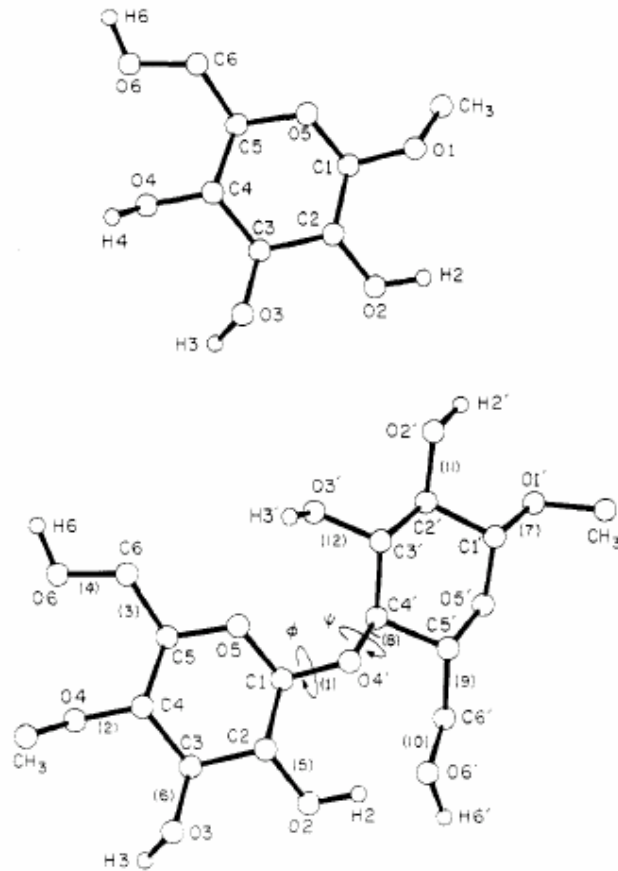


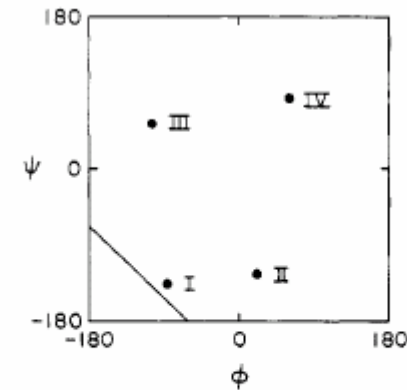
# Makromolekulák 10.

Simon István

# A béta-glikozidos kötés konfigurációja



**Figure 1.** Nomenclature used for the atoms and dihedral angles in the mono- and disaccharide: top, methyl  $\beta$ -D-glucopyranoside (for glucose, the terminal  $\text{CH}_3$  group is replaced by an H atom designated as H1); bottom, dimethyl  $\beta$ -D-diglucofuranoside (for cellobiose, the two terminal  $\text{CH}_3$  groups are replaced by H atoms, designated as H4 and H1').



**Figure 2.** Location of the four energy minima and the line corresponding to the values of  $\phi$  and  $\psi$  for a two-fold screw axis (a second portion of this line, near minimum IV, has been omitted). Relative energies in kcal/mol: I, 0.0; II, 18; III, 33; IV, 224.

# A CVFF forcefield

$$\begin{aligned}
 E_{pot} = & \sum_b D_b \left[ 1 - e^{-\alpha(b-b_0)^2} \right] + \frac{1}{2} \sum_{\theta} H_{\theta} (\theta - \theta_0)^2 + \frac{1}{2} \sum_{\phi} H_{\phi} [1 + s \cos(n\phi)] + \\
 & \frac{1}{2} \sum_x H_x \chi^2 + \sum_b \sum_{b'} F_{bb'} (b - b_0)(b' - b'_0) + \sum_{\theta} \sum_{\theta'} F_{\theta\theta'} (\theta - \theta_0)(\theta' - \theta'_0) + \\
 & \sum_b \sum_{\theta} F_{b\theta} (b - b_0)(\theta - \theta_0) + \sum_{\phi} F_{\phi\theta\theta'} \cos\phi (\theta - \theta_0)(\theta' - \theta_0) + \sum_x \sum_{x'} F_{xx'} \chi\chi' \\
 & + \sum \varepsilon \left[ \left( \frac{r^*}{r} \right)^{12} - 2 \left( \frac{r^*}{r} \right)^6 \right] + \sum \frac{q_i q_j}{\varepsilon r_{ij}}
 \end{aligned}$$

