

Chapter 21

Clues for the origin of comet Hale-Bopp

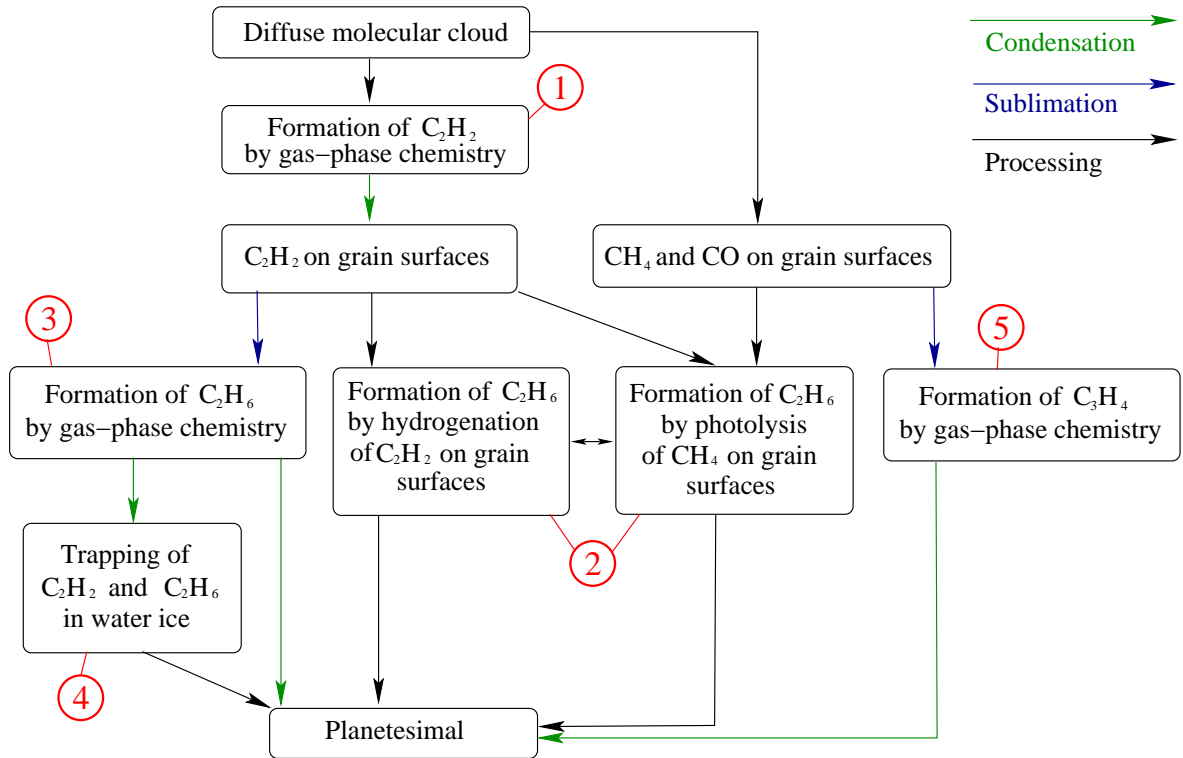
To study the formation processes of comets there are three main sources of information: laboratory studies of analog material, numerical simulations of the chemistry in the protoplanetary disk and the prenatal molecular cloud, and observations of dense molecular clouds in star forming regions.

Laboratory studies of cometary analog material can provide information on the processes in interstellar materials under the conditions of the early solar system or its precursor states as dense and diffuse molecular clouds. Three recent relevant examples for laboratory studies are Moore and Hudson [1998], Notesco *et al.* [1997] and Hiraoka *et al.* [2000]. Moore and Hudson have irradiated water ice mixtures containing (small) hydrocarbons to study the formation of larger hydrocarbons and other molecules. Hiraoka *et al.* [2000] studied the hydrogenation of C_2H_2 , C_2H_4 and C_2H_6 at cryogenic temperatures. Notesco *et al.* [1997] studied the temperature dependence of the efficiency of the trapping of various species in water ice. An overview of the laboratory work done in this field is given by Cottin *et al.* [1999] in their review.

A recent example for numerical simulations is the work by Aikawa and Herbst [1999]; Aikawa *et al.* [1999] and by Gail [2002]. They simulated the molecular abundances in protoplanetary disks under a number of different conditions.

