Chapter 15

Abundance ratios of the C_2 and C_3 parent molecules

The following step-by-step example explains how the ComChem model is used to determine abundance ratios for C_2H_2, C_2H_6 and C_3H_4. The process is illustrated using data obtained on Dec. 19, 1997 at the ESO 1.5m telescope. This special night was chosen as an example, because the profiles have a good S/N ratio and the ESO 1.5m telescope does not suffer from the contamination seen in the spectra from the Danish 1.54m telescope. The heliocentric distance for the comet was 3.78AU. The same procedure was repeated for all other nights.

The basic principle as shown in figure 15.1 is straightforward. The ComChem model is used to generate model column density profiles for the C_2 and C_3 radical and these are compared to the measured profiles. The nucleus composition is changed until modeled and measured profiles agree. In practice this is done by two iterations, the first iteration for the C_3H_4 abundance and the second one for the C_2H_2 and C_2H_6 abundances. It is important to keep this order of iterations, because based on the chemistry discussed in sections 11.1 and 11.2 C_3H_4 is, via C_3, a grand-parent of C_2, while C_2H_2 and C_2H_6 have little or no influence on the C_3 formation.

The assumption that C_3H_4 is the sole dominant parent molecule of the C_3 radical in this model, while C_2 has two dominant parent molecules has an important consequence. The abundance of C_3H_4 can be derived directly by adjusting the model abundance until the model yields a C_3 profile which is in agreement with the measurements. This method is based on the assumption that the reaction rates mainly affect the shape of the profile, while the abundance of C_3H_4 yields a shift of the resulting profile. Therefore it is valid to derive the reaction rates for the photodissociation of C_3H_2 and C_3 and the production rate for C_3H_4 in separate fits. The effects of variations of the reactions rates in the C_3 chemistry on the resulting C_3H_4 abundance are discussed in details in section 19. In a sense the determination of C_3H_4 production rates used here is similar to using a multi-step Haser model.

For the C_2 parent molecules however the influence of the two parent molecules has to be separated. Fortunately, the spatial column density profiles provide enough information for this task. The profile yields the absolute numbers for the column densities and the shape e.g. the spatial distribution of the C_2 radical. The abundances of both parent molecules has

