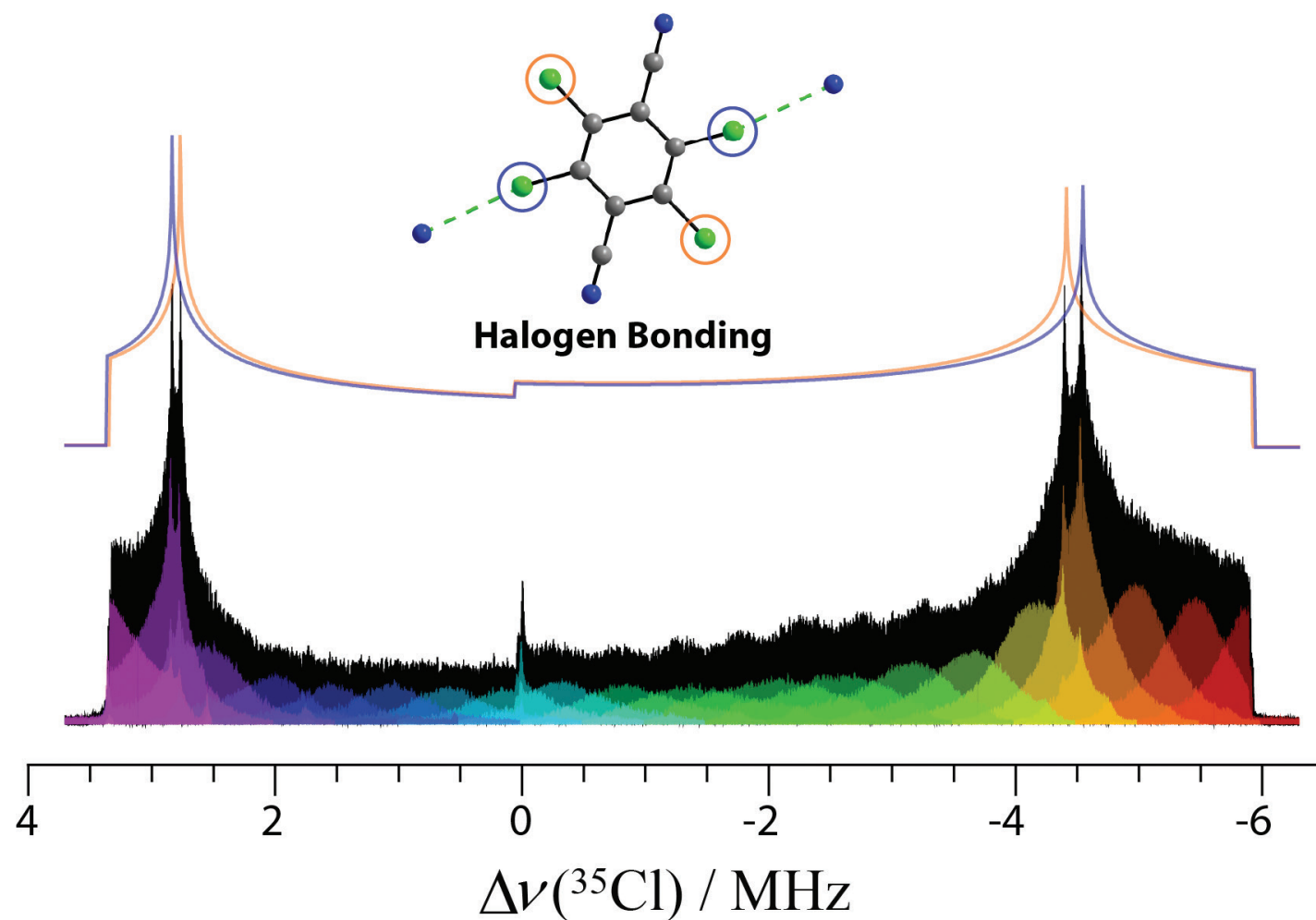




nmr is science



Tetrachloroterephthalonitrile

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Field strength: 21.1 T

Why is this your favorite spectrum?

Although this chlorine-35 spectrum is 8 MHz broad, it looked fantastic. This acquisition required a specialized probe, an ultra-high magnetic field (21.1 T), a set of 20 sub-spectra using variable-offset cumulative acquisition, and the use of the WURST-QCPMG pulse sequence. This ultra-wideline ^{35}Cl solid-state NMR spectrum is amongst the broadest spectra acquired to date. Due to the crystallographic symmetry of this compound, there are only two chlorine sites in the asymmetric unit: the site exhibiting a halogen bond to nitrogen (in blue) and the non-halogen bonded site (in orange). Fitting the spectrum with QUEST (Quadrupolar Exact SoftWare) elegantly shows the effect that the halogen bond can have on the quadrupolar coupling parameters of chlorine.