Finally the observation of interstellar material and especially dense molecular clouds around protostellar objects and young stars, can give insights on the conditions leading to the formation of our solar system. Irvine [1999] presented a review of the composition of interstellar clouds. Unfortunately the abundances for C_2H_2 and C_2H_6 given in this paper are only upper limits. Boudin *et al.* [1998] presented a combined laboratory and observational study on the abundance of various molecules in interstellar ices. Lhuis and van Dishoeck [2000] reported the observation of gas-phase C_2H_2 toward a number of massive young stellar objects.

Figure 21.1 is an extremely simplified view of the processes leading to the formation of C_2H_2 and C_2H_6 until it is finally incorporated into planetesimals and cometary nuclei. It is summary of the results from the publications listed above.

Figure 21.1: Scenarios for the formation of C_2H_2 and C_2H_6

- 1 Energy source is UV radiation and galactic cosmic rays
- 2 Most efficient for $T < 10 - 50$ K
- 3 Energetically possible only for high temperatures
- 4 High ethane abundance only for $T > 65$ K
- 5 Most efficient inside the sublimation front of CH_4 and CO ($T > 25$ K)

C_2H_2 and C_2H_6 ice have not yet been detected in the interstellar medium. The problem in observing solid C_2H_2 and C_2H_6 ices is a blend with the signature of H_2O ice which masks the C_2H_6 and C_2H_2 bands [Boudin *et al.*, 1998]. Only upper limits for their abundance can be derived. Of course the ratio of the upper limits for $Q(C_2H_2)$ and $Q(C_2H_6)$ is not directly comparable with the abundance ratio of $Q(C_2H_2)$ to $Q(C_2H_6)$ as derived in this study, although this has been done in the literature. A better approach is to compare the abundance ratios of C_2H_2 and C_2H_6 relative to CO with the upper limits derived for the interstellar medium.

In molecular clouds C_2H_2 is formed by gas-phase ion-molecule reactions. Lahuis and van Dishoeck [2000] have reported the observation of C_2H_2 in the gas-phase toward a number of massive young stellar objects. There are no observations of solid C_2H_2 until today. Strong evidence for the presence of C_2H_2 ice on grain surfaces is the enhanced abundance of C_2H_2 in the gas-phase towards the warmer regions of dense molecular clouds (Lahuis and van Dishoeck [2000]). This C_2H_2 is most probably formed by sublimation of ice from grain surfaces. Lahuis and van Dishoeck derived under this assumption an abundance ratio of

C_2H_2 to water ice of $\sim (1 - 5) 10^{-3}$. This is in rough agreement with the values of $(6.23 \pm 0.42) 10^{-3}$ obtained for Hale-Bopp at perihelion by Dello Russo *et al.* [2001].

In section 20.1 an abundance ratio of C_2H_2 relative to CO of $Q(\text{C}_2\text{H}_2)/Q(\text{CO}) = 0.01 \pm 0.004$ was determined. This is in agreement with the upper limit for the dense molecular cloud NGC 7538:IRS9 as determined by Boudin *et al.* [1998] (see section 17).

For the abundance ratio of C_2H_6 relative to CO a value of $Q(\text{C}_2\text{H}_6)/Q(\text{CO}) = 0.03 \pm 0.01$ was determined in section 20.1. This is about a magnitude larger than the value of $Q(\text{C}_2\text{H}_6)/Q(\text{CO}) \leq 0.002$ as determined by Boudin *et al.* [1998] for NGC 7538:IRS9 (see above). This indicates that C_2H_6 is indeed overabundant in comet Hale-Bopp compared to a dense molecular cloud which is similar to the precursor of our solar system [Boudin *et al.*, 1998]. While the abundance ratio of C_2H_2 to CO (and C_2H_2 to H_2O) is in agreement with an pristine origin of this molecule, the abundance ratio of C_2H_6 to CO indicates a formation of C_2H_6 during the early stage of our solar system.