to be varied until the shape and the absolute column densities of the modeled profile fit to the observed profile. Basically this is a two dimensional parameter space which has to be scanned in a most effective way. The details of this technique are presented below in **Step 3**.
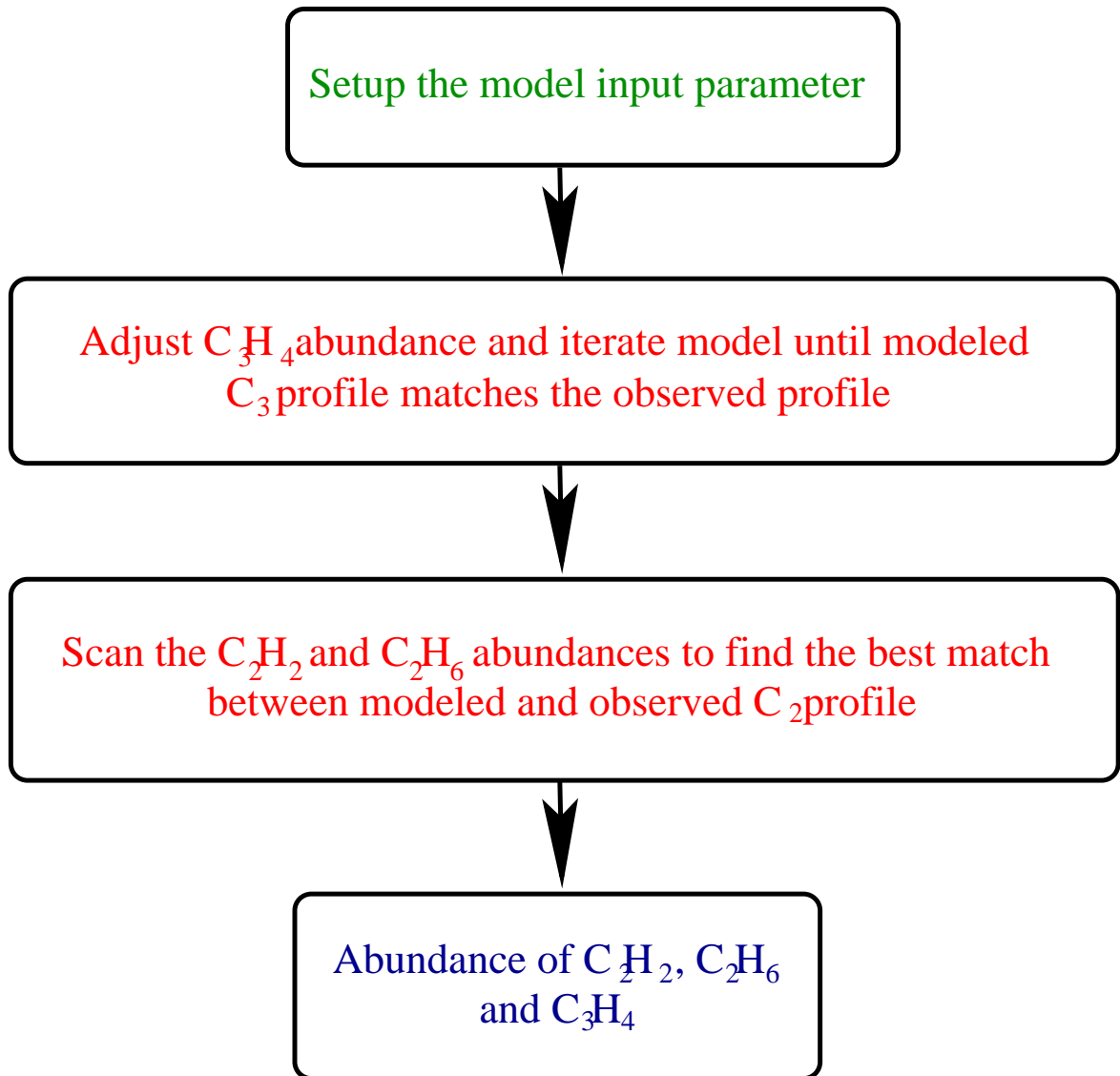

Figure 15.1: Flowchart for obtaining abundance ratios using the ComChem model

Step 1: Initial setup

To start the process, the observational data and a set of model input parameters are needed.
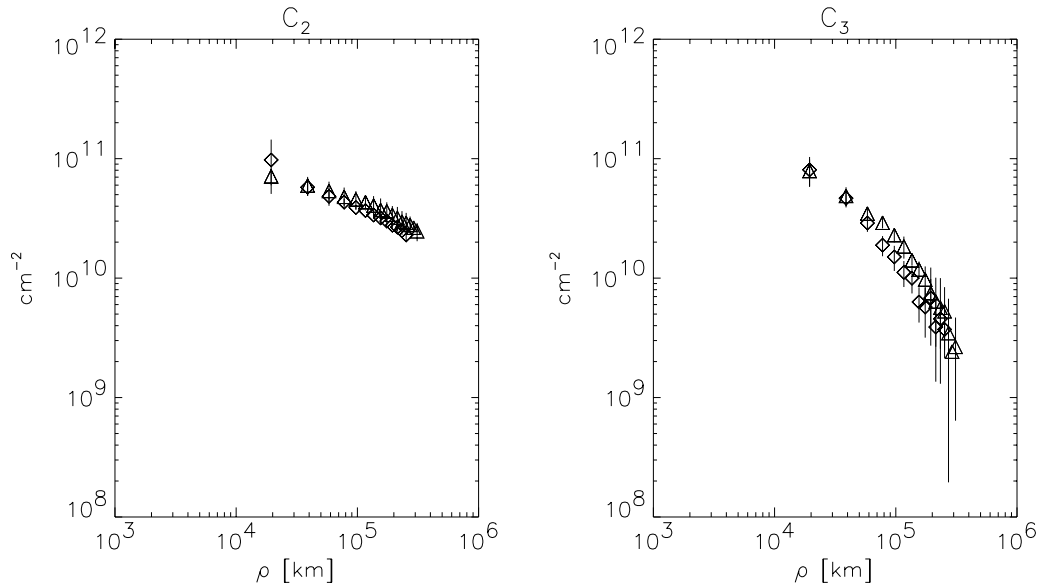

