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Advances in biochemical applications of β-detected NMR

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Since the implementation of β-detected NMR (β-NMR) at TRIUMF, it has mainly been used to study condensed matter systems ranging from metals to superconductors to topological insulators. In the last few years, there has been a desire to extend the applications of β-NMR to include the study of biochemical problems. For a number of metal ions in our body, such as Mg(II), Zn(II) and Cu(I), the absence of convenient physical and spectroscopic properties limits our ability to characterize their role in health and disease using conventional techniques, such as classical NMR. However, β-NMR has the possibility to help address these gaps in our knowledge by aiding in the elucidation of metal coordination in biomolecules.

In this presentation, I demonstrate that we are able to observe ^{31}Mg binding to the biomolecule adenosine 5'-triphosphate (ATP) in solution. The resonance spectrum shows two distinct peaks which indicates that we observe not one, but two distinct complexes between Mg^{2+} and ATP. We identify these complexes with ^{31}Mg β-NMR complemented by ^{31}P NMR and DFT calculations. This represents the first measurement of a β-NMR probe binding to a biomolecule and is an important milestone in applying β-NMR to the study of biochemical problems[1].

1. R. M. L. McFadden et al., Angew. Chem. Intl. Ed. e202207137 (2022)

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