

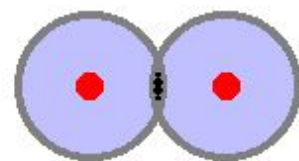
PROTEIN PHYSICS

LECTURES 3-4

**Elementary interactions:
Van der Waals
&
H-bonds**



**repulsion at
small distances**

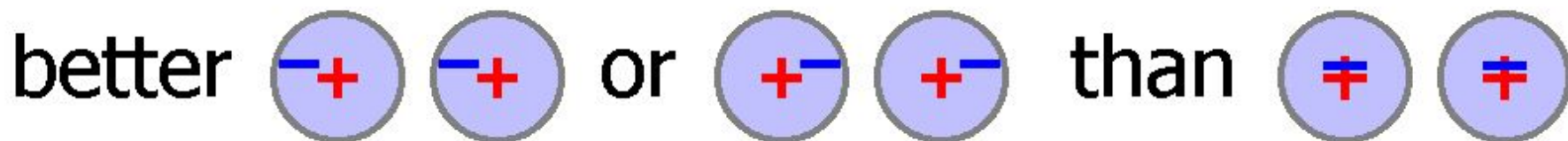


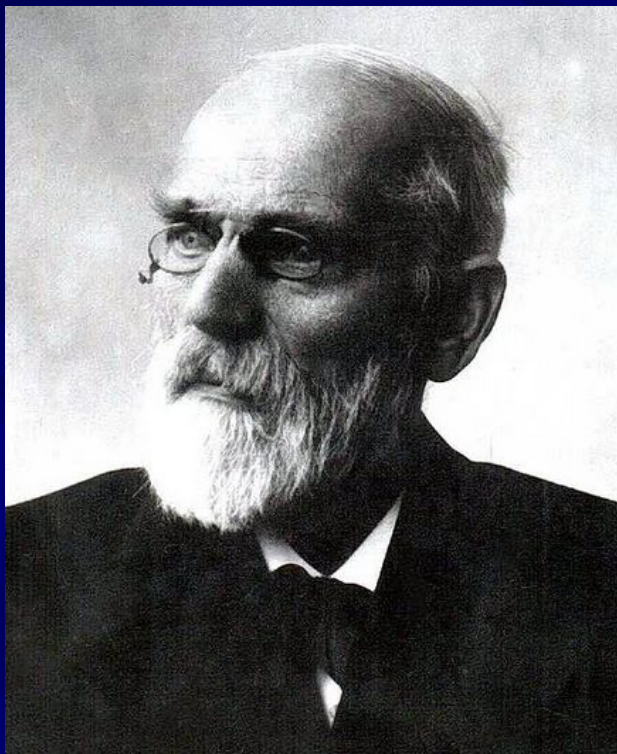
BUT:

Van der Waals

attraction at larger distances

due to coordination of e vibrations





Johannes Diderik van der Waals
(1837 – 1923)
— Nobel Prize 1910

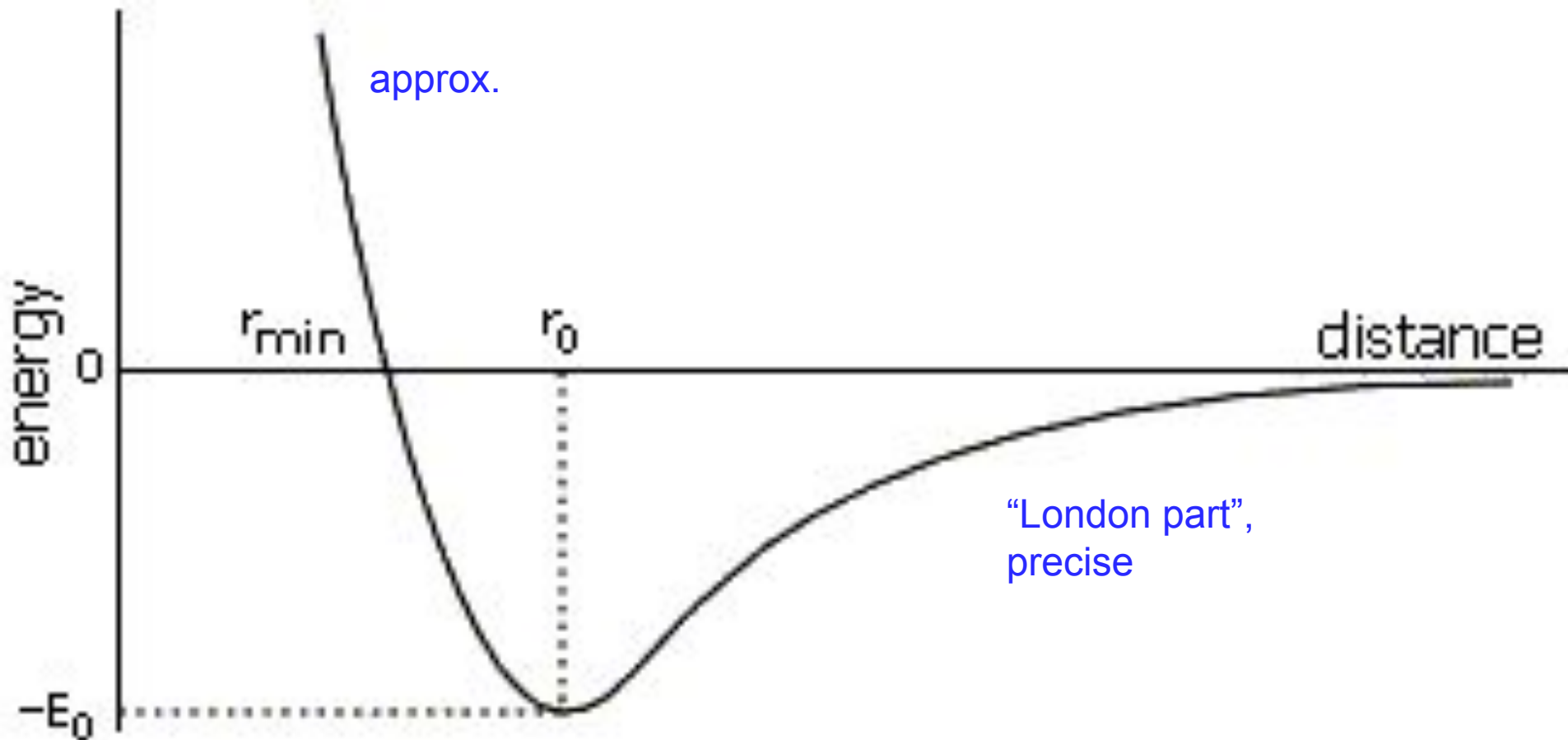


Fritz Wolfgang London
(1900 – 1954)

Lennard-Jones potential:

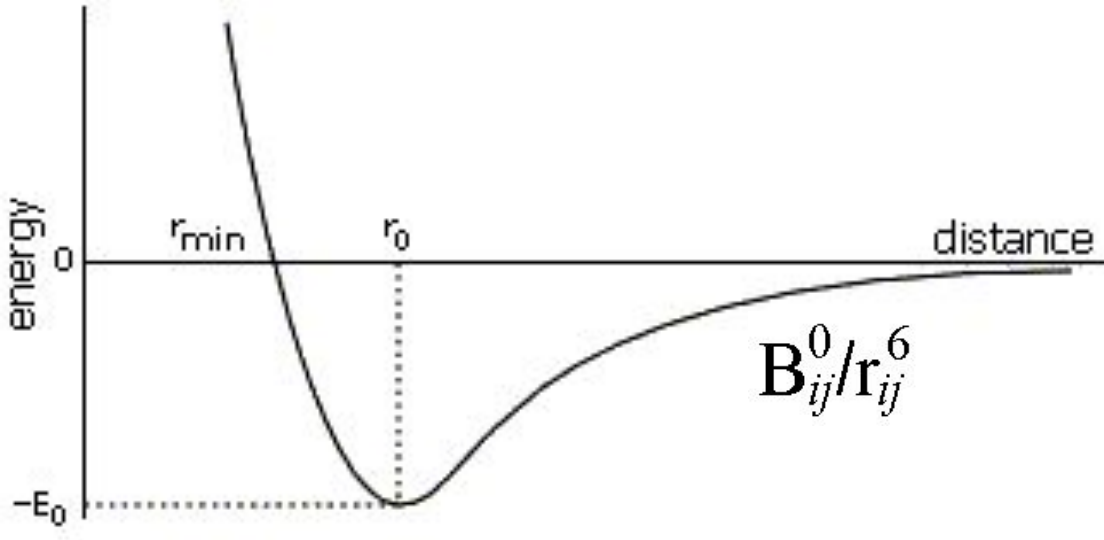
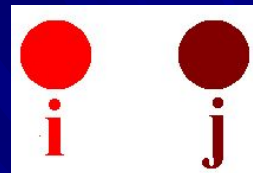
$$U_{\text{LJ}}(r) = E_0[(r_0/r)^{12} - 2(r_0/r)^6]$$

