  ($c+$a*cos($v1))*sin($u1)]
                              set z3 [expr  $a*sin($v1)]

                              draw  triangle "$x0 $y0 $z0" "$x1 $y1 $z1" "$x2 $y2 $z2"
                              draw  triangle "$x2 $y2 $z2" "$x1 $y1 $z1" "$x3 $y3 $z3"
                    }
          }
}
```