# Uncertainty in UDfA?

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**The UMIST Database for Astrochemistry**

Woodall, Agúndez, Markwick-Kemper, Millar

*RATE06 - 4th publicly available version*

*10% bigger than rate99*

*cleaner than rate99*

*23 new species, inc. F-bearing*

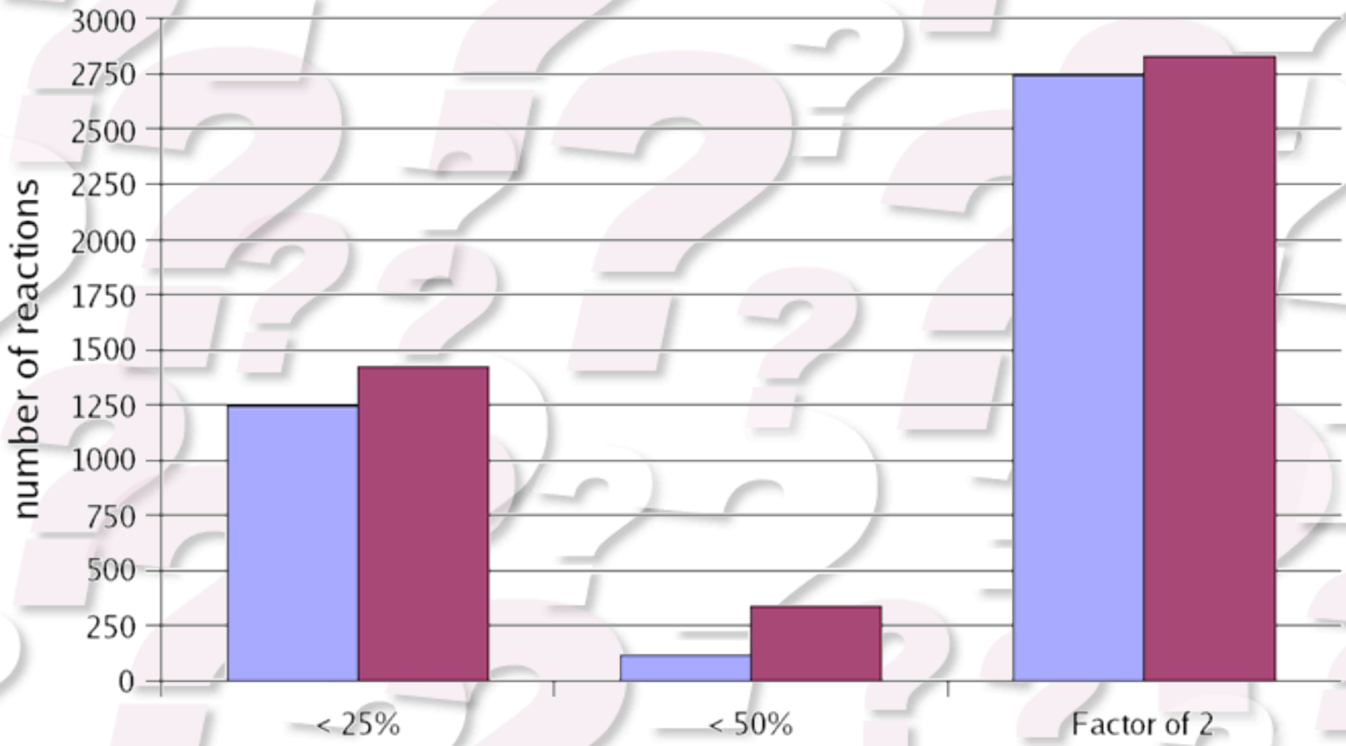
*over 1100 new or revised rate coefficients*