(1)
(2)
(3)

(4)
(5)
(6)

(7)
(8)
(9)

(10)
(11)

# Az ECEPP forcefield

Coulomb term:

$$U_e = \frac{332 q_i q_j}{D r_{ij}}$$

Lennard-Jones 6-12 potencial:

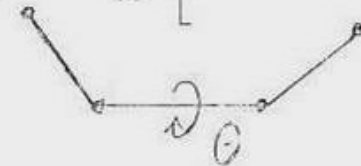
$$U_{6-12} = \epsilon_{ij} \left[ F \left( \frac{r_{ij}^0}{r_{ij}} \right)^{12} - 2 \left( \frac{r_{ij}^0}{r_{ij}} \right)^6 \right]$$

Hydrogen-bonding potencial:

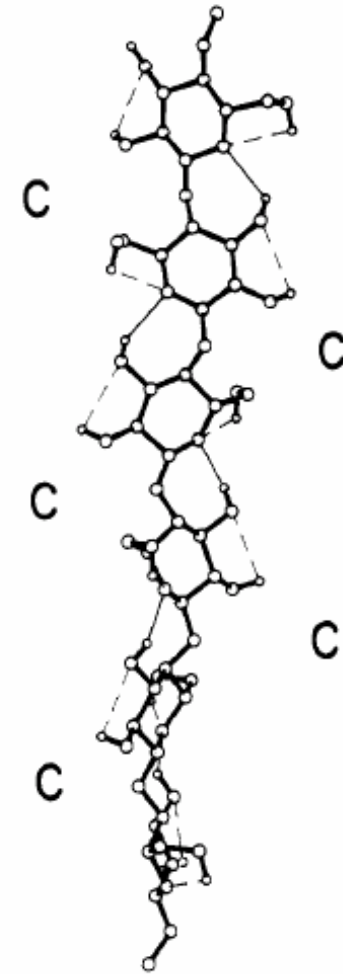
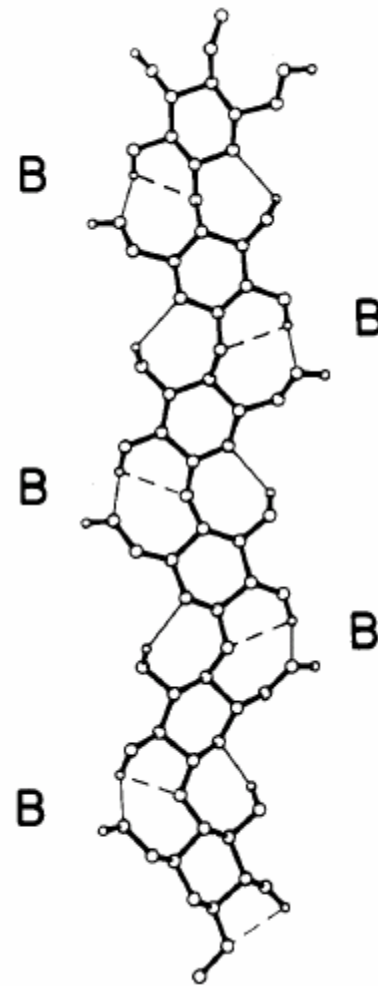
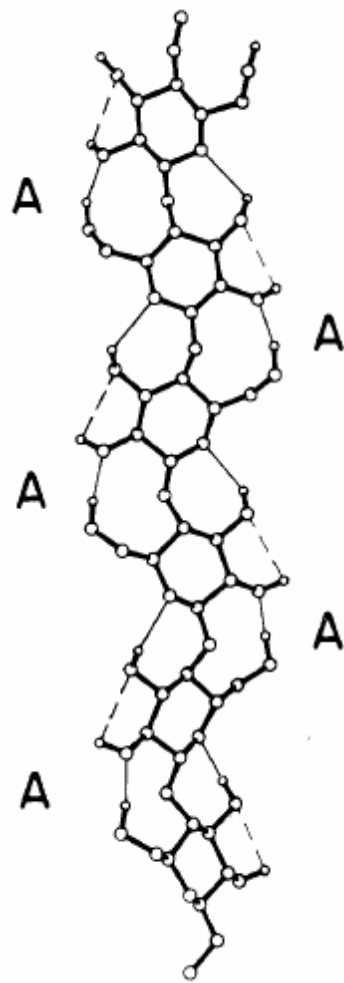
$$U_{HB} = \epsilon_{ij} \left[ \left( \frac{r_{ij}^0}{r_{ij}} \right)^{12} - 2 \left( \frac{r_{ij}^0}{r_{ij}} \right)^{10} \right]$$

