

Singlet H-cCNC-C: A Potential Interstellar Molecule

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Abstract: A new planar isomer of HNC₃ system, H-cCNC-C, is theoretically predicted by means of B3LYP and CCSD(T) methods. The suggested species can isomerize into other five kinetically more stable isomers, which have been experimentally identified, with relatively higher reaction barriers. In view of its higher kinetic stability, we can reasonably believe that the obtained species H-cCNC-C can be experimentally observed in future studies.

Keywords: HNC₃ system, stability, isomer, isomerization.

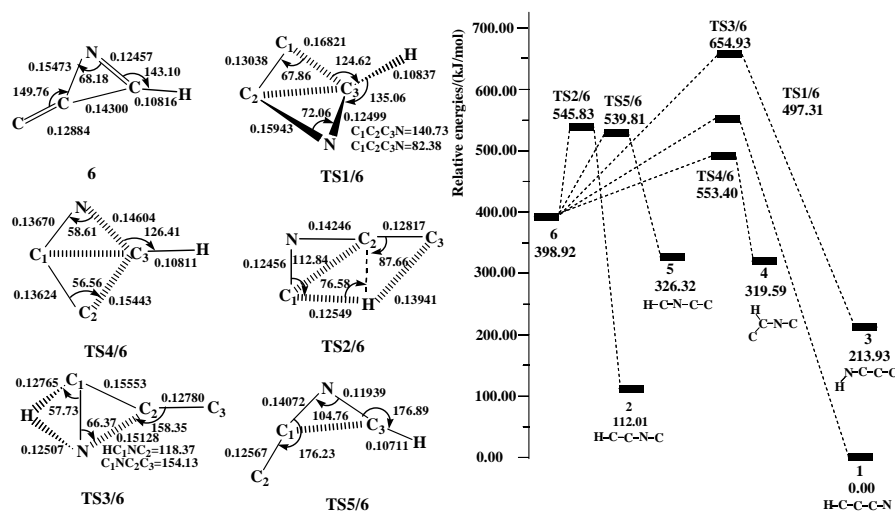
HNC₃ is a typical interstellar molecular system, and three isomers, HCCCN (**1**, cyanoacetylene)¹, HCCNC (**2**, isocyanoacetylene)², and HNCCC (**3**, imine isomer)^{3,4}, have been detected in the atmosphere of titan or in the taurus molecular cloud. Furthermore, other two isomers, chain branched CC(H)CN **4**^{5,6} and HCNCC **5**^{7,8}, have also been theoretically and experimentally suggested to exist as potential interstellar molecules. In our recent theoretical study, another planar isomer, H-cCNC-C **6** with a CNC three-membered ring and exocyclic C-H and C-C bonding, has been found to be possible to exist because of its higher kinetic stability.

All calculations are carried out with Gaussian 98 package running on the SGI/Origin300 server. The geometries of stationary points are optimized using B3LYP method with 6-311++G(d,p) basis set followed by the frequency analyses for confirming the nature of the obtained local minima and saddle points. The B3LYP geometries are used to calculate CCSD(T) single-point energies with 6-311++G(2df,p) basis set.

Calculated five transition states and isomer **6** are shown in **Figure 1**, and a sketch-map of the potential energy surface profile is also plotted in **Figure 1**.

In isomer **6**, the H-site C-N bond (0.12457 nm) is a rather strong double bond and the C-site C-N bond (0.15473 nm) is a somewhat weak single bond in view of the normal C-N double and single bond lengths 0.12670 nm and 0.14670 nm in CH₂NH and CH₃NH₂ molecules, respectively. Furthermore, the normal C-C single, double, and triple bonds are 0.15309 nm, 0.13289 nm, and 0.11993 nm in C₂H₆, C₂H₄, and C₂H₂ species. Therefore, we can consider the C-C bond (0.14300 nm) in NCC ring and the terminal C-C bond (0.12884 nm) as two intermediates between single and double bonding and between

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Figure 1 Calculated stationary points and isomerization channels

double and triple bonding, respectively.

Based on the reaction pathways shown in **Figure 1**, we can easily find that isomer **6** can isomerize into other five isomers *via* several different reaction channels. No other isomerization channels were found in spite of a lot of work has been paid. It should be pointed out that the isomerization reaction connecting species **6** and **5** with the lowest barrier height 140.89 kJ/mol hardly happens *via* the suggested transition state **TS5/6** in the atmosphere of titan with lower temperature. Certainly, other reaction, processing with higher barriers, also can not happen. Furthermore, we also considered all possible dissociate patterns and found that the energies of these direct dissociate fragments are higher than optimized transition states. Therefore, we can safely consider that the obtained isomer **6** is a kinetic stable species, and it can be experimentally observed in future studies.

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