

60th anniversary NMR-DG Oct 31, Nijmegen

NMR Crystallography of Cannabinoids

Andreas Brinkmann, National Research Council Canada

The Organic Chemical Metrology Team at the Metrology Research Centre at the National Research Council Canada develops and provides certified reference materials (CRMs) to laboratories performing cannabinoid analysis of cannabis and hemp. In this contribution we present our recent progress in characterizing selected cannabinoids by NMR crystallography, the combined approach of solid-state NMR, X-ray diffraction, and density functional theory (DFT) calculations. We performed natural abundance ^{13}C cross-polarization magic-angle spinning (CP-MAS) experiments and determined the ^{13}C chemical shift anisotropies (CSAs) by CSA recoupling experiments. First results on our efforts to label cannabinoids with ^{18}O and ^{17}O and subsequent ^{17}O NMR experiments will be presented. The experimental results are complemented by calculations of the NMR parameters by periodic DFT using geometry-optimized structures and structures generated by molecular dynamics (MD) and path-integral MD calculations.