*‘historical data’*

*www.udfa.net*

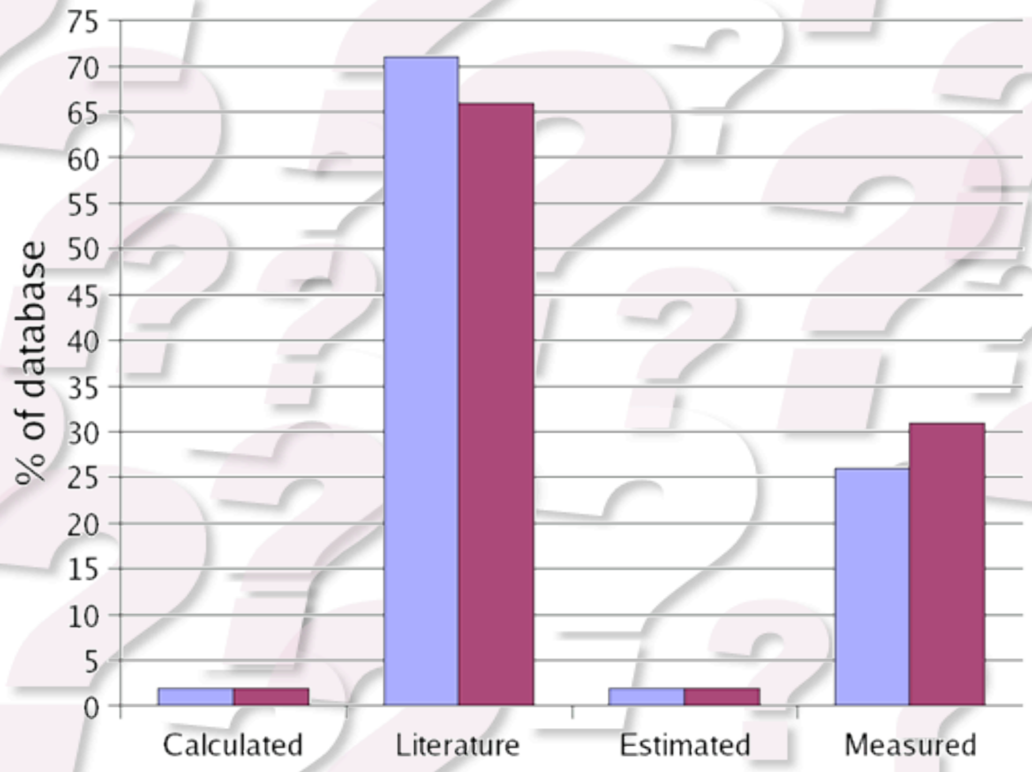
*future?*

***Comparison of rate coefficient ‘accuracy’***



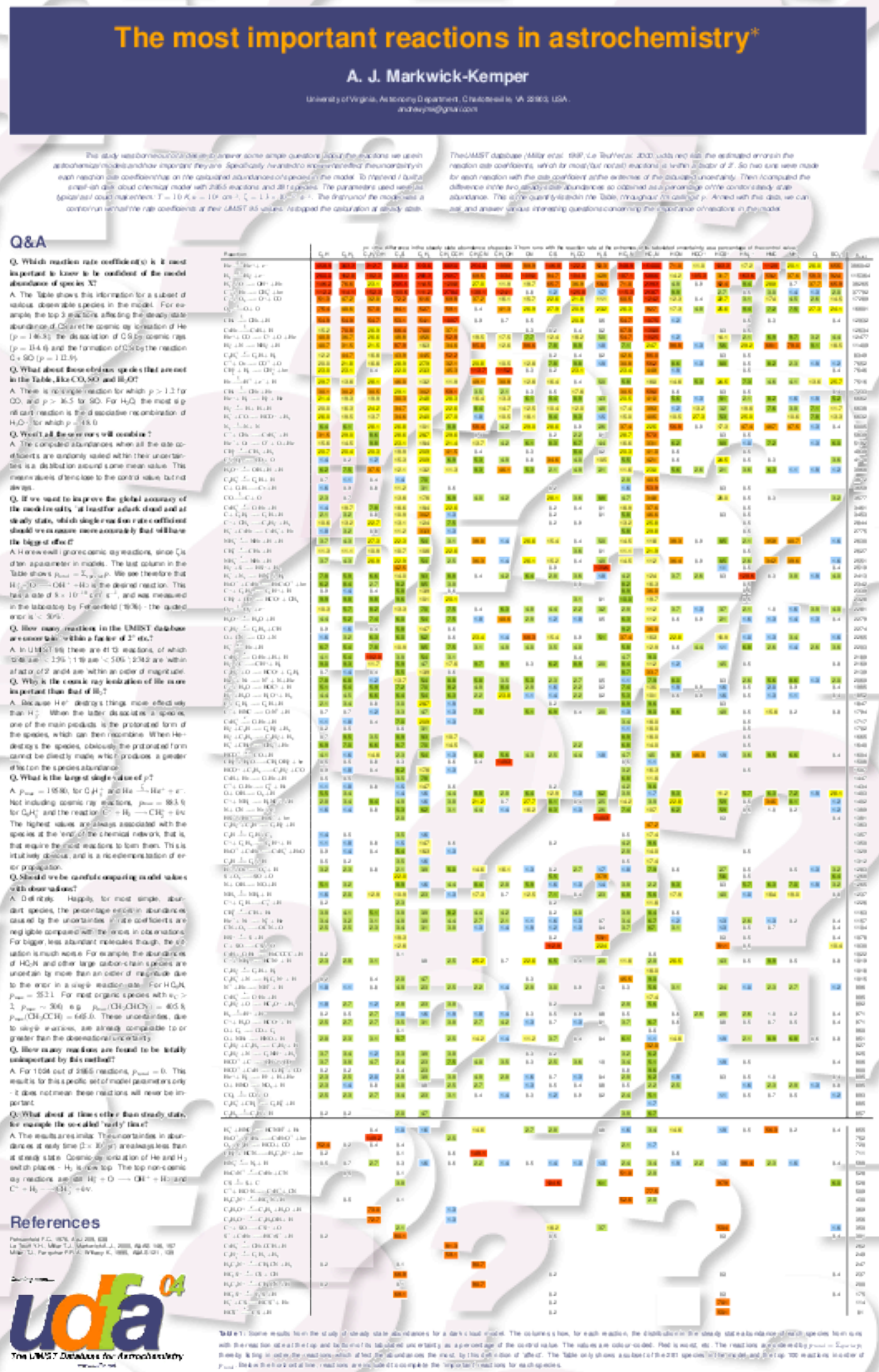

***blue = rate99, purple = rate06***

## *Comparison of rate coefficient source*




***blue = rate99, purple = rate06***

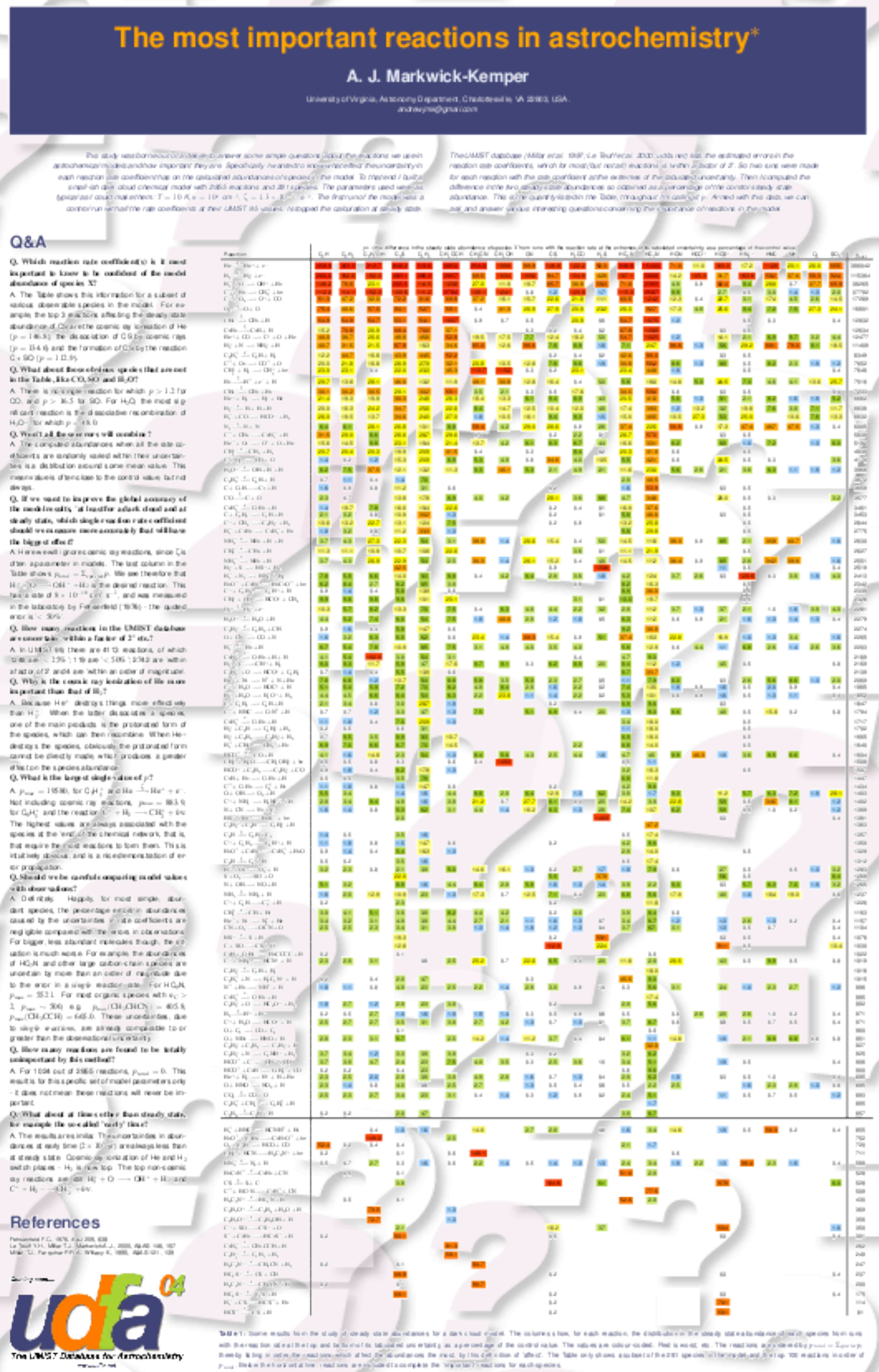
