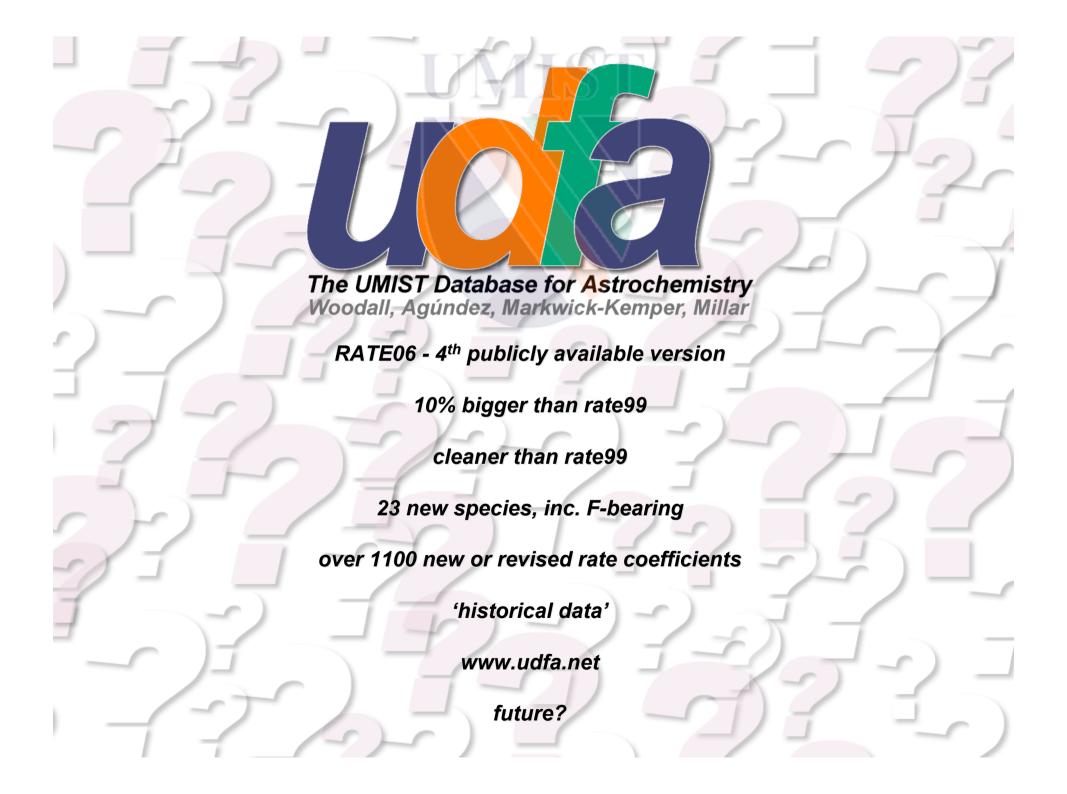
andrew markwick-kemper university of manchester

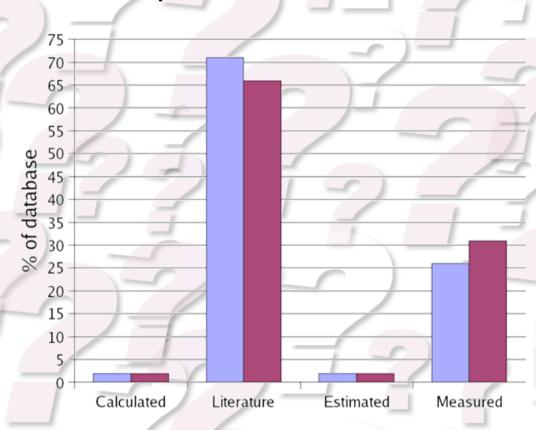






blue = rate99, purple = rate06

Comparison of rate coefficient source



blue = rate99, purple = rate06

The most important reactions in astrochemistry

A. J. Markwick-Kemper

The start ventor record the entire of the property of the entire of the

Q&A

O. Which reaction rate coefficient's is it most

Q. Which reaction rate conflicted to it is not important in those is no conflicted to it is model absorbance of species X? A. The likely independent in the product of the state of the st

efficients are cardiomly varied within their uncertain-ties is a distribution around some mean value. This eany size is often close to the control value, but not

reason about the extent to the control values builded as as.

If the control is a proper was placed as assument of the most investigation proper was placed as consistent of the most investigation and the extent of the control value of the extent of the

are concertain within a factor of 3" etc."

A in UMST on these are of the explore, of which
the last 1.295 1.19 are '< 500 1.230 are within
afractor of 2 mind are within an order of registrate.

Q. Why is the count is ray isolatation of the more
in pertant than that of \$1.5?

is persist than flad of \$1.7.