Intrinsic torsional potencial:

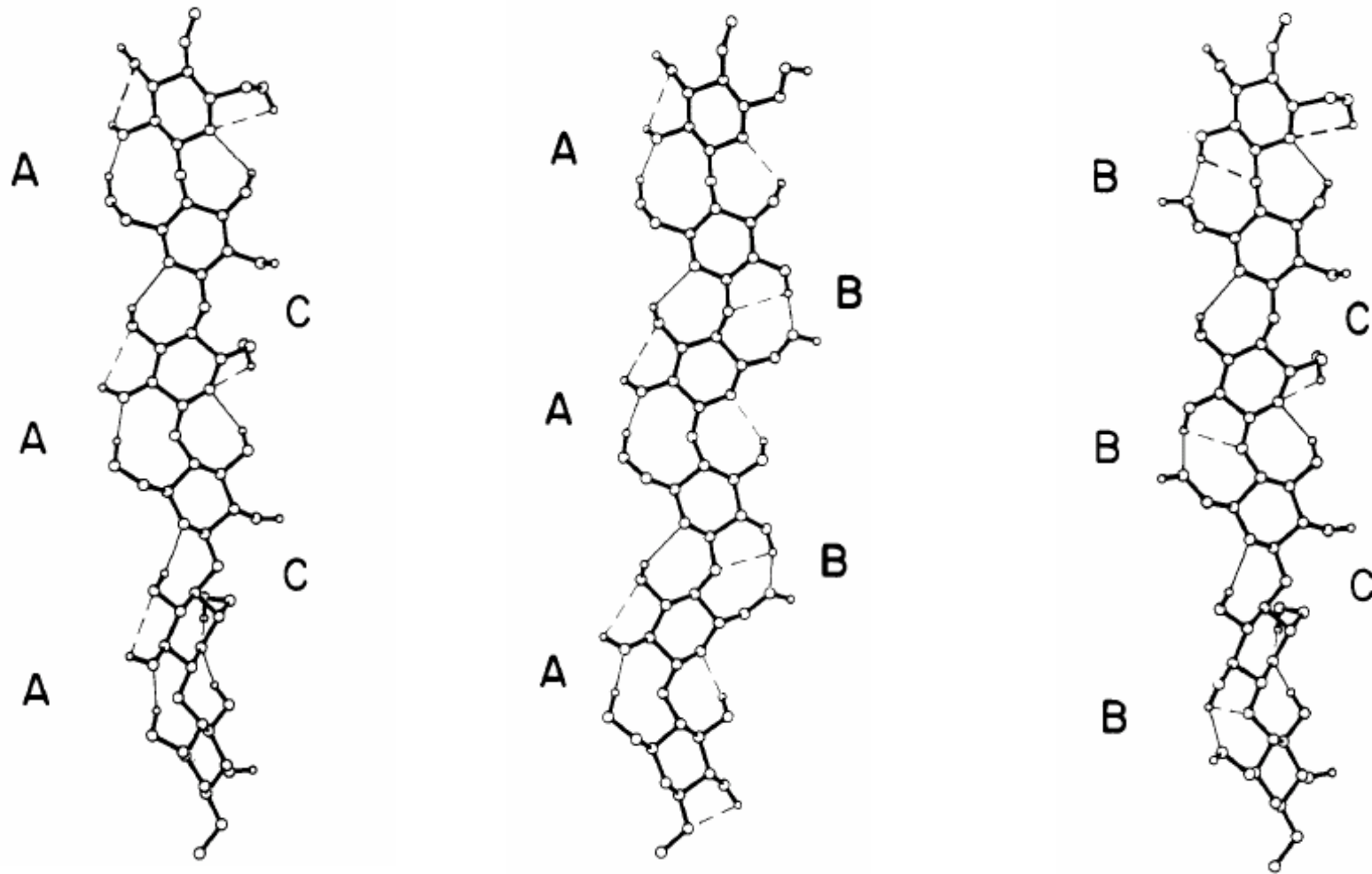
$$U_t = \frac{U_0}{2} \left[ 1 + k \cos(n\theta) \right]$$



