The C–H···O Hydrogen Bonding Effects on the ^{17}O Electric Field Gradient and Chemical Shielding Tensors in Crystalline 1-Methyluracil: A DFT Study

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A density functional study was carried out to investigate the C–H···O hydrogen bonding effects on the ^{17}O electric field gradient and chemical shielding tensors in crystalline 1-methyluracil. Since the structural coordinates were obtained from a neutron diffraction study, no geometry optimization was needed in performing the calculations. It is demonstrated that C–H···O hydrogen bonding has different influences on O2 and O4 EFG and CS tensors. In the tetramer model of 1-methyluracil, which is much closer to the real crystalline phase, the influence of C–H···O on the O4 EFG and CS tensors is significant, whereas this influence is negligible for O2.

Key words: DFT; C–H···O Hydrogen Bonding; Electric Field Gradient Tensor; Chemical Shielding Tensor; 1-Methyluracil.