Sorption of poly(hexamethylenbiguanide) on cellulose: Mechanism of binding and molecular recognition

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SUPPORTING INFORMATION
Figure S.1. Experimentally determined structure of cellulose I\(\beta\) (a) 2 unit cells (b) layer of 2 \(\times\) 2 unit cells.
Figure S.2. The modified cellulose surface: introduced COO$^-$ group is indicated (‡).
Figure S.3. The volume of water inaccessible to molecules of increasing size: (– –) non-dried celluloses, (- - -) dried and re-swollen celluloses. Reprinted, by permission, from Stone, J. E.; Treiber, E.; Abrahamson, B. Tappi J. 1969, 52, 109.
Figure S.4. Hydrogen-bonding of the PHMB oligomer with different types of oxygen in the cellulose surface.
Figure S.5. Interacting PHMB trimers: a) side-to-side interactions; b) sheets of interacting trimers.
Figure S.6. Hydrogen-bonding interactions for PHMB in solution at 300 K.