A. Dick saw th' destroys those infect inly true in \$1.7.

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Q. What it the larged single value of p? A $p_{\rm cos} = 1080$, to $O(\frac{1}{2})^2$ with e^{-1} . Here e^{-1} . Not including counter $p_{\rm cos}$ storm, $p_{\rm cos} = 83$. No $C(\frac{1}{2})^2$ with e^{-1} . On the largest values a replication as the CCO e^{-1} to the largest values are placed as a successful of the Constant of the Largest values of the Constant o

or or operation.

For or operation contribute regarding model value of Chills abservable of Chill abservable of Chill abservable of Child abservab

partied. Q. What should all times either from more the time Q_{ij} . What should all times either from the shortly distinct to example the overallest "ordy" filtract.

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References



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simple questions simple study

(downloadable at asilomar.caltech.edu)

The most important reactions in astrochemistry

A. J. Markwick-Kemper

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O. Which reaction rate coefficient's is it most

Q. Which matches rate coefficient's it is most important in loss in its confident of the smooth discolution of species N. A The Value from the internation for a size of national discolution process in the model. For example, the top D within substant price consists of national discolution and Geoletic states of the (D - B + B) with the states of D of (D - B + B). The states of D of (D - B + B) with the formulation of Geoletic strengths on the (D - B + B) with the formulation of Geoletic strengths of the first (D - B + B) with the formulation of (D - B) with (D - B + B) with (D - B) with (

A. There is no unplie reaction for which p>1.21 for 0.00, as p>1.55 for 9.0. For H₂O, the most sign of card reaction is the dissociative recombination of H₂O₂ for which p=48.0

Q. Woolf all the over nors will combine?

A. The computed abundances when all the rate co floorts are andonly sailed with their uncertain servaluels oftensione to the control value, but not

Now we want to keep over the global accuracy of the model models, "a function which decide and a deal and why data, which decide was the representation of the second model of the second

O'DE IS 20%.

Q. How many reactions in the UMIST database are smooth, in within a factor of 2" etc.?

A in UMST66 there are 41th reactions, of which to 40 are < 195 \110 are < 505 \2342 are within at acts of 2 and 4 are within an order of magnitude.

Q. Why is the count's ray lenkration of the more in meeting than that of 18-2.

Q. What is the large display value of p? A $p_{\rm cor} = 1800$, to $O(\frac{1}{4})^2$, while $O(\frac{1}{4})^2$, while $O(\frac{1}{4})^2$ and $O(\frac{1}{4})^2$. The "extraction for the processing of the processing of the CDQF and the results of $O(\frac{1}{4})^2$, where the results of $O(\frac{1}{4})^2$, which is the processing a supersystem of the processing a three values of $O(\frac{1}{4})^2$ for the results of which is that expire the value reaction to be the Processing of the results of the processing of the results of the results

to distinct our conflict comparing model values (Shi show values). A Did stop (Happil), for most comparing control of Did stop). Happil, for most comparing control of the property and of the conflict of th