# The most important reactions*



# The most important reactions*

*simple questions*

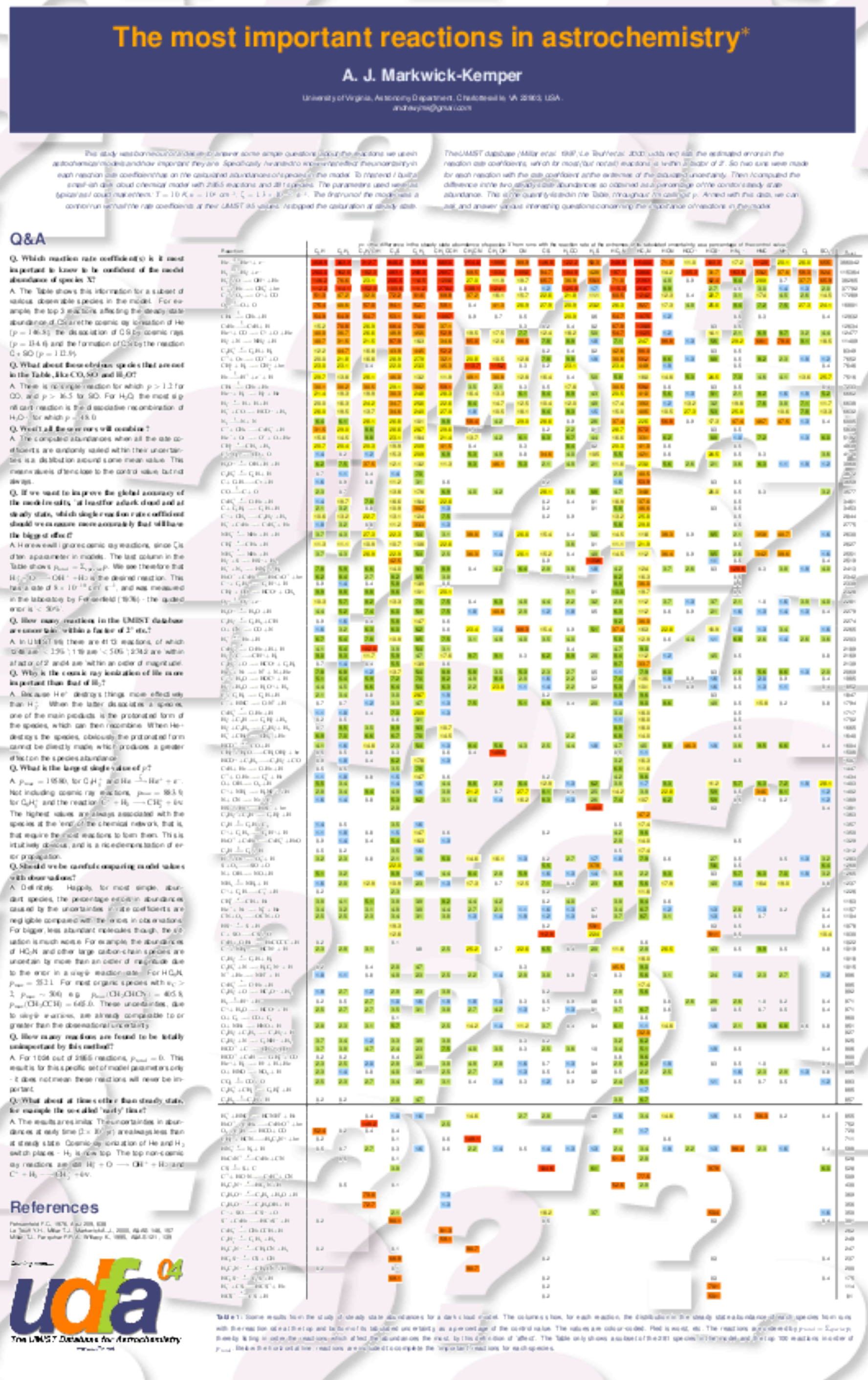
*simple study*




***( downloadable at asilomar.caltech.edu )***

# The most important reactions*

*observers put errors on their abundances, so why don't we put errors on our calculated abundances?*