Figure 15.2: Spatial column density profiles for the C_2 and C_3 radicals (Diamonds sunward, triangles tailward profiles)

The spatial profiles for C_2 and C_3 for the example night are a mean of the profiles derived from 3 spectra each with an exposure time of 1200 sec (see section 8 for details). The spatial column density profiles are shown in figure 15.2. Triangles mark the tailward directions, diamonds the sunward directions. Within the error bars sunward and tailward profiles show good agreement.

The model parameters for the nucleus are set as described in section 14. The production rates for some of the species used in the modeling are given in table 15.1 (the complete set of production rates is given in table 14.1). As has been discussed before, the abundance of water is set to 1. and all other abundances are given relative to this value. The values are calculated for the heliocentric distance of the example night. The C_3H_4 abundance is a mixture of 50% allene and 50% propyne.

For the initial setup a mixing ratio of 1:3 was assumed for C_2H_2 : C_2H_6 . These values for C_2H_2, C_2H_6 and C_3H_4 are only start parameters. For the abundances of all other minor species see table 14.1.

Step 2: Getting the C_3H_4 abundance

Using the initial nucleus composition ComChem computes the profile shown as solid line in the left plot of figure 15.3. Compared to the observation this composition produces too much C_3. Using a fitting routine (Levenberg-Marquardt least-squares weighted fit [Stoer and Bulirsch, 1980]) the linear factor k between the observed column density N_{obs} and the model column density N_{mod} can be determined as

Total production	$3.3005 \cdot 10^{15} \text{cm}^{-2}\text{s}^{-1}$	
Molecule	Abundance	Q [s^{-1}]
H_2O	1.000000	$4.00000 \cdot 10^{28}$
CO_2	0.680000	$2.72000 \cdot 10^{28}$
CO	2.017500	$8.07000 \cdot 10^{28}$
C_3H_4	0.013472	$5.38880 \cdot 10^{26}$
C_2H_2	0.015787	$6.31480 \cdot 10^{26}$
C_2H_6	0.045412	$1.81648 \cdot 10^{27}$

Table 15.1: An extract of the composition (the complete composition is given in table 14.1)

$$N_{\text{obs}}(\rho) = k \cdot N_{\text{mod}}(\rho) \tag{15.1}$$

By adjusting the abundance of $A(C_3H_4)$ with the factor k

$$A'(C_3H_4) = k \cdot A \tag{15.2}$$

the abundance of C_3H_4 can be derived in an iterative process.