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FC 200 OFF +Bir		•	-				22	-	18.7	-	-			48	1.7	-	•	4 🚃	1.7	-	-	200705
C 300 DC 14m C 300 D' 4 DD						-			1.8	12		101				100		2.0	14	2.5	2.0	57794 57988
C-3/0, 0 1 00	100	67.2	10.0	70.0	100	100.0	10.0	186.1	182	20.0		100		12.3	8.4	2.7	2.0	100		2.6	116.6	1778
0, -0+0	200	-	100	100	Sec.	100	8.4	100	290.00	87.8 (II)	-	200	100	17.8	4.0	2.1	8.00	2.0	2.8	20.00	26.1	10001
	100	Sec. 8	66.7	100	No.	100	1.7	8.7	8.5		20.0	an se		10			1.6	8.3			8.4	12902
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C46 - C41 H Bert D - D + 0 + He Hg + N - Heg + H	-	M-7	26.6	-	1000	500.00	18.5	17.6	22	19.4	18.2	100		152		-	2.1	8.8	8.75	22	18.5	1927
H2 +H MH2 +H	-	31.5	21.5	M218	150	26.6	100	12.6		280	11	NR. B	M 200	-	5.2	580	28.2	100			18.5	111400
CAC III GALLAL	10.0	867	16.6	-	100	100		_	_	1.2	34	io io		_	10	107	8-6	_	2.3	100	_	10-9
CH + H (D) +hr	20.0	-	/ TA	20.0	200	100.0	-	10.0	12.8	12		NR.	-		11.20		1.5	8.2	2.3	11.00	쁜	769
Brand State H	-	_	-	_	-	-	_	_	12.8	18.4	_		-		6.0	_	28	4.6	_		PE 2	700 /
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N ₁ − N ₂ − N ₃ − N ₄ − N	-	-	-	=	-		-	1 162	-	-		-		100	1.1	-		-		11.00	14	riot !
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CRY SECTION AND	20.7	20.0	20.0	188	200	40.0	8.4		1-3		16	W 20		1-6 1-6		20	8.5					4000
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C+GHC+H	H.B		1.0	111.2	241	8.6				(12)			K 100			10	8.6				_	ENG.
COC.L.O	2.3	8.7		10.6	178	8.8	4.0	4.2	- 4		3.6					2.1	1.5	1.3			32/	1677
$\begin{array}{c} CdC \stackrel{f}{\longrightarrow} Cdb \rightarrow H \\ C+C_1H \longrightarrow C_1H+H \\ C \hookrightarrow CH_1 \longrightarrow C_2H_2 \rightarrow H_1 \\ H_1^* \rightarrow Cdb \longrightarrow CdC_2 \rightarrow H_2 \end{array}$	2.0	19.7	28	18.6	1704	10 A 10 A 10 A 10 A 10 A			100	12	8.4	F .	100			10	1.5				40	3401
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Contract Charles	5.3		8.4	22.0	148	1,5		_									Ä				- 1	2000
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BUT THE HE	18.3	6.7	82.6	10.0	74	28	8.4	16.3	16.80	6.6	22	100		8.7	11.20	92	2.1	1.8	10.00	2.0	100	2001
	16.6	100	2.6	8.8	544	2.8	5.80	-	2.8	1120	N. H.	MS S		11.6	1.3	200	15.00	36.20	514	100	14	2079
CHC SCHLICH	1.3	12	2.4	-	1007	8.6	_	_	_			- 4	2 100				E	_	_			2074
0+00+N	98		6.30	6.0	100	8.6	20.4	16.4	100.0	15.4				20.8		4.1	HH	16.20	3.6			2015
C AN _ C GA, LCN CA _ D D AN CC _ D D AN	8.7	6.4	-	10.0	85	2.8	3.4	16.88	16.00	3.6	4.0	_	10.0		44	MI	100	2.6	5.6	2.6	3.6	2290
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CHOOL STORY	1.7		10.7	-	100	10.6	8.7		8.0	6.0	-	-	110	52		100	2.5				11	2100
March and A Sales	-	6.6 6.6 6.5	12		-	-	100	3.5		2.9	9.7			-			2.0	100	100	10	22	200
CONTRACT HOD + H	2.6 6.6 2.1		6.0	200 200 200	76	11 A	4.0	2.5	2.0	2.0	22	NE N	_/65	-	1.1		2.6	2.0		100		7000
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F 5 G H G H+H	2.1	3.4	1.8	3.8	200	15.88				1.2						101						1847
ET HING ONT LIN	8.7	8.7	11.21	2.2	167	16.2	7.8		16.10	6.0	9.4	200	2 11	8.6		48	8.6	15.6	8.2		14	1794
CAC DBr+H Rt+CH QR+H _c	18.2	115	8.4	7.0	200	11.2							18.1				1.5				- 1	100 108
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A. J. Markwick-Kemper

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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

we contain productive extracts in users.

The delical displaces (Mail rest 1887 to Berlinet) accounts on the contained minus in the medical accounts which is the contained account of the contained accounts which is the contained account of the contained accounts accounts accounts accounts accounts account of the contained accounts account account of the contained accounts account account accounts accounts account account accounts accounts account account accounts account account accounts account account accounts account account account account accounts account account account accounts account accoun

O. Which reaction rate coefficient's is it most

Q. Which matches rate coefficient's it is most important in loss in its confident of the smooth discolution of species N. A The Value from the internation for a size of national discolution process in the model. For example, the top D within substant price consists of national discolution and Geoletic states of the (D - B + B) with the states of D of (D - B + B). The states of D of (D - B + B) with the formulation of Geoletic strengths on the (D - B + B) with the formulation of Geoletic strengths of the first (D - B + B) with the formulation of (D - B) with (D - B + B) with (D - B) with (

A. There is no implementation by which $p>1.2 \, {\rm fm}$ 00, and $p>8.5 \, {\rm fm}$ 90. For Hy0, the most slip in little reaction is the dissociative recombination of Hy0-, for which p=48.0

Q. Woolf all the over nors will combine?

A. The computed abundances when all the rate co floorts are andonly sailed with their uncertain servalue's oftensione to the control value, but not

deep. Of the word in improve the global assumpty of the model investity, at leastful adult of each and and at the only often, which deep least the real and at the only often, which deep least the real action of the old provided by the same one content of the old provided by the same one content of the old provided by the ol

O'DE IS 20%.