# The most important reactions in astrochemistry*

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## Q&A

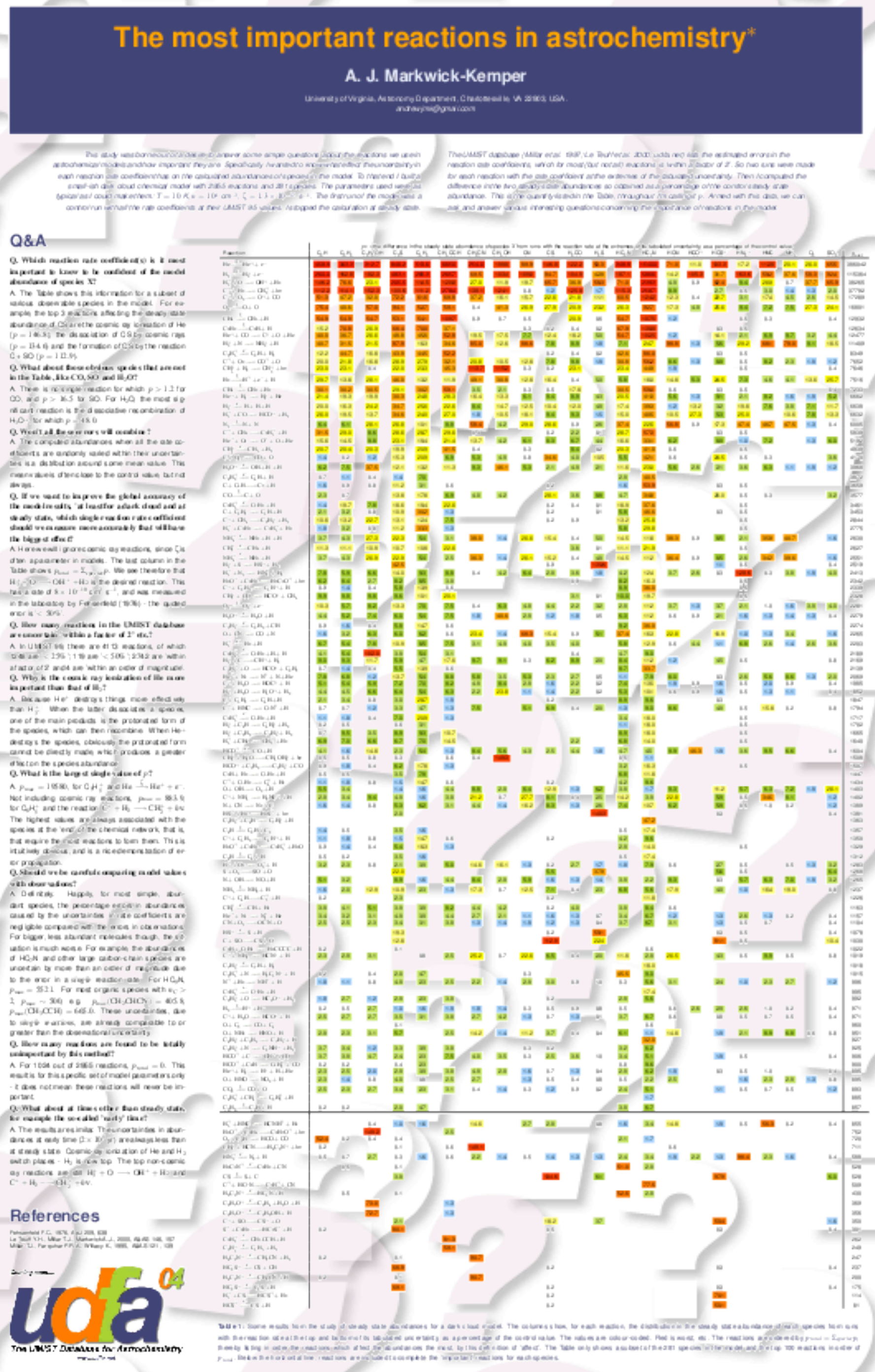
## References

# The most important reactions*

*which reaction affects the model abundances the most?*

*which reaction would I most like to be better quantified?*

*etc.*



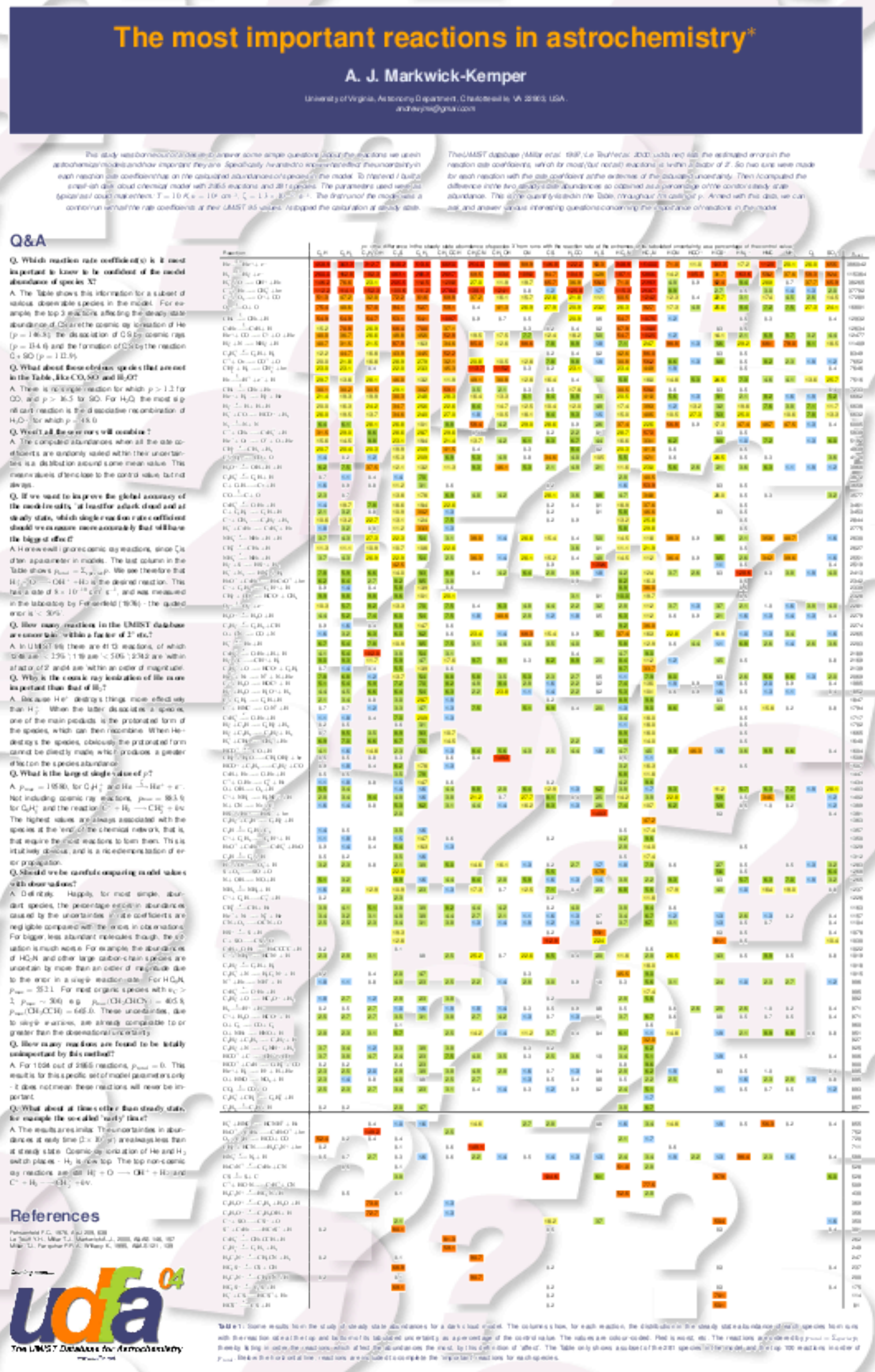
# The most important reactions*

*about the asterisk:*

*dark cloud*

*steady state*

*choice of ‘p’*



# *Methodology*

*One control model: ‘standard’ parameters*

*Run one model at the extremes of each reaction rate coefficient’s tabulated uncertainty*

*Compute the difference between the results so obtained as a percentage of the control value ( = p ), on a species by species basis.*

*e.g. if p = 0, there was no effect on the species abundance by varying the reaction rate coefficient.*

*The bigger p is, the more significant the reaction is for that species*

*Summing p over all species, we can work out the ‘most important reaction’ * caveat caveat etc etc*

***What is the most important reaction by these standards?***

# A

$$He + \zeta \rightarrow He^{+} + e^{-}$$

*OK, why isn't it*

$$H_2 + \zeta \rightarrow H_2^+ + e^-?$$

***Forget about cosmic rays…***
***what is the most important reaction***
***by these standards?***

***Or.. What single reaction rate coefficient can we measure that will improve the overall accuracy of the model the most?***

# A

$$H_3^+ + O \rightarrow OH^+ + H_2$$

*measured by Fehsenfeld (1976)*

*$k = 8 \times 10^{-10}$ cm$^3$s$^{-1}$*

*quoted error '< 50%'*

***Show me the whole list!!***

$p_X$ = the difference in the steady state abundance of species $X$ from runs with the reaction rate at the extremes of its tabulated uncertainty, as a percentage of the control value.

