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Photochemistry of C_2 parent species in cometary comae

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Abstract

The to date most established compositional classification of comets is based on the Haser production rates of C_2 and OH or CN. A link between the Haser production rate of C_2 and the abundances of realistic parent species in comets is still missing. In this work, a model for photochemistry is used to predict radial column densities of C_3 and C_2. These predictions are compared to observed column densities. Markov-Chain Monte-Carlo (MCMC) techniques [1] are used to determine the production rates of parent species, and the rates of photochemical reactions required to reproduce the observations. The role of the potential C_2 and C_3 parent species C_3H_4, C_3H_2O, C_4H_2, C_2H_6, C_2H_2, and HC_3N are discussed with respect to their role in producing the observed cometary C_2.

1. Introduction

A'Hearn et al. (1995) introduced a classification scheme for comets, dividing them into two groups [2]. The "typical" comets show a correlation between the Haser production rates of C_2 and OH or CN. The group of the "depleted" comets present no such correlation, having in general a lower abundance of C_2 with respect to OH or CN, as compared to typical comets. The existence of these two groups was confirmed by later work (e.g. [3][4]). To interpret the existence of the two compositionally distinct groups of comets with respect to their origins, and to link this classification to emerging classification schemes based on observations of parent species in comets, the origin of cometary C_2 has to be understood. By now suggested formation mechanisms for C_2 [5] fail to explain the radial distribution of C_2 in a number of comets. However, electron impact reactions seem to play no important role in the production of C_2, allowing further studies to focus on photochemical processes. In this work we use a simple but fast model for photochemical processes in cometary coma to compare the predicted radial column density profiles of C_2 and C_3 with observations. MCMC is used to determine the reaction rates and parent species production rates and their uncertainties. The results are compared to reaction rates and observed parent species production rates where available. The role of C_3H_4, C_3H_2O, C_4H_2, C_2H_6, C_2H_2, and HC_3N in producing C_2 is evaluated this way.

2. The model

The model used in this work is a complex version of a multistep Haser model. Parent species are assumed to be released from the nucleus and to expand with constant velocity into a spherically symmetric coma. They can undergo photodissociation, photoionization, and photoionization dissociation reactions. Different chemical reaction networks are evaluated with respect to they capability to reproduce the observed column density profiles of C_2 and C_3 in the coma of comets. Fig. 1 shows one of the networks, including C_2H_6, C_2H_2, and C_3H_4 as parent species for C_2.

3. Analysis

For the different reaction networks studied in this work, MCMC was used to determine the best fitting values for the reaction rates and the parent species production rates. Fig. 2 shows the best-fiting profiles for comet 9P/Tempel 1 (observed Jul 3, 2005, at $r_h = 1.5$ AU), as obtained with the reaction network presented in Fig. 1. The use of MCMC does not only allow for the determination of the best-fiting parameters, but also provides information on the uncertainties of the parameters and their complex correlations. The outputs can therefore be compared with values available in the literature.

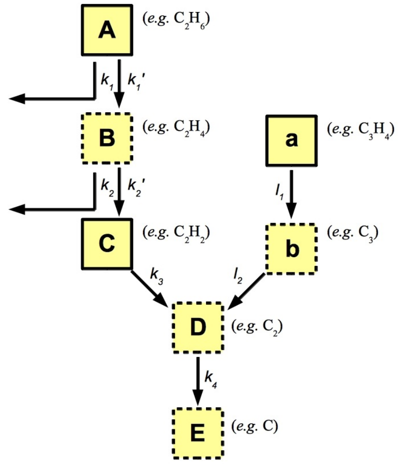

Figure 1: Example of a simple reaction network for the production of C_3 and C_2 in the cometary coma studied in this work. Parent species are shown in solid boxes, daughter species in boxes with dashed frames.

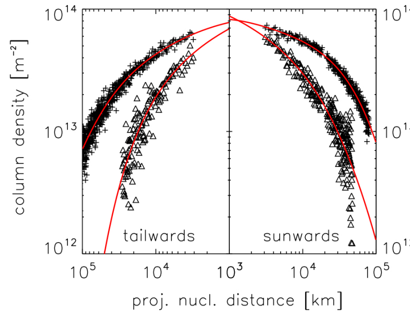

Figure 2: Radial column density profiles of C_3 (triangles) and C_2 (crosses) for comet 9P/Tempel 1. The red lines show the profiles predicted by the reaction network of Fig. 1, after adjusting the reaction rates and parent species production rates.

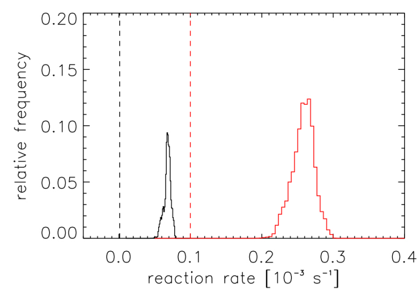

Figure 3: Relative frequencies of the reaction rates for $C_3 \rightarrow C_2$ (l_2 in Fig. 1, red curve) and $C_2 \rightarrow C$ (k_4 in Fig. 1, black curve) in the Markov Chain after burn-in, for the sunward side of comet 9P/Tempel 1. The reaction rates from Huebner et al. [6] are shown as dashed lines.

4. Summary and Conclusions

An example for comparing parameters and their uncertainties as obtained from fitting the observed column density profiles using MCMC is presented in Fig. 3. The distributions of two reaction rates from the network in Fig. 1 after burn-in of the MCMC is presented, together with their literature values taken from [6]. The two example reactions for which the results are shown are $C_3 \rightarrow C_2 + C$ and $C_2 \rightarrow 2\,C$ / C_2^+. The results obtained are not in agreement with the literature values, making the reaction network from Fig. 1 unlikely to represent the formation of C_2 in the cometary coma. From the full studies, further conclusions can be drawn, e.g. that C_2H_6 as no significant influence on the observed C_2, and that C_2H_2, together with a parent species for C_3, is unlikely to be the sole parent species of C_2.

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