

The background of the slide is filled with numerous question marks of varying sizes and colors, including shades of purple, pink, and white, creating a sense of uncertainty and inquiry.

Uncertainty? in UDfA!

***andrew markwick-kemper
university of manchester***



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

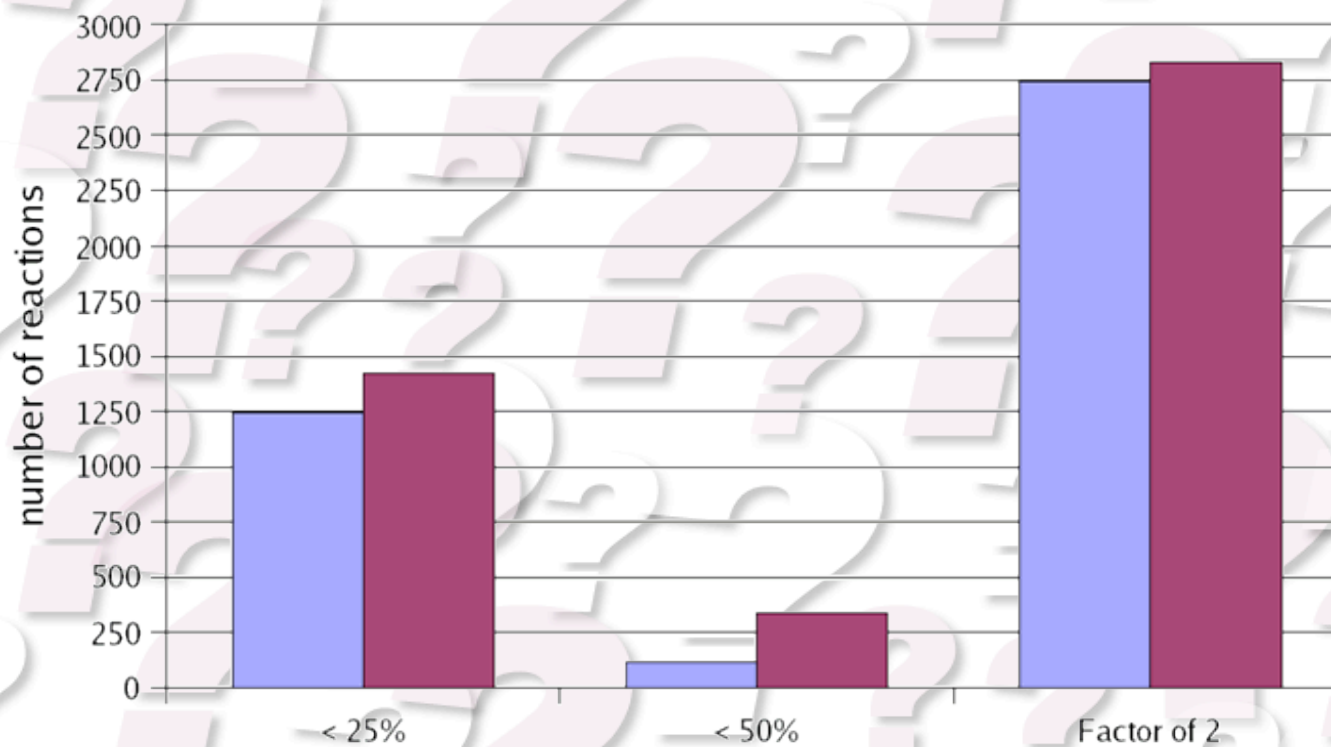
over 1100 new or revised rate coefficients

