# Chapter 16

# Determining the production rates for $C_2H_2$, $C_2H_6$ and $C_3H_4$

On the following pages the results for the studies with the ComChem model are shown. For each night the results are presented on two pages. The first page shows a table with the results of the iterations and a table with the resulting production rates as discussed in section 15. The second page shows the plots used to derive the production rates as described in Figure 15.6. It should be noted that these are only the results of the iterations, no intermediate steps are listed. As a general guideline, each row in the first table is calculated with about 10 iteration steps.

The table for the results of the iterations shows in each row the results of a complete iteration run for $C_2H_2$, $C_2H_6$ and $C_3H_4$ for a given ratio of $Q(C_2H_2)/Q(C_2H_6)$. The table lists in the first two columns the resulting abundance of $C_2H_2$ and $C_2H_6$ after the iteration, the third column gives the ratio of $Q(C_2H_2)/Q(C_2H_6)$ for convenience. The fourth column shows the resulting abundance of $C_3H_4$ after the iterations. The fifth and sixth column lists the resulting values for k and $\chi^2$ for $C_2$ as determined from the iterations. The seventh and eighth column gives the same information for $C_3$.

The second table for each night lists production rates for $C_2H_2$, $C_2H_6$ and $C_3H_4$, derived from the information given in the first table and from the plots as explained in section 15. The errors given for the production rates are only statistical errors derived from the standard deviation of the results for the iterations. They do not include errors introduced by uncertainties in the initial composition or the reaction rates. In order to discuss the uncertainties due to poorly known reaction rates it is first necessary to identify the main reactions. This is done in section 18. Based on this discussion the resulting errors are discussed in section 19. The final results for the productionrates with more meaningful errors are then given in section 17.

The profiles obtained in the night of Jan. 20, 1998 show a slight but distinct offset between the two spatial directions. This offset is observed in all species and is also seen in the dust (see also Weiler [2002]). The coma showed an unusually high asymmetry. Because the model assumes a symmetric coma the sunward and tailward profiles have been treated separately as a test. The results of this test will be discussed in section 19.

Figures 16.9 and 16.10 show the best fitting profiles for the $C_2$ and the $C_3$ profiles obtained in each night. These figures show that the ComChem model yields very good agreement with the observational data over the whole dataset.

# 17.8.1996

## Results of the iterations

| $A(C_2H_2)$ | $A(C_2H_6)$ | Ratio $\left(\frac{Q(C_2H_2)}{Q(C_2H_6)}\right)$ | $A(C_3H_4)$ | k $(C_2)$ | $\chi^2$ $(C_2)$ | k $(C_3)$ | $\chi^2$ $(C_3)$ |
|---|---|---|---|---|---|---|---|
| 0.017463 | 0.000000 | 1:0 | 0.009457 | 1.029 | 148.914 | 0.992 | 446.718 |
| 0.017463 | 0.017463 | 1:1 | 0.009457 | 1.027 | 132.725 | 1.004 | 448.306 |
| 0.017463 | 0.032299 | 1:2 | 0.009457 | 1.015 | 132.583 | 1.004 | 449.318 |
| 0.017463 | 0.052389 | 1:3 | 0.009457 | 1.013 | 132.883 | 1.005 | 449.319 |
| 0.017363 | 0.087315 | 1:5 | 0.009457 | 1.002 | 138.583 | 1.004 | 449.315 |
| 0.017323 | 0.174630 | 1:10 | 0.009457 | 1.021 | 142.583 | 1.004 | 449.320 |
| 0.000000 | 0.734055 | 0:1 | 0.009220 | 1.050 | 243.414 | 1.002 | 474.359 |