| Reaction | $C_2H$ | $C_2H_2$ | $C_2H_5OH$ | $C_3S$ | $C_3H_2$ | $CH_3CCH$ | $CH_3CN$ | $CH_3OH$ | CN | CS | $H_2CO$ | $H_2S$ | $HC_3N$ | $HC_7N$ | HCN | $HCO^+$ | $HCS^+$ | $HN_2^+$ | HNC | $NH_3$ | $O_2$ | $SO_2$ | $p_{total}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $He \xrightarrow{\zeta} He^+ + e^-$ | 458.9 | 343.3 | 312.7 | 846.2 | 513.6 | 665.0 | 254.0 | 199.9 | 89.9 | 146.8 | 122.2 | 53.3 | 348.9 | 1540.0 | 71.0 | 11.0 | 133.3 | 17.2 | 112.8 | 20.1 | 26.0 | 65.5 | 386042 |
| $H_2 \xrightarrow{\zeta} H_2^+ + e^-$ | 260.0 | 162.8 | 182.3 | 483.1 | 280.3 | 265.7 | 69.5 | 103.4 | 109.0 | 94.7 | 104.9 | 42.8 | 187.1 | 586.6 | 14.2 | 105.3 | 31.7 | 163.6 | 59.2 | 37.6 | 58.3 | 92.4 | 115364 |
| $H_3^+ + O \longrightarrow OH^+ + H_2$ | 146.2 | 76.6 | 23.1 | 205.5 | 114.5 | 120.8 | 27.0 | 11.9 | 19.7 | 65.7 | 36.9 | 58.3 | 71.0 | 239.3 | 4.9 | 0.9 | 62.4 | 9.4 | 28.9 | 0.7 | 37.7 | 65.9 | 38265 |
| $C^+ + H_2 \longrightarrow CH_2^+ + h\nu$ | 112.2 | 114.1 | 152.3 | 100.6 | 111.2 | 278.4 | 138.1 | 124.1 | 0.8 | 1.2 | 125.8 | 1.7 | 115.3 | 258.7 | 9.9 | | 2.7 | 0.5 | 3.0 | 1.4 | 1.3 | 2.0 | 37792 |
| $C^+ + O_2 \longrightarrow O^+ + CO$ | 51.3 | 47.2 | 32.0 | 72.2 | 61.6 | 69.8 | 37.2 | 16.1 | 15.7 | 22.6 | 21.8 | 11.1 | 60.5 | 124.2 | 12.3 | 0.4 | 22.7 | 3.1 | 17.4 | 4.5 | 2.6 | 14.5 | 17289 |
| $O_2 \xrightarrow{\zeta} O + O$ | 75.4 | 40.6 | 57.0 | 94.1 | 52.7 | 59.1 | 0.4 | 41.3 | 26.9 | 27.9 | 20.9 | 23.2 | 26.3 | 92.7 | 17.3 | 4.8 | 25.6 | 9.4 | 7.2 | 7.5 | 27.3 | 24.1 | 16801 |
| $CH_4 \xrightarrow{\zeta} CH_3 + H$ | 54.9 | 54.9 | 54.7 | 53.1 | 54.1 | 109.7 | 0.9 | 0.7 | 0.5 | | 20.9 | 0.6 | 54.7 | 107.5 | 1.2 | | | 0.5 | 0.3 | | | 0.4 | 12932 |
| $C_2H_2 \xrightarrow{\zeta} C_2H + H$ | 15.2 | 70.8 | 26.9 | 68.4 | 70.0 | 37.1 | | | 0.3 | 0.2 | 0.4 | 0.2 | 67.9 | 138.8 | | | 0.3 | 0.5 | | | | | 12634 |
| $He^+ + CO \longrightarrow C^+ + O + He$ | 40.0 | 36.7 | 26.6 | 48.8 | 45.6 | 52.8 | 19.5 | 17.5 | 7.7 | 12.4 | 18.2 | 5.0 | 54.7 | 102.5 | 1.2 | | 14.1 | 2.1 | 6.9 | 9.7 | 3.2 | 4.4 | 12477 |
| $H_3^+ + N \longrightarrow NH_2^+ + H$ | 40.7 | 31.5 | 21.5 | 87.9 | 16.3 | 34.6 | 85.0 | 12.6 | 88.6 | 7.8 | 8.9 | 1.8 | 7.1 | 24.7 | 98.8 | 1.3 | 5.6 | 29.2 | 68.1 | 79.0 | 9.1 | 18.5 | 11409 |
| $C_2H_3^+ \xrightarrow{e^-} C_2H + H_2$ | 12.2 | 44.7 | 16.8 | 43.9 | 44.5 | 52.2 | | | | 0.2 | 0.4 | 0.2 | 42.6 | 86.0 | | | 0.3 | 0.5 | | | | | 8349 |
| $C^+ + O_2 \longrightarrow CO^+ + O$ | 20.0 | 21.8 | 16.8 | 28.9 | 27.9 | 32.1 | 20.8 | 10.5 | 12.8 | 7.8 | 9.8 | 1.9 | 30.8 | 56.2 | 8.6 | 1.3 | 8.0 | 0.5 | 8.2 | 2.3 | 1.9 | 1.2 | 7652 |
| $CH_3^+ + H_2 \longrightarrow CH_5^+ + h\nu$ | 23.0 | 23.1 | 0.4 | 22.0 | 23.3 | 45.3 | 113.7 | 115.2 | 0.3 | 0.2 | 23.1 | | 23.4 | 44.9 | 1.9 | | | 0.5 | | | | 0.4 | 7646 |
| $H_2 \xrightarrow{\zeta} H^+ + e^- + H$ | 29.7 | 13.8 | 28.1 | 46.0 | 13.2 | 11.9 | 49.1 | 30.8 | 12.8 | 16.4 | 0.4 | 5.0 | 5.8 | 18.0 | 14.8 | 5.3 | 24.5 | 7.3 | 4.6 | 4.1 | 13.6 | 25.7 | 7516 |
| $CH_4 \xrightarrow{\zeta} CH_2 + H_2$ | 30.1 | 30.2 | 30.5 | 29.1 | 30.2 | 59.1 | 3.5 | 2.1 | 0.3 | 0.5 | 17.8 | | 30.5 | 59.0 | 0.6 | | 0.3 | 0.5 | | | | 0.4 | 7233 |
| $He^+ + H_2 \longrightarrow H_2^+ + He$ | 21.4 | 19.3 | 19.9 | 30.3 | 24.8 | 28.3 | 16.4 | 13.3 | 6.1 | 9.4 | 8.9 | 4.3 | 20.5 | 41.0 | 5.6 | 1.3 | 9.1 | 2.1 | 8.2 | 1.6 | 1.9 | 5.2 | 6662 |
| $H_3^+ \xrightarrow{e^-} H + H + H$ | 20.0 | 16.3 | 24.2 | 34.7 | 25.6 | 22.6 | 8.4 | 14.7 | 12.5 | 10.4 | 12.0 | 4.8 | 17.4 | 39.3 | 1.2 | 13.2 | 3.2 | 19.8 | 7.6 | 3.8 | 7.1 | 11.7 | 6638 |
| $H_3^+ + CO \longrightarrow HCO^+ + H_2$ | 26.0 | 19.5 | 13.7 | 34.6 | 24.0 | 27.0 | 1.8 | 10.5 | 18.1 | 9.4 | 9.3 | 1.5 | 15.0 | 40.5 | 10.5 | 27.3 | 5.3 | 25.0 | | 10.6 | 7.8 | 13.3 | 6632 |
| $N_2 \xrightarrow{\zeta} N + N$ | 6.4 | 6.1 | 28.1 | 26.8 | 10.1 | 8.8 | 58.4 | 4.2 | 29.0 | 28.6 | 0.9 | 2.6 | 37.4 | 22.5 | 56.8 | 0.9 | 17.3 | 47.4 | 46.7 | 47.5 | 1.3 | 0.4 | 6005 |
| $C^+ + CH_4 \longrightarrow C_2H_3^+ + H$ | 31.5 | 29.0 | 8.6 | 28.6 | 28.7 | 29.6 | 0.4 | | | 0.2 | 2.2 | 0.1 | 28.7 | 57.3 | | | 0.3 | 0.5 | | | | | 5839 |
| $He^+ + O_2 \longrightarrow O^+ + O + He$ | 15.6 | 14.5 | 9.8 | 23.1 | 19.4 | 21.4 | 13.7 | 4.2 | 6.1 | 8.3 | 6.7 | 4.4 | 16.6 | 33.1 | 6.2 | | 8.0 | 1.0 | 7.2 | | 1.3 | 6.0 | 5192 |
| $CH_5^+ \xrightarrow{e^-} CH_3 + H_2$ | 20.7 | 20.4 | 20.3 | 19.9 | 20.9 | 41.5 | 0.4 | | 0.3 | | 8.4 | 0.2 | 20.3 | 41.0 | 0.6 | | | 0.5 | | | | | 4939 |
| $C + O_2 \longrightarrow CO + O$ | 1.4 | 0.2 | 1.2 | 15.3 | 20.9 | 6.9 | 5.3 | 4.9 | 0.8 | 34.6 | 4.0 | 10.5 | 5.5 | 42.1 | 0.6 | | 24.5 | 0.5 | 0.3 | | | 3.6 | 4170 |
| $H_3O^+ \xrightarrow{e^-} OH + H + H$ | 6.2 | 7.5 | 37.5 | 12.1 | 13.2 | 11.3 | 9.3 | 46.1 | 5.3 | 2.1 | 4.9 | 2.1 | 11.6 | 23.0 | 5.6 | 2.6 | 2.1 | 3.6 | 6.3 | 1.1 | 1.9 | 1.2 | 3968 |
| $C_4H_2^+ \xrightarrow{e^-} C_4H + H$ | 0.7 | 1.1 | 0.4 | 1.4 | 7.0 | | | | | | | | 2.9 | 40.5 | | | | | | | | | 3872 |
| $C + C_4H \longrightarrow C_5 + H$ | 1.6 | 0.9 | 0.8 | 11.2 | 3.1 | 0.6 | | | | 0.2 | | | 1.6 | 53.9 | | | 0.3 | 0.5 | | | | | 3659 |
| $CO \xrightarrow{\zeta} C + O$ | 2.3 | 0.7 | | 13.8 | 17.8 | 6.9 | 4.0 | 4.2 | | 28.1 | 3.6 | 8.8 | 4.7 | 34.8 | | | 20.0 | 0.5 | 0.3 | | | 3.2 | 3577 |
| $C_2H_3^+ \xrightarrow{e^-} C_2H_2 + H$ | 1.4 | 19.7 | 7.8 | 18.6 | 19.4 | 22.6 | | | | 0.2 | 0.4 | 0.1 | 18.9 | 37.6 | | | | 0.5 | | | | | 3461 |
| $C + C_2H_2 \longrightarrow C_3H + H$ | 2.1 | 3.2 | 0.8 | 10.9 | 30.2 | 1.3 | | | | 0.2 | | 0.1 | 5.8 | 46.6 | | | 0.3 | 0.5 | | | | | 3453 |
| $C^+ + CH_4 \longrightarrow C_2H_2^+ + H_2$ | 10.6 | 13.2 | 22.7 | 13.1 | 12.4 | 7.5 | | | | 0.2 | 0.9 | | 13.2 | 25.8 | | | | 0.5 | | | | | 2844 |
| $H_3^+ + C_3H_2 \longrightarrow C_3H_3^+ + H_2$ | 1.8 | 3.2 | 0.8 | 11.2 | 33.3 | 1.3 | | | | | | | 5.8 | 29.8 | | | | 0.5 | | | | | 2775 |
| $NH_4^+ \xrightarrow{e^-} NH_2 + H + H$ | 3.7 | 4.3 | 27.3 | 22.3 | 5.4 | 3.1 | 38.0 | 1.4 | 26.6 | 15.4 | 0.4 | 5.0 | 14.5 | 11.8 | 38.3 | 0.9 | 8.5 | 2.1 | 35.9 | 40.7 | | 1.6 | 2630 |
| $CH_5^+ \xrightarrow{e^-} CH_4 + H$ | 11.3 | 11.1 | 10.9 | 10.7 | 10.8 | 22.6 | | | | | 3.6 | 0.1 | 11.1 | 21.9 | | | | 0.5 | | | | | 2627 |
| $NH_4^+ \xrightarrow{e^-} NH_3 + H$ | 3.7 | 4.3 | 26.9 | 22.9 | 5.4 | 2.5 | 36.3 | 1.4 | 26.1 | 15.2 | 0.4 | 4.8 | 14.5 | 11.2 | 36.4 | 0.9 | 8.5 | 2.6 | 34.2 | 39.6 | | 1.6 | 2551 |
| $H_3^+ + S \longrightarrow HS^+ + H_2$ | | | | 42.5 | | | | | | 0.9 | | 130.6 | | | | | 1.1 | 0.5 | | | | 0.4 | 2519 |
| $H_3^+ + N_2 \longrightarrow HN_2^+ + H_2$ | 7.8 | 5.9 | 6.6 | 14.0 | 9.3 | 8.8 | 0.4 | 4.2 | 6.4 | 2.8 | 3.6 | 1.8 | 4.2 | 12.4 | 3.7 | 2.6 | 0.3 | 128.6 | 0.3 | 3.8 | 1.9 | 4.0 | 2413 |
| $H_3O^+ + C_2H_2 \longrightarrow H_5C_2O^+ + h\nu$ | 6.2 | 8.4 | 2.7 | 8.2 | 8.5 | 3.8 | | | | | 0.9 | | 8.2 | 16.3 | | | | 0.5 | | | | | 2342 |
| $C^+ + C_2H_2 \longrightarrow C_3H^+ + H$ | 0.9 | 1.4 | 0.4 | 5.8 | 13.9 | 0.6 | | | | | | | 8.9 | 36.0 | | | | 0.5 | | | | | 2339 |
| $CH_5^+ + CO \longrightarrow HCO^+ + CH_4$ | 9.9 | 9.8 | 9.8 | 9.6 | 10.1 | 20.1 | | | | | 3.1 | 0.1 | 10.0 | 19.7 | | | | 0.5 | | | | | 2328 |