'historical data'

www.udfa.net

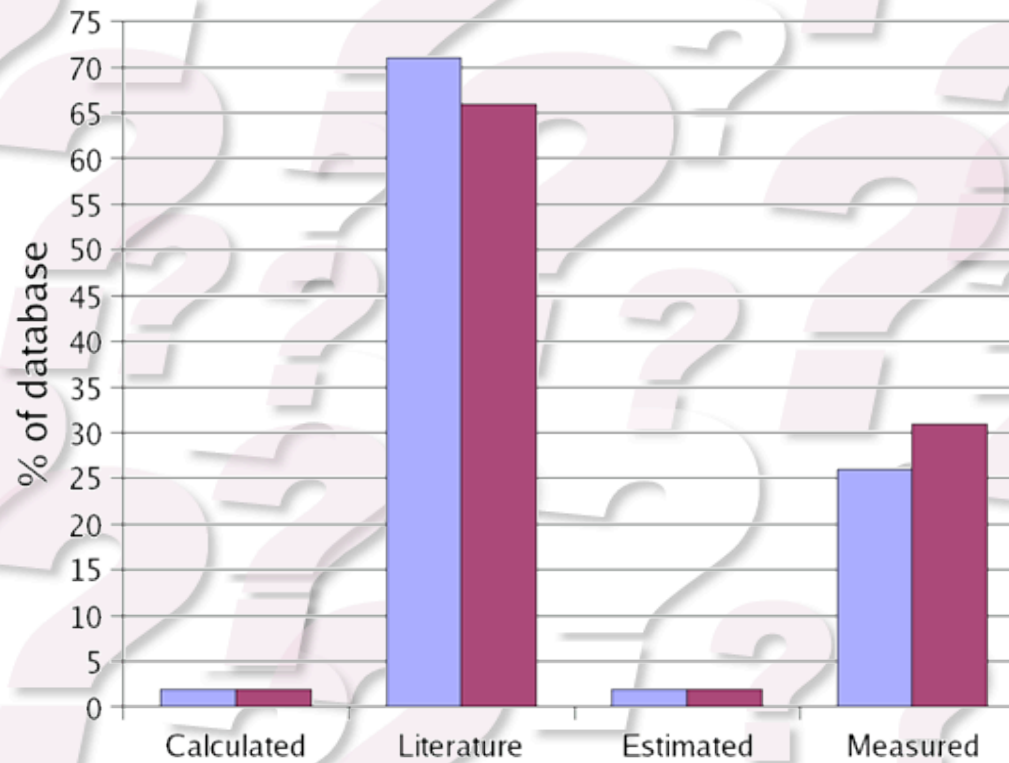
future?

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 in astrochemistry*

A. J. Markwick-Kemper

University of Virginia, Astronomy Department, Charlottesville, VA 22904, USA,
amk3j@virginia.edu

The data was compiled from the JPL astrochemical kinetics database (http://www.astrochem.org) and the IUPAC kinetic data bank. The reactions were selected based on their importance in the ISM, as determined by the reaction rate coefficients. The reactions were selected based on their importance in the ISM, as determined by the reaction rate coefficients.

The IUPAC database (http://www.astrochem.org) was used to determine the reaction rate coefficients, which were then used to determine the importance of each reaction in the ISM. The reactions were selected based on their importance in the ISM, as determined by the reaction rate coefficients.

Q&A

Q. Which reaction rate coefficients are most important to know to be confident of the model abundance of species X?

A. The table shows the information for a subset of relevant, observable species in the model. For example, the top 3 reactions affecting the steady-state abundance of CO are the reaction of He ($p = 18.3$), the dissociation of CS by cosmic rays ($p = 24.4$) and the formation of CO by cosmic rays ($p = 60$) ($p = 12.9$).

Q. What about dissociation, species that are not in the table, like CO, H₂O and H₂O⁺?

A. These are included in the table for which $p > 1.2$ for CO, $p = 8.5$ for H₂O. For H₂O, the most significant reaction is the dissociation recombination of H₂O⁺ for which $p = 2.0$.

Q. What all the numbers in the table mean?

A. The numbers in the table are the importance coefficients, which are calculated as follows: $p = 10 \log_{10}(k_{\text{max}}/k_{\text{min}})$ for the dissociation recombination of H₂O⁺, $p = 10 \log_{10}(k_{\text{max}}/k_{\text{min}})$ for other reactions. The table also shows the reaction rate coefficients, k , and the temperature T for the reaction.

