Title: Collision of DCN with He: Isotopic effects and ro-vibrational rate coefficients

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Abstract:

The study of the deuterated molecules can be useful to understand the physical properties and chemical history of the molecular clouds. We have analysed the effects to replace H by D in the collision of HCN with He. We solve the close coupling equations in the space fixed frame using the potential energy surface recently published for the HCN-He system. These calculations were done treating the triatomic molecule within the rigid rotor and rigid bender approaches. Ro-vibrational rate coefficients of DCN in collision with He were computed and compared with those for HCN-He. For the first *l*-doubling transitions, we found that the behaviour of the rate coefficients with the temperature is of the same order of magnitude than the rate coefficients for pure rotational transitions. The ratio of the rate coefficients between both isotopologues varies from 0.4 to 3.9 in the ground vibrational level. These results show that the collisional rate coefficients of deuterated species cannot be evaluated by simply using extrapolated rates of hydrogenated species.