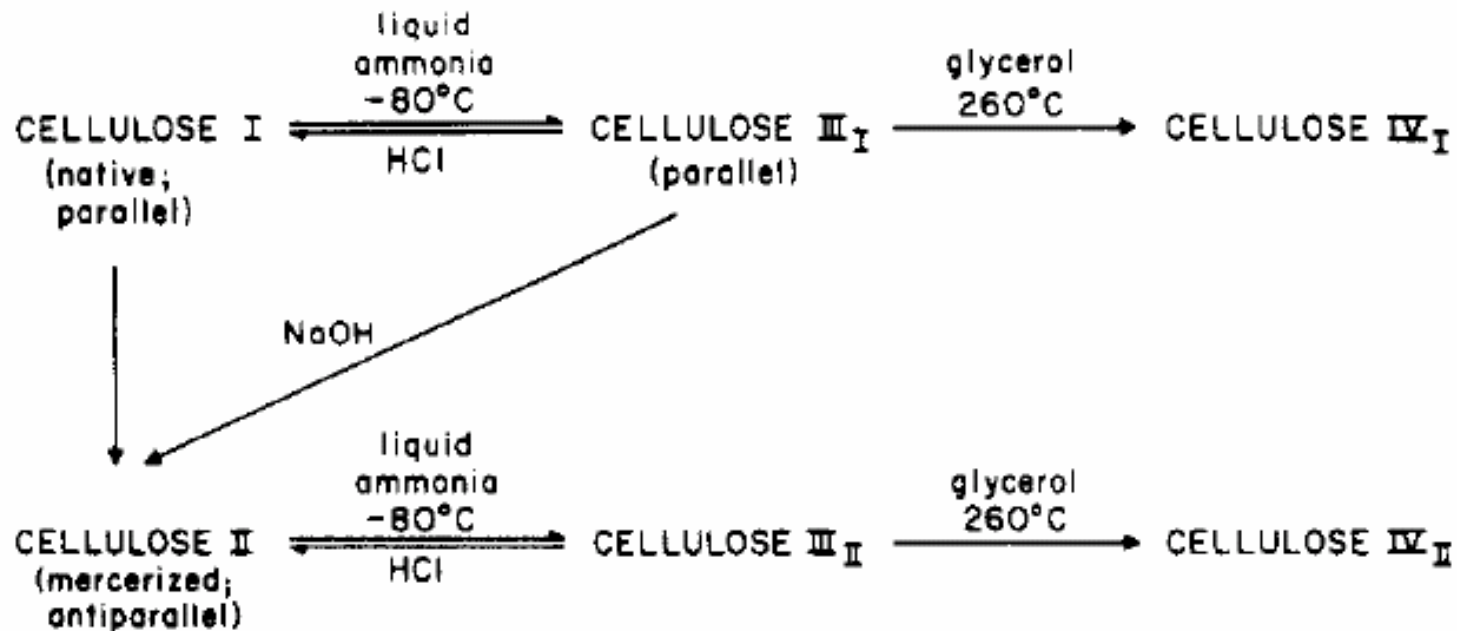
# Azonos diszaccharidokból felépülő hexaszaccharid



