

Chair interconversion and reactivity of mannuronic acid esters

Jerk Rönnols,^a Marthe T. C. Walvoort,^b Gijsbert A. van der Marel,^b

Jeroen D. C. Codée,^b and Göran Widmalm^a

^aDepartment of Organic Chemistry
Stockholm University
S-106 91 Stockholm (Sweden)

^bLeiden Institute of Chemistry
Leiden University, P.O. Box 9502
2300 RA Leiden (The Netherlands)

Supporting information

Table of contents

DNMR spectra of compound 1	S1
DNMR spectra of compound 4	S2
DNMR spectra of compound 5	S3
DNMR spectra of compound 6	S4
DNMR spectra of compound 7	S5
NMR spectra from competition between 1 and 2	S6

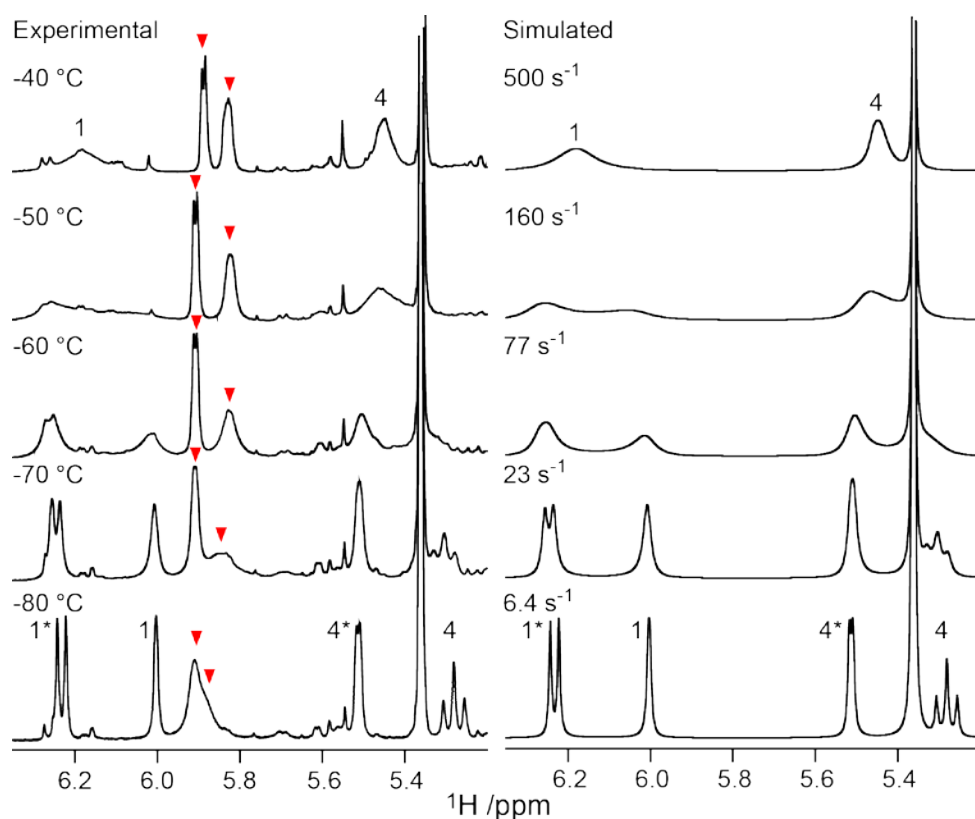


Figure S1. Experimental and simulated ^1H NMR spectra of the H1 and H4 signals of anomeric triflate **1**. Signals arising from the $^1\text{C}_4$ conformer are marked with asterisks. Signals marked with red triangles pointing downwards are unknown by-products formed upon activation. The signal at 5.36 ppm originates from residual dichloromethane-*d*.