The simplest form



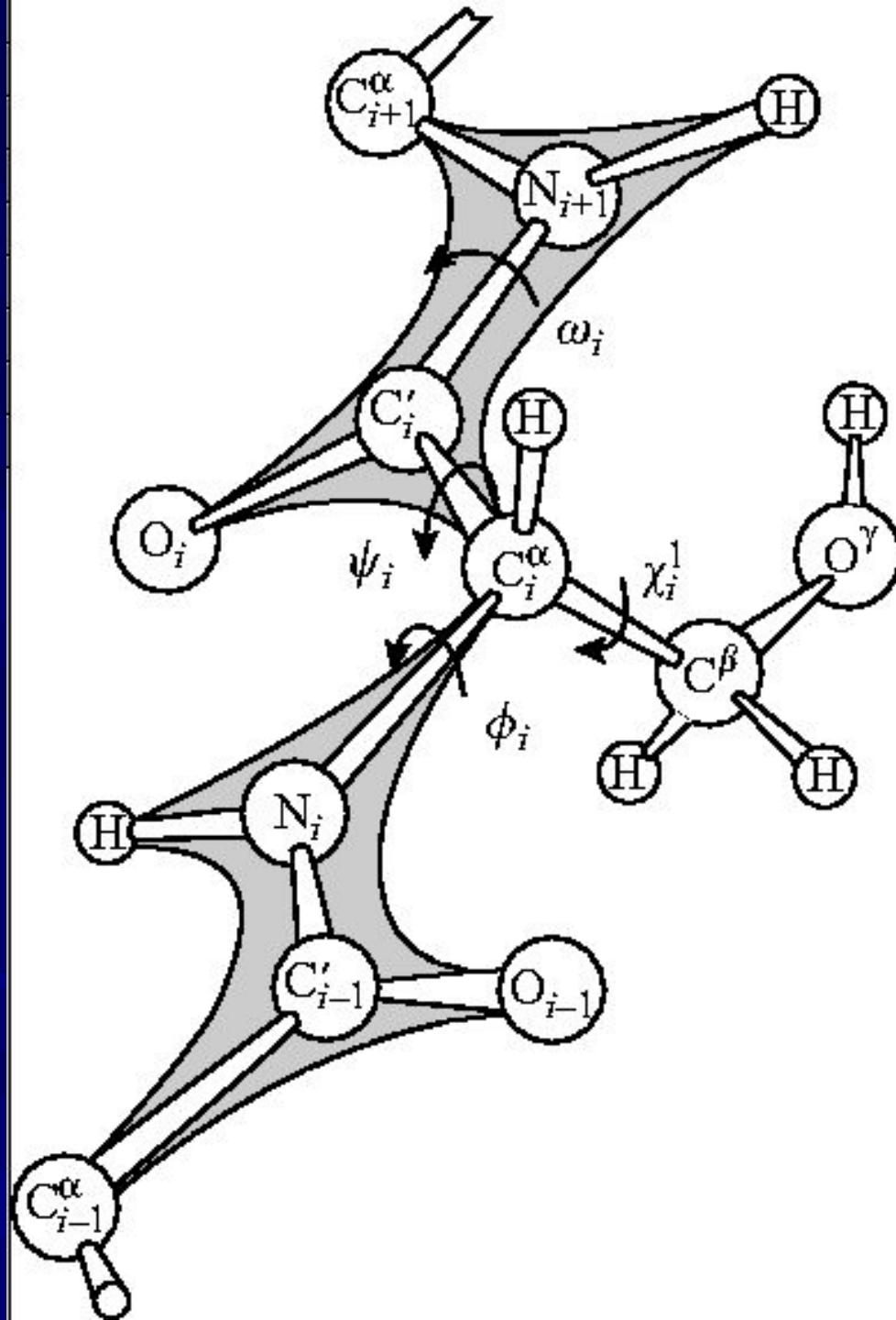
In vacuum

$$B_{ij}^0 = \beta_i \beta_j$$



Typical parameters of van der Waals interaction potentials.

Interaction	$E_0, \frac{\text{kcal}}{\text{mol}}$	$r_0, \text{\AA}$	$r_{\min}, \text{\AA}$	Min. v. d. Waals radii of atoms, $\text{\AA}$
H H	0.12	2.4	2.0	H: 1.0
H C	0.11	2.9	2.4	
C C	0.12	3.4	3.0	C: 1.5
O O	0.23	3.0	2.7	O: 1.35
N N	0.20	3.1	2.7	N: 1.35
CH ₂ . . . CH ₂	≈ 0.5	≈ 4.0	≈ 3.0	CH ₂ : ≈ 1.5

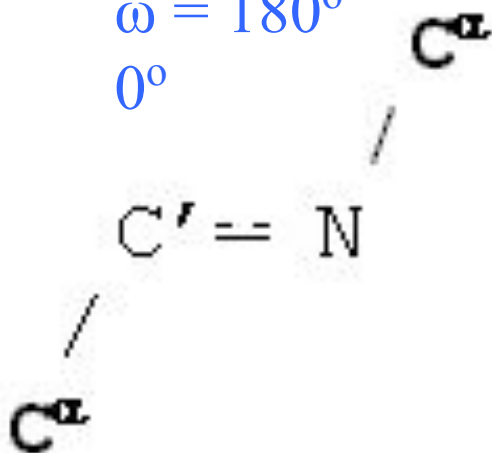


Main-chain:

ϕ (N-C α) ,
 ψ (C α -C')

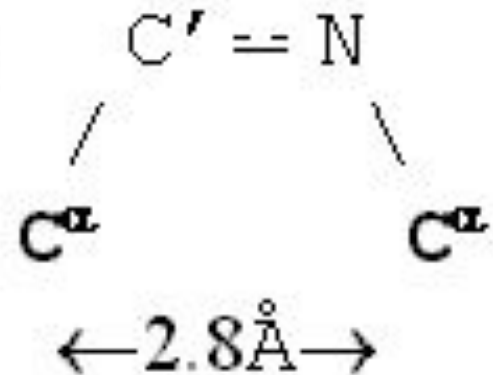
$$\omega = 180^\circ$$

trans:

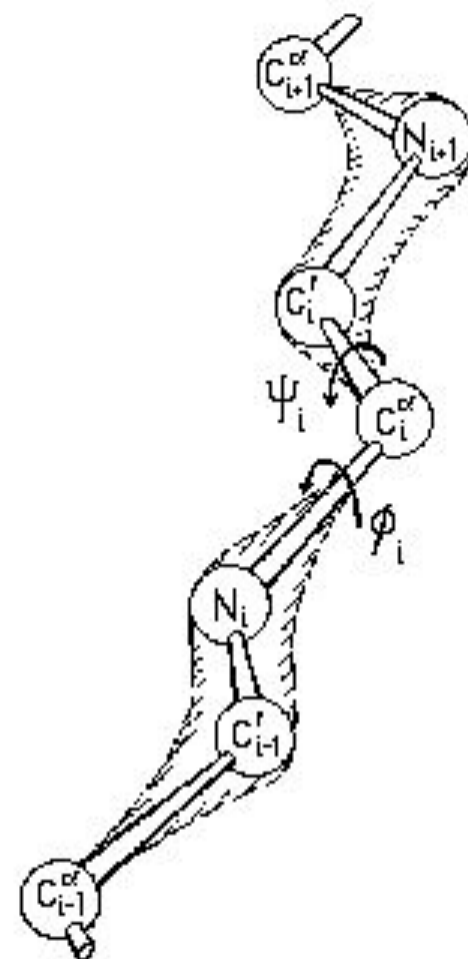
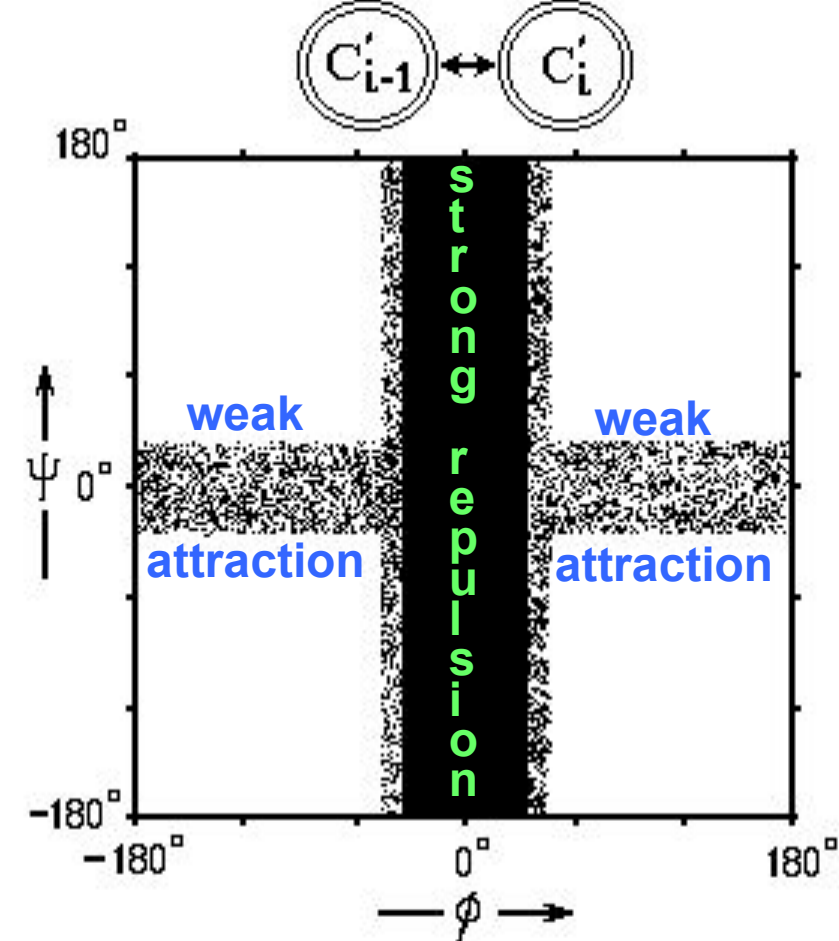


$$\omega =$$

cis:

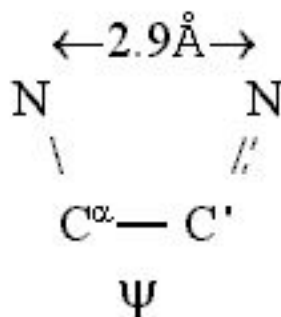
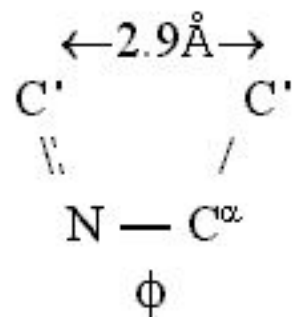


$2.8\text{\AA} < r_{\min}(\text{C}\dots\text{C}) = 3.0\text{\AA}$
strong repulsion

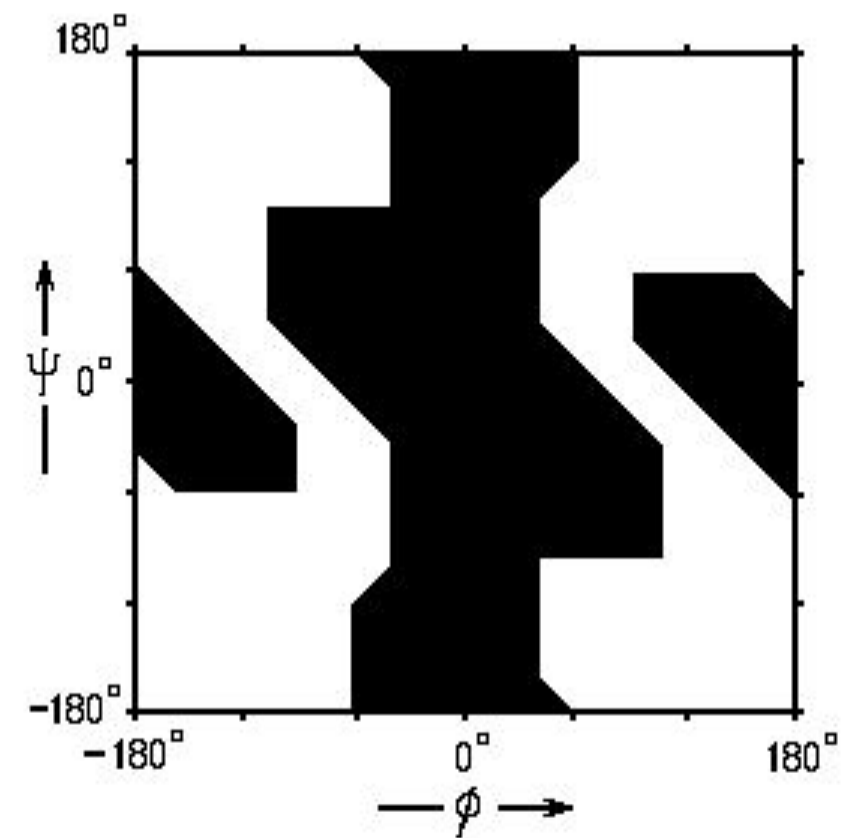


$$2.9\text{\AA} < r_{\min}(C \dots C) = 3.0\text{\AA}$$

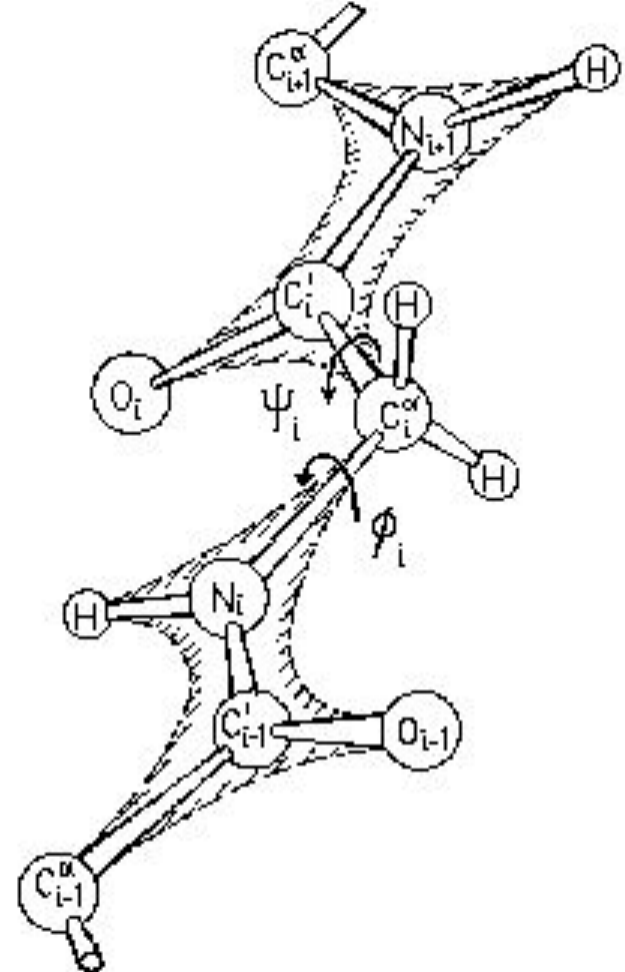
$$2.9\text{\AA} > r_{\min}(N \dots N) = 2.7\text{\AA}$$

