Constrains of abiotic Thioester chemistries in origins of life

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Thioesters such as thioacetic acid (TAA) and methyl thioacetic acid (MTA) are often invoked as a key prebiotic reagent for the establishment of self-propagating metabolic reactions or as a reducing agent for the abiotic synthesis of deoxyribonucleotides. The esters would be acting as an activated form of acetate (i.e. acetyl-CoA) allowing C-insertions to form C_3 compounds such as pyruvate. Despite its interest in prebiotic chemistry, data related to kinetic and thermodynamic properties of thioacetic acid are scarce, making it difficult to evaluate its relevance in a geochemical context.

Here, using a combination of laboratory measurements, literature data, and thermochemical models, we examine the constrains of the accumulation of sufficient amounts of this compound to participate in these types of chemistry. We find that the equilibrium constant for the formation of TAA is extraordinarily low, and there are unlikely to be many environments where this compound could have formed abiotically to any significant extant. These problems in the synthesis of TAA may call into question the plausibility of higher order chemistry which requires it as a reactant.