Figure 15.3 shows the iteration steps for the C_3H_4 profiles of the example night. A deviation of less than 5% between modeled and measured profiles is defined as the exit condition for the iteration. This condition is equivalent to $0.95 < k < 1.05$. The iteration process yields a production rate for C_3H_4 of $Q(C_3H_4) = 5.38880 \cdot 10^{26}$ s^{-1}. The resulting production rate is independent of the starting value for $Q(C_3H_4)$ as will be shown in section 19.
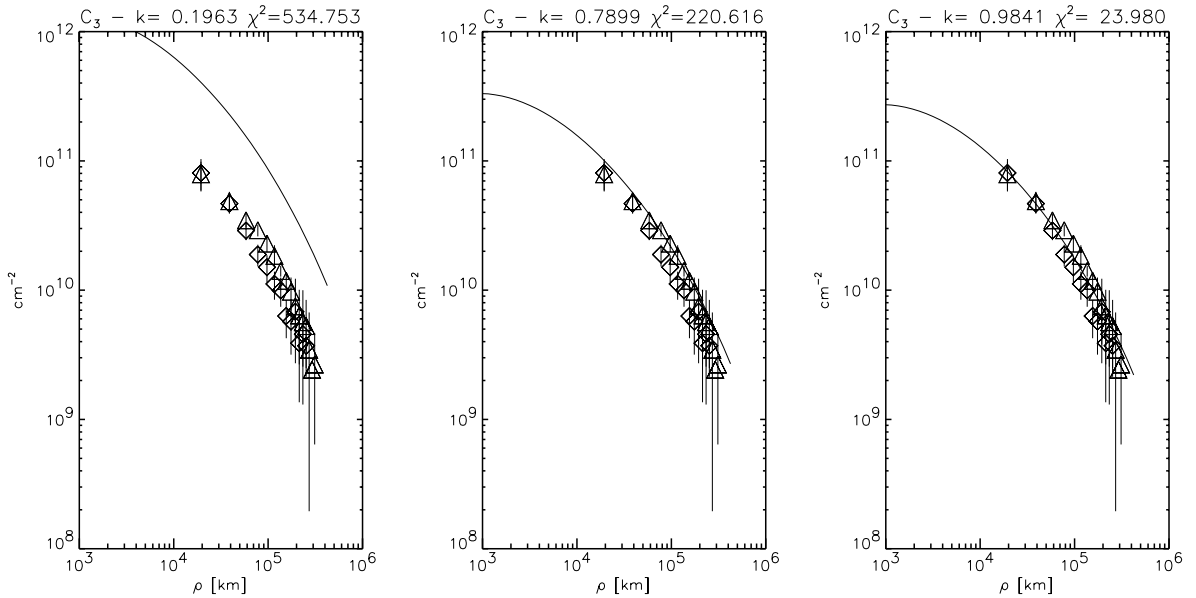
Figure 15.3: Weighted fit of the C_3 column density profile (From left to right results of Iteration 0,1,2)

Step 3: Getting the C_2H_2 and C_2H_6 abundance

Deriving the abundance of C_2H_2 and C_2H_6 using the ComChem model is difficult. Both parent molecules produce the C_2 radical via a number of intermediate steps as has been discussed in section 11.1.

Fortunately, the spatial column density profiles provide two informations. The modeled profiles can be fitted to match the absolute values for the column densities and to match the shape of the profiles. The fit to the absolute values is mainly determined by the abundance, whereas the fit to the shape is governed by the abundance ratio of $Q(C_2H_2):Q(C_2H_6)$. The parameter space is scanned in two subsequent steps and the task of the optimization is to minimize the factor k between modeled and measured profiles, as a measure for the match of the absolute values for the column densities, and to minimize the χ^2 error as a measure for the fit to the shape of the profile.

In the first step an initial abundance ratio is assumed and the absolute values of $Q(C_2H_2)$ and $Q(C_2H_6)$ are varied to find the best matching profile. This is shown by the green arrows in figure 15.4. The values of $Q(C_2H_2)$ and $Q(C_2H_6)$ and χ^2 for this fit are derived. This procedure is repeated for different ratios. This is shown by the red arrow in figure 15.4.

Figure 15.5 shows an example of the first step for a ratio of 1:1. For this ratio the models yields after 3 iterations a profile which fits within 5% to the column densities of the measured profile as well as to the shape. The point marked as number 3 on the plot has the minimal χ^2. This procedure is repeated for the other ratios. For all nights at least 7 ratios have been scanned: 1:0,1:1,1:2,1:3,1:5,1:10,0:1. The ratios 1:0 and 0:1 are cases where C_2H_2 or C_2H_6 respectively is the sole parent of C_2. These are the extreme cases. For some nights even more intermediate ratios have been used.

The result of the iteration for a fixed abundance ratio is not influenced by starting values (as is shown in section 19.3). The starting values for the first iteration for each night is based on a rough estimate of the production rates. To save time, the iteration for the next abundance ratio starts with the result from the previous iteration, e.g. the iteration for the 1:3 ratio starts with the result from the 1:1 ratio.

The iterative fit for each ratio results in a triplet $(Q(C_2H_2), Q(C_2H_6), \chi^2)$. These triplets are displayed in a two panel diagram as shown in figure 15.6.

The general question addressed here is, to determine the abundance of C_2H_2 and C_2H_6 for the heliocentric distance of the observation. This is equivalent to finding the global minimum of the error χ^2 of the fit in the parameter space spanned by $Q(C_2H_2)$ and $Q(C_2H_6)$. The technique (see Figure 15.4) used to scan the parameter space automatically yields the minimal χ^2 for each scan with a fixed ratio.

