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PII: S0009-2614(17)30209-9
DOI: http://dx.doi.org/10.1016/j.cplett.2017.02.079
Reference: CPLETT 34592

To appear in: *Chemical Physics Letters*

Received Date: 5 January 2017
Accepted Date: 27 February 2017

Please cite this article as: H.M. Lee, J.C. Choe, Formation of glycine from HCN and H_2O: A computational mechanistic study, *Chemical Physics Letters* (2017), doi: http://dx.doi.org/10.1016/j.cplett.2017.02.079

Formation of glycine from HCN and H_2O: A computational mechanistic study

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Abstract

The potential energy surfaces for the formation of glycine from HCN and H_2O were determined from CBS-QB3 calculations. After the formation of a HCN trimer, amino malononitrile, amino malononitrile monoamide (**3**) was formed by a water addition reaction. Two pathways were found for the subsequent reaction, **3** + $2H_2O$ → glycine + HNCO + NH_3. 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