Q. How many reactions in the UMINT database are smooth is within a factor of 2° etc.?

A in UMST66 there are 41th reactions, of which to 40 are < 195 \110 are < 505 \2342 are within at act or of 2 and 4 are 'within an order of magnitude.

Q. Why is the countie may lenkration of the more immediate than that of 16-2.

Q. What is the large display (Gines dy.? Q. What is the large display (Gines dy.? Constitute year. Not including committing as times, $p_{max} = 1800$, $p_{max} = 1800$, and the CoLLY and the relation (b = 0), $p_{max} = 0.00$. The highest values are display associated with the gaussian of the world (b = 0) for the chemical density. But is, that expairs the first exact as both the latter produced of the chemical density in the first exact as the latter of the constitution of the constitution of the chemical density of a reference in this in the constitution of the constituti

to distinct our conflict comparing model values (Shi show values). A Did stop (Happil), for most comparing control of Did stop). Happil, for most comparing control of the property and of the conflict of th

points: (V, W) about at these other has deady data, he complet the one also leady these. A This ensular results if the control leady these is the control of the control

References

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the Section of the		-	-	-		- /	= :	_		8.4			-	63					W 267	79/8	1
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$H_{i_1}^{C} \perp CO \longrightarrow HCD^- \perp H_{i_1}$ $H_{i_2} \stackrel{f}{\longrightarrow} Hc_1 Hc$ $C^- \perp CD \longleftarrow CHC_1 Hc$ $He^+ \perp O \longrightarrow O' \perp O \perp Hc$ $CH_{i_1}^{C} \stackrel{f}{\longrightarrow} CH_{i_2} \perp H_{i_3}$	26.0	18.5	10.7	26.0	200	27.8	<u> </u>	9.5		16.70		C. I	18.6	20.0	SE .		_		10.0	1800	
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CO _ C+ O	23	12	- 11	19.6	-	E.B		62	400	2.0		27 100					1.2		12	100	
DAC COM-N					100		-	- 4		8.4							6-4		-	100	
C+CH CHIN	2.5	82	28	10.0	100	20 A		- 4	12		P 1	100				1.6				3-63	
$\begin{array}{c} \mathbb{C}d\mathbb{C} \stackrel{f}{\leftarrow} \mathbb{C}Bb + \mathbb{H} \\ \mathbb{C} + \mathbb{I}_{0} \mathbb{H}_{1} & = \mathbb{I}_{0} \mathbb{H} + \mathbb{H} \\ \mathbb{C}^{+} + \mathbb{C}B_{1} & = \mathbb{C}B_{1} + \mathbb{H}_{1} \\ \mathbb{H}_{1}^{+} + \mathbb{C}db & = \mathbb{C}d\mathbb{C} + \mathbb{H}_{1} \end{array}$	18.8	102	20.7	10.1	104	53			1.2	1.0		12 251				1.6				3401 3463 2844 2775	
$B_{ij}^{*} : ACAb \longrightarrow CAB_{ij}^{*} : Bb$ $BB_{ij}^{*} : - Bb : B : B$ $CB_{ij}^{*} : - CBb : B$ $BB_{ij}^{*} : - Bb : B$ $BC_{ij}^{*} : - Bb : B$ $BC_{ij}^{*} : - BB_{ij}^{*} : B$ $BC_{ij}^{*} : - BCC_{ij}^{*} : BCC_$	153	3.2	190	111.2	100	16.20	_	_ /_	_		_ :		_			1.6			_	5775	
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Hr + 5 100 107				100			_	-,-	1.1				_				_	-	1.4	2001	
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O+ th: tO+N	HX		6.0	6.0	107	8.6	20.4	14	15.4	1.0	100 M	150	22.8		4.1		1.3	1.6	11.80	2265	
NC TOTAL LAN	8.7	5.6	2.86	10.0	165		3.1	48	3.5	4.0		10.8	14.5	6.6	W .		2.6	14	8.0	2290	
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C"+ O.Hr C" + Hr	88	111	1.0	14	1167	1.6			12			12 15								1604	
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CHILDR THOUGH	1.2			8.4					_			14			_					1922	
C-2,005 - HC10 1 H	2.3	28	38.40		100	2.5	25.2	8.7 20.	6.00	8.4	-	18 28	26.5		a	1.6		1.5	1.0		
$C_iH_i^* \stackrel{\mathcal{L}}{\sim} G_iH_i \cdot H_i$	1		14	_	_		8.					18.1								10/4	
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$CR_1 \stackrel{L}{\hookrightarrow} CR_1 \cdot R_1$ $CR_2 \stackrel{L}{\hookrightarrow} CR_1 \cdot R_2 \stackrel{L}{\hookrightarrow} L_1$ $R^2 \cdot R^2 \stackrel{L}{\hookrightarrow} R_