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Formation of glycine from HCN and H₂O: A computational mechanistic study

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Abstract

The potential energy surfaces for the formation of glycine from HCN and H₂O were determined from CBS-QB3 calculations. After the formation of a HCN trimer, amino malonitrile, amino malonitrile monoamide (**3**) was formed by a water addition reaction. Two pathways were found for the subsequent reaction, **3** + 2H₂O → glycine + HNCO + NH₃. One pathway involving an amino ketone was much more favored than the other pathway involving glycinamide. Addition of a water molecule as a catalyst greatly enhanced steps occurring by hydrogen rearrangement.

Keywords: Reaction pathway, CBS calculation, Prebiotic chemistry, Astrophysics, Astrobiology

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