THEORETICAL STUDY OF AMINO ACID PRECURSOR FORMATION IN INTERSTELLAR MEDIUM.
1. REACTION OF METHYLEMININE WITH HYDROGEN CYANIDE.

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Introduction: Search for amino acids and their precursors in interstellar medium is one of the most challenging tasks for modern radio astronomy and astrobiology. Although no convincing detections of even the simplest amino acid glycine have been reported so far, rich organic chemistry of molecular clouds gives hope to expect even more complex species of prebiotic interest to be present in interstellar medium. Methylenimine (HN=CH\textsubscript{2}), definitively detected in several Galactic objects \cite{1}, has been suggested as a possible precursor for glycine and its nitrile \cite{1-3}. One can imagine different reaction pathways, but the most probable are those involving abundant, commonly found organic species. One of such species is hydrogen cyanide (HCN). From common considerations, its interaction with methylenimine might produce glycine nitrile (H\textsubscript{2}NCH\textsubscript{2}CN). Here we present the results of \textit{ab initio} quantum chemical study of this reaction.

Calculation Details: All calculations were performed with the Gaussian 98W \cite{4} suite of programs. All the geometry optimizations, vibration frequency calculations and transition state searches were done using the hybrid B3LYP functional and 6-31++G** basis set.

Results and Discussion: The potential energy surface for the reaction HN=CH\textsubscript{2} + HCN $\rightarrow$ H\textsubscript{2}NCH\textsubscript{2}CN is very complicated, with several transition structures found.

The initial step is the formation of a van der Waals complex I (Fig. 1). Its energy is below than that of the reactants by 6.8 kcal mol\textsuperscript{-1} (by 5.5 kcal mol\textsuperscript{-1} with zero-point energy correction found from vibration frequency calculations). The first transition structure II forms due to proton transfer from HCN molecule to the N-atom of methylenimine. Already TS1 has a high energy barrier of +27.1 (+27.9 ZPE-corrected) kcal mol\textsuperscript{-1}, but the next TS2 (III) has even higher energy of +32.3 (+34.6 ZPE-corrected) kcal mol\textsuperscript{-1}. The latter structure corresponds to an intermediate transfer of CN\textsuperscript{-} anion formed from the protonated imino group of HN=CH\textsubscript{2} to its C-atom. After complete CN\textsuperscript{-} transfer, the third transition structure forms, IV, where the C—C distance is 2.066 Å (vs. 1.472 Å in glycine nitrile V); its energy is +22.1 (+24.9 ZPE-corrected) kcal mol\textsuperscript{-1}.

The overall reaction exothermicity calculated is 24.4 (20.0 ZPE-corrected) kcal mol\textsuperscript{-1}. However, the presence of the three high-energy transition states makes the reaction discussed hardly feasible in the gas phase, leaving grain-surface chemistry the only possible way of a direct glycine nitrile formation from methylenimine and hydrogen cyanide (if any).

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Fig. 1. Relative energies (kcal mol$^{-1}$) for the van der Waals complex (I), transition states (II-IV) and glycine nitrile (V) computed at B3LYP/6-31++G** level (in parenthesis, zero-point energy corrected values), with some important distances in angstroms (Å).