The upper part of figure 15.6 is a plot of the resulting normalized $\overline{\chi^2}$ versus $Q(C_2H_2):Q(C_2H_6)$ ratio for all scans. $\overline{\chi^2}$ is defined as

$$\overline{\chi^2} = \frac{\chi^2}{\min\left(\bigwedge_{\text{Ratios}} \chi^2\right)} \tag{15.3}$$

This normalization by the minimal χ^2 removes effects due to the different data quality of the observations and yields the relative quality of the fit within the night. The values for $\overline{\chi^2}$
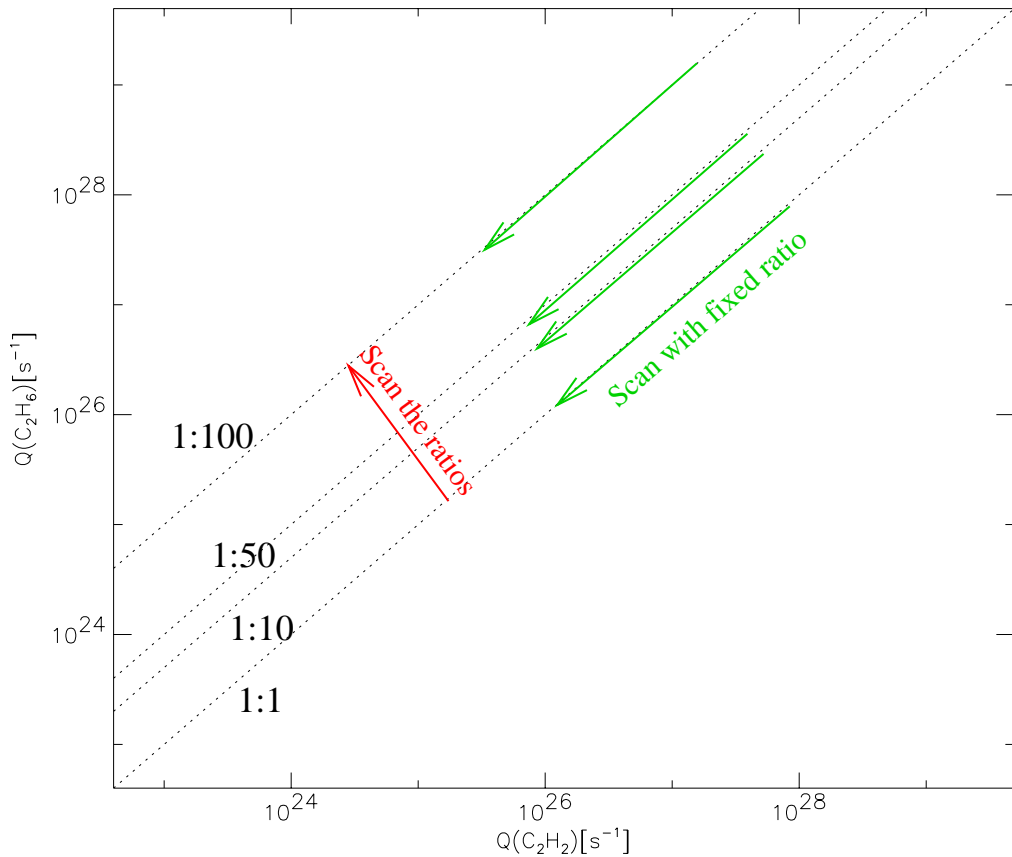
Figure 15.4: Scanning the $Q(C_2H_2)/Q(C_2H_6)$ parameter space. Each dotted lines mark the abundance ratios $Q(C_2H_2)/Q(C_2H_6)$ 1:1, 1:10, 1:50 and 1:100.

are to the first order comparable between different nights.

