Modeling of negative Poisson's ratio (auxetic) crystalline cellulose Iβ

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Modeling of negative Poisson's ratio (auxetic) crystalline cellulose I_β

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Online Resource Table 1. Unit-cell parameters for cellulose I_β: comparison between experiment (Nishiyama et al. 2002) and predictions from force fields employed by *Materials Studio* and *Cerius*[2].

	V (Å^3)	*a* (Å)	*b* (Å)	*c* (Å)	γ(°)
Experiment	658.3(1)	7.784(8)	8.201(8)	10.380(1)	96.5
Materials Studio					
Compass	628.6	7.563	8.049	10.432	98.1
Dreiding	723.4	8.105	8.604	10.633	102.7
Universal	767.9	8.704	8.637	10.267	95.8
CVFF	656.1	7.652	8.136	10.615	96.8
PCFF	679.8	7.737	8.368	10.625	98.8
Cerius[2]					
CVFF	656.1	7.652	8.136	10.615	96.8
PCFF	679.8	7.736	8.368	10.625	98.8

Online Resource Table 2. Bond lengths for cellulose I_β: comparison between experiment (Nishiyama et al. 2002) and predictions from force fields employed by *Materials Studio*.

	Expt	Universal	Dreiding	Compass	PCFF	CVFF
Corner chain						
c4-o1	1.44	1.427	1.446	1.422	1.433	1.42
o1-c1	1.415	1.421	1.442	1.428	1.436	1.418
c1-c2	1.53	1.534	1.55	1.513	1.548	1.552
c2-c3	1.51	1.546	1.551	1.501	1.537	1.546
c3-c4	1.516	1.55	1.557	1.508	1.548	1.562
c4-c5	1.497	1.555	1.562	1.515	1.555	1.564
c5-o5	1.441	1.417	1.445	1.429	1.432	1.45
o5-c1	1.426	1.413	1.442	1.427	1.427	1.449
c5-c6	1.52	1.532	1.549	1.514	1.548	1.536
c6-o6	1.416	1.397	1.425	1.427	1.425	1.428
c2-o2	1.43	1.403	1.427	1.437	1.438	1.426
c3-o3	1.442	1.404	1.425	1.435	1.434	1.426
Centre chain						
c4-o1	1.439	1.432	1.442	1.424	1.433	1.424
o1-c1	1.429	1.416	1.44	1.426	1.433	1.42
c1-c2	1.525	1.537	1.547	1.51	1.544	1.549
c2-c3	1.514	1.543	1.55	1.504	1.54	1.553
c3-c4	1.53	1.554	1.559	1.511	1.551	1.565
c4-c5	1.538	1.549	1.562	1.513	1.552	1.559
c5-o5	1.416	1.416	1.445	1.428	1.43	1.443
o5-c1	1.406	1.414	1.44	1.419	1.419	1.431
c5-c6	1.559	1.533	1.55	1.516	1.549	1.532
c6-o6	1.415	1.4	1.426	1.426	1.424	1.428
c2-o2	1.426	1.406	1.42	1.432	1.432	1.418
c3-o3	1.417	1.405	1.426	1.436	1.434	1.427

Online Resource Table 3. Force-field bond angle predictions compared with the experimental data of Nishiyama et al. 2002.

	χ (°)	χ' (°)	ψ (°)	ϕ (°)
Corner chain				
Expt	170.3	-70	-142.3	-98.5
Dreiding	176.3	-62	-156	-88.6
Universal	172	-67.4	-153	92.4
PCFF	167.8	-71.5	-148.9	-92.6
Compass	170.3	-67.1	-153.1	-87.5
CVFF1	169.4	-69.3	-144.7	-94.7
Centre chain				
Expt	158	-83	-147.1	-88.7
Dreiding	170	-68.6	-150.3	-91.3
Universal	167.7	-71.3	-157.6	-91.1
PCFF	168	-69.6	-146.2	-97
Compass	173.1	-50.2	-154.9	-83.6
CVFF1	178.8	-59.3	-142.4	-92.5

Online Resource Table 4. Compliance coefficients (GPa^{-1}) for cellulose I_β predicted using the CVFF1, CVFF2 and CVFF3 models.

s_{ij}	CVFF1	CVFF2	CVFF3
s_{11}	0.047635	0.057615	0.477859
s_{12}	-0.014451	-0.017566	-0.300745
s_{13}	-0.001113	-0.001026	0.002259
s_{22}	0.025547	0.030879	0.231860
s_{23}	-0.001177	-0.001193	-0.003469
s_{33}	0.005376	0.004963	0.005567
s_{44}	0.109768	0.161612	0.156454
s_{55}	0.309345	0.677733	1.645820
s_{66}	0.211735	0.314473	0.523760

Online Resource Figure 1. Hydrogen bonding networks in the corner (left) and center (right) sheets of cellulose I_β predicted from the CVFF1 model. Carbon, oxygen and hydrogen atoms are colored grey, red and white, respectively. Hydrogen bonds are indicated by dotted lines. For clarity, only the oxygen atoms participating in the hydrogen bonding are identified.