Chapter 22

Results and outlook

22.1 Summary of the results on the formation of C_2 and C_3

The aim of this study was to analyse the formation of C_2 and C_3 in a cometary coma at large heliocentric distances. For this purpose a chemical model for the formation of C_2 and C_3 from C_2H_2, C_2H_6 and C_3H_4 is presented, based on the observations of C_2 and C_3 column densities obtained during the optical longterm-monitoring program of comet Hale-Bopp [Rauer *et al.*, 2002]. The chemical model was developed using and extending the ComChem model by Huebener and Boice (Giguere and Huebner [1978], Boice *et al.* [1986, 1998], Huebner *et al.* [1987], Schmidt *et al.* [1988]).
The chemical model contains the most complete reaction network used until today to study the formation processes of the C_2 and C_3 radicals in a cometary coma. At the heliocentric distance range $r_h > 2.86$ AU covered in this study the formation of the C_2 radical is dominated by photodissociation and electron impact dissociation of C_2H_2. C_2H_6 has been identified as a minor parent of C_2.
The observed C_3 column density profiles can be explained by C_3H_4 as the parent molecule. However it is not possible to distinguish between the isomeric forms allene and propyne. Both isomers can form C_3 via the same intermediate product C_3H_2. C_3 is formed by electron impact and photodissociation reactions. Although the reaction network for the formation of C_3 shows a good agreement with the observed C_3 column density profiles it is still preliminary. For the photodissociation of C_3H_2 and C_3 reaction rates had to be derived in this work from fits to the observed data. The reaction pathways for the electron impact dissociation of allene and propyne are still unknown. For this reason a hypothetical reaction is included describing the direct dissociation of C_3H_4 by electron impact to form C_3. Due to all these uncertainties, the results for C_3 and its parent C_3H_4 have not the same quality as the results for C_2 and its parents C_2H_2 and C_2H_6. Nevertheless the C_3 formation model presented here is the first model to include a detailed photochemical reaction scheme, in addition to a simplified electron impact reaction, linking allene and propyne with C_3.
The chemical model allows to derive the abundances for C_2H_2, C_2H_6 and C_3H_4 using the

observations of the C_2 and C_3 radicals in the optical wavelengths range. The derived production rates for C_2H_2 and C_2H_6 are in very good agreement with values obtained by Dello Russo *et al.* [2001] from infrared observations at heliocentric distance $r_h \leq 3$ AU. The derived C_3H_4 production rate is consistent with an upper limit for propyne derived by Crovisier [2000] near perihelion. The values presented here extend the heliocentric distance range over which hydrocarbons can be studied in the coma of comet Hale-Bopp to almost 5AU, a range presently not accessible by infrared observations.

The abundance ratios of C_2H_2, C_2H_6 and C_3H_4 relative to water and carbon monoxide have been studied for large heliocentric distances. They show that the abundance of C_2H_2 relative to carbon monoxide is comparable to interstellar molecular clouds, while the C_2H_6 to CO ratio indicates an overabundance in comet Hale-Bopp. Furthermore the abundance ratios show that all three molecules have a high volatility. This is especially noteworthy for C_3H_4. Little is known about the volatility of allene or propyne, but the values for the latent heat of this molecules indicate a high volatility. The almost constant ratio of C_3H_4 to CO is therefore an additional indicator for the identification of allene or propyne as the likely C_3 parents.

It was possible for the first time to derive abundance ratios of C_3H_4 to C_2H_2 and C_2H_6. The values have a large error, because they include all uncertainties in the modeling of the C_2 and C_3 formation. Nevertheless they are an important indicator showing that C_3H_4 is underabundant by a factor of about 2 compared to C_2H_2 and C_2H_6.

Using the results from the modeling an attempt was made to derive indications for the formation region of comet Hale-Bopp. The idea was primarily to show how abundance ratios for C_2H_2, C_2H_6 and C_3H_4 determined with the model for the formation of C_2 and C_3 allows to derive conclusions about the condition during the formation of the nucleus of comet Hale-Bopp. A distance range of approximately 10 – 30 AU from the earlier Sun has been proposed as a possible formation region. However, one has to be very careful with this estimate, as it is based on a number of assumptions.