## Resulting production rates in $[10^{25}\ s^{-1}]$

| | | |
|---|---|---|
| $Q(C_2H_2)$ | = | 120.3±3.3 |
| $Q(C_2H_6)$ | = | 360.0±119.0 |
| $Q(C_3H_4)$ | = | 66.2±1. |

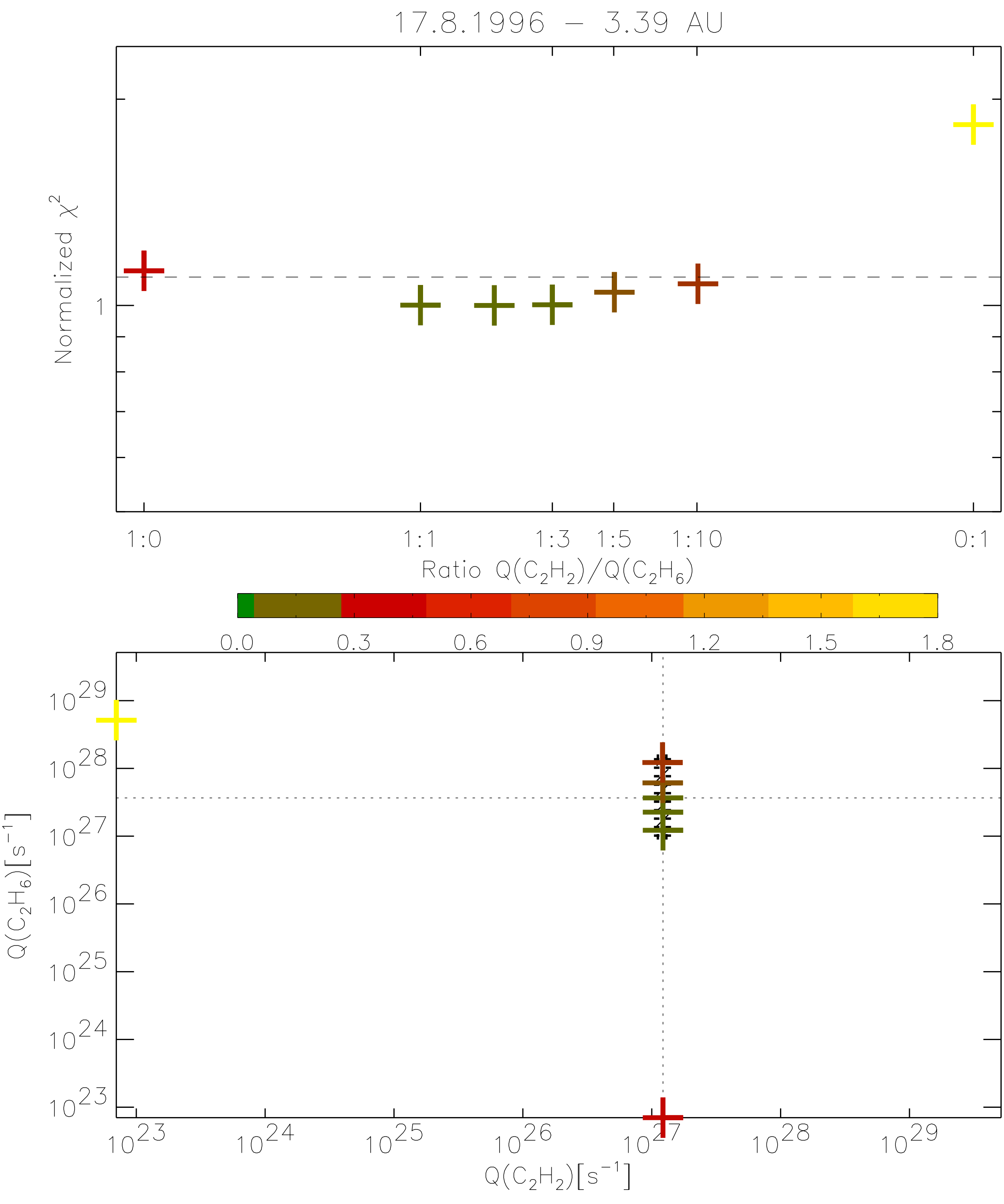


Figure 16.1: 17.8.1996

# 2.10.1996

## Results of the iterations

| $A(C_2H_2)$ | $A(C_2H_6)$ | Ratio $\left(\frac{Q(C_2H_2)}{Q(C_2H_6)}\right)$ | $A(C_3H_4)$ | k ($C_2$) | $\chi^2$ ($C_2$) | k ($C_3$) | $\chi^2$ ($C_3$) |
|---|---|---|---|---|---|---|---|
| 0.018258 | 0.000000 | 1:0 | 0.012390 | 1.054 | 0.251 | 1.056 | 0.250 |
| 0.016258 | 0.016258 | 1:1 | 0.012250 | 0.996 | 0.209 | 1.061 | 0.250 |
| 0.016258 | 0.032516 | 1:2 | 0.012250 | 0.982 | 0.207 | 1.061 | 0.251 |
| 0.016258 | 0.048774 | 1:3 | 0.012250 | 0.966 | 0.217 | 1.071 | 0.250 |
| 0.016258 | 0.081291 | 1:5 | 0.012250 | 0.973 | 0.231 | 1.071 | 0.250 |
| 0.016258 | 0.162580 | 1:10 | 0.012250 | 0.982 | 0.239 | 1.061 | 0.250 |
| 0.000000 | 0.723122 | 0:1 | 0.011250 | 0.982 | 10.113 | 1.022 | 0.291 |

## Resulting production rates in $[\mathbf{10^{25}\ s^{-1}}]$

$$Q(C_2H_2) = 260.1 \pm 2.4$$
$$Q(C_2H_6) = 520.0 \pm 50.1$$
$$Q(C_3H_4) = 20.2 \pm 1.$$

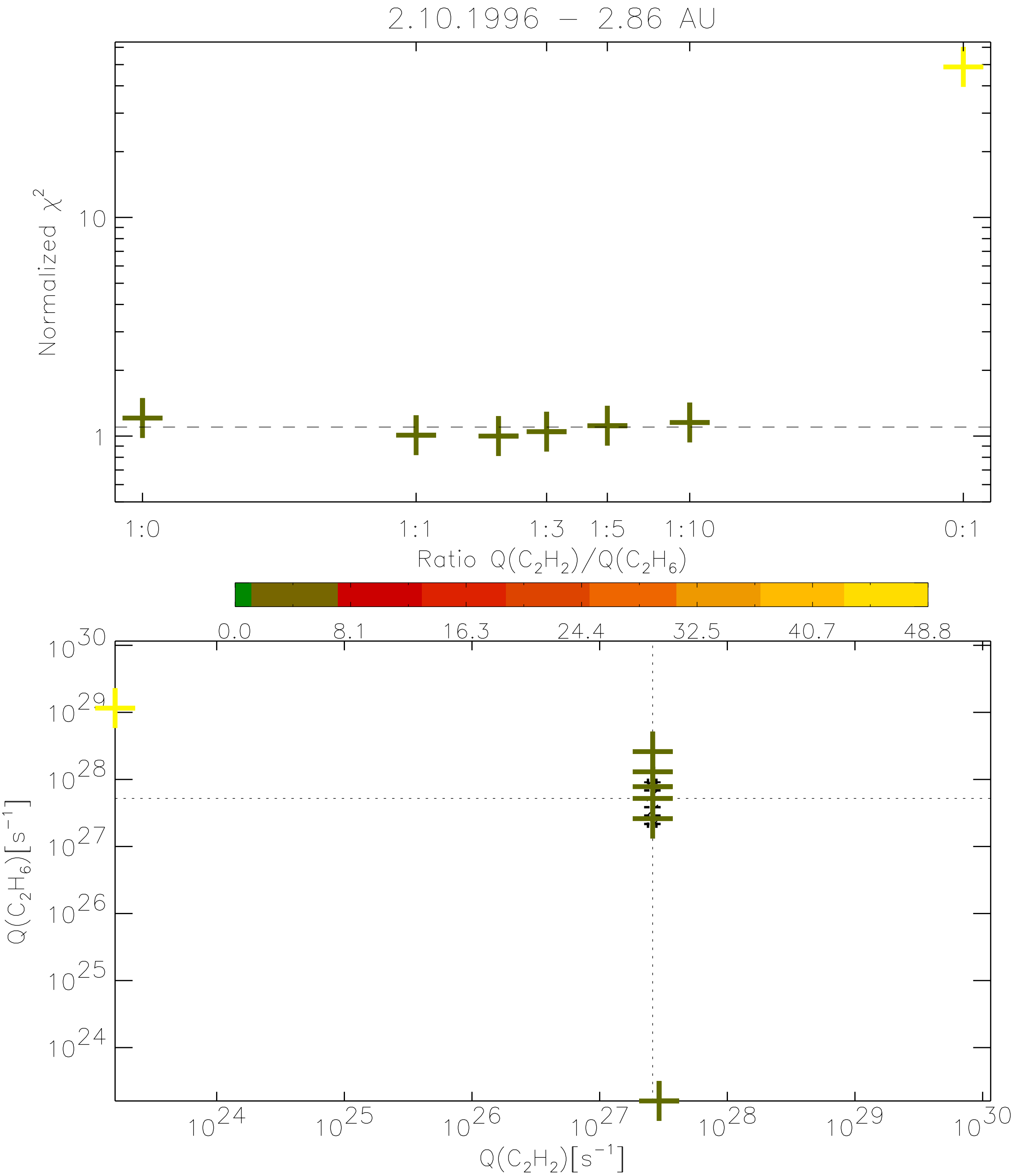


Figure 16.2: 2.10.1996

# 6.12.1997

## Results of the iterations

| $A(C_2H_2)$ | $A(C_2H_6)$ | Ratio $\left(\frac{Q(C_2H_2)}{Q(C_2H_6)}\right)$ | $A(C_3H_4)$ | k ($C_2$) | $\chi^2$ ($C_2$) | k ($C_3$) | $\chi^2$ ($C_3$) |
|---|---|---|---|---|---|---|---|
| 0.023362 | 0.000000 | 1:0 | 0.010771 | 1.011 | 11.298 | 1.000 | 70.630 |
| 0.022755 | 0.022755 | 1:1 | 0.010921 | 1.021 | 9.833 | 0.986 | 70.622 |
| 0.022755 | 0.044346 | 1:2 | 0.010921 | 1.006 | 9.594 | 0.986 | 70.615 |
| 0.022755 | 0.067646 | 1:3 | 0.010921 | 1.012 | 9.614 | 0.986 | 70.614 |
| 0.021617 | 0.108086 | 1:5 | 0.010812 | 0.993 | 10.232 | 0.995 | 70.604 |
| 0.019797 | 0.197968 | 1:10 | 0.010812 | 1.029 | 12.621 | 0.994 | 70.591 |
| 0.000000 | 0.970639 | 0:1 | 0.010718 | 0.963 | 36.009 | 1.004 | 70.628 |