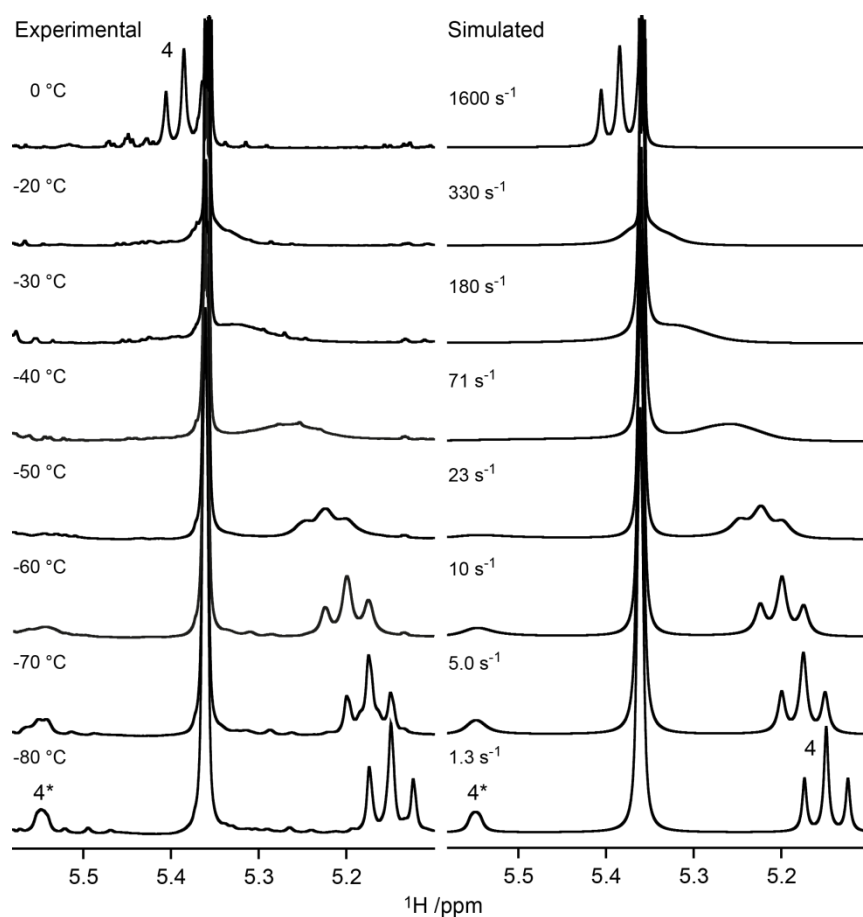


Figure S2. Experimental and simulated ^1H NMR spectra of the signals from H4 of methyl glycoside **4**. The signal arising from the $^1\text{C}_4$ conformer is marked with an asterisk. The signal at 5.36 ppm originates from residual dichloromethane-*d*.