***What about obvious important species, like CO, SO or $H_2O$?***

A

***There is no single reaction for which $p > 1.2$ for CO, or $p > 16.5$ for SO. For water, $p_{max} = 48.0$ for dissociative recombination of $H_3O^+$.***

***What is the largest single value of p?***

# A

*it's 19580, for $C_9H_5^+$ and the reaction*

*$He + \zeta \rightarrow He^+ + e^-$*

*'end chain' species*

***What about other times in the model, for example at 'early time'?***

# A

***The results are similar.***

***The uncertainties are always less than at steady state.***

***The cri reactions for $H_2$ and He switch places.***

***The top non cr reactions are still***

$H_3^+ + O \rightarrow OH^+ + H_2$

***and***

$C^+ + H_2 \rightarrow CH_2^+ + h\nu$

***Won't all these errors cancel out?***


A
CS
Formations: 34
Destructions: 13
Reactions: 47
Control: −7.9000001
Mean: −7.9140000
Std Dev: 0.093390003
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−8.430
−8.329
−8.227
−8.126
−8.024
−7.923
−7.821
−7.720
log f

***Should we be careful comparing models with observations?***

**Absolutely.**

***Simple species are OK***
***but bigger molecules are definitely not***

***e.g. $HC_7N$ abundance uncertain to an order of magnitude because of a single rate!***

***For $HC_9N$, $p_{max} = 5521$!***

***For most species with $n_C > 2$, $p_{max} \sim 500$***

***How many reactions were found to be totally unimportant by this method?***

# A

***$p_{total}$ = 0 for about a third of them.***

***But that doesn't mean those reactions will never be important under any conditions***

***How can we get a handle on ζ?***

$p_X$ = the difference in the steady state abundance of species $X$ from runs with the reaction rate at the extremes of its tabulated uncertainty, as a percentage of the control value.

