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Hydrocarbon Chemistry in Cometary Comae

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Abstract

The radicals C_3 and C_2 belong to the longest known species in cometary comae. The by now most detailed compositional taxonomy of comets is based on these species [1], making the origin of these daughter products an important problem for the understanding of comet formation and classification. C_3 and C_2 are believed to be formed by chemical and photochemical reactions from hydrocarbon species sublimating from the comet's nucleus. A detailed mechanism for the formation of C_3 and C_2 from C_3H_4, C_2H_6, and C_2H_2 has been suggested and used to determine the production rates for the parent hydrocarbons in the coma of comet C/1995 O1 (Hale-Bopp) at large heliocentric distances [2]. In this work we present a chemical reaction model for cometary comae and it's application to interpret the observed radial column density profiles of C_3 and C_2 in the comae of four comets. It turns out that the reaction network used to reproduce the observational data on C_3 and C_2 of comet Hale-Bopp fails for three other comets observed at lower heliocentric distances. The reason for this failure is discussed and possible alternative formation mechanisms for C_3 and C_2 are briefly discussed.

1. Introduction

In previous studies it was assumed that C_3 in cometary comae is formed from C_3H_4 (which exists in two isomers, allene and propyne) via photodissociation reactions in the solar radiation field, as well as by an electron impact reaction, producing C_3 in one step from C_3H_4:

$$C_3H_4 + e^- \rightarrow C_3 + 2\ H_2 + e^- \qquad (1)$$

C_2 is then formed by a further photodissociation process of C_3, as well as by photodissociation reactions of C_2H_6 and C_2H_2. With these assumptions, it was possible to reproduce the radial column density profiles of C_3 and C_2 in comet Hale-Bopp, observed at heliocentric distances larger than 2.9 AU, and to determine the production rates of the hydrocarbon parent species.

In this work we present a model for chemical processes in cometary comae. This model is employed in attempts to reproduce the observed C_3 and C_2 abundances in the coma of comet Hale-Bopp at a heliocentric distance of 3.8 AU, as well as in the comae of the comets C/2001 Q4 (NEAT), C/2002 T7 (LINEAR), and 9P/Tempel 1. The later three comets were observed at heliocentric distances between 1 and 1.5 AU.

2. The model

We used a three-fluid model for the hydrodynamics and chemical processes in the coma of a comet. It assumes spherical symmetry and allows us to solve the coupled hydrodynamical and chemical reaction equations for three fluids (neutral fluid, ion fluid, and electron fluid) in the coma. This model includes various types of chemical reactions, such as photoreactions, electron impact reactions, and neutral-neutral and neutral-ion reactions. The model uses production rates of parent species from the nucleus as starting values and computes the densities of these species as well as of daughter species as a function of nucleocentric distance. These densities are converted to column densities and can be compared to observed column densities. The observed column densities are fitted by varying the parent species production rates, using a downhill-simplex algorithm.

3. The data set

Radial column density profiles of C_3 and C_2 were obtained simultaneously by means of low-resolution long-slit spectroscopy. The observations of four comets were performed using ESO telescopes. An overview of the observations is presented in Table 1.

Table 1: Overview of the observations used in this work. r_h and Δ denote the heliocentric and geocentric distances, respectively.

Comet	Date 2	Telescope / Instrument	r_h [AU]	Δ [AU]
C/1995 O1 Hale-Bopp	19 Dec 1997	ESO 1.5m / B&C	3.78	3.60
C/2001 Q4 NEAT	13 Jun 2004	ESO 3.6m / EFOSC2	1.00	0.39
C/2002 T7 LINEAR	30 Apr 2004	ESO 3.6m / EFOSC2	1.20	1.03
9P/Tempel 1	04 Jul 2005	VLT1 / FORS2	1.51	0.89

4. Results

With the model used, we can confirm the results for comet Hale-Bopp published before [2]. With the suggested reaction network we obtain acceptable fits of the C_3 and C_2 column density profiles with reasonable parent hydrocarbon production rates. However, for the other three comets studied, no acceptable fit of the observed column density profiles could be obtained. The reason for this failure is the electron impact reaction (1) included in the reaction network by [2]. This reaction becomes significant when the water density in the coma of a comet is sufficiently low. For Hale-Bopp at large heliocentric distances this occurs very close to the nucleus, at a distance not resolved by the observations. For the other comets, this distance is within the range of observed column densities, and the reaction causes features in the modeled column densities of C_3 which are not in agreement with our observations. Recent publications [3] on the reaction rate for reaction (1) suggest that this reaction is indeed overestimated in the reaction network presented by [2]. However, with a lower reaction rate for this reaction, still the observations cannot be reproduced.

Furthermore, our model shows no significant influence of the parent species C_2H_6 upon the column densities of C_2. Although C_2 is formed from C_2H_6, this process is too slow to significantly produce C_2 at projected nucleocentric distances covered by our observations.

Thus the by now assumed formation scheme for C_3 and C_2 fails to explain the data for comets other than Hale-Bopp at large distances from the Sun.

5. Other potential parent species

Since the by now suggested formation mechanism for cometary C_3 and C_2 fails to explain our observations, other parent species than C_3H_4, C_2H_2, and C_2H_6 should be taken into consideration. Candidates are C_4H_2, C_3H_2O, and HC_3N. For these species the production rates and reaction rates are poorly constrained. Although further studies are required, by now it was not possible to reproduce the C_3 and C_2 observations simultaneously with any of these potential parent species.

6. Summary and Conclusions

We present a model for chemical processes in the cometary coma. The model was used to study the formation of C_3 and C_2 in the coma. For this purpose, we compared the model outputs to observations of C_3 and C_2 in four different comets. It could be shown that the model can reproduce results published elsewhere for comet Hale-Bopp, but it fails to reproduce the observations in other comets. This is caused by an overestimated electron impact reaction rate. With a lower rate for this reaction it is still not possible to reproduce the observations. Therefore, the formation of C_3 and C_2 in the coma of comets remains unexplained by now. Other parent species should be taken into consideration in future work to explain the formation of C_3 and C_2.

References

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