

Photodissociation of HNC and HNC isomers in the UV, from 7 to 13 eV

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In regions with high UV flux, photodissociation is a fundamental event destroying molecules. HCN and its isomer HNC are widely detected in space, and in photodissociation regions the HNC/HCN ratio presents anomalies. In order to understand their photostability the photodissociation cross section for both isomers in a wide range of excitation energies will be presented [1,2]. For this purpose, 21 electronic states have been calculated in a three-dimensional grid, 12 ¹A' and 9 ¹A'', at icMRCI level. The individual spectra to each of the excited state are obtained with a wave packet method using the ab initio transition dipole moments.

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References

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