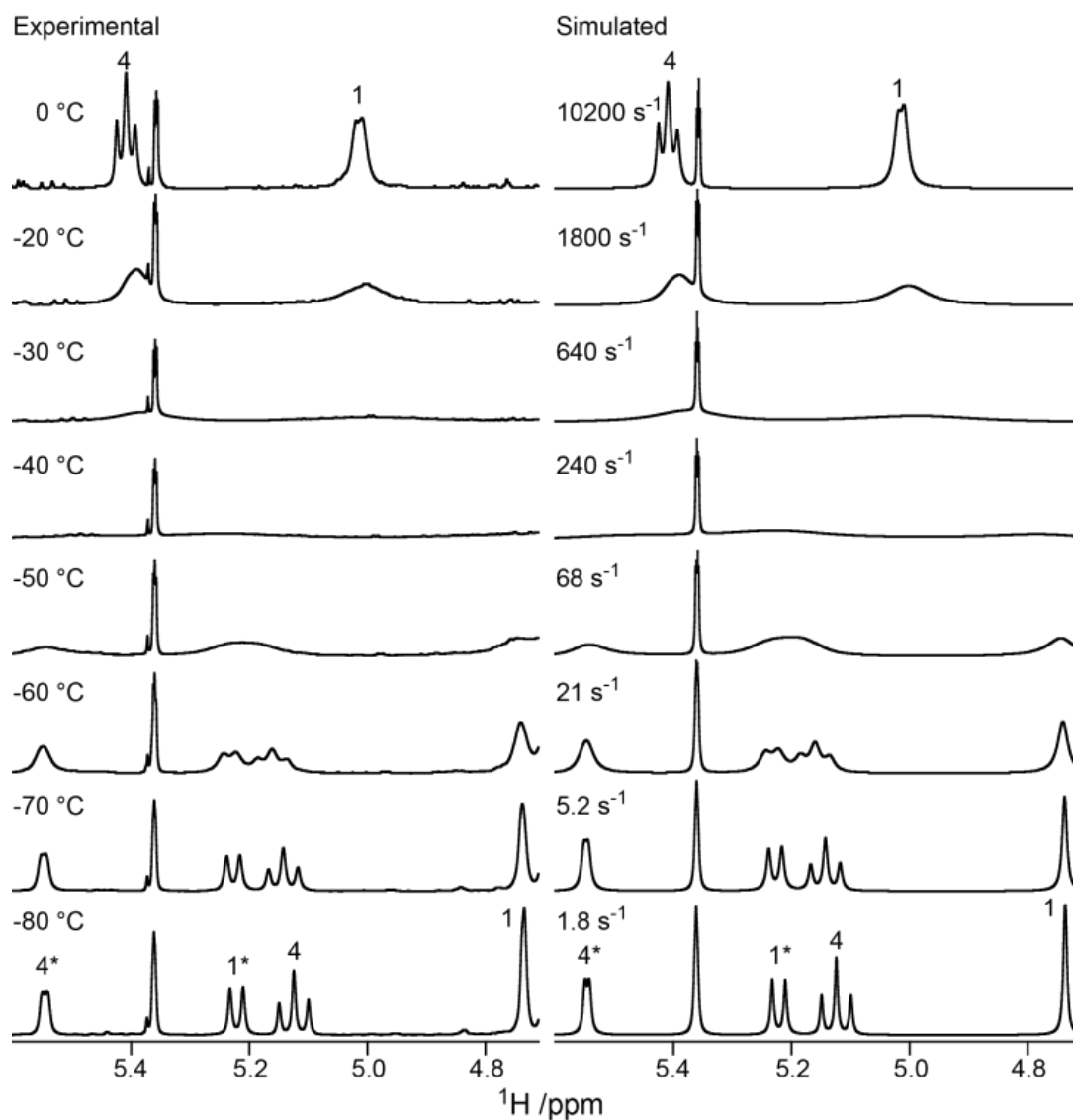


Figure S3. Experimental and simulated ¹H NMR spectra of the H1 and H4 signals of methyl glycoside **5**. The signals arising from the ¹C₄ conformer are marked with asterisks (*). The signal at 5.36 ppm originates from residual dichloromethane-*d*.