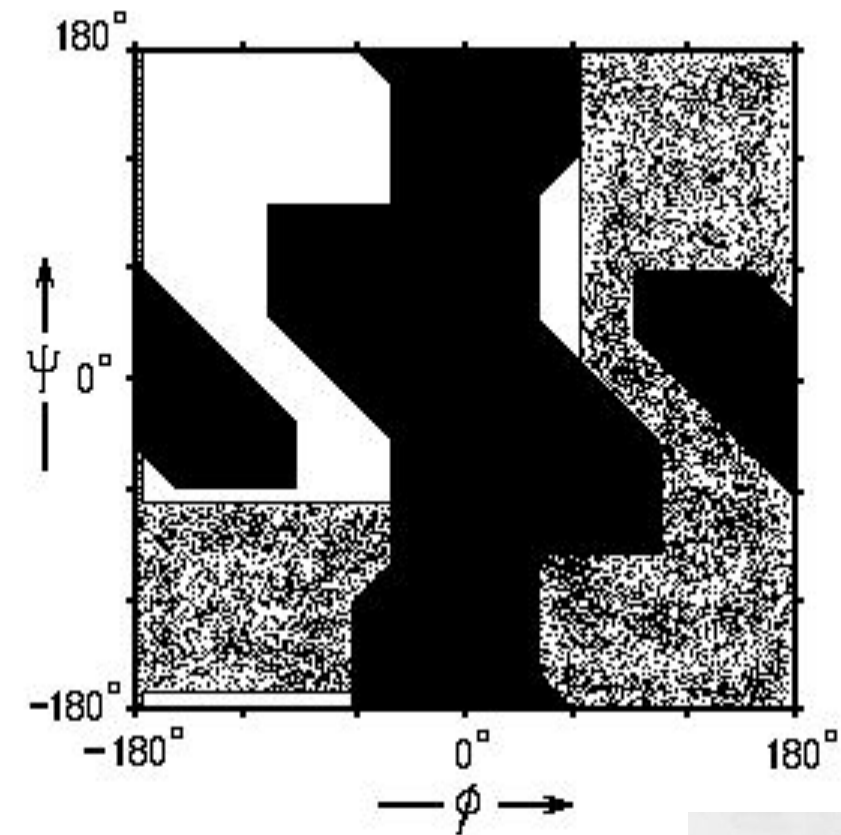


$$r_0(N \dots N) = 3.1\text{\AA}$$

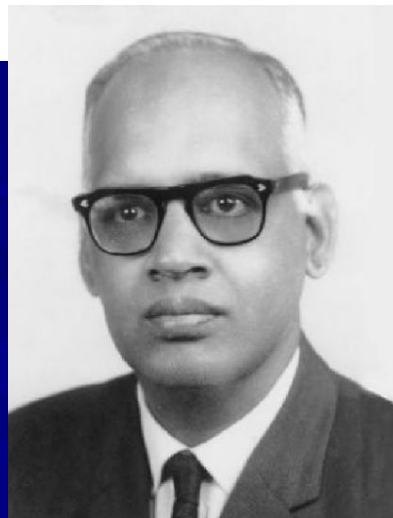
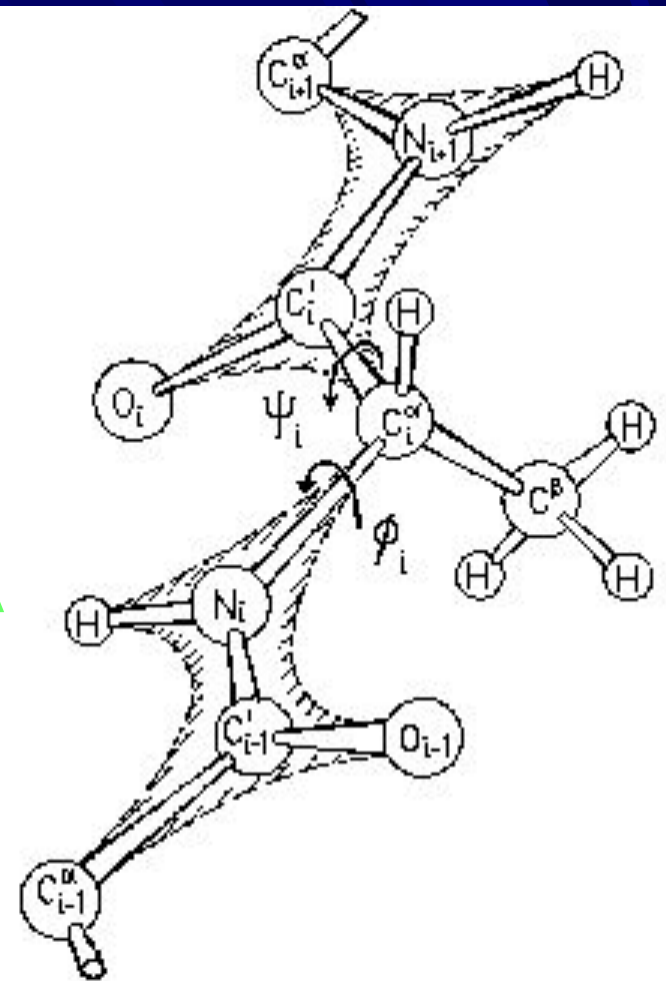


