AU Talbi, D, Le Padellec, A, Mitchell, JBA
TI Quantum chemical calculations for the dissociative recombination of HCN+ and HNC+
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AB A theoretical investigation of the dissociative recombination (DR) of HCN+(X (2)Pi), HNC+(X (2)Sigma) and HCN+(A (2)Sigma) has been undertaken in order to complement the recent experimental measurement (Sheehan C, Le Padellec A, Lennard WN, Talbi D and Mitchell J B A 1999 J. Phys. B: At. Mel. Opt. Phys. 32 3347) of the DR of [CHN](+). Using quantum chemical methods, we have shown that the dissociative recombination of HNC+(X (2)Sigma) should involve the indirect mechanism while that of HCN+(X (2)Pi) and HCN+(A (2)Sigma) should be possible through both direct and indirect processes. Our theoretical study therefore suggests that HCN+(X (2)Pi) and HCN+(A (2)Sigma) should recombine much more rapidly than HNC+(X (2)Sigma) explaining the large rate coefficient measured for the DR of HCN+ compared with the HNC+ case.
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