Q. Why is the cosmic ray ionization of the main important than He?

A. Because the cosmic ray ionization of the main important than He, because the cosmic ray ionization of the main important than He, because the cosmic ray ionization of the main important than He.

Q. What is the largest single value of p ?

A. $p = 18.8$, for $\text{C}^+ + \text{He} \rightarrow \text{C} + \text{He}^+$. This reaction is important because of its high rate coefficient and its role in the ionization of the ISM.

Q. How many reactions are listed to be totally unimportant?

A. For 1008 out of 1888 reactions, $p = 0$. These reactions are unimportant because their rate coefficients are very low and they do not significantly affect the chemistry of the ISM.

References
 O'Dell, G. L., & Walmsley, C. M. (1998). *Journal of Chemical Kinetics*, 20, 1045-1070.
 JPL astrochemical kinetics database (http://www.astrochem.org)
 IUPAC kinetic data bank (http://kin.nist.gov)

Species	H	He	Li	Be	B	C	N	O	F	Ne	Ar	Si	S	Fe	Ca	Mg	Al	K	V	Mn	Zn	Cu	Ni	Co	Nb	Mo	Ru	Rh	Ir	Os	As	Sb	Bi	Pb	Ba	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Hf	Ta	W	Re	Os	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
CO			

*Note: Some results from the study of steady-state abundances for a set of 1000 reactions. The columns show, for each reaction, the importance coefficient for the reaction in the ISM, which is determined by the reaction rate coefficient and the abundance of the reactants. The values are sorted in descending order of importance. The reactions are listed in the table only if they are important. The table only shows a subset of the reactions in the ISM, as determined by the reaction rate coefficients.



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 in astrochemistry
A. J. Markwick-Kemper
University of Virginia, Astronomy Department, Charlottesville, VA 22904, USA
markwick@jina.com

The above reactions were obtained from a model using a simple quantitative analysis of the reactions between the most abundant molecules and atoms. The most important reactions in astrochemistry are those that affect the abundances of the most abundant molecules and atoms. The results are shown in the table below. The table lists the reaction rate coefficients at 10 K, 100 K, and 1000 K, and the change in the abundance of the reactants and products. The table also lists the reaction rate coefficients at 10 K, 100 K, and 1000 K, and the change in the abundance of the reactants and products. The table also lists the reaction rate coefficients at 10 K, 100 K, and 1000 K, and the change in the abundance of the reactants and products.

Q&A

Q: Which reaction rate coefficients are it most important to know to be modified in the revised abundance of species X?
A: The table shows the information for a subset of various chemical species in the model. For example, the top 3 reactions affecting the abundance of CO are: $CO + H \rightarrow C + OH$ ($k = 1.0 \times 10^{-10}$), $CO + C \rightarrow C_2 + O$ ($k = 1.0 \times 10^{-10}$), and $CO + O \rightarrow CO_2$ ($k = 1.0 \times 10^{-10}$). The rate coefficient for the reaction $CO + H \rightarrow C + OH$ is 1.0×10^{-10} cm³ molecule⁻¹ s⁻¹. The rate coefficient for the reaction $CO + C \rightarrow C_2 + O$ is 1.0×10^{-10} cm³ molecule⁻¹ s⁻¹. The rate coefficient for the reaction $CO + O \rightarrow CO_2$ is 1.0×10^{-10} cm³ molecule⁻¹ s⁻¹.

Q: How many reactions in the UMIST database are essential to the model?
A: In the UMIST database, there are 41 reactions, of which 38 are essential to the model. The reactions are listed in the table below. The table lists the reaction rate coefficients at 10 K, 100 K, and 1000 K, and the change in the abundance of the reactants and products.

