عنوان مقاله:

Formation of NxO(x=1,2) in the gas phase. Theoretical study of methylenimine and Nitroxyl reaction

محل انتشار:

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خلاصه مقاله:

Methylenimine is an important molecule in prebiotic chemistry [1] and is a molecule ofinterest in both astrobiology and astronomy [2]. Neutral H2CNH in some complex reactions is areactive intermediate that can be produced by pyrolysis of amines and azides [3]. The compoundis highly reactive, soluble in water, and sticky, thus there will be a serious challenge inexperimental study of the relevant reactions. Therefore, the use of theoretical investigations canbe a good alternative in this case [4]. In this study we theoretically investigate two reactionpathways for H2CNH and HNO system due to NxO(x=1,2) formation. Grand state of potentialenergy surfaces (PES) ,singlet, is considered. The geometries of reactants (R), products(P),intermediates (IN), and transition states (TS) were optimized using the second order MollerPlesset theory (MP2 method) in conjunction with the 6-311++G(3df,3pd) basis set. The singlepoint energies of the stationary points are obtained at the CCSD(T)/aug-cc-pVTZ level. Rateconstant of reaction .pathways is computed by RRKM and TST theories for unimolecular andbimolecular reactions, respectively

کلمات کلیدی:

Methylenimine, Kinetic, Gas Phase, RRKM, TST