

Influence of nucleobase structures on goethite-catalyzed dephosphorylation of ribonucleotides

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Strong adsorption of phosphorus (P) species to iron (Fe) oxide minerals is well documented. Recent studies have brought attention to the possible role of Fe oxides in catalyzing the dephosphorylation of organic P (P_{org}) to produce inorganic P (P_{i}). However, much remains unknown about the influence of different P_{org} structures on the extent of this catalytic reactivity. Here we investigated the reactivity of goethite (1g L^{-1}) towards two ribonucleotide compounds ($50\ \mu\text{mol L}^{-1}$) containing different nitrogenous bases: adenosine triphosphate (ATP) with a purine nucleobase, and cytosine triphosphate (CTP) with a pyrimidine nucleobase. We tracked the inorganic (i.e. P_{i}) and organic (i.e., dephosphorylated ribonucleotides) hydrolysis products using UV-visible spectroscopy and liquid-chromatography mass spectrometry, respectively. After 48-h reactions, we found that the goethite-ATP mixture yielded approximately 50% more P_{i} in solution than the goethite-CTP mixture (**Fig. 1a**). We performed molecular modeling simulations to determine the adsorbate conformations for the different ribonucleotide-goethite complexes (**Fig. 1b**). The findings of this study led us to hypothesize that differences in the structure and functional groups of P_{org} compounds would dictate interactions on the Fe oxide surfaces to result in different extent of hydrolytic cleavage by the mineral.

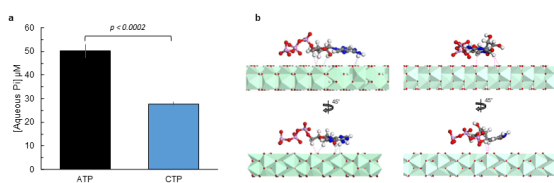


Figure 1. Catalytic reactivity and adsorption interactions for ribonucleotide reactions with goethite. (a) Total P_{i} generated after 48-h goethite reaction with ATP or CTP. (b) Adsorbate conformations of (left) ATP and (right) CTP binding on the surface of goethite. Atom color legend in b: Hydrogen (white), oxygen (red), nitrogen (blue), phosphorus (pink), Fe (green), and carbon (gray).