GLY

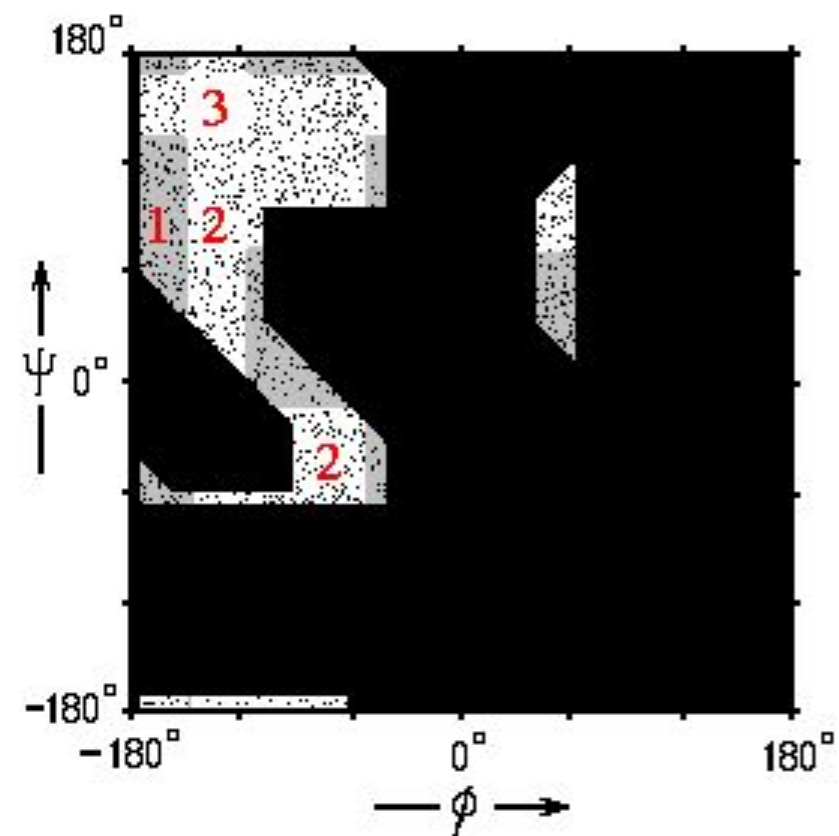




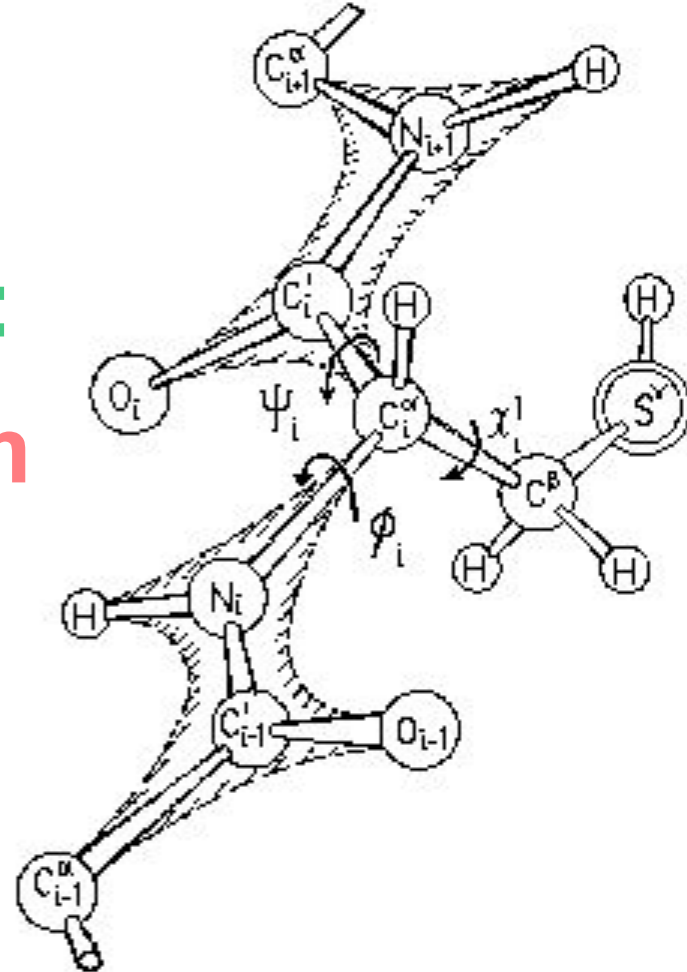
ALA



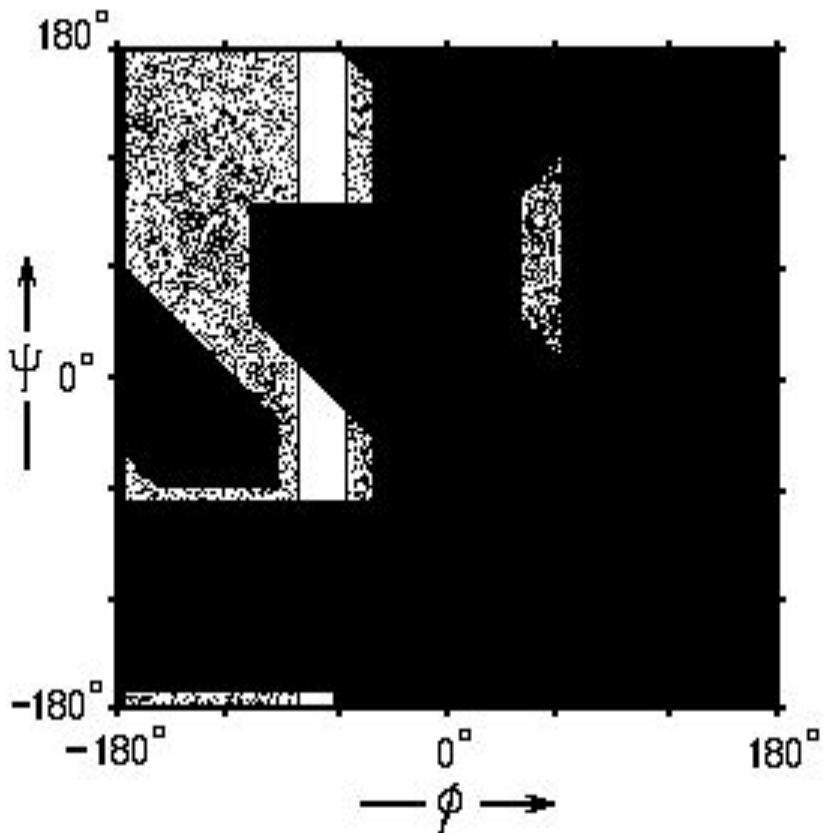
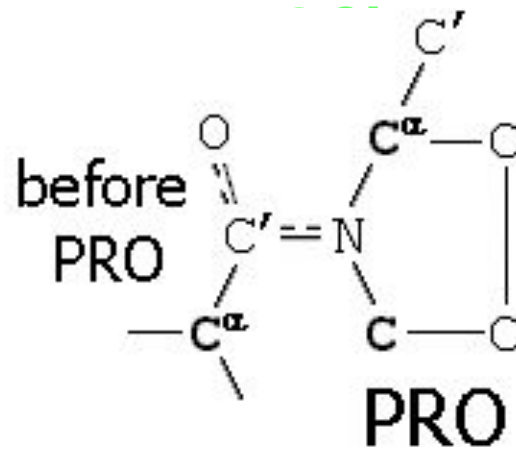
Gopalasamudram Narayana Iyer
Ramachandran(1922-2001)



