**Table S1.** Geometric parameters and electronic density values regarding the non-covalent interactions found in the minimized Complex 1 (CA\_*βO4*\_SA\_*β5*\_CA – 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 | 1.76 | 2.74 | 171.0 | 0.040 | **a** |
| OH | O | 1.78 | 2.71 | 155.7 | 0.038 | **b** |
| OH | O | 2.10 | 3.06 | 175.3 | 0.019 | **c** |
| O | HC | 2.21 | 3.19 | 150.1 | 0.018 | **d** |
| O | HO | 2.18 | 2.96 | 136.8 | 0.016 | **e** |
| CH | O | 2.30 | 3.15 | 133.7 | 0.015 | **f** |
| CH | O | 2.30 | 3.25 | 144.6 | 0.015 | **g** |
| O | HC | 2.63 | 3.69 | 164.6 | 0.008 | **h** |
| O | HC | 2.71 | 3.40 | 121.4 | 0.007 | **i** |
| CH | O | 2.73 | 3.72 | 152.0 | 0.006 | **j** |
| O | HC | 2.75 | 3.42 | 119.3 | 0.006 | **k** |
| OH | O | 3.06 | 3.93 | 149.5 | 0.002 | **l** |
| CH | O | 3.35 | 3.93 | 114.4 | 0.002 | **m** |

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

 to those shown in Fig. 5.