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PENTAMETAPHOSPHATE: ACCESS TO NUCLEOSIDE HEXA- AND HEPTA-PHOSPHATES AND STUDY OF THEIR INTERACTION WITH RIBONUCLEASE A

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The first synthesis of the anhydride of dihydrogen pentametaphosphate, $[\text{PPN}]_2[\text{TBA}][\mathbf{1}]$ is reported in this paper. (PPN = bis(triphenylphosphine)iminium, TBA = tetra-*n*-butylammonium, $\mathbf{1} = \text{P}_5\text{O}_{14}^{3-}$). Here, we investigate the utility of $[\text{PPN}]_2[\text{TBA}][\mathbf{1}]$ as a novel reagent for pentaphosphorylation in the first syntheses of nucleoside hexa- and heptaphosphates. These syntheses are aided by the use of an organometallic complex, $\text{Mo}(\text{NCMe})_3(\text{CO})_3$, which binds to the condensed phosphate and activates it towards pentaphosphorylation. Furthermore, we delve into a detailed investigation of the interaction between their polyanionic constructs and ribonuclease A (RNase A), a model protein containing a polycationic active site. Our experimental assays of enzymatic inhibition and co-crystal structures with RNase A are interpreted with the aid of modern quantum chemical methods (QM1/QM2), including the combination of the ONIOM approach with the DLPNO-CCSD(T)-based local energy decomposition algorithm.