Q: What are the essential reactions in the model?
A: The essential reactions in the model are those that affect the abundances of the most abundant molecules and atoms. The results are shown in the table below. The table lists the reaction rate coefficients at 10 K, 100 K, and 1000 K, and the change in the abundance of the reactants and products.

References

McKee, J. C., & O'Dell, S. L. (2007). The UMIST Database for Astrochemistry. *Journal of Chemical Physics*, 127, 124301. doi:10.1063/1.2803062

Reaction	10 K	100 K	1000 K	Change in Reactants	Change in Products	10 K	100 K	1000 K	Change in Reactants	Change in Products	10 K	100 K	1000 K	Change in Reactants	Change in Products
CO + H	1.0e-10	1.0e-10	1.0e-10	-0.5	0.5	CO	H	C	OH		CO	H	C	OH	
CO + C	1.0e-10	1.0e-10	1.0e-10	-1.0	1.0	CO	C	C2	O		CO	C	C2	O	
CO + O	1.0e-10	1.0e-10	1.0e-10	-1.0	1.0	CO	O	CO2			CO	O	CO2		
...

*The table shows results from the study of steady state abundances for a set of 41 reactions. The columns show, for each reaction, the change in the abundance of the reactants and products. The table lists the reaction rate coefficients at 10 K, 100 K, and 1000 K, and the change in the abundance of the reactants and products.



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





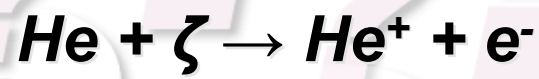
Q

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



?

A





Q

OK, why isn't it



?



Q

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



?



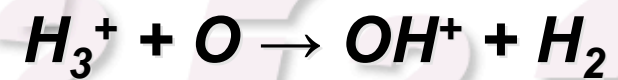
Q

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



?

A



measured by Fehsenfeld (1976)

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

quoted error '< 50%'



Q

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 ₂ H	C ₂ H ₂	C ₂ H ₃ OH	C ₂ S	C ₃ H ₂	CH ₃ CCH	CH ₃ CN	CH ₃ OH	CN	CS	H ₂ CO	H ₂ S	HC ₃ N	HC ₇ N	HCN	HCO ⁺	HCS ⁺	HN ₂ ⁺	HNC	NH ₃	O ₂	SO ₂	<i>P_{total}</i>	
He $\xrightarrow{\gamma}$ 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 $\xrightarrow{\gamma}$ 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 \rightarrow 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 \rightarrow CH ₂ ⁺ + hν	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 \rightarrow 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 $\xrightarrow{\gamma}$ 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 $\xrightarrow{\gamma}$ 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 ₂ H ₂ $\xrightarrow{\gamma}$ C ₂ H + 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 \rightarrow 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 \rightarrow 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 ₂ H ₃ ⁺ $\xrightarrow{e^-}$ C ₂ H + 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 \rightarrow 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 \rightarrow CH ₃ ⁺ + hν	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 $\xrightarrow{\gamma}$ 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 $\xrightarrow{\gamma}$ 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 \rightarrow 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 \rightarrow 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 $\xrightarrow{\gamma}$ 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 \rightarrow C ₂ H 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 \rightarrow 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 ₃ ⁺ $\xrightarrow{e^-}$ 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 \rightarrow 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 ₃ O ⁺ $\xrightarrow{e^-}$ 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 ₄ H ₂ ⁺ $\xrightarrow{e^-}$ C ₄ H + H	0.7	1.1	0.4	1.4	7.0								2.9	40.5									3872	
C + C ₄ H \rightarrow 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 $\xrightarrow{\gamma}$ 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 ₂ H ₃ ⁺ $\xrightarrow{e^-}$ C ₂ H 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 ₂ H ₂ \rightarrow C ₃ H + 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 \rightarrow C ₂ H 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 ₃ H ₂ \rightarrow C ₃ H 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 ₃ ⁺ $\xrightarrow{e^-}$ 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 \rightarrow HS ⁺ + H ₂				42.5													1.1	0.5					2519	
H ₃ ⁺ + N ₂ \rightarrow 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 ₃ O ⁺ + C ₂ H ₂ \rightarrow H ₅ C ₂ O ⁺ + hν	6.2	8.4	2.7	8.2	8.5	3.8					0.9		8.2	16.3				0.5					2342	
C ⁺ + C ₂ H ₂ \rightarrow C ₃ H ⁺ + H	0.9	1.4	0.4	5.8	13.9	0.6							8.9	36.0				0.5					2339	
CH ₃ ⁺ + CO \rightarrow 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	