22.2 Outlook

It has been stated various times in this work, that the results are affected by a number of uncertainties. One of the main concerns are the uncertainties on the various reaction rates. Unfortunately, even for well-known species not all of the required rates are known. The situation is especially difficult for the electron impact reactions of C_2H_6 and C_3H_4. For these molecules even the reaction pathways are unknown. For C_2H_2 only very limited information is available based mainly on theoretical work. All this can easily lead to large discrepancies in determining abundances for the parent molecules. The good agreement of the production rates for C_2H_2 and C_2H_6 obtained in this work with the results by Dello Russo *et al.* [2001] indicates, that the effects of the uncertainties on the results in this case are small and well within the errors given for the production rates. For C_3H_4 there is no direct comparison available, therefore the results have be be viewed with more caution.

For future work it would be highly valuable to know more photodissociation rate coefficients, electron impact dissociation rates and all the relevant branching ratios to be able to minimize the error on the abundance of the parent molecules. Hopefully some of the missing information can be supplied from laboratory measurements in the near future. The reaction network can be updated as soon as new data becomes available. It would be useful to engage collaborations with laboratory groups to obtain reaction rates under the condition needed for cometary application, especially at low temperatures.

The results obtained in this work are strictly valid only for comet Hale-Bopp and only for the heliocentric distance range covered in this study. The fact that the derived production rates for C_2H_2 and C_2H_6 are consistent with direct measurements at smaller heliocentric distances, indicates that the model might be valid for this distance range as well. To prove this assumption, the next step in the verification of the formation model of C_2 and C_3 has to be an analysis of the data obtained near perihelion. Comet Hale-Bopp was a very active comet. Some of the assumptions used in this study may not hold for small heliocentric distances. For example the inner coma of comet Hale-Bopp was most likely optical thick at perihelion. The densities in the coma are much higher at perihelion, therefore the probability of collisions and molecule-molecule reaction is increased. This all can lead to some changes in the reaction network for the formation of C_2 and C_3.

Even more crucial is a verification using data of different comets. Hale-Bopp was an exceptionally active comet. Therefore it has to be verified that results obtained for the coma of this comet are applicable to more typical comets. At the distance range covered in this work the activity of comet Hale-Bopp was comparable to the activity of 'normal' comets near their perihelion. If the model is able to show equally good results for different and less active comets, it can be assumed as a valid general model for the formation of C_2 and C_3 in a cometary coma.

Until now production rates for C_2H_2 and C_2H_6 could only be derived from infrared observations of bright comets. They were limited to small heliocentric distances. C_3H_4 as the likely parent of C_3 has not been detected in a cometary coma up to now. On the other hand C_2 and C_3 have been observed in many comets and over a wide range of heliocentric distances. The model can be used to obtain the abundances for C_2H_2, C_2H_6 and C_3H_4 over the same range of heliocentric distances, after it has been verified. It will allow a systematic study of the hydrocarbon inventory of cometary nuclei including short period comets which are usually too faint for a direct detection of C_2H_2 or C_2H_6. Of special interest for this kind of study would be carbon-chain depleted comets. Using this model it might be possible to determine whether these comets are depleted in C_2H_2 and C_2H_6 or only in one of these molecules. If they are depleted in only one of the two parent molecules of C_2, this would be an indication for a different formation region of this type of comets compared to the 'normal' comets.

The final verification for this model will be obtained from future in-situ measurements of the coma and nucleus composition. Especially the Rosetta mission to comet Wirtanen with its spectrometer and the surface elements will provide ground truth for models like the one presented here. However the work presented here is a proof of concept, for the fact that optical spectroscopy of comets can provide valuable information on the cometary nucleus, its formation and therefore can give clues on the conditions in the early solar system.

One of the joys of science is turning data into knowledge

Marc Rayman, Deep Space 1 Project Manager