Examining the plot two things are obvious. $\overline{\chi^2}$ increases dramatically for high abundances of C_2H_6, which rules out the possibility that C_2H_6 is the sole parent of C_2. There is no distinct global minimum for $\overline{\chi^2}$. Nevertheless there is a well defined region where $\overline{\chi^2}$ is minimal. This region has been defined by an upper limit $\overline{\chi}_u$, with

$$\overline{\chi}_u = 1.1 \cdot \min\left(\overline{\chi^2}\right)$$

All profiles with a $\overline{\chi^2}$ within 10% of the minimal $\overline{\chi^2}$ are considered good fits. This region is called the confidence area. The 10% deviation was chosen because all small scale variations within the minimal area for $\overline{\chi^2}$ are smaller than this margin.

To determine $Q(C_2H_2)$ and $Q(C_2H_6)$ for the observed heliocentric distance the mean $\overline{Q(C_2H_2)}$ and $\overline{Q(C_2H_6)}$ of the production rates for C_2H_2 and C_2H_6 are obtained from all values within the confidence area. The lower part of figure 15.6 is a plot of $Q(C_2H_2)$ versus $Q(C_2H_6)$, with the $\overline{\chi^2}$ values indicated by the color of the crosses. The confidence area is marked as
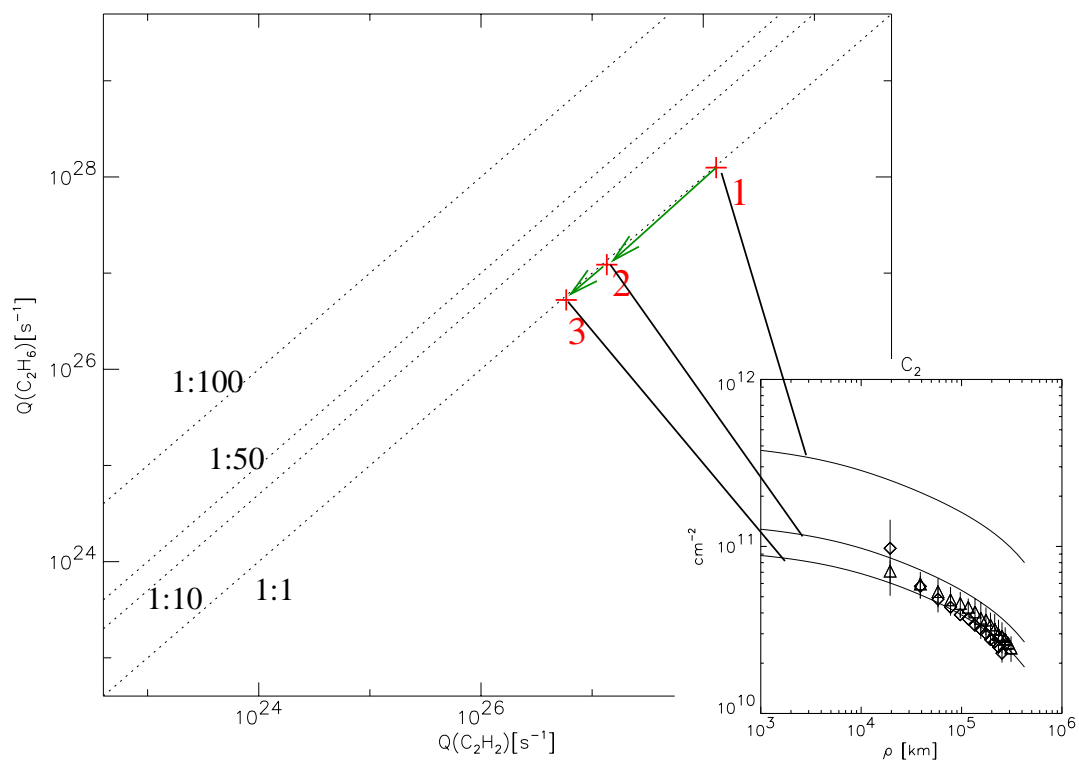
Figure 15.5: Iteration for the ratio $Q(C_2H_2)$:$Q(C_2H_6)$ 1:1

