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Modeling of negative Poisson’s ratio (auxetic) crystalline cellulose $I_\beta$

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Online Resource Table 1. Unit-cell parameters for cellulose Iβ: comparison between experiment (Nishiyama et al. 2002) and predictions from force fields employed by Materials Studio and Cerius².

|                  | \( V (\text{Å}^3) \) | \( a (\text{Å}) \) | \( b (\text{Å}) \) | \( c (\text{Å}) \) | \( \gamma(\text{°}) \) |
|------------------|----------------------|-------------------|-------------------|-------------------|-------------------|
| **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              |
| **Cerius²**      |                      |                   |                   |                   |                   |
| 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 \( I_\beta \): 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.

|                 | $\chi$ (°) | $\chi'$ (°) | $\psi$ (°) | $\phi$ (°) |
|-----------------|------------|-------------|------------|------------|
| **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\(_\beta\) 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$_\beta$ 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.