| Reaction | $C_2H$ | $C_2H_2$ | $C_2H_5OH$ | $C_3S$ | $C_3H_2$ | $CH_3CCH$ | $CH_3CN$ | $CH_3OH$ | CN | CS | $H_2CO$ | $H_2S$ | $HC_3N$ | $HC_7N$ | HCN | $HCO^+$ | $HCS^+$ | $HN_2^+$ | HNC | $NH_3$ | $O_2$ | $SO_2$ | $p_{total}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $He \xrightarrow{\zeta} He^+ + e^-$ | 458.9 | 343.3 | 312.7 | 846.2 | 513.6 | 665.0 | 254.0 | 199.9 | 89.9 | 146.8 | 122.2 | 53.3 | 348.9 | 1540.0 | 71.0 | 11.0 | 133.3 | 17.2 | 112.8 | 20.1 | 26.0 | 65.5 | 386042 |
| $H_2 \xrightarrow{\zeta} H_2^+ + e^-$ | 260.0 | 162.8 | 182.3 | 483.1 | 280.3 | 265.7 | 69.5 | 103.4 | 109.0 | 94.7 | 104.9 | 42.8 | 187.1 | 586.6 | 14.2 | 105.3 | 31.7 | 163.6 | 59.2 | 37.6 | 58.3 | 92.4 | 115364 |
| $H_3^+ + O \longrightarrow OH^+ + H_2$ | 146.2 | 76.6 | 23.1 | 205.5 | 114.5 | 120.8 | 27.0 | 11.9 | 19.7 | 65.7 | 36.9 | 58.3 | 71.0 | 239.3 | 4.9 | 0.9 | 62.4 | 9.4 | 28.9 | 0.7 | 37.7 | 65.9 | 38265 |
| $C^+ + H_2 \longrightarrow CH_2^+ + h\nu$ | 112.2 | 114.1 | 152.3 | 100.6 | 111.2 | 278.4 | 138.1 | 124.1 | 0.8 | 1.2 | 125.8 | 1.7 | 115.3 | 258.7 | 9.9 | | 2.7 | 0.5 | 3.0 | 1.4 | 1.3 | 2.0 | 37792 |
| $C^+ + O_2 \longrightarrow O^+ + CO$ | 51.3 | 47.2 | 32.0 | 72.2 | 61.6 | 69.8 | 37.2 | 16.1 | 15.7 | 22.6 | 21.8 | 11.1 | 60.5 | 124.2 | 12.3 | 0.4 | 22.7 | 3.1 | 17.4 | 4.5 | 2.6 | 14.5 | 17289 |
| $O_2 \xrightarrow{\zeta} O + O$ | 75.4 | 40.6 | 57.0 | 94.1 | 52.7 | 59.1 | 0.4 | 41.3 | 26.9 | 27.9 | 20.9 | 23.2 | 26.3 | 92.7 | 17.3 | 4.8 | 25.6 | 9.4 | 7.2 | 7.5 | 27.3 | 24.1 | 16801 |
| $CH_4 \xrightarrow{\zeta} CH_3 + H$ | 54.9 | 54.9 | 54.7 | 53.1 | 54.1 | 109.7 | 0.9 | 0.7 | 0.5 | | 20.9 | 0.6 | 54.7 | 107.5 | 1.2 | | | 0.5 | 0.3 | | | 0.4 | 12932 |
| $C_2H_2 \xrightarrow{\zeta} C_2H + H$ | 15.2 | 70.8 | 26.9 | 68.4 | 70.0 | 37.1 | | | 0.3 | 0.2 | 0.4 | 0.2 | 67.9 | 138.8 | | | 0.3 | 0.5 | | | | | 12634 |
| $He^+ + CO \longrightarrow C^+ + O + He$ | 40.0 | 36.7 | 26.6 | 48.8 | 45.6 | 52.8 | 19.5 | 17.5 | 7.7 | 12.4 | 18.2 | 5.0 | 54.7 | 102.5 | 1.2 | | 14.1 | 2.1 | 6.9 | 9.7 | 3.2 | 4.4 | 12477 |
| $H_3^+ + N \longrightarrow NH_2^+ + H$ | 40.7 | 31.5 | 21.5 | 87.9 | 16.3 | 34.6 | 85.0 | 12.6 | 88.6 | 7.8 | 8.9 | 1.8 | 7.1 | 24.7 | 98.8 | 1.3 | 5.6 | 29.2 | 68.1 | 79.0 | 9.1 | 18.5 | 11409 |
| $C_2H_3^+ \xrightarrow{e^-} C_2H + H_2$ | 12.2 | 44.7 | 16.8 | 43.9 | 44.5 | 52.2 | | | | 0.2 | 0.4 | 0.2 | 42.6 | 86.0 | | | 0.3 | 0.5 | | | | | 8349 |
| $C^+ + O_2 \longrightarrow CO^+ + O$ | 20.0 | 21.8 | 16.8 | 28.9 | 27.9 | 32.1 | 20.8 | 10.5 | 12.8 | 7.8 | 9.8 | 1.9 | 30.8 | 56.2 | 8.6 | 1.3 | 8.0 | 0.5 | 8.2 | 2.3 | 1.9 | 1.2 | 7652 |
| $CH_3^+ + H_2 \longrightarrow CH_5^+ + h\nu$ | 23.0 | 23.1 | 0.4 | 22.0 | 23.3 | 45.3 | 113.7 | 115.2 | 0.3 | 0.2 | 23.1 | | 23.4 | 44.9 | 1.9 | | | 0.5 | | | | 0.4 | 7646 |
| $H_2 \xrightarrow{\zeta} H^+ + e^- + H$ | 29.7 | 13.8 | 28.1 | 46.0 | 13.2 | 11.9 | 49.1 | 30.8 | 12.8 | 16.4 | 0.4 | 5.0 | 5.8 | 18.0 | 14.8 | 5.3 | 24.5 | 7.3 | 4.6 | 4.1 | 13.6 | 25.7 | 7516 |
| $CH_4 \xrightarrow{\zeta} CH_2 + H_2$ | 30.1 | 30.2 | 30.5 | 29.1 | 30.2 | 59.1 | 3.5 | 2.1 | 0.3 | 0.5 | 17.8 | | 30.5 | 59.0 | 0.6 | | 0.3 | 0.5 | | | | 0.4 | 7233 |
| $He^+ + H_2 \longrightarrow H_2^+ + He$ | 21.4 | 19.3 | 19.9 | 30.3 | 24.8 | 28.3 | 16.4 | 13.3 | 6.1 | 9.4 | 8.9 | 4.3 | 20.5 | 41.0 | 5.6 | 1.3 | 9.1 | 2.1 | 8.2 | 1.6 | 1.9 | 5.2 | 6662 |
| $H_3^+ \xrightarrow{e^-} H + H + H$ | 20.0 | 16.3 | 24.2 | 34.7 | 25.6 | 22.6 | 8.4 | 14.7 | 12.5 | 10.4 | 12.0 | 4.8 | 17.4 | 39.3 | 1.2 | 13.2 | 3.2 | 19.8 | 7.6 | 3.8 | 7.1 | 11.7 | 6638 |
| $H_3^+ + CO \longrightarrow HCO^+ + H_2$ | 26.0 | 19.5 | 13.7 | 34.6 | 24.0 | 27.0 | 1.8 | 10.5 | 18.1 | 9.4 | 9.3 | 1.5 | 15.0 | 40.5 | 10.5 | 27.3 | 5.3 | 25.0 | | 10.6 | 7.8 | 13.3 | 6632 |
| $N_2 \xrightarrow{\zeta} N + N$ | 6.4 | 6.1 | 28.1 | 26.8 | 10.1 | 8.8 | 58.4 | 4.2 | 29.0 | 28.6 | 0.9 | 2.6 | 37.4 | 22.5 | 56.8 | 0.9 | 17.3 | 47.4 | 46.7 | 47.5 | 1.3 | 0.4 | 6005 |
| $C^+ + CH_4 \longrightarrow C_2H_3^+ + H$ | 31.5 | 29.0 | 8.6 | 28.6 | 28.7 | 29.6 | 0.4 | | | 0.2 | 2.2 | 0.1 | 28.7 | 57.3 | | | 0.3 | 0.5 | | | | | 5839 |
| $He^+ + O_2 \longrightarrow O^+ + O + He$ | 15.6 | 14.5 | 9.8 | 23.1 | 19.4 | 21.4 | 13.7 | 4.2 | 6.1 | 8.3 | 6.7 | 4.4 | 16.6 | 33.1 | 6.2 | | 8.0 | 1.0 | 7.2 | | 1.3 | 6.0 | 5192 |
| $CH_5^+ \xrightarrow{e^-} CH_3 + H_2$ | 20.7 | 20.4 | 20.3 | 19.9 | 20.9 | 41.5 | 0.4 | | 0.3 | | 8.4 | 0.2 | 20.3 | 41.0 | 0.6 | | | 0.5 | | | | | 4939 |
| $C + O_2 \longrightarrow CO + O$ | 1.4 | 0.2 | 1.2 | 15.3 | 20.9 | 6.9 | 5.3 | 4.9 | 0.8 | 34.6 | 4.0 | 10.5 | 5.5 | 42.1 | 0.6 | | 24.5 | 0.5 | 0.3 | | | 3.6 | 4170 |
| $H_3O^+ \xrightarrow{e^-} OH + H + H$ | 6.2 | 7.5 | 37.5 | 12.1 | 13.2 | 11.3 | 9.3 | 46.1 | 5.3 | 2.1 | 4.9 | 2.1 | 11.6 | 23.0 | 5.6 | 2.6 | 2.1 | 3.6 | 6.3 | 1.1 | 1.9 | 1.2 | 3968 |
| $C_4H_2^+ \xrightarrow{e^-} C_4H + H$ | 0.7 | 1.1 | 0.4 | 1.4 | 7.0 | | | | | | | | 2.9 | 40.5 | | | | | | | | | 3872 |
| $C + C_4H \longrightarrow C_5 + H$ | 1.6 | 0.9 | 0.8 | 11.2 | 3.1 | 0.6 | | | | 0.2 | | | 1.6 | 53.9 | | | 0.3 | 0.5 | | | | | 3659 |
| $CO \xrightarrow{\zeta} C + O$ | 2.3 | 0.7 | | 13.8 | 17.8 | 6.9 | 4.0 | 4.2 | | 28.1 | 3.6 | 8.8 | 4.7 | 34.8 | | | 20.0 | 0.5 | 0.3 | | | 3.2 | 3577 |
| $C_2H_3^+ \xrightarrow{e^-} C_2H_2 + H$ | 1.4 | 19.7 | 7.8 | 18.6 | 19.4 | 22.6 | | | | 0.2 | 0.4 | 0.1 | 18.9 | 37.6 | | | | 0.5 | | | | | 3461 |
| $C + C_2H_2 \longrightarrow C_3H + H$ | 2.1 | 3.2 | 0.8 | 10.9 | 30.2 | 1.3 | | | | 0.2 | | 0.1 | 5.8 | 46.6 | | | 0.3 | 0.5 | | | | | 3453 |
| $C^+ + CH_4 \longrightarrow C_2H_2^+ + H_2$ | 10.6 | 13.2 | 22.7 | 13.1 | 12.4 | 7.5 | | | | 0.2 | 0.9 | | 13.2 | 25.8 | | | | 0.5 | | | | | 2844 |
| $H_3^+ + C_3H_2 \longrightarrow C_3H_3^+ + H_2$ | 1.8 | 3.2 | 0.8 | 11.2 | 33.3 | 1.3 | | | | | | | 5.8 | 29.8 | | | | 0.5 | | | | | 2775 |
| $NH_4^+ \xrightarrow{e^-} NH_2 + H + H$ | 3.7 | 4.3 | 27.3 | 22.3 | 5.4 | 3.1 | 38.0 | 1.4 | 26.6 | 15.4 | 0.4 | 5.0 | 14.5 | 11.8 | 38.3 | 0.9 | 8.5 | 2.1 | 35.9 | 40.7 | | 1.6 | 2630 |
| $CH_5^+ \xrightarrow{e^-} CH_4 + H$ | 11.3 | 11.1 | 10.9 | 10.7 | 10.8 | 22.6 | | | | | 3.6 | 0.1 | 11.1 | 21.9 | | | | 0.5 | | | | | 2627 |
| $NH_4^+ \xrightarrow{e^-} NH_3 + H$ | 3.7 | 4.3 | 26.9 | 22.9 | 5.4 | 2.5 | 36.3 | 1.4 | 26.1 | 15.2 | 0.4 | 4.8 | 14.5 | 11.2 | 36.4 | 0.9 | 8.5 | 2.6 | 34.2 | 39.6 | | 1.6 | 2551 |
| $H_3^+ + S \longrightarrow HS^+ + H_2$ | | | | 42.5 | | | | | | 0.9 | | 130.6 | | | | | 1.1 | 0.5 | | | | 0.4 | 2519 |
| $H_3^+ + N_2 \longrightarrow HN_2^+ + H_2$ | 7.8 | 5.9 | 6.6 | 14.0 | 9.3 | 8.8 | 0.4 | 4.2 | 6.4 | 2.8 | 3.6 | 1.8 | 4.2 | 12.4 | 3.7 | 2.6 | 0.3 | 128.6 | 0.3 | 3.8 | 1.9 | 4.0 | 2413 |
| $H_3O^+ + C_2H_2 \longrightarrow H_5C_2O^+ + h\nu$ | 6.2 | 8.4 | 2.7 | 8.2 | 8.5 | 3.8 | | | | | 0.9 | | 8.2 | 16.3 | | | | 0.5 | | | | | 2342 |
| $C^+ + C_2H_2 \longrightarrow C_3H^+ + H$ | 0.9 | 1.4 | 0.4 | 5.8 | 13.9 | 0.6 | | | | | | | 8.9 | 36.0 | | | | 0.5 | | | | | 2339 |
| $CH_5^+ + CO \longrightarrow HCO^+ + CH_4$ | 9.9 | 9.8 | 9.8 | 9.6 | 10.1 | 20.1 | | | | | 3.1 | 0.1 | 10.0 | 19.7 | | | | 0.5 | | | | | 2328 |

