**Table S4.** Geometric parameters and electronic density values regarding the non-covalent interactions found in the minimized Complex 3 (CA\_*ββ*\_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 |
| O | HO | 2.00 | 2.79 | 137.7 | 0.023 | **a** |
| O | HC | 2.38 | 3.36 | 149.4 | 0.012 | **b** |
| O | HC | 2.68 | 3.69 | 155.3 | 0.007 | **c** |
| O | HC | 2.76 | 3.16 | 100.8 | 0.007 | **d** |
| CH | O | 2.77 | 3.69 | 141.6 | 0.005 | **e** |
| CH | O | 2.81 | 3.64 | 131.9 | 0.005 | **f** |
| Cπ | HC | 2.89 | 3.87 | 150.2 | 0.005 | **g** |
| CπH | O | 3.12 | 3.90 | 129.2 | 0.003 | **h** |

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

 to those shown in Fig. 5.