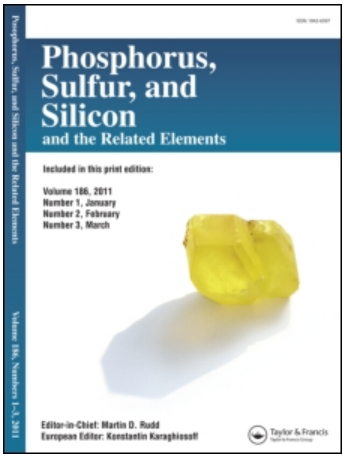

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^{1}H AND ^{13}C NMR SPECTRA OF 1-DEOXY-1-THIOGLYCOPYRANOSIDES

Gilbert Hamus[a]; Ivan K. Nielsen[a]; Peter Laur[a]
[a] Institute of Inorganic Chemistry, Aachen, Fed. Rep. of Germany

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^{1}H AND ^{13}C NMR SPECTRA OF 1-DEOXY-1-THIOGLYCOPYRANOSIDES

Gilbert Hamus, Ivan K.Nielsen, and Peter Laur
Institute of Inorganic Chemistry, Rheinisch-Westfälische Technische Hochschule (Technical University), Aachen, Fed.Rep.of Germany

In the absence of previous systematic investigations, we have embarked on the study of the NMR spectra of thioglycosides, as we needed structural information in connection with our work on the spectroscopic properties of these compounds. In this sommunication, data will be presented on alkyl α- and β-thiogluco- and -thiogalactopyranosides and some related compounds, including certain natural products like lincomycin, sinigrin, and glucocapparin. The ^{1}H spectra of the strongly coupled carbohydrate portion can readily be analyzed at 270 MHz in the case of the thiogalactosides, whereas the spectrum of the thioglucose moiety in, e.g., thioglucose sodium salt, remains a system of higher order even at 360 MHz, giving rise to multiple lines and virtual coupling. The assignment of the ^{13}C spectra proceeded basically via selective or via frequency dependant off-resonance heteronuclear double resonance experiments at 68 MHz; the C-H coupling pattern (triplet) directly reveals the position of C-(6). Application of the increment method of the ^{13}C chemical shift in connection with the thioalkyl grouping presented no complications. Tetraacetylation of the thioglycosides shifts the ring ^{13}C resonances in a systematic manner and is, therefore, an additional aid. All the compounds investigated adopt the $^{4}C_{1}$ conformation; in the α-series, $^{3}J(H\text{-}1/H\text{-}2)$ = ca. 5.5 Hz, i.e., relatively large. Long range $^{13}C\text{-}^{1}H$ coupling constants were measured in a few cases only. Values of $^{1}J(^{13}C\text{-}^{1}H)$ were also obtained from satellite lines in the appropriate high-field ^{1}H spectra. From the spectra of the fully or partly analyzed compounds rules can be deduced that are especially helpful in the examination of ^{13}C spectra of other thioglycosides, employing, e.g., chemical shift data, coupling constants, and T_1 data.