For the formation of C_2H_6 there are at least two possible scenarios. At low temperature $T=10-50$ K C_2H_6 can not be formed by gas-phase chemistry because all relevant reactions are endothermic [Herbst, 1983]. However in this temperature range grain surface chemistry is very efficient. Moore and Hudson [1998] and Cottin *et al.* [1999] showed that ices consisting of mixtures of $\text{H}_2\text{O}+\text{C}_2\text{H}_2$ and $\text{H}_2\text{O}+\text{CH}_4+\text{C}_2\text{H}_2$ can produce C_2H_6 efficiently when irradiated with UV or gamma rays. According to Hiraoka *et al.* [2000] the yield of C_2H_6 is largely enhanced at temperatures below $T < 35$ K and the process is most efficient at temperatures of about 10 K (see Figure 21.2). Moore and Hudson noted also that in none of their experiments C_2H_2 was formed in a significant amount. This is consistent with a pristine origin of C_2H_2 . Furthermore in these experiments only trace amounts of C_2H_4 are detected. While C_2H_4 is formed by hydrogenation of C_2H_2 it is even more efficient in adsorbing additional H atoms than C_2H_2 . Therefore C_2H_4 is only an intermediate step in the formation of C_2H_6 from C_2H_2 . This is consistent with the fact that no C_2H_4 has been detected in comets up to now. The formation of C_2H_6 by hydrogenation of C_2H_2 on grain surfaces could be a possible explanation for the high abundance of C_2H_6 relative to C_2H_2 as observed in comet Hale-Bopp. While C_2H_6 can not be formed by gas-phase chemistry at low temperature, Notesco *et al.* [1997] noted that it can be formed by CH_4 photolysis under high temperature ($T \gtrsim 100$ K), high density conditions (see Figure 21.2). These conditions can be found in the Jupiter region of the protoplanetary disk. The overabundance of C_2H_6 can be explained by a very efficient trapping of C_2H_6 in water ice for temperatures of 64 – 66 K (see Figure 21.2). An open question in this scenario is the achievable C_2H_6 to CH_4 ratio. While Bar-Nun [1979] found a ratio $> 1.5 10^{-2}$, Mumma *et al.* [1996] (and references therein) state that the C_2H_6 to CH_4 ratio is $< 10^{-3}$. Assuming this low ratio the trapping of C_2H_6 in water ice would not be efficient enough to explain the overabundance of C_2H_6 . Further laboratory and theoretical work is urgently needed on this topic. Notesco *et al.* [1997] predict also the formation of C_3H_8 with an abundance comparable to C_2H_6 .

An important clue for the formation location of comet Hale-Bopp may be derived from the abundance of C_3H_4 , which has been estimated for the first time in this work. Aikawa *et al.* [1999] showed in their numerical simulations of the evolution of molecular abundances in protoplanetary disks that C_3H_4 is readily formed by gas-phase chemistry from CH_4 and CO

(see Figure 21.2). The relative yield is largely increased in the inner regions of the disks for $r_h \leq 20$ AU. In this region the temperatures are high enough to sublime large amounts of CH_4 and CO from the icy mantles of dust grains. Outside of the sublimation front of CH_4 and CO the C_3H_4 abundance decrease rapidly with heliocentric distance.

In order to put limits on the formation region of comet Hale-Bopp all the pieces of information need to be combined to form a coherent picture. In order to do so the key points should be repeated:

1. The abundance of C_2H_2 relative to H_2O and to CO is in agreement with values for dense molecular clouds. Therefore it is well possible that the C_2H_2 observed in comet Hale-Bopp is of pristine origin.
2. There are no observations in molecular clouds of C_2H_6 either as solid ice or in the gas-phase. Therefore it is not possible to derive a 'typical' abundance ratio of C_2H_2 to C_2H_6 for this regions. However, the abundance of C_2H_6 relative to CO is by an order of magnitude larger than the the upper limit derived for dense molecular clouds. As stated above the C_2H_2 to CO ratio observed in the same region is in agreement with the value derived for comet Hale-Bopp. Based on this evidence C_2H_6 seems indeed to be overabundant in comet Hale-Bopp.
3. A formation of C_2H_6 by gas-phase chemistry is possible only for a high temperature, high density regime, because the reactions are endothermic. The overabundance of C_2H_6 can be explained in this scenario by trapping in water ice at temperature $T > 65\text{K}$.
4. A formation of C_2H_6 by grain surface chemistry is efficient for a temperature range of $T \sim 10\text{--}50$ K.
5. C_3H_4 is slightly less abundant than C_2H_2 and C_2H_6 .
6. The formation of C_3H_4 is possible by gas-phase chemistry from CH_4 and CO . The formation is most efficient inside the sublimation front of CH_4 and CO , e.g. in a distance from the early Sun where CH_4 and CO can sublime from the grain surfaces. Here the abundance of these molecules in the gas-phase is high enough to produce C_3H_4 with the observed abundance ratio.