# Változó szerkezetű diszaccharidokból felépülő hexaszaccharid



# A cellulóz különböző módosulatai

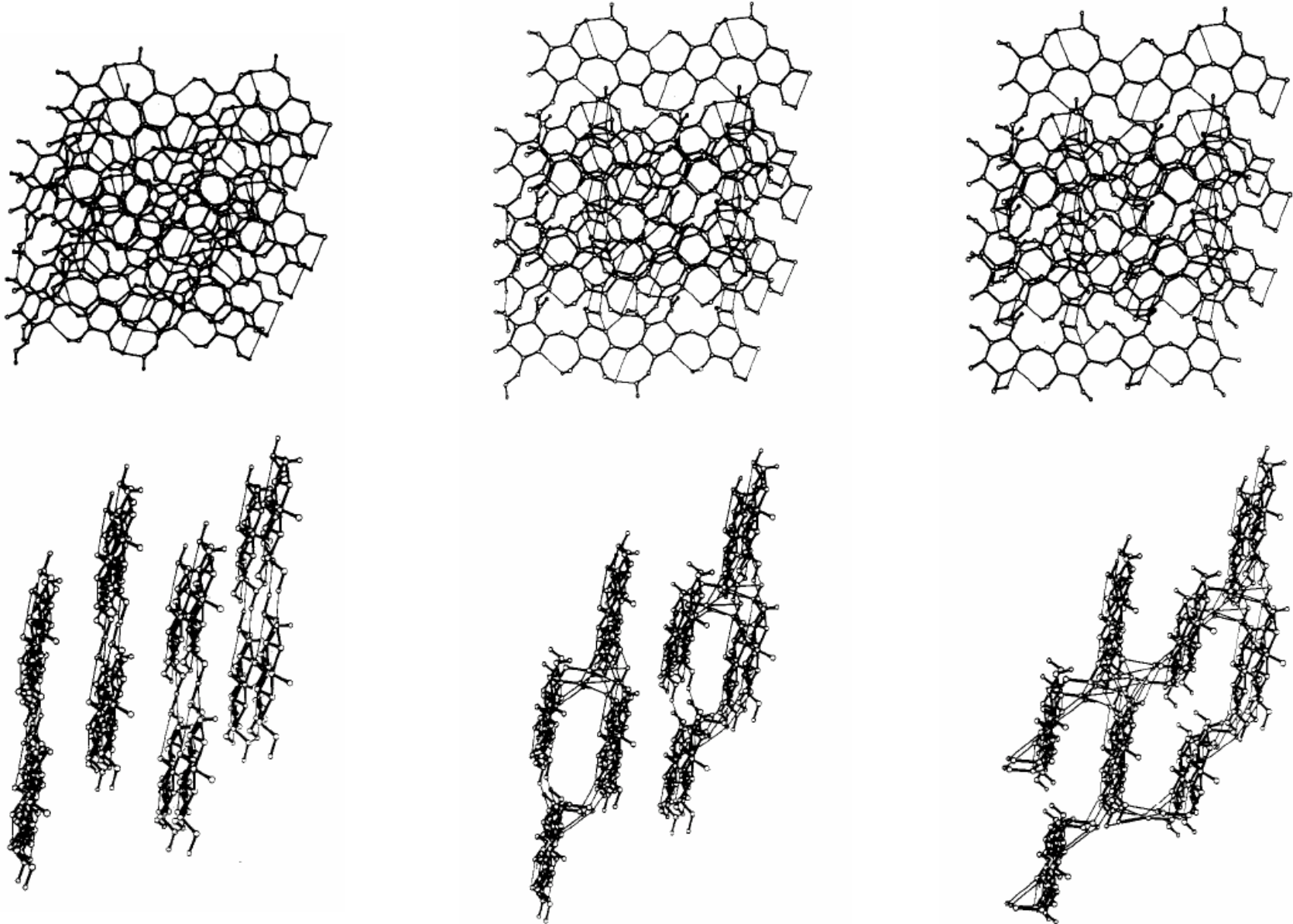


# Alacsony energiájú parallel és antiparallel elrendezésű cellulóz elemi cellák

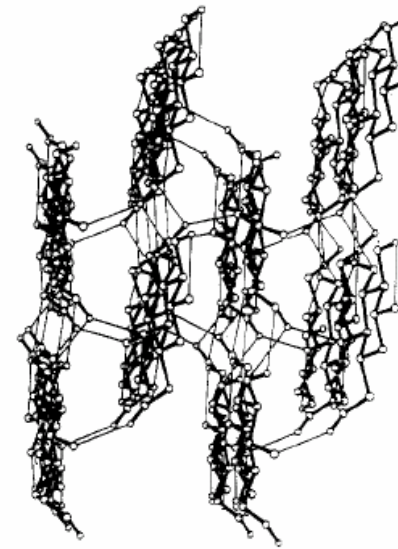
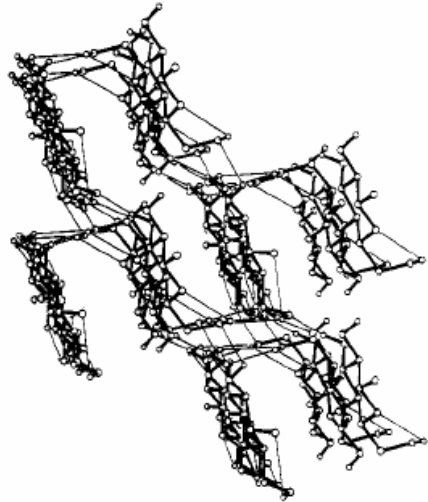
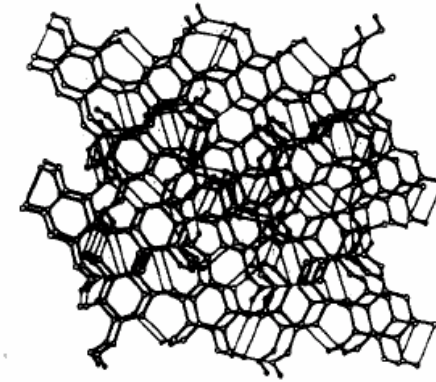
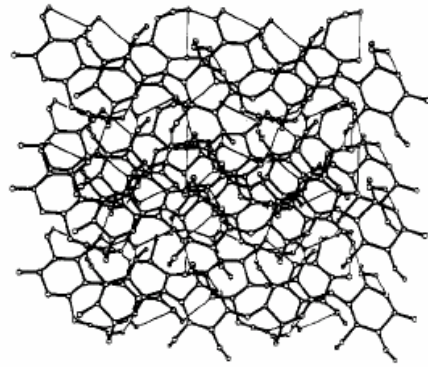
	corner/center	$\Delta E$	$a$	$b$	$c$	$\alpha$	$\beta$	$\gamma$	$x_0$	$y_0$	$z_0$	$D$
						Parallel						
	cellulose I (X-ray) <sup>1</sup>		10.3	8.35	7.90	84°	90°	90°				
1	(BB) <sub>n</sub> /(BB) <sub>n</sub>	0.00	(10.23) <sup>c</sup>	8.28	8.22	76.15°	90.74°	89.85°	0.241	0.487	0.505	2.57°
2 <sup>b</sup>	(CB) <sub>n</sub> /(BB) <sub>n</sub>	0.49	(10.23)	8.13	9.66	58.70°	91.43°	89.33°	0.228	0.491	0.505	-9.90°
3	(CC) <sub>n</sub> /(BB) <sub>n</sub>	1.34	(10.23)	8.07	9.62	58.68°	91.00°	89.83°	0.228	0.491	0.503	11.57°
						Antiparallel						
	cellulose II (X-ray) <sup>3</sup>		10.36	8.01	9.04	117.1°	90°	90°				
4	(AA) <sub>n</sub> /(CC) <sub>n</sub>	-5.95	(10.23)	7.74	9.75	122.46°	90.09°	89.66°	0.620	0.613	0.457	12.15°
5	(BB) <sub>n</sub> /(BB) <sub>n</sub>	-2.07	(10.23)	8.24	7.71	90.18°	89.99°	90.32°	0.623	0.664	0.500	0.89°