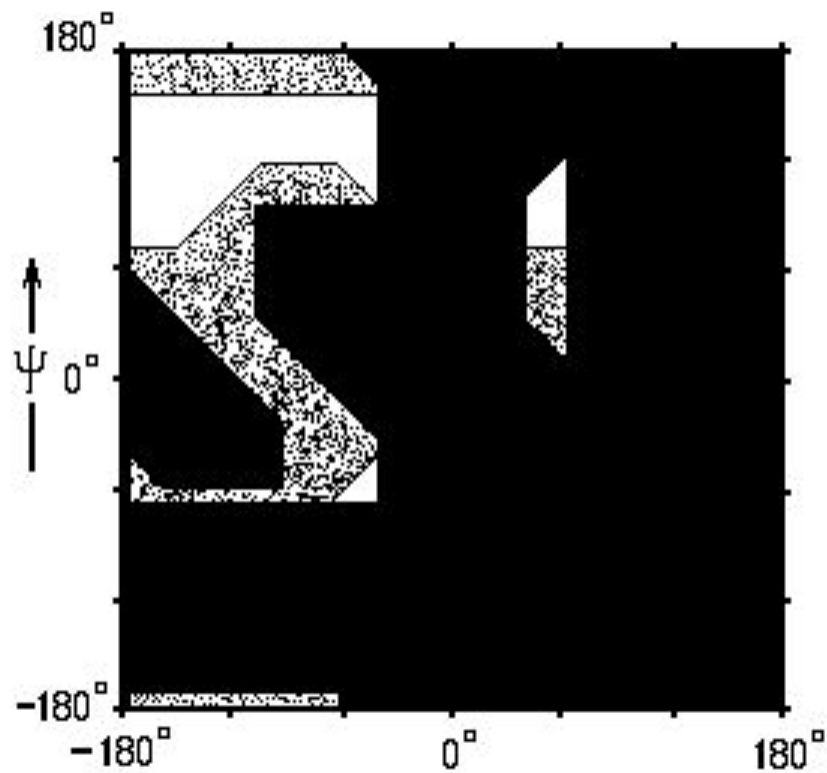
>ALA:
 γ -atoms



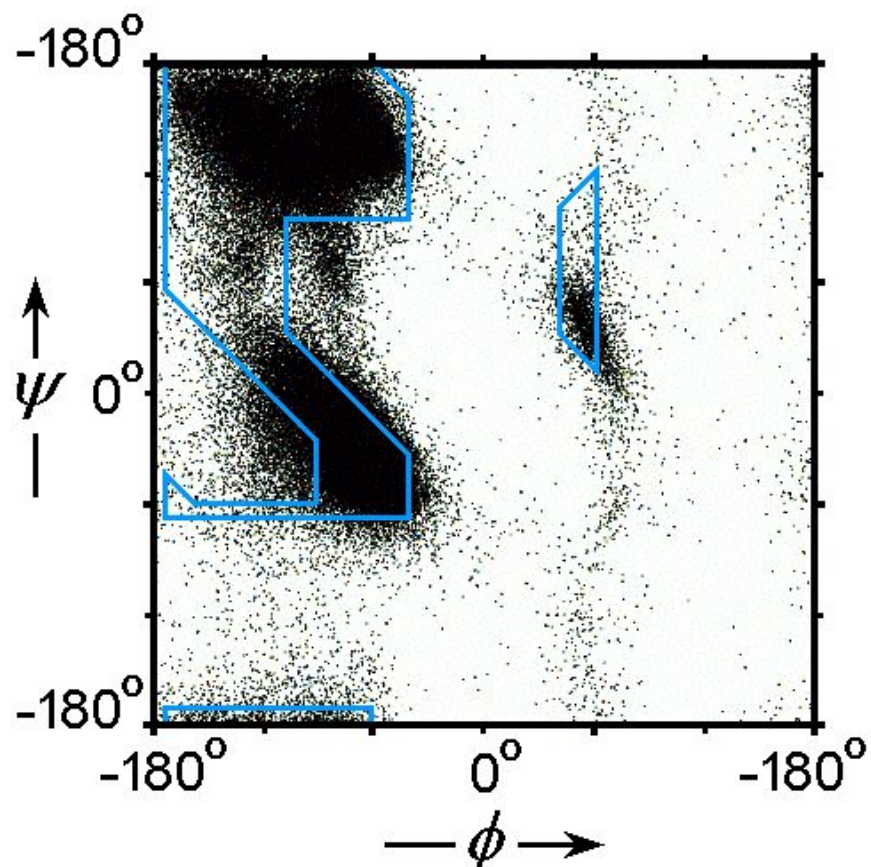
PRO ($\phi =$



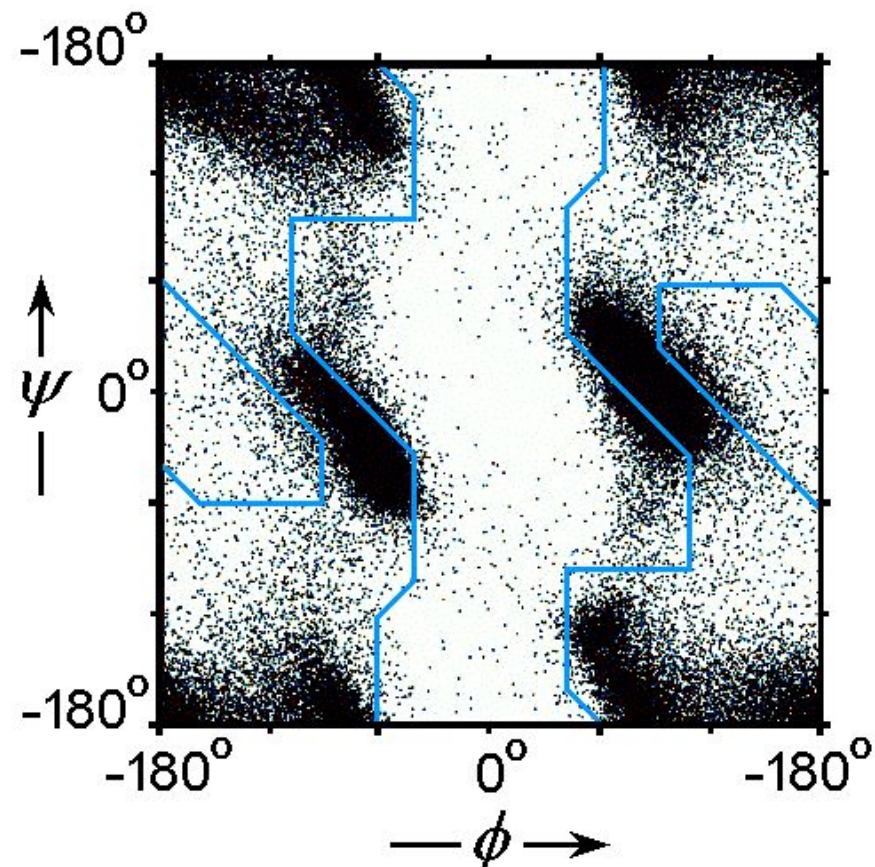
Before PRO



ALA, etc.

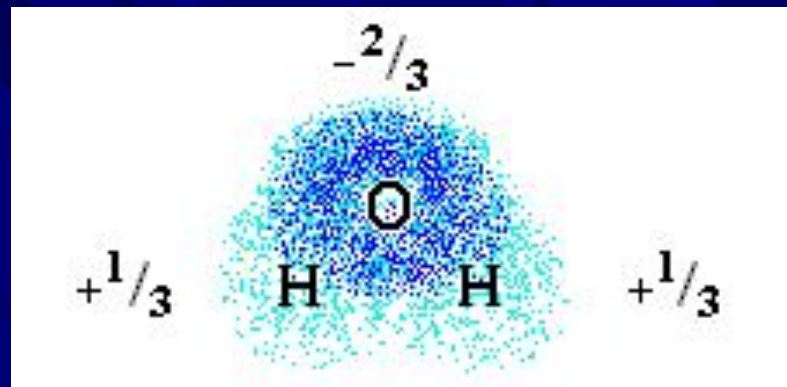


GLY only



HYDROGEN BONDS

WATER molecule:



H-bond energy: 5 kcal/mol

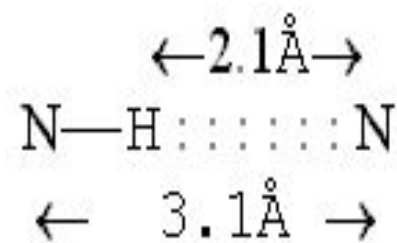
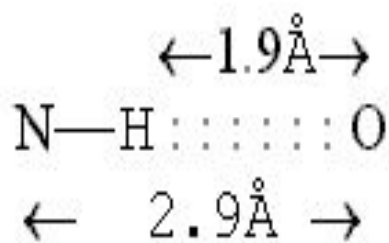
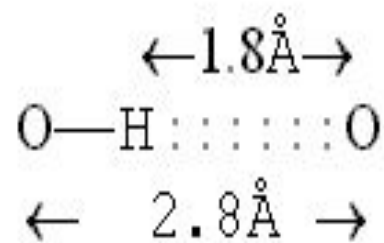
ICE sublimation: (12 kcal/mol - 2 kcal/mol[vdW])/2
10 kcal/mol[CH₃-CH₂-OH] - 5 kcal/mol[CH₃-O-CH₃]

$$U = q_1 q_2 / r$$

$$\varepsilon = e \cdot e / 1\text{\AA} = 330 \text{ kcal/mol}$$

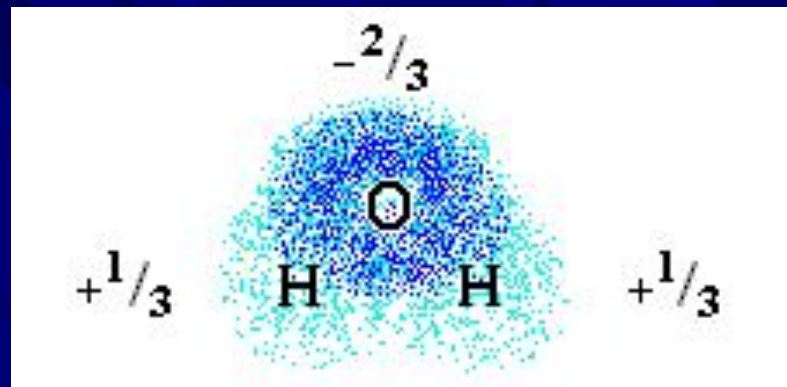
$$(\text{HO})^{-1/3} - \text{H}^{+1/3} \text{ } \text{O}^{-2/3} - \text{H}_2^{+2/3} : \quad \varepsilon \cdot \frac{1}{3} \cdot \frac{2}{3} \cdot (-\frac{1}{2} - \frac{1}{4} + 2 \cdot \frac{1}{3})$$

~ 6 kcal/mol



HYDROGEN BONDS

WATER molecule:



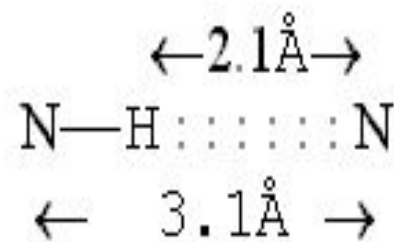
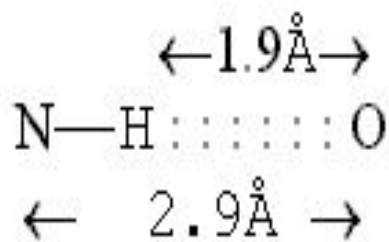
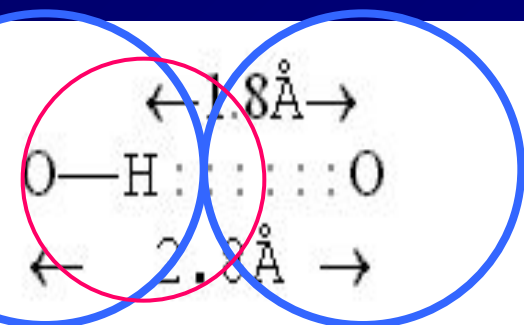
H-bond energy: 5 kcal/mol

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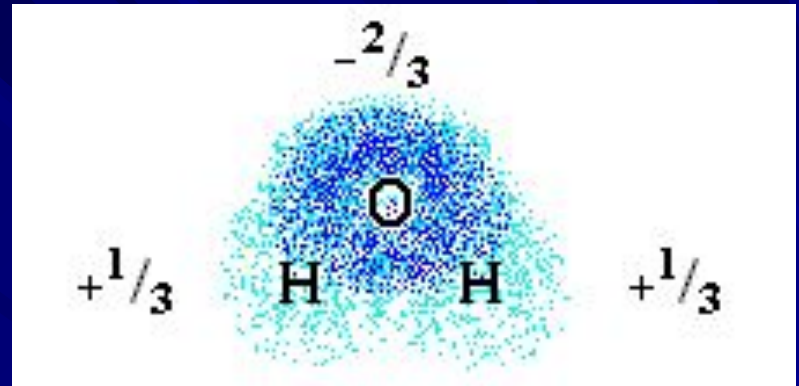
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HYDROGEN BONDS

WATER molecule:



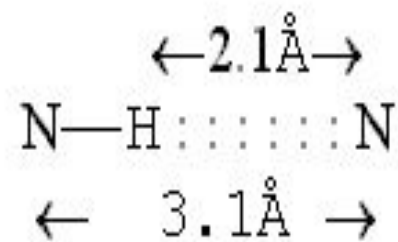
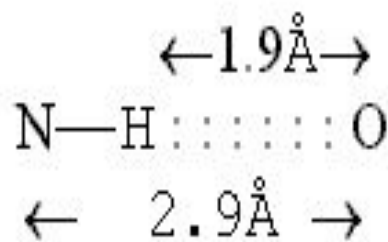
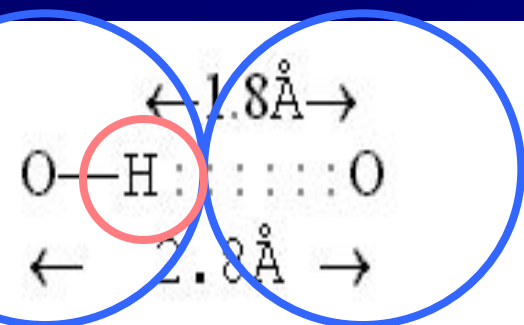
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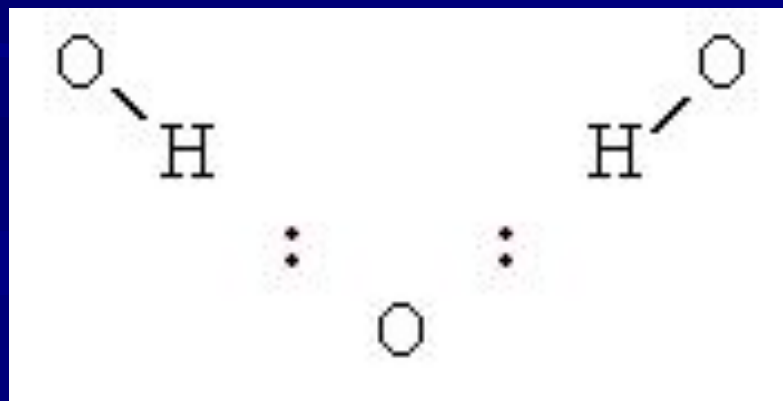
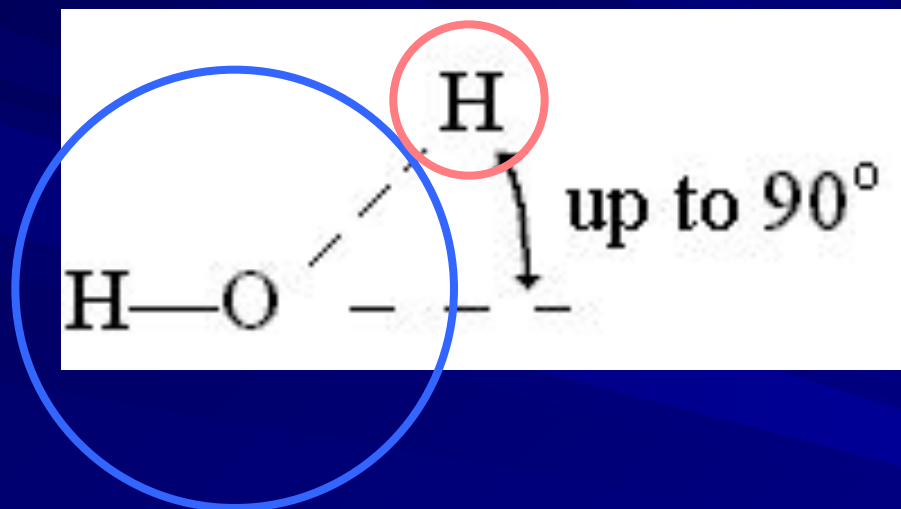
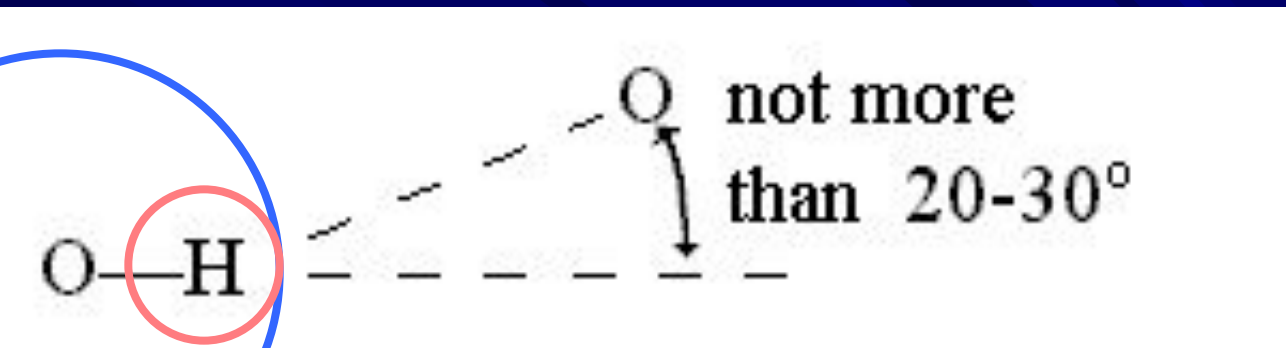
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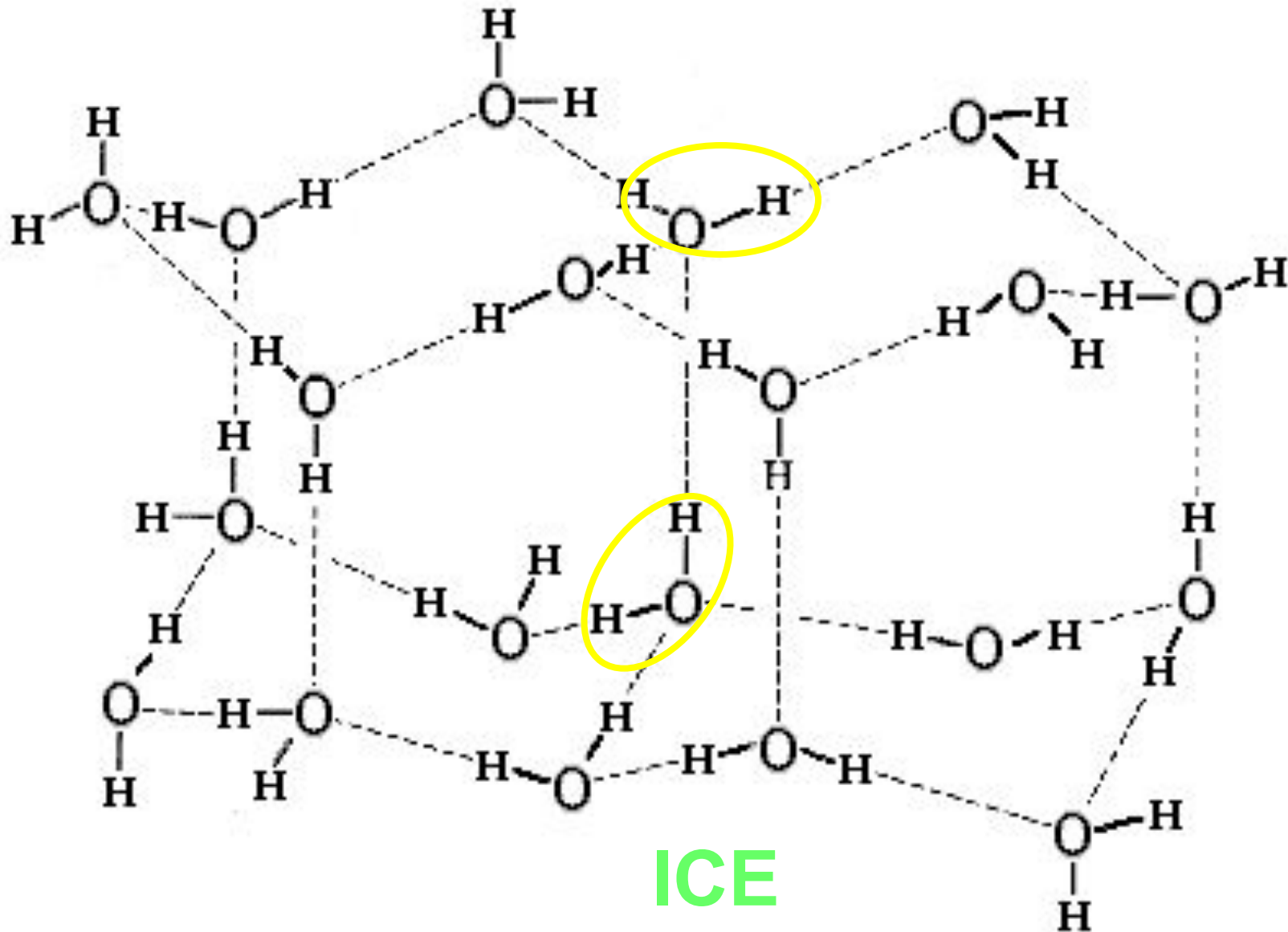
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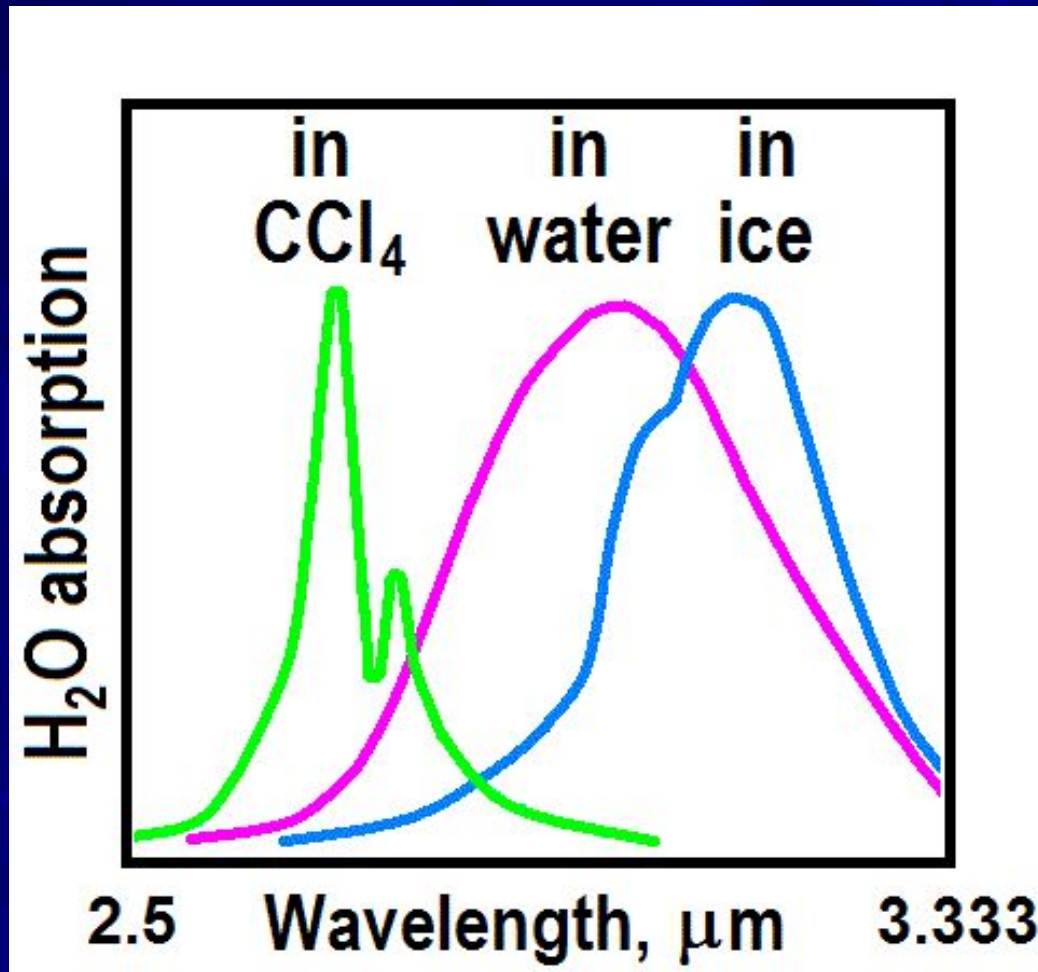
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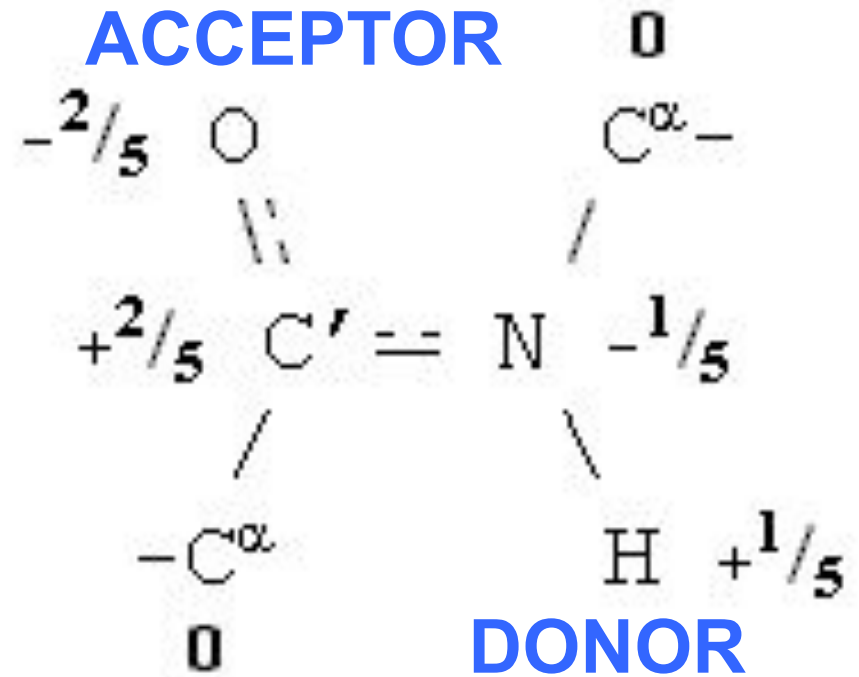


