**Table S2.** Geometric parameters and electronic density values regarding the non-covalent interactions found in the minimized Complex 2 (CA\_*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 |
| OH | O | 1.81 | 2.64 | 141.6 | 0.036 | **a** |
| O | HO | 1.99 | 2.77 | 136.4 | 0.025 | **b** |
| CH | O | 2.29 | 3.23 | 142.7 | 0.014 | **c** |
| O | HO | 2.25 | 2.92 | 125.9 | 0.013 | **d** |
| O | HC | 2.45 | 3.35 | 139.1 | 0.011 | **e** |
| O | HC | 2.45 | 3.47 | 155.7 | 0.010 | **f** |
| O | HC | 2.49 | 3.43 | 144.6 | 0.009 | **g** |
| O | HC | 2.59 | 3.55 | 147.0 | 0.008 | **h** |
| O | HC | 2.58 | 3.41 | 144.1 | 0.006 | **i** |
| CH | O | 2.83 | 3.38 | 110.6 | 0.005 | **j** |
| O | HC | 2.89 | 3.73 | 134.2 | 0.004 | **k** |
| O | HC | 2.91 | 3.78 | 137.9 | 0.004 | **l** |
| CH | O | 2.99 | 3.85 | 135.4 | 0.003 | **m** |
| CH | O | 3.00 | 3.86 | 136.0 | 0.003 | **n** |
| CH | O | 3.05 | 3.63 | 113.3 | 0.003 | **o** |
| CH | O | 3.13 | 3.90 | 127.9 | 0.003 | **p** |
| CπH | O | 3.16 | 4.02 | 137.4 | 0.002 | **q** |
| O | HC | 3.36 | 4.16 | 131.7 | 0.001 | **r** |
| O | HC | 3.44 | 4.03 | 115.8 | 0.001 | **s** |

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

 to those shown in Fig. 5.