**Table S3.** Geometric parameters and electronic density values regarding the non-covalent interactions found in the minimized Complex 3 (SA\_*βO4*\_SA\_*ββ*\_SA – cellulose Iβ).*a*

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Lignol | Cellulose | d(A..H)($\dot{A}$) | d(A..D)($\dot{A}$) | α(D..H..A) | $$ρ(r\_{c})$$(a.u.) | Label |
| O | HO | 1.87 | 2.80 | 162.4 | 0.031 | **a** |
| CH | O | 2.38 | 3.32 | 143.2 | 0.012 | **b** |
| CH | O | 2.42 | 3.41 | 150.3 | 0.011 | **c** |
| CH | O | 2.40 | 3.45 | 158.9 | 0.011 | **d** |
| CH | O | 2.43 | 3.41 | 118.4 | 0.011 | **e** |
| CH | O | 2.43 | 3.41 | 148.9 | 0.011 | **f** |
| O | HC | 2.48 | 3.49 | 153.5 | 0.010 | **g** |
| CH | O | 2.51 | 3.34 | 132.2 | 0.010 | **h** |
| CH | O | 2.54 | 3.03 | 106.0 | 0.009 | **i** |
| CH | O | 2.57 | 3.38 | 130.4 | 0.008 | **j** |
| CH | O | 2.61 | 3.55 | 144.6 | 0.008 | **k** |
| CH | O | 2.66 | 3.59 | 143.0 | 0.007 | **l** |
| O | HC | 2.69 | 3.54 | 134.4 | 0.007 | **m** |
| O | HC | 2.71 | 3.74 | 156.8 | 0.006 | **n** |
| CH | O | 2.74 | 3.33 | 113.7 | 0.006 | **o** |
| O | HC | 2.82 | 3.33 | 108.6 | 0.006 | **p** |
| CπH | O | 2.89 | 3.43 | 110.4 | 0.005 | **q** |
| O | HC | 2.93 | 3.80 | 137.1 | 0.004 | **r** |
| CH | O | 3.16 | 4.12 | 147.0 | 0.002 | **s** |
| O | HC | 3.28 | 4.10 | 132.8 | 0.002 | **t** |
| CH | O | 3.36 | 4.38 | 155.8 | 0.001 | **u** |

*a* Acceptor-H and acceptor-donor distances, donor-H-acceptor angle. The labels correspond

 to those shown in Fig. 5.