## Resulting production rates in $[10^{25}\ s^{-1}]$

$$Q(C_2H_2) = 112.1 \pm 2.5$$

$$Q(C_2H_6) = 340.1 \pm 53.9$$

$$Q(C_3H_4) = 54.6 \pm 1.$$

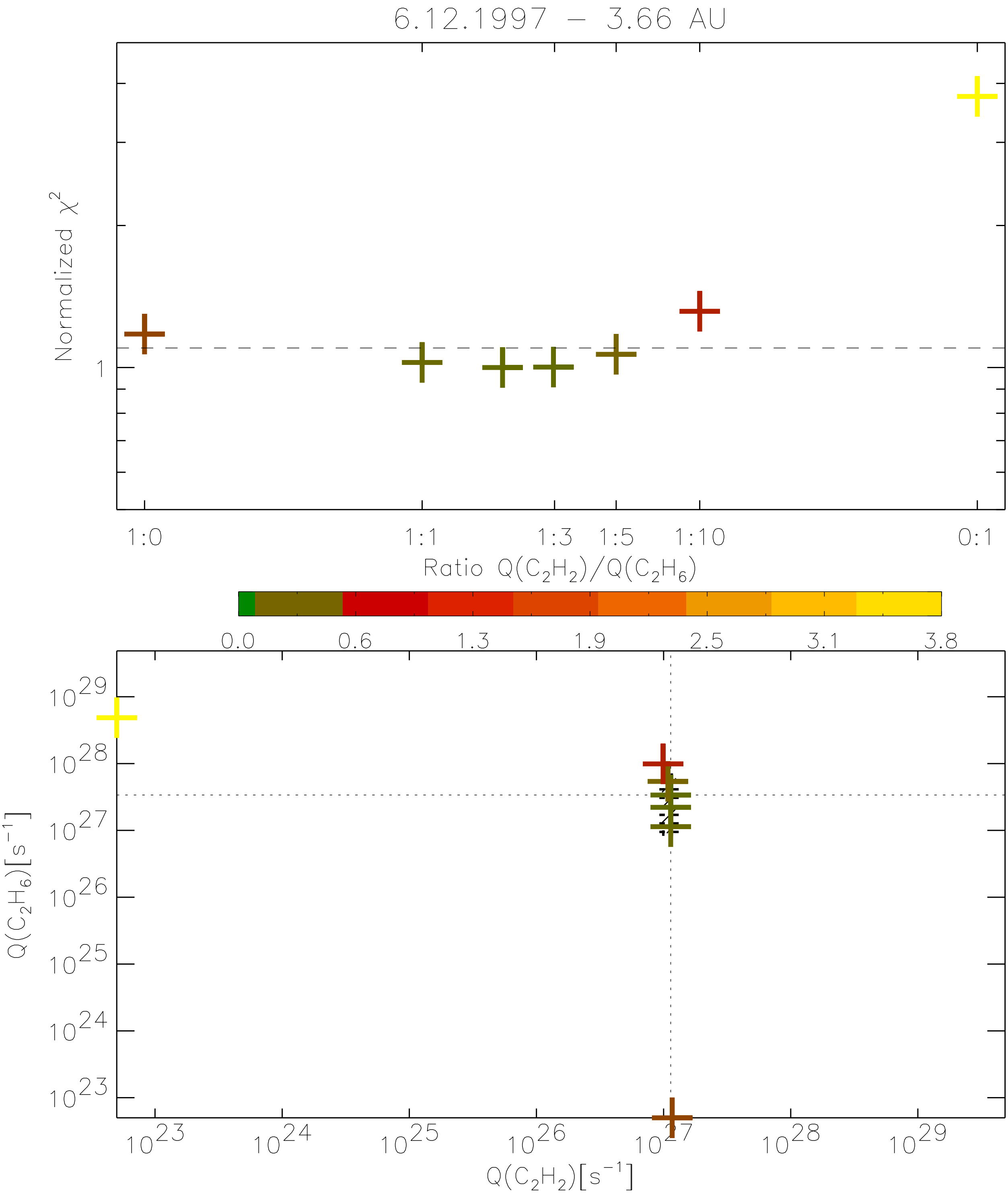


Figure 16.3: 6.12.1997

# 19.12.1997

## Results of the iterations

| $A(C_2H_2)$ | $A(C_2H_6)$ | Ratio $\left(\frac{Q(C_2H_2)}{Q(C_2H_6)}\right)$ | $A(C_3H_4)$ | k $(C_2)$ | $\chi^2$ $(C_2)$ | k $(C_3)$ | $\chi^2$ $(C_3)$ |
|---|---|---|---|---|---|---|---|
| 0.017362 | 0.000000 | 1:0 | 0.013974 | 1.011 | 1.091 | 1.003 | 24.033 |
| 0.017366 | 0.017366 | 1:1 | 0.013472 | 1.000 | 0.982 | 1.039 | 24.030 |
| 0.017366 | 0.024977 | 1:1.5 | 0.013472 | 1.000 | 0.972 | 1.039 | 24.030 |
| 0.016523 | 0.033047 | 1:2 | 0.014011 | 1.029 | 1.009 | 1.000 | 24.032 |
| 0.016110 | 0.048325 | 1:3 | 0.014011 | 1.039 | 1.021 | 0.999 | 24.031 |
| 0.016358 | 0.065432 | 1:4 | 0.014011 | 1.015 | 1.107 | 1.000 | 24.034 |
| 0.016110 | 0.161100 | 1:10 | 0.014011 | 0.964 | 1.465 | 1.001 | 24.042 |
| 0.010306 | 0.515277 | 1:50 | 0.014011 | 1.002 | 4.450 | 0.997 | 24.039 |
| 0.000000 | 1.236752 | 0:1 | 0.013710 | 1.022 | 15.981 | 1.010 | 24.066 |