Figure 21.2 gives a graphical summary of the formation processes discussed in this chapter. The figure shows the different formation scenarios for C_2H_2 , C_2H_6 and C_3H_4 versus the temperature. Green shaded areas denote formation in the gas-phase, blue areas formation on grain surfaces (light blue marks less efficient processes). The pink box shows an enrichment by trapping in ice.

In this work an abundance ratio of $Q(\text{C}_2\text{H}_6)/Q(\text{C}_2\text{H}_2)=2.3\pm 1.0$ has been derived (see section 20.2 and point 2 in the list above). C_2H_6 is clearly overabundant, which indicates an efficient formation process. Based in Figure 21.2 this would be possible for temperatures higher than 100K by gas-phase chemistry. This hot time period has to be followed by a cooler time period

with $T \approx 65\text{K}$, where efficient trapping of C_2H_6 in water ices would lead to the observed overabundance of C_2H_6 . This would put the formation region of comet Hale-Bopp in the Jupiter region at $r_h \approx 5\text{--}10\text{ AU}$ [Notesco *et al.*, 1997]. There are no observations of C_2H_6 in the gas-phase in the interstellar medium or in dense molecular clouds as might be expected for a formation by gas-phase chemistry. Although the reason for this might be the observational difficulties to detect the C_2H_6 emission bands.

The second possibility for the formation of C_2H_6 is by grain surface chemistry at temperatures below 50K . As discussed before the efficiency of the processes is greatly enhanced below 35K (indicated by the light and dark blue areas in Figure 21.2). Based on the simulations by Aikawa *et al.* [1999] these conditions are best matched in the Uranus and Neptune region at $r_h \geq 10\text{--}20\text{ AU}$. Further out the H atom density decreases rapidly, further inward the temperature increases leading to a reduced efficiency of the grain surface chemistry. Hydrogenation of C_2H_2 on grain surfaces is also favored by Gail [2002] as the mechanism explaining the high abundance of C_2H_6 in comet Hale-Bopp.

Based only on the abundance of C_2H_6 relative to C_2H_2 it is difficult to decide between the two formation scenarios for C_2H_6 and therefore between the two formation regions for the nucleus of comet Hale-Bopp. In this work however the abundance ratios of C_3H_4 relative to C_2H_2 and C_2H_6 could be estimated for the first time in a cometary coma. With this additional information the second scenario seems more likely. As discussed in section 20.2 values of $Q(\text{C}_3\text{H}_4)/Q(\text{C}_2\text{H}_2)=0.65\pm 0.37$ and $Q(\text{C}_3\text{H}_4)/Q(\text{C}_2\text{H}_6)=0.28\pm 0.18$ have been estimated. This indicates that C_3H_4 is slightly underabundant compared to C_2H_2 and C_2H_6 . However as discussed before the formation of C_3H_4 is more efficient for higher temperatures [Aikawa *et al.*, 1999]. If the nucleus of Hale-Bopp has been formed at temperatures of $T \geq 65\text{K}$ one would expect a high abundance of C_3H_4 . Furthermore in this scenario a formation of C_3H_8 would be expected. There has been no detection of C_3H_8 in comet Hale-Bopp or any other comet. It has been search for by Dello Russo *et al.* [2001] but they were unable to obtain an upper limit due to the observational difficulties in observing the possible C_3H_8 emission bands.

On the other hand the formation of C_2H_6 on grain surfaces for temperatures below 50K would be in agreement with the underabundance of C_3H_4 . In the temperature range between 25K and 50K the formation of C_3H_4 is possible but not very efficient, while the formation of C_2H_6 is possible and efficient. A lower limit for the temperature is in the case given by the sublimation temperature of CO at 24K . Considering that C_2H_6 is clearly overabundant in comet Hale-Bopp one might even consider an upper limit for the formation temperature at $T \approx 35\text{K}$, because as Hiraoka *et al.* [2000] have shown the efficiency for the formation on grain surfaces is largely increased below this temperature.