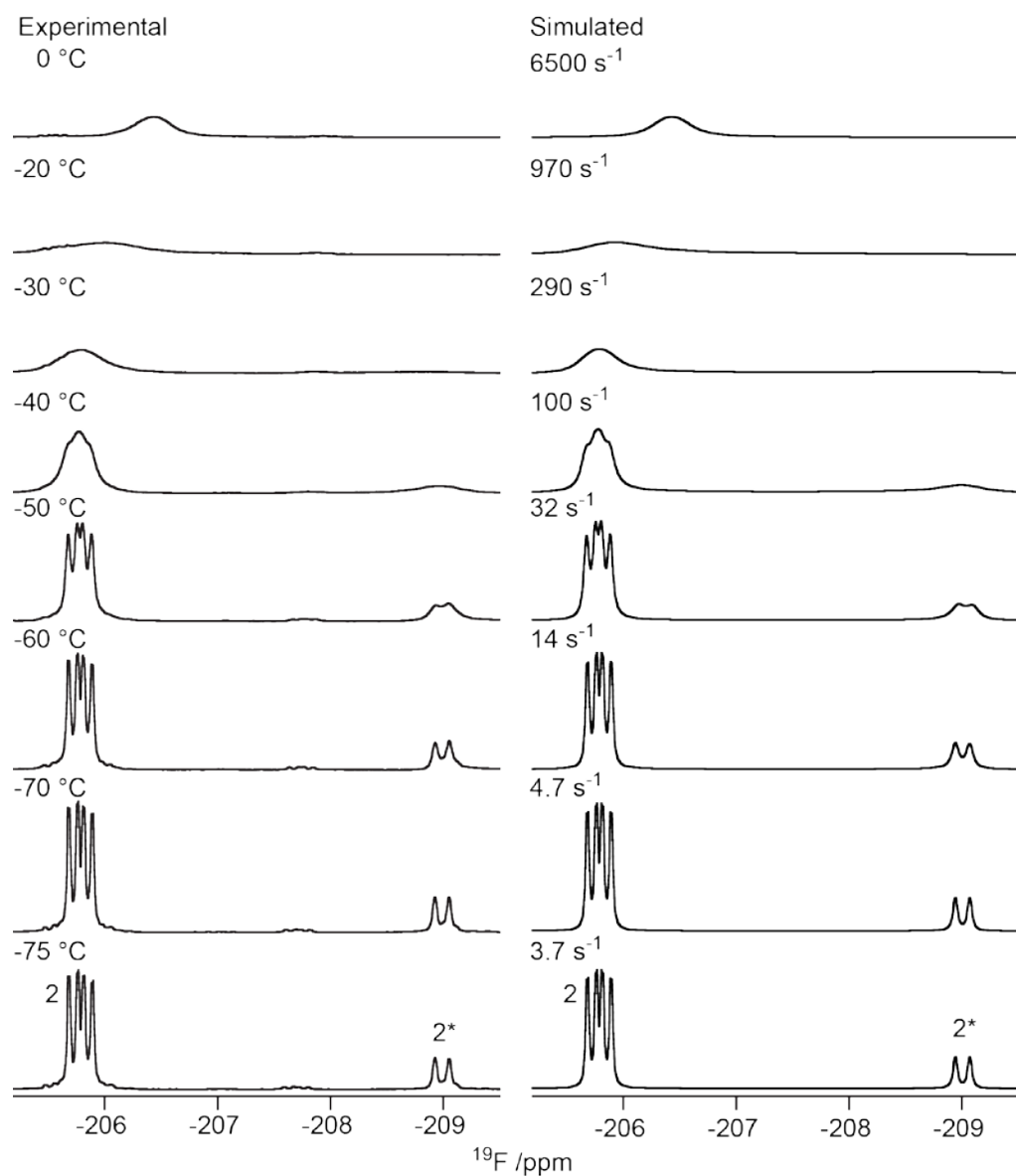


Figure S4. Experimental and simulated ¹⁹F NMR spectra of methyl glycoside **6**.