Q

What about obvious important species, like CO, SO or H₂O?



?

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^+ .



Q

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



Q

***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 H₂ and He switch places.

The top non cr reactions are still



and





Q

Won't all these errors cancel out?



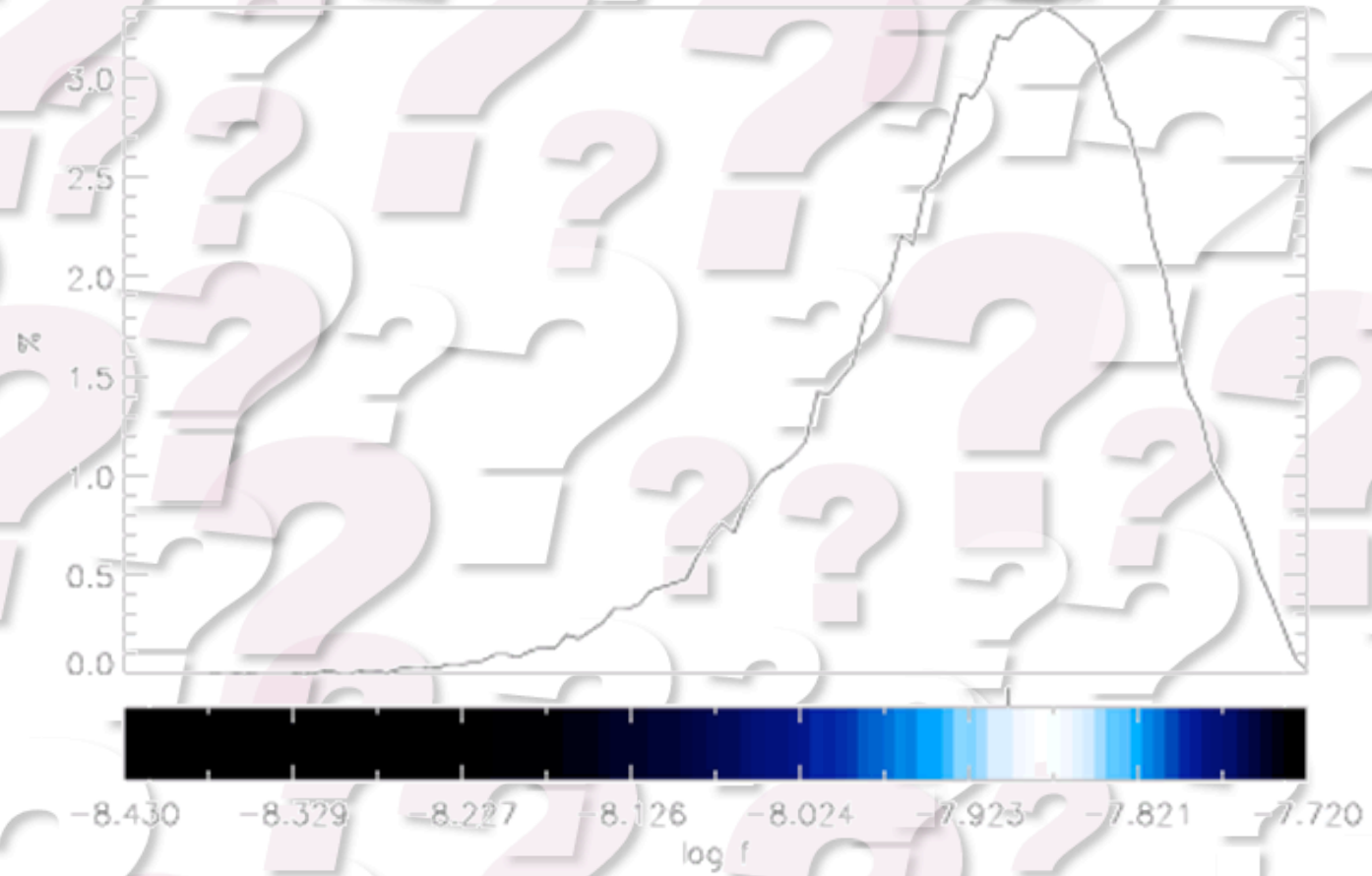
?

