Laboratory Astrophysics: from Observations to Interpretation
Proceedings IAU Symposium No. 350, 2019
F. Salama & H. Linnartz, eds.
doi:10.1017/S1743921319009335

Gas-phase reactivity of $CH_3C(O)CH_3$ with OH radicals at interstellar temperatures (T = 11.7 – 64.4 K) using the CRESU technique

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Abstract. The rate coefficients, $k(T = 11.7–64.4$ K), for the gas-phase reaction between OH radicals and acetone, $CH_3C(O)CH_3$, have been measured using the pulsed CRESU (French acronym for Reaction Kinetics in a Uniform Supersonic Flow) technique, the most suitable one to cool down gases below the freezing point without gas condensation. The experimental $k(T)$ was found to increase as temperature was lowered and is several orders of magnitude higher for low temperature than k(300 K). No pressure dependence of k(20 K) and k(64 K) was observed, while k(50 K) at the largest gas density is twice higher than the average values found at lower gas densities. The obtained values of k(11.7 K) and k(21.1 K) were 2.45×10^{-10} and 1.39×10^{-10} cm^3 molecule^{-1} s^{-1}, respectively.

Keywords. astrochemistry, methods: laboratory, ISM: molecules

1. Introduction

Hydroxyl (OH) radicals and acetone ($CH_3C(O)CH_3$) were detected for the first time in Cassiopeia A (Weinreb *et al.* (1963)) and in Sagittarius B2 molecular cloud (Combes *et al.* (1987)), respectively. Since then, these species have been detected in several interstellar environments. The gas-phase kinetics of the reaction of acetone with OH radicals (R1) has not been widely investigated at temperatures in star-forming regions of the interstellar medium (T = 10−100 K), only the Leeds group reported the rate coefficients, $k(T)$, for reaction (R1) down to 79 K (Shannon *et al.* (2010); Shannon *et al.* (2014)).

$$OH + CH_3C(O)CH_3 \rightarrow H_2O + CH_3C(O)CH_2 \quad \text{(R1)}$$

Acharyya *et al.* (2015) used a gas-phase network to evaluate the role of reaction (R1) in the chemistry of interstellar clouds. At 10 K and 50 K, the estimated $k(T)$ was 1.0×10^{-10} cm^3 molecule^{-1} s^{-1}, based on the work of Shannon *et al.* (2014). These authors observed a strong pressure dependence of k at around 80 K, while at 140 K the p-dependence of k was less pronounced. Shannon *et al.* (2014) computed the pressure dependence of $k(T)$ using MESMER code and predicted a k of 10^{-11} cm^3 molecule^{-1} s^{-1}

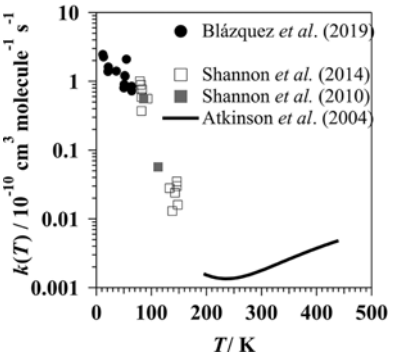

Figure 1. Rate coefficients for the $CH_3C(O)CH_3$ + OH reaction as a function of temperature.

for reaction (R1) at 20 K. In this work, we have experimentally determined $k(T)$ in an extended temperature range (11.7−64.4 K) by employing the pulsed CRESU technique to confirm the current rate coefficients used in gas-phase astrochemistry models at 10 K and 20 K. Additionally, the potential P-dependence of k has been explored at 20 K, 50 K and 64 K.

2. Experimental part

The pulsed CRESU system in Ciudad Real (Spain) allows us to perform kinetic measurements in the range of 11.7−64.4 K by using different Laval nozzles and buffer gases (He and N_2 and binary mixtures). The CRESU technique is coupled to the pulsed laser photolysis and the laser induced fluorescence techniques (Jiménez *et al.* (2015).

3. Results, Discussion and Implications

As can be seen in Figure 1, the rate coefficients obtained in this work increase when decreasing the temperature from 64.4 to 11.7 K. This increase is less pronounced than that observed by Shannon *et al.* (2010) and Shannon *et al.* (2014) from 148 to 79 K. No pressure dependence of k(20 K) and k(64 K) was observed, while k(50 K) at the largest gas density is twice higher than the average values found at lower densities. These kinetic results are the first determination of $k(T)$ in that temperature range and the first investigation of the pressure dependence of $k(T)$ at temperatures below 80 K, widely developed and discussed in Blázquez *et al.* (2019).

The obtained rate coefficients of k(11.7 K) and k(21.1 K) are 2.45×10^{-10} and 1.39×10^{-10} cm^3 molecule^{-1} s^{-1} respectively. These values are of the same order of magnitude as the estimated values at 10 K by Acharyya *et al.* (2015) in their gas-phase astrochemical model (1.0×10^{-10} cm^3 molecule^{-1} s^{-1}), however k(20 K) is one order of magnitude lower than that calculated by Shannon *et al.* (2014) at pressure conditions typical for the interstellar molecular clouds (10^6 cm^{-3}).

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https://doi.org/10.1017/S1743921319009335 Published online by Cambridge University Press

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https://doi.org/10.1017/S1743921319009335 Published online by Cambridge University Press