# Parallel elrendezésű elemi cellák



# Antiparallel elrendezésű elemi cellák

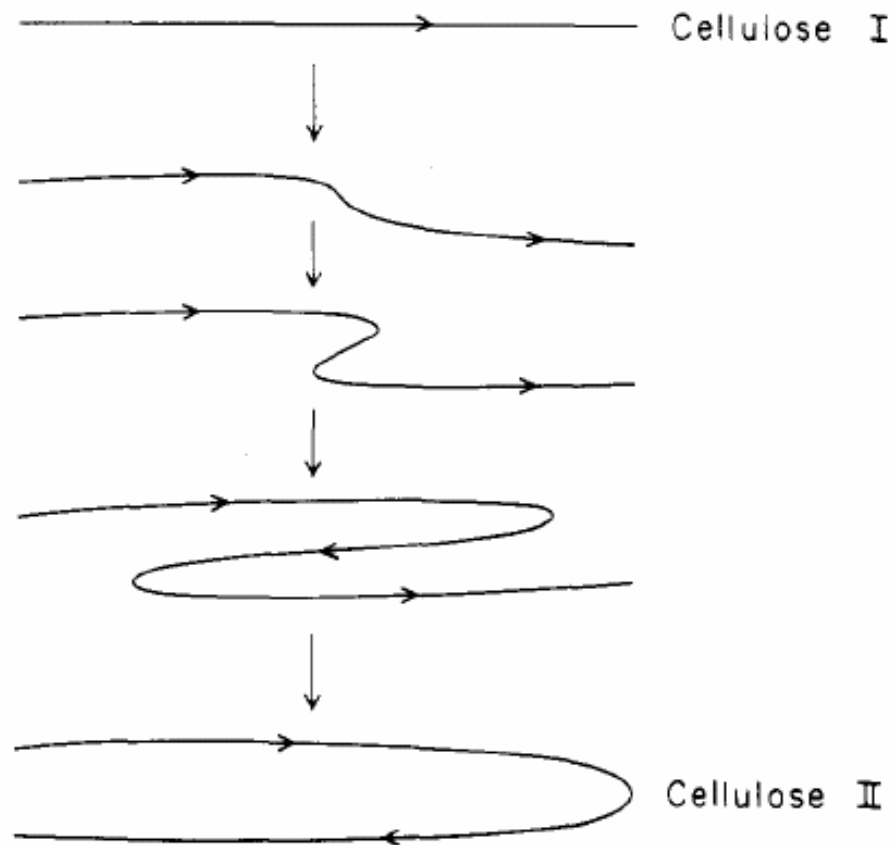


# Cellulóz szerkezetek azonosítása

**Lengths (Å) of Hydrogen Bonds<sup>a</sup> Stabilizing Cellulose Structures**

struct <sup>b</sup>	intrachain <sup>c</sup>	intrasheet <sup>d</sup>	intersheet <sup>d</sup>
Parallel (Cellulose I)			
1	O4...H2 (2.62) O5...H3 (2.15) O6...H2 (1.76)	O3...H6 (1.79)	none
2	O4...H2 (2.62) O5...H3 (2.27) O5...H6 (2.44) O6...H2 (1.75)	O3...H6 (1.76)	O3...H6 (2.61) O6...H2 (1.87) O6...H3 (2.23) O6...H6 (1.84)
3	O4...H2 (2.71) O5...H3 (2.30) O5...H6 (2.40) O6...H2 (1.85)	O3...H6 (1.77)	O3...H6 (2.61) O6...H2 (1.87) O6...H3 (2.23) O6...H6 (1.84)
Antiparallel (Cellulose II)			
4	O2...H6 (1.73) O3...H2 (2.69) O4...H2 (2.80) O4...H6 (2.80) O5...H3 (2.56) O5...H6 (2.58)	none	O2...H2 (1.80) O2...H6 (2.33) O6...H3 (1.73) O6...H6 (2.74)
5	O4...H2 (2.59) O5...H3 (2.35) O6...H2 (1.74)	O3...H6 (2.67) O6...H3 (2.66)	O4...H6 (2.18)

# Antiparallel cellulóz szerkezet kialakulása



# Parallel és antiparallel cellulóz-triacetát