a rectangular box, as well as the resulting values for $\overline{Q(C_2H_2)}$ and $\overline{Q(C_2H_6)}$. The values for $Q(C_2H_2)=0$ and $Q(C_2H_6)=0$ are indicated by the crosses plotted directly on the axes.
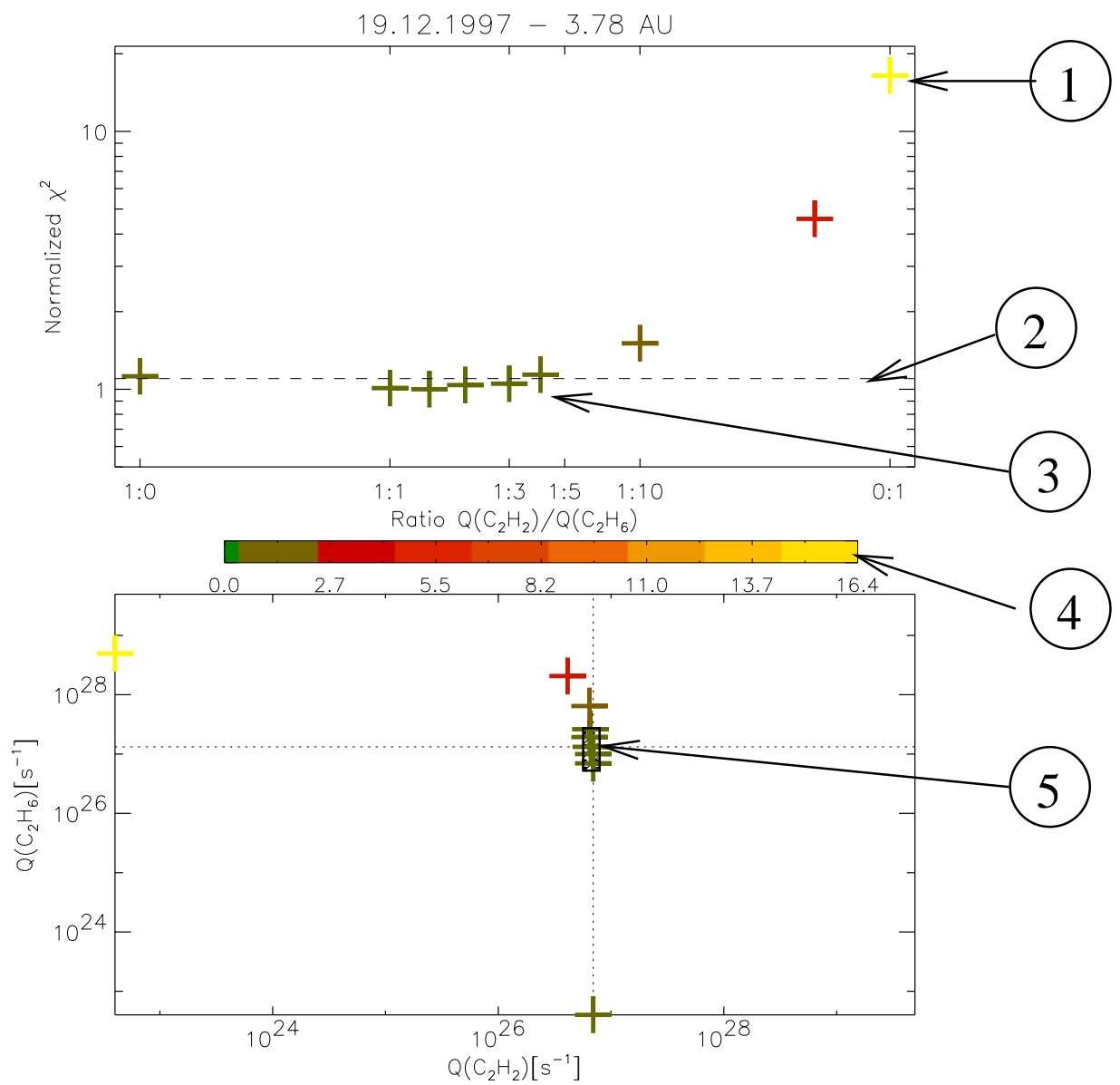
Figure 15.6: The results of the iterations are presented in this type of plot

1 Result outside the confidence area
2 upper limit $\overline{\chi}_u = 1.1 \cdot \min\left(\overline{\chi^2}\right)$ of the confidence area
3 Result inside the confidence area
4 Color coding of the χ values
5 Confidence area