## Resulting production rates in $[10^{25}\ s^{-1}]$

| | | |
|---|---|---|
| $Q(C_2H_2)$ | = | 69.5±3.6 |
| $Q(C_2H_6)$ | = | 132.3±40.1 |
| $Q(C_3H_4)$ | = | 55.8±1. |

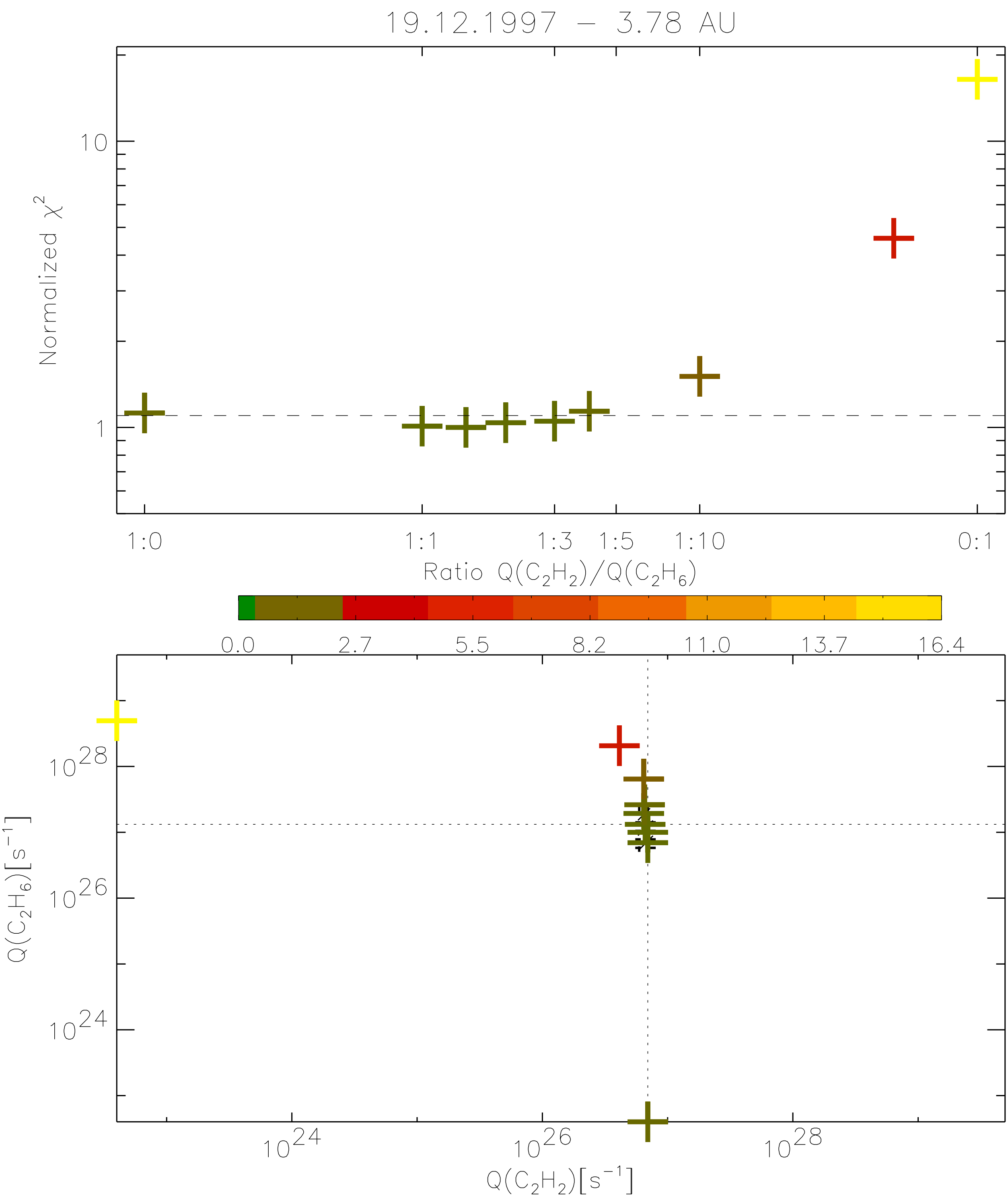


Figure 16.4: 19.12.1997

## 20.1.1998 - sunward profile

## Results of the iterations

| $A(C_2H_2)$ | $A(C_2H_6)$ | Ratio $\left(\frac{Q(C_2H_2)}{Q(C_2H_6)}\right)$ | $A(C_3H_4)$ | k ($C_2$) | $\chi^2$ ($C_2$) | k ($C_3$) | $\chi^2$ ($C_3$) |
|---|---|---|---|---|---|---|---|
| 0.036671 | 0.000000 | 1:0 | 0.052985 | 1.014 | 1.734 | 1.000 | 18.382 |
| 0.036671 | 0.036671 | 1:1 | 0.052985 | 1.003 | 1.531 | 1.000 | 18.395 |
| 0.036671 | 0.073342 | 1:2 | 0.052985 | 0.992 | 1.581 | 1.000 | 18.408 |
| 0.035143 | 0.099846 | 1:3 | 0.052985 | 1.016 | 1.624 | 0.998 | 18.452 |
| 0.036548 | 0.182741 | 1:5 | 0.052985 | 0.955 | 1.707 | 1.000 | 18.837 |
| 0.034148 | 0.341481 | 1:10 | 0.052985 | 0.985 | 2.244 | 1.012 | 18.634 |
| 0.000000 | 2.677742 | 0:1 | 0.052985 | 1.042 | 20.064 | 1.002 | 21.368 |

## Resulting production rates in [$10^{25}$ $s^{-1}$]

$$Q(C_2H_2) = 90.4 \pm 2.4$$
$$Q(C_2H_6) = 183.3 \pm 43.2$$
$$Q(C_3H_4) = 132.4 \pm 1.$$