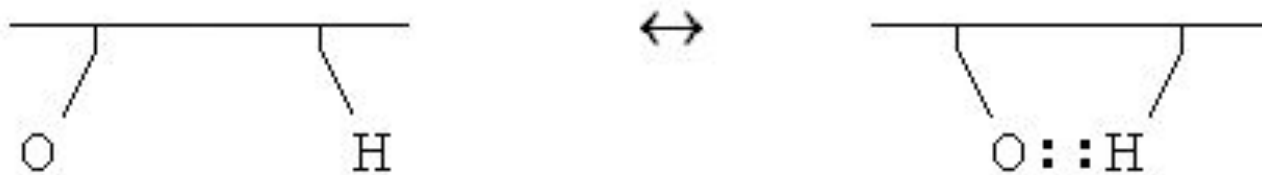


MODEL OF “FORMED” and “BROKEN” H-BONDS IN WATER IS VERY ROUGH



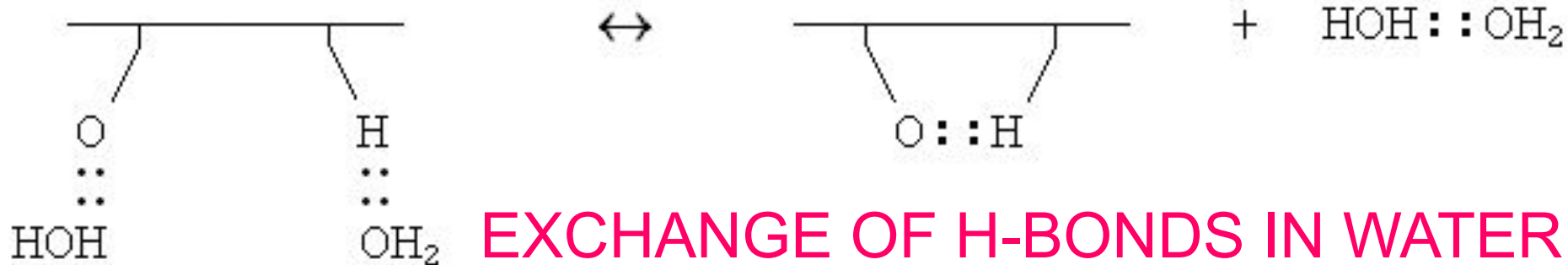
PEPTIDE GROUP ALSO FORMS H-BONDS





FORMATION OF H-BOND IN VACUUM

ENERGY E decreases



EXCHANGE OF H-BONDS IN WATER

ENERGY $E = \text{const}$ ENTROPY $S \sim \ln(\text{pos.})$ increases
 FREE ENERGY $F = E - TS$ decreases: water moves

**Just because H-bonds have large energy,
 only their ENTROPIC part
 plays a role in water surrounding**