AICAr (5-amino-1-(β-D-ribofuranosyl)imidazole-4-carboxamide) is cumulated in AICAr transformylase/IMP cyclohydrolase deficiency (ATIC deficiency[1]). During the synthesis of AICAr, we obtained products with two sets of NMR signals, with very similar chemical shifts. From the mechanism of reaction it is known that three products can be obtained: 2’,3’,5’-Tri-O-acetyl-1-(2,4-dinitrophenyl)inosine (A), 2’,3’,5’-tri-O-acetyl-3-(2,4-dinitrophenyl)inosine (B) or 2’,3’,5’-Tri-O-acetyl-6[(2,4-dinitrophenyl)]inosine (C). Besides, compounds (A) and (B) can occur in two diasteroisomeric forms. In our investigation, analysis of experimental NMR spectra and theoretical GIAO - DFT calculations (PCM; Gaussian 03W) were performed to obtain information about the reaction products. All these results will be presented in the poster.