A

CS

Formations: 34
Destructions: 13
Reactions: 47

Control: -7.9000001
Mean: -7.9140000
Std Dev: 0.093390003





Q

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



?

A

bsolutely.

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

**e.g. HC₇N abundance uncertain to an order of
magnitude because of a single rate!**

For HC₉N, $p_{\max} = 5521!$

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



Q

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



?

A

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

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



Q

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 ₂ H	C ₂ H ₂	C ₂ H ₃ OH	C ₂ S	C ₃ H ₂	CH ₃ CCH	CH ₃ CN	CH ₃ OH	CN	CS	H ₂ CO	H ₂ S	HC ₃ N	HC ₇ N	HCN	HCO ⁺	HCS ⁺	HN ₂ ⁺	HNC	NH ₃	O ₂	SO ₂	<i>P_{total}</i>	
He $\xrightarrow{\gamma}$ 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 $\xrightarrow{\gamma}$ 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 \rightarrow 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 \rightarrow CH ₂ ⁺ + hν	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 \rightarrow 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 $\xrightarrow{\gamma}$ 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 $\xrightarrow{\gamma}$ 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 ₂ H ₂ $\xrightarrow{\gamma}$ C ₂ H + 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 \rightarrow 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 \rightarrow 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 ₂ H ₃ ⁺ $\xrightarrow{e^-}$ C ₂ H + 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 \rightarrow 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 \rightarrow CH ₂ ⁺ + hν	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 $\xrightarrow{\gamma}$ 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 $\xrightarrow{\gamma}$ 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 \rightarrow 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 \rightarrow 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 $\xrightarrow{\gamma}$ 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 \rightarrow C ₂ H 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 \rightarrow 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 ₃ ⁺ $\xrightarrow{e^-}$ 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 \rightarrow 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 ₃ O ⁺ $\xrightarrow{e^-}$ 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 ₄ H ₂ ⁺ $\xrightarrow{e^-}$ C ₄ H + H	0.7	1.1	0.4	1.4	7.0								2.9	40.5									3872	
C + C ₄ H \rightarrow 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 $\xrightarrow{\gamma}$ 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 ₂ H ₃ ⁺ $\xrightarrow{e^-}$ C ₂ H 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 ₂ H ₂ \rightarrow C ₃ H + 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 \rightarrow C ₂ H 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 ₃ H ₂ \rightarrow C ₃ H 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 ₃ ⁺ $\xrightarrow{e^-}$ 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 \rightarrow HS ⁺ + H ₂				42.5														1.1	0.5				2519	
H ₃ ⁺ + N ₂ \rightarrow 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 ₃ O ⁺ + C ₂ H ₂ \rightarrow H ₅ C ₂ O ⁺ + hν	6.2	8.4	2.7	8.2	8.5	3.8					0.9		8.2	16.3				0.5					2342	
C ⁺ + C ₂ H ₂ \rightarrow C ₃ H ⁺ + H	0.9	1.4	0.4	5.8	13.9	0.6							8.9	36.0				0.5					2339	
CH ₃ ⁺ + CO \rightarrow 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	

A

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*