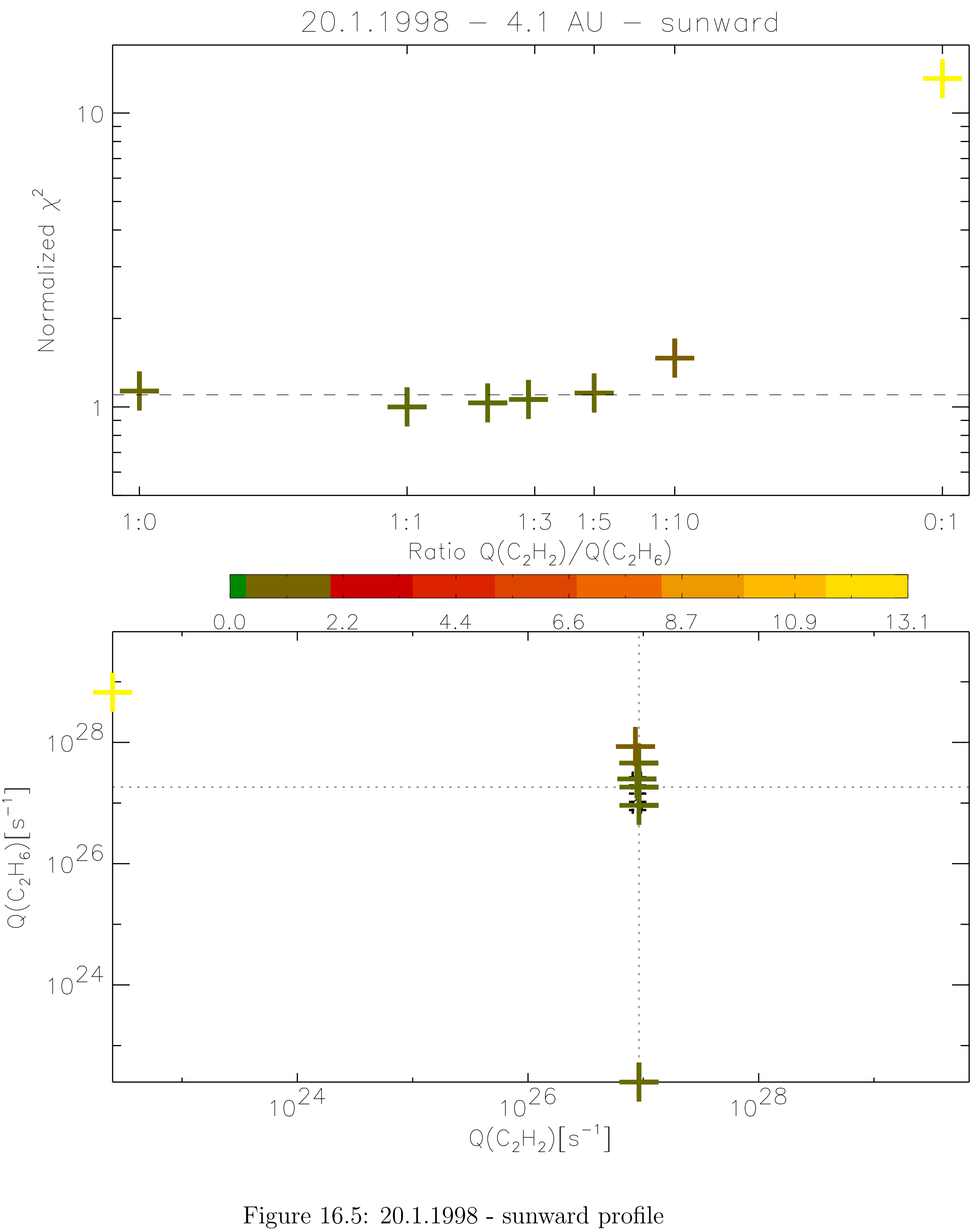


Figure 16.5: 20.1.1998 - sunward profile

# 20.1.1998 - tailward profile

## Results of the iterations

| A($C_2H_2$) | A($C_2H_6$) | Ratio $\left(\frac{Q(C_2H_2)}{Q(C_2H_6)}\right)$ | A($C_3H_4$) | k ($C_2$) | $\chi^2$ ($C_2$) | k ($C_3$) | $\chi^2$ ($C_3$) |
|---|---|---|---|---|---|---|---|
| 0.029997 | 0.000000 | 1:0 | 0.028612 | 1.000 | 0.359 | 1.012 | 3.337 |
| 0.029337 | 0.029337 | 1:1 | 0.028612 | 0.990 | 0.259 | 1.015 | 3.339 |
| 0.029337 | 0.058674 | 1:2 | 0.028612 | 0.980 | 0.268 | 1.015 | 3.339 |
| 0.028114 | 0.079877 | 1:3 | 0.028612 | 1.006 | 0.276 | 1.014 | 3.334 |
| 0.027870 | 0.139351 | 1:5 | 0.028612 | 0.991 | 0.366 | 1.013 | 3.333 |
| 0.025584 | 0.255837 | 1:10 | 0.027468 | 0.988 | 0.415 | 0.992 | 2.911 |
| 0.000000 | 2.026126 | 0:1 | 0.027468 | 0.982 | 10.264 | 1.022 | 11.367785 |

