

## O4: Detection of polymorphism using $^{14}\text{N}$ NQR spectroscopy

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To demonstrate good and reliable selective property of  $^{14}\text{N}$  nuclear quadrupole resonance ( $^{14}\text{N}$  NQR) spectroscopy and its applicability in determination of polymorphism, a study of sulfanilamide polymorphism was undertaken. Three known polymorphs of sulfanilamide were examined. Two sets of three  $^{14}\text{N}$  NQR transition frequencies, corresponding to two different nitrogen sites in the crystal structure for each of three polymorphs, were found at room temperature (Figures 1 and 2). One of the three  $^{14}\text{N}$  NQR frequencies is recognized to be enough to characterize the polymorph (Figure 3). This quick and reliable proof of polymorphism appearance was successfully applied also in several other compounds containing nitrogen and could become a secondary standard in determination and/or confirmation of polymorphism.

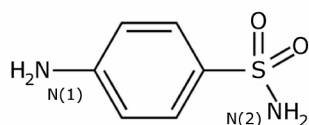


Figure 1 Sulfanilamide structure.

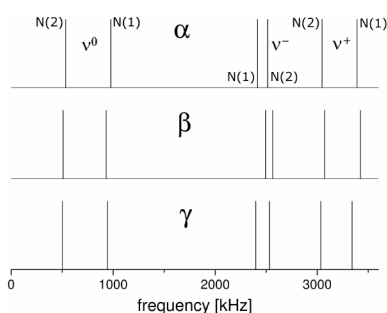


Figure 2  $^{14}\text{N}$  NQR transition frequencies for N(1) and N(2) atoms in  $\alpha$ ,  $\beta$  and  $\gamma$  polymorphs of sulfanilamide.

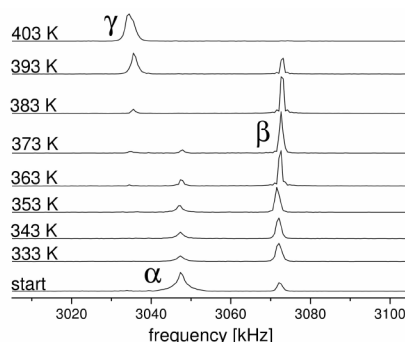


Figure 3  $^{14}\text{N}$  NQR spectra of nitrogen N(2) ( $v^+$  line) displaying a transition of the initial  $\alpha$  polymorph at 295 K (with traces of  $\beta$  form) to the final  $\gamma$  polymorph. The sulfanilamide sample was thermally treated at different temperatures, written at the left side of each  $^{14}\text{N}$  NQR scan, prior to the  $^{14}\text{N}$  NQR measurements.