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Unique energetic properties of Adenosine Tri-Phosphate in comparison to similar compounds using density functional theory KEVIN MURASZKO, THOMAS HALLORAN, SVETLANA MALINOVSKAYA, PHILIP LEOPOLD, Stevens Inst of Tech — Adenosine Tri-Phosphate (ATP) is arguably the most critical compound to all life known on Earth, serving as the main energy transport and storage in cellular biology. Why in particular did nature "choose" ATP instead of a similar compound? We are seeking to answer this question by comparing the energetic properties of ATP to similar compounds. We discuss 3-D models for ATP, variants of the molecule based on all of the separate nucleobases, and ATP's twin molecule Adenosine Di-Phosphate. All calculations were done using Density Functional Theory. The results showed that purine compounds like Adenosine and Guanosine produce similar bond angles, making these viable unlike the other nucleobases. We have analyzed the chiral properties of ATP by comparing the ground-state-energies of ATP-cis and ATP-trans and have shown that ATP-cis is the more energetically favorable of the two. This is consistent with observations in nature.

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