***Maybe with $HCO^+$***

***Maybe we should actually measure fractional abundances rel. $HCO^+$***

## Some random thoughts in conclusion

*Sensitivity analysis squared:*
*how sensitive is a sensitivity analysis?*

*Not clear that any results are transferrable*

*What IS an important reaction / species ?*

*Matching observations?*

# The most important reactions*

$$He \xrightarrow{\zeta} He^+ + e^-$$
$$H_2 \xrightarrow{\zeta} H_2^+ + e^-$$
$$H_3^+ + O \longrightarrow OH^+ + H_2$$
$$C^+ + H_2 \longrightarrow CH_2^+ + h\nu$$
$$C^+ + O_2 \longrightarrow O^+ + CO$$
$$O_2 \xrightarrow{\zeta} O + O$$
$$CH_4 \xrightarrow{\zeta} CH_3 + H$$
$$C_2H_2 \xrightarrow{\zeta} C_2H + H$$
$$He^+ + CO \longrightarrow C^+ + O + He$$
$$H_3^+ + N \longrightarrow NH_2^+ + H$$
$$C_2H_3^+ \xrightarrow{e^-} C_2H + H_2$$
$$C^+ + O_2 \longrightarrow CO^+ + O$$
$$CH_3^+ + H_2 \longrightarrow CH_5^+ + h\nu$$
$$H_2 \xrightarrow{\zeta} H^+ + e^- + H$$
$$CH_4 \xrightarrow{\zeta} CH_2 + H_2$$
$$He^+ + H_2 \longrightarrow H_2^+ + He$$
$$H_3^+ \xrightarrow{e^-} H + H + H$$
$$H_3^+ + CO \longrightarrow HCO^+ + H_2$$
$$N_2 \xrightarrow{\zeta} N + N$$
$$C^+ + CH_4 \longrightarrow C_2H_3^+ + H$$
$$He^+ + O_2 \longrightarrow O^+ + O + He$$
$$CH_5^+ \xrightarrow{e^-} CH_3 + H_2$$
$$C + O_2 \longrightarrow CO + O$$
$$H_3O^+ \xrightarrow{e^-} OH + H + H$$