## Resulting production rates in [$10^{25}$ $s^{-1}$]

| | | |
|---|---|---|
| Q($C_2H_2$) | = | 73.3±2.1 |
| Q($C_2H_6$) | = | 146.7±43.0 |
| Q($C_3H_4$) | = | 91.5±1. |

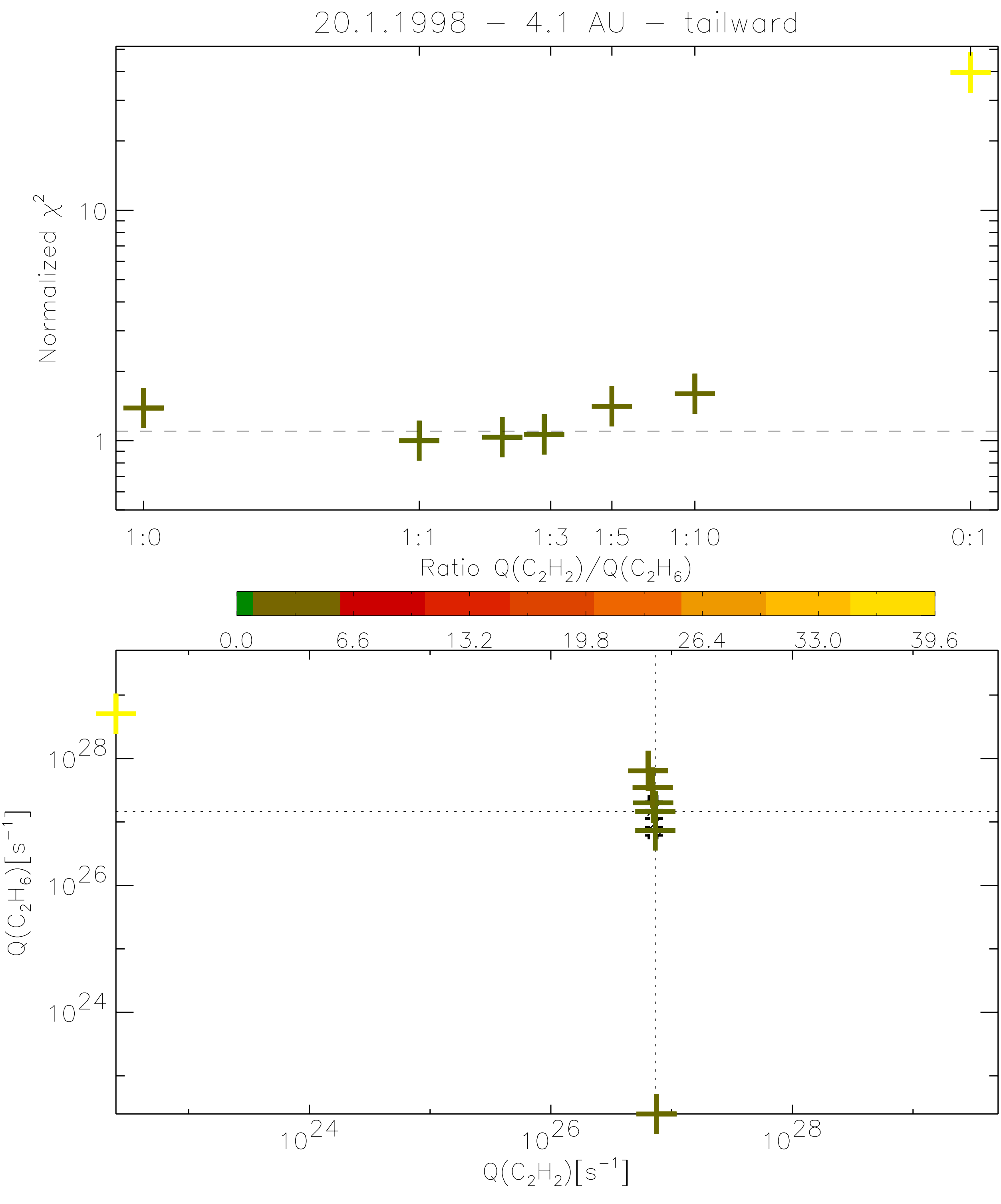


Figure 16.6: 20.1.1998 - tailward profile

# 22.1.1998

## Results of the iterations

| $A(C_2H_2)$ | $A(C_2H_6)$ | Ratio $\left(\frac{Q(C_2H_2)}{Q(C_2H_6)}\right)$ | $A(C_3H_4)$ | k ($C_2$) | $\chi^2$ ($C_2$) | k ($C_3$) | $\chi^2$ ($C_3$) |
|---|---|---|---|---|---|---|---|
| 0.030925 | 0.000000 | 1:0 | 0.017224 | 1.057 | 20.488 | 1.013 | 10.419 |
| 0.030925 | 0.030925 | 1:1 | 0.017224 | 1.044 | 18.321 | 1.012 | 10.419 |
| 0.030925 | 0.062850 | 1:2 | 0.017224 | 1.044 | 18.221 | 1.002 | 10.419 |
| 0.030925 | 0.087865 | 1:3 | 0.017224 | 1.008 | 18.734 | 1.004 | 10.420 |
| 0.030925 | 0.154625 | 1:5 | 0.017224 | 0.993 | 19.244 | 1.012 | 10.422 |
| 0.028888 | 0.288874 | 1:10 | 0.017396 | 0.994 | 20.349 | 1.000 | 10.428 |
| 0.027214 | 0.544280 | 1:20 | 0.017741 | 0.977 | 25.242 | 0.994 | 10.515 |
| 0.020720 | 1.035987 | 1:50 | 0.017741 | 0.965 | 29.987 | 0.988 | 10.547 |
| 0.000000 | 2.350389 | 0:1 | 0.018946 | 1.007 | 47.465 | 1.009 | 10.362 |

