The Unexpected Role of Molecular Chirality in CP-MAS Solid State NMR Spectroscopy

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Abstract: I will discuss a rather unexpected behavior in the intensity pattern of optical isomers obtained using hydrogen/nitrogen cross-polarization magic angle spinning (CP-MAS) NMR for a series of aminoacids. In all molecules considered, the D isomer yields higher intensity than the L form, including a case where, one of the two optical isomers is essentially undetectable within the experimental limits. Such an effect cannot be explained as due to structural differences, and we attribute this striking behavior to the onset of electron spin polarization, accompanying bond charge polarization, due to the chiral-induced spin selectivity effect (CISS), recently described in the literature. CISS, induces a chirality-dependent non-zero local electron spin density that influences the molecular magnetic environment, causing a change in the nuclear chemical shift, affecting the nuclear polarization transfer mechanism, and ultimately provoking the observed asymmetry.