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POTENTIAL ENERGY SURFACE OF C_3H_3N.

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Azetes (C_3H_3N, $C_2H_2N_2$, CHN_3 and N_4) are group of species derived from cyclobutadiene **(**CBD) by means of substituting the C-H groups with N atoms. Azetes are extremely reactive, as is their parent compound, CBD. There are few theoretical studies on nitrogen substituted analogues of CBD or tetrahedrane (TH) [1, 2]. The bonds in the azetes are rather strained, but the strain in the molecule decreases as the number of nitrogen atoms in structure increases.

There have been some attempts to synthesize unsubstituted azete (C_3H_3N). Due to it is high reactivity, its preparation has been problematic. In the 1970s, azete was produced in matrix preparation at low temperatures by Maier and Schaefer [3]. Decades later the very same experiment was verified computationally by Neumann and Jug [4].

The derivatives of azete are known to be stable under normal conditions. Probably the most known is azete with stabilizing *tert*-butyl groups; first attempt to prepare it was made by Vogelbacher *et al* using pyrolysis [5]. Like CBD, kinetically stabilized azete will participate readily in cycloaddition reactions with different available partners, meaning that it could be used in organic synthesis [6].

We have investigated potential energy surface (PES) of ground state singlet C_3H_3N. We intend to discuss some of the interesting reactions occurring on the PES of C_3H_3N as well as some of the isomers of azete. To our knowledge PES of C_3H_3N has never been studied before, although some of the isomers present on the surface have been investigated. However, there have been recently some studies on the PES of $C_3H_3N^+$ [7] which is of interest due to new data available on interstellar chemistry. We hope that our contribution will provide new knowledge on processes in the interstellar space and dust clouds.

In our study two levels of theory was used: 1) density functional theory B3LYP functional with 6-311+G** basis set for preliminary PES scan and 2) second order Møller–Plesset perturbation theory (MP2(Full)/aug-cc-pvtz) to verify data obtained. Minima (reactant and product) corresponding to specific transition state (TS) were determined using the intrinsic reaction coordinate (IRC) calculations and also the vibrational frequencies were calculated for each optimized structure and to identify the minima and TS character of the stationary points found in the geometry optimization.

Though the system studied appears to be very simple the PES of C_3H_3N is very complicated and rich in different species: at MP2 level of theory altogether 52 different minima was found.

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