Zenodo data deposit description related to the publication:

Spatial distribution of functional groups in cellulose ethers by DNP Enhanced Solid-State NMR Spectroscopy

Pierrick Berruyer,[a] Pinelopi Moutzouri, [a] Martin Gericke, [b] Dörthe Jakobi, [b] Michel Bardet, [a,c] Thomas Heinze, [b] Leif Karlson, [d] Staffan Schantz, [e] and Lyndon Emsley[a]*

[a] Dr. Pierrick Berruyer, Dr. Pinelopi Moutzouri, Dr. Michel Bardet, Prof. Dr. Lyndon Emsley
Institut des Sciences et Ingénierie Chimiques, École Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland

[b] Dr. Martin Gericke, Dörthe Jakobi, Prof. Dr. Thomas Heinze
Institute of Organic Chemistry and Macromolecular Chemistry, Friedrich Schiller University of Jena, Centre of Excellence for Polysaccharide Research, Humboldtstraße 10, D-07743 Jena, Germany

[c] Dr. Michel Bardet
Univ. Grenoble Alpes, CEA, IRIG-MEM, Laboratoire de Résonance Magnétique, Grenoble F-38000, France

[d] Dr. Leif Karlson
Nouryon Functional Chemicals AB, SE-444 31 Stenungsund, Sweden

[e] Dr. Leif Karlson
Oral Product Development, Pharmaceutical Technology & Development, Operations, AstraZeneca, Gothenburg, Sweden

Cite original research publication is re-used at DOI: 10.1021/acs.macromol.2c00061

Details of methods and materials are available from DOI : 10.1021/acs.macromol.2c00061

Folder "Figure1_matlab_simulation_code" includes the Matlab (The MathWorks, Inc) code used to perform the steady-state enhancement simulation of panel (e) of the figure.

Folder "Figure3_data" includes all NMR raw data used to produce Figure 3. The experiments are organized as described in the table below. If two or more experiments numbers are indicated, the raw data have been added to each to increase s/n before processing. Raw data are available in topspin and JCAMP-DX v6 format.

Sample	{^{1}H}-^{13}C CPMAS µw ON	{^{1}H}-^{13}C CPMAS µw OFF	{^{1}H}-^{13}C CPMAS echo µw ON	{^{1}H}-^{13}C CPMAS echo µw OFF
HMPC-1,1	11	111	21	121, 122
HMPC-1,2	11	111	21	121, 122
HMPC-1,3	11	111	21	121, 122
HMPC-2,1	11	111	21	121
HMPC-2,2	11	111	21	121
HMPC-2,3	11	111	21	121

Folder "Figure4_data" includes all NMR raw data used to produce Figure 4. The experiments are organized as described in the table below. If two or more experiments numbers are indicated, the raw data have been added to each to increase s/n before processing. Raw data are available in topspin and JCAMP-DX v6 format.

Sample	{¹H}-¹³C CPMAS μw ON	{¹H}-¹³C CPMAS μw OFF	{¹H}-¹³C CPMAS echo μw ON	{¹H}-¹³C CPMAS echo μw OFF
HMPC-1,1	31	131	41	141
HMPC-1,4	31	131	41	141,142,143
HMPC-2,2	31	131	41	141,142
HMPC-2,3	31	131	41	141

Folder "Figure5 data" includes all NMR raw data used to produce Figure 5. The experiments are organized as described in the table below. If two or more experiments numbers are indicated, the raw data have been added to each to increase s/n before processing. Raw data are available in topspin and JCAMP-DX v6 format.

Sample	{¹H}-¹³C CPMAS μw ON	{¹H}-¹³C CPMAS μw OFF	{¹H}-¹³C CPMAS echo μw ON	{¹H}-¹³C CPMAS echo μw OFF
3-O-MC,1	3	24,25,26	103	113
3-O-MC,2	110	120	111	121