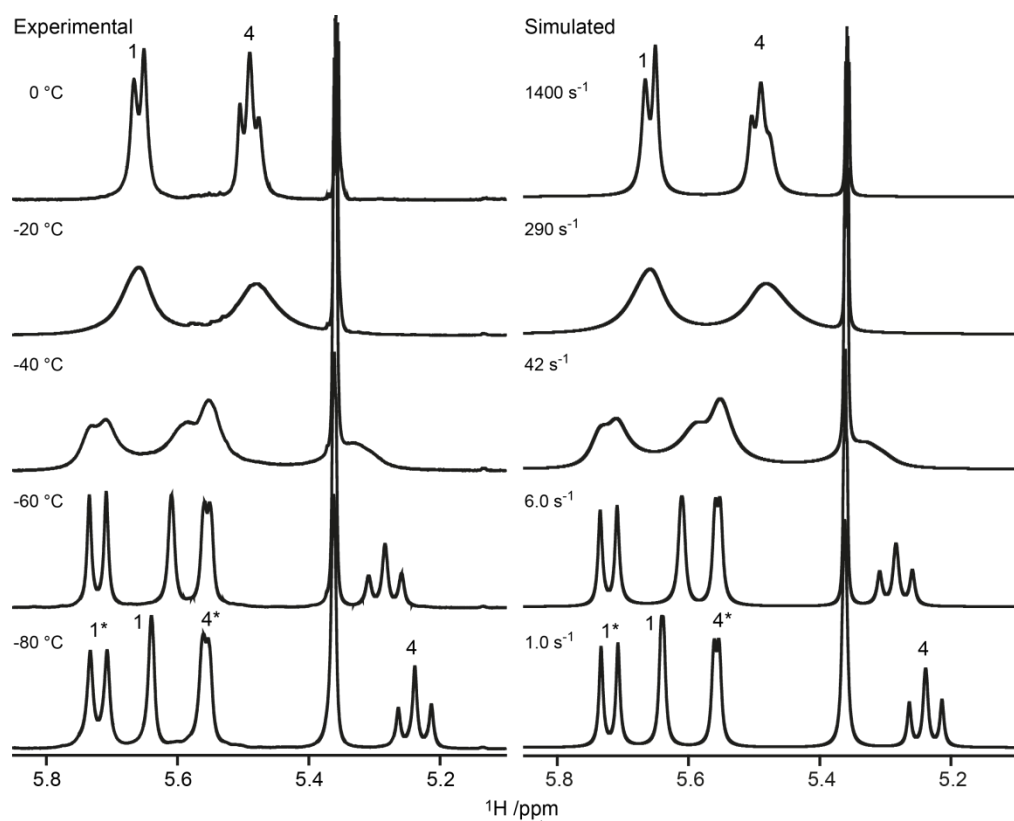


Figure S5. Experimental and simulated ^1H NMR spectra of the H1 and H4 signals of compound **7**. Signals arising from the $^1\text{C}_4$ conformer are marked with asterisks. The signal at 5.36 ppm originates from residual dichloromethane-*d*.

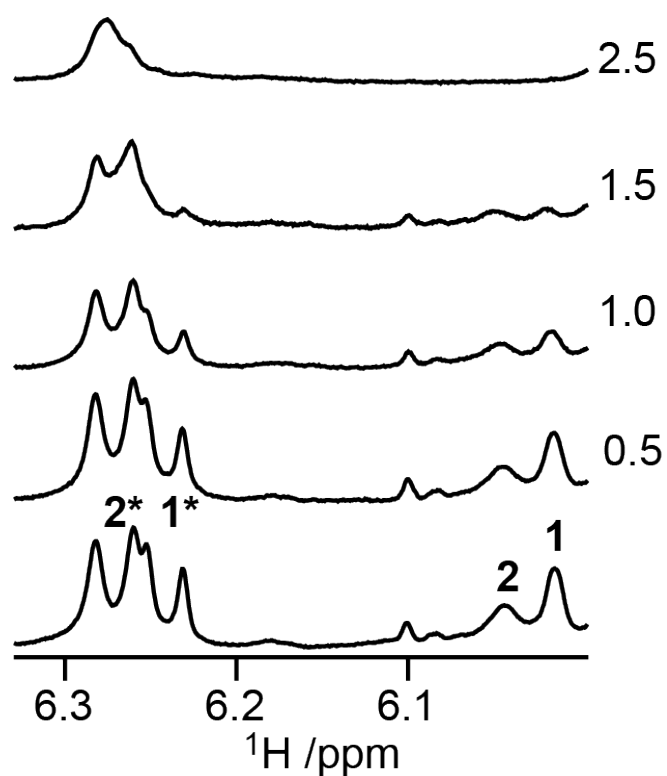


Figure S6. Anomeric region of the ^1H NMR spectra from the competition experiment of anomeric triflates **1** and **2**. The numbers in the right margin denote the number of methanol equivalents added. Signals arising from the $^1\text{C}_4$ conformer are marked with asterisks.