Therefore based on the abundance ratios of C_2H_2 , C_2H_6 and C_3H_4 derived in this work a temperature range of $T \approx 25\text{--}35\text{K}$ seems likely for the formation of the nucleus of comet Hale-Bopp. This range has been marked by a red dashed box in Figure 21.2. This temperature range is in agreement with the results by several other groups giving a formation temperature for comet Hale-Bopp of $T \sim 30\text{ K}$. These results are based on different observational methods, for example Crovisier [1997] based on H_2O ortho-para ratio, Krasnopolsky *et al.* [1997] based on the abundances of the noble gas Neon, Meier *et al.* [1998] based on the D/H ratio and

recently Stern *et al.* [2000] based on the detection of Argon in the coma of comet Hale-Bopp. Based on the results of this work and in combination with previous studies there are some indications for the assumption that comet Hale-Bopp has been formed in a range from 10 - 30 AU from the early Sun. This would put the birthplace of comet Hale-Bopp somewhere in the region between Saturn and Uranus. However the whole argumentation is based on a number of assumption and poorly known quantities. While a high degree of uncertainty remains, the discussion presented here shows, how the observations of radicals could be used to deduce informations about the nucleus and its formation.

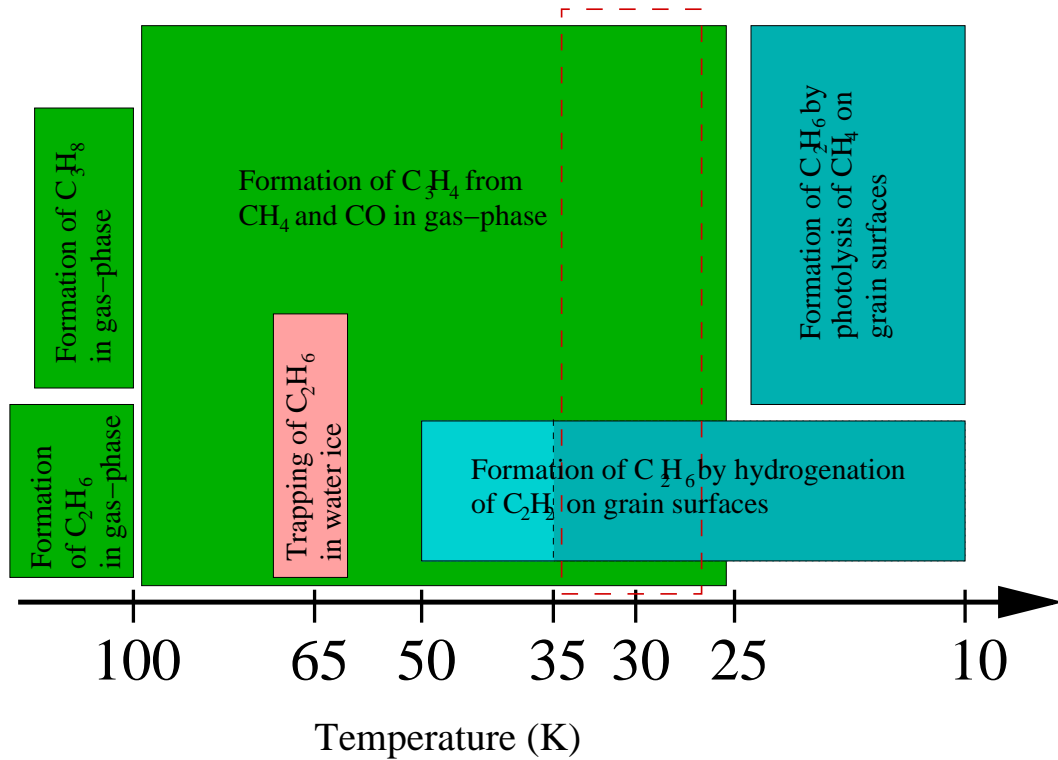


Figure 21.2: Temperature ranges for the formation processes of C_2H_2 , C_2H_6 and C_3H_4 . Green shaded areas denote formation in the gas-phase, blue areas formation on grain surfaces (light blue marks less efficient processes). The pink box shows an enrichment by trapping in ice.