## Resulting production rates in [$10^{25}$ $s^{-1}$]

| | | |
|---|---|---|
| $Q(C_2H_2)$ | = | 77.3±1.5 |
| $Q(C_2H_6)$ | = | 219.7±59.7 |
| $Q(C_3H_4)$ | = | 43.0±1. |

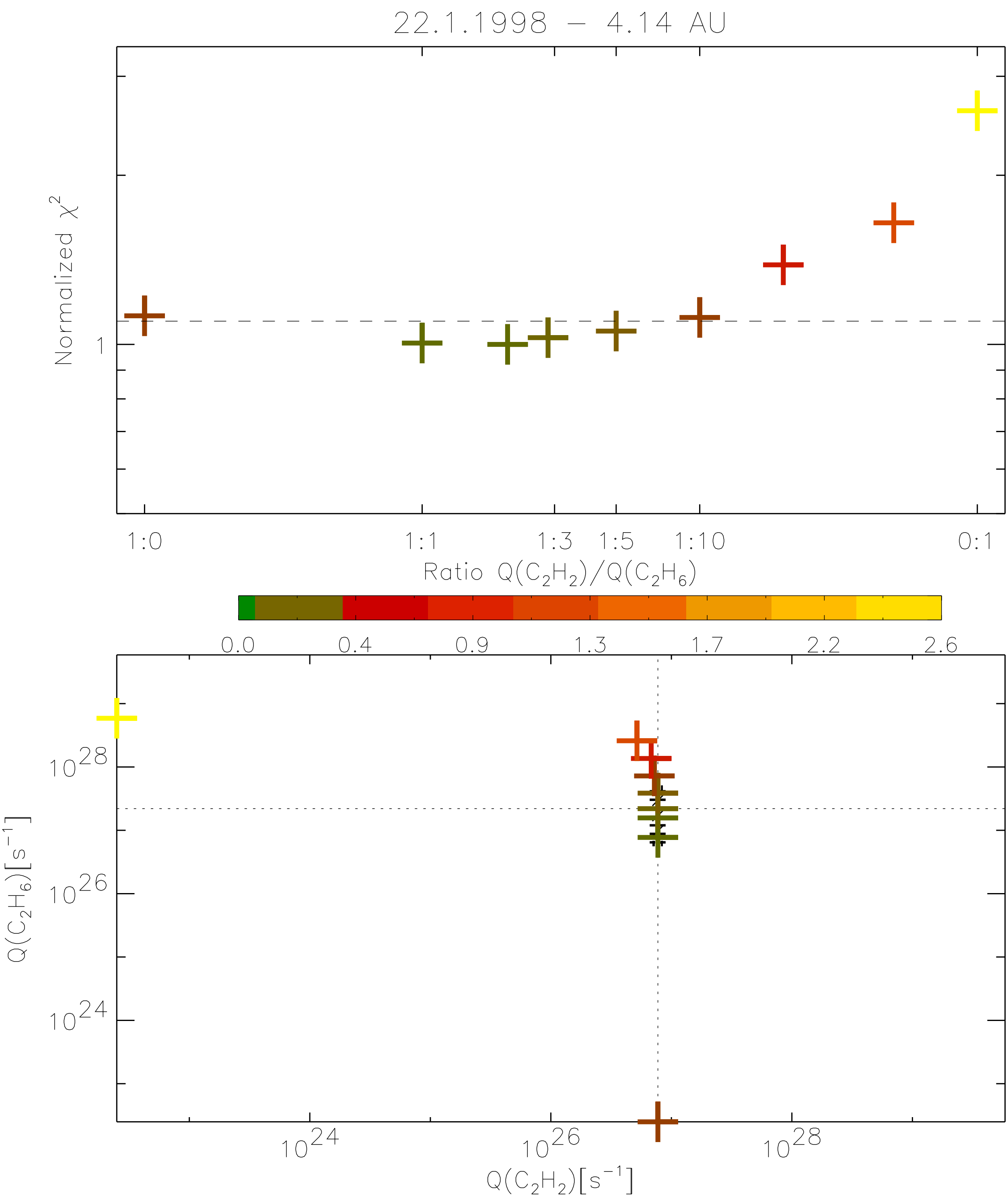


Figure 16.7: 22.1.1998

# 21.3.1998

## Results of the iterations

| $A(C_2H_2)$ | $A(C_2H_6)$ | Ratio $\left(\frac{Q(C_2H_2)}{Q(C_2H_6)}\right)$ | $A(C_3H_4)$ | k ($C_2$) | $\chi^2$ ($C_2$) | k ($C_3$) | $\chi^2$ ($C_3$) |
|---|---|---|---|---|---|---|---|
| 0.135273 | 0.000000 | 1:0 | 0.130507 | 1.025 | 2.238 | 1.005 | 36.241 |
| 0.140191 | 0.140191 | 1:1 | 0.130507 | 0.984 | 2.102 | 1.007 | 36.188 |
| 0.135985 | 0.271971 | 1:2 | 0.130507 | 0.997 | 2.109 | 1.006 | 36.230 |
| 0.128509 | 0.371379 | 1:3 | 0.130507 | 1.034 | 2.086 | 1.004 | 36.306 |
| 0.130693 | 0.392080 | 1:3 | 0.130507 | 1.018 | 2.082 | 1.004 | 36.283 |
| 0.127129 | 0.635644 | 1:5 | 0.130507 | 1.018 | 2.014 | 1.004 | 36.318 |
| 0.118812 | 1.188117 | 1:10 | 0.130507 | 1.020 | 1.936 | 1.002 | 36.398 |
| 0.111089 | 2.221781 | 1:20 | 0.130507 | 0.977 | 2.060 | 1.000 | 36.467 |
| 0.086257 | 4.312869 | 1:50 | 0.130507 | 0.947 | 3.232 | 0.995 | 36.708 |
| 0.000000 | 9.995694 | 0:1 | 0.125287 | 1.058 | 13.931 | 1.045 | 39.744 |

## Resulting production rates in $[10^{25}\ s^{-1}]$

| | | |
|---|---|---|
| $Q(C_2H_2)$ | = | 64.3±1.1 |
| $Q(C_2H_6)$ | = | 196.0±19.0 |
| $Q(C_3H_4)$ | = | 65.2±1. |

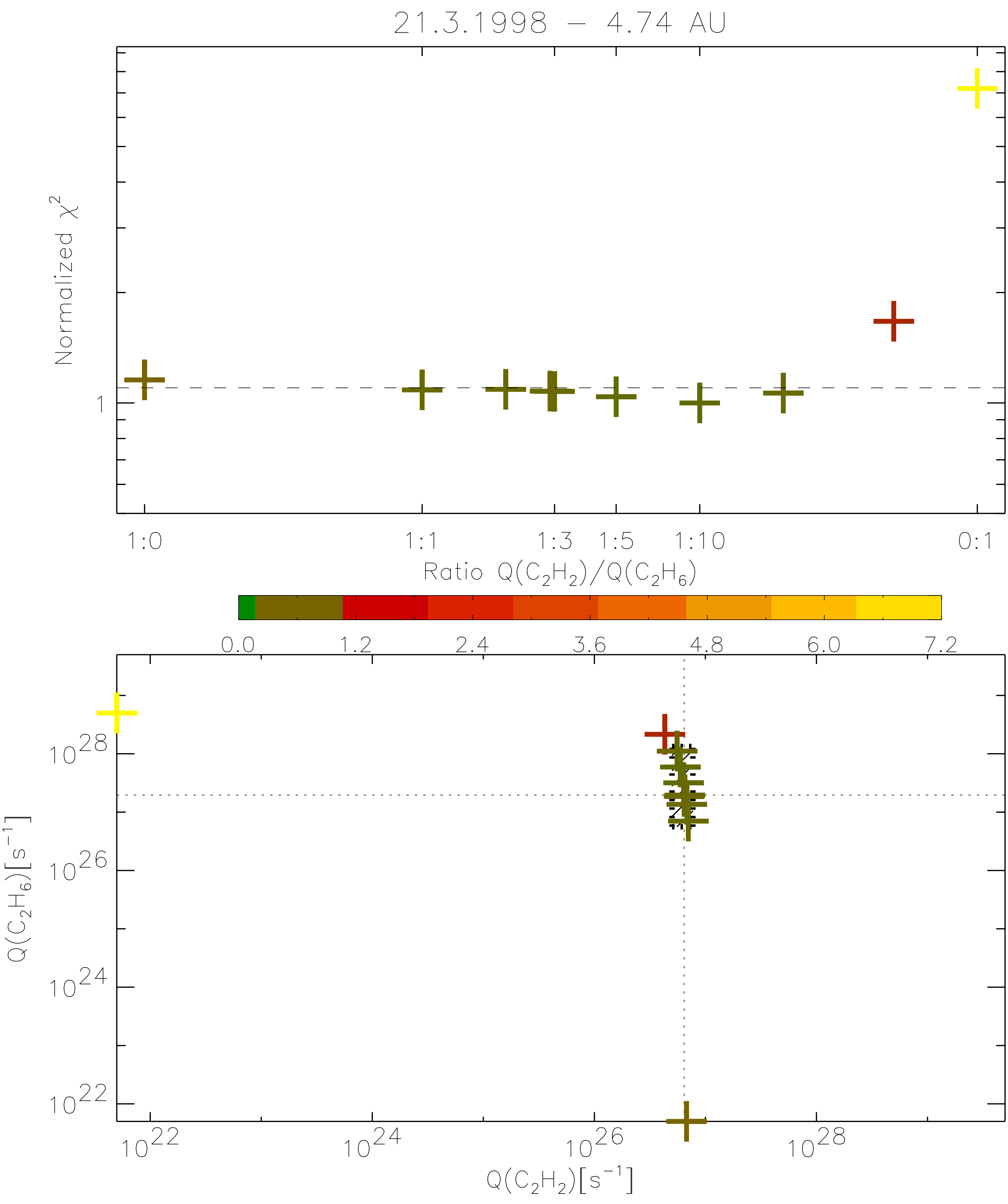


Figure 16.8: 21.3.1998

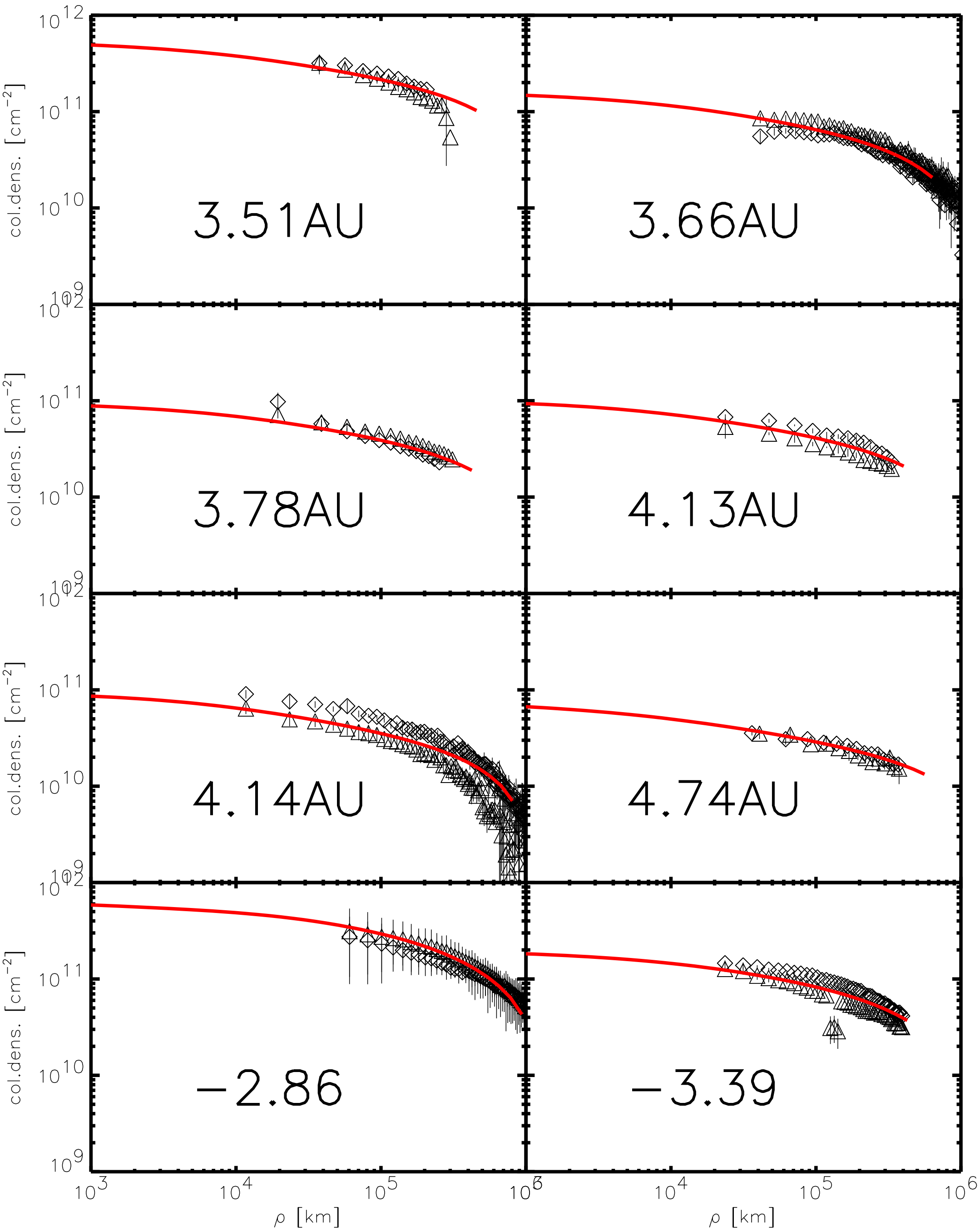


Figure 16.9: Overview of the best fitting $C_2$ profiles

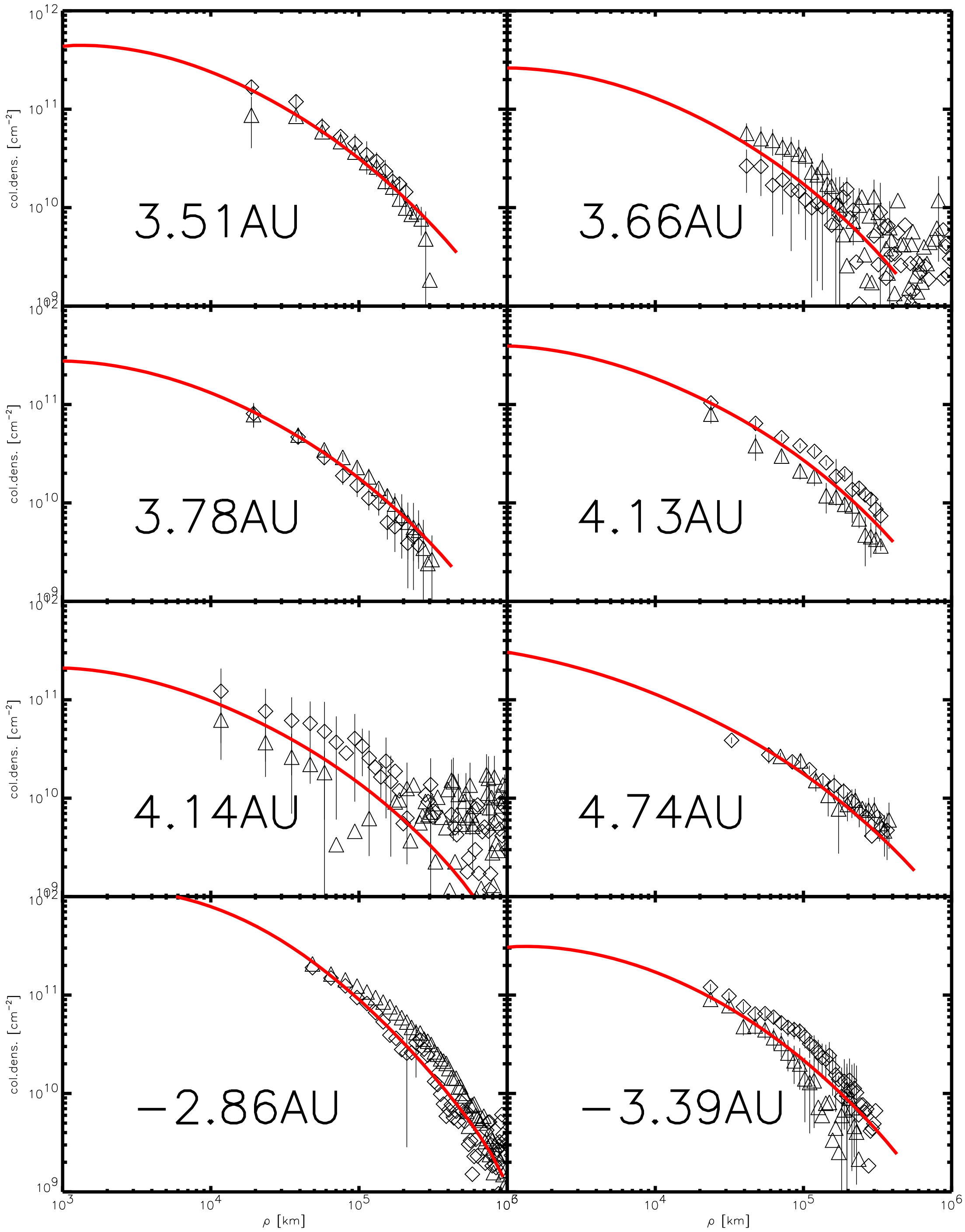


Figure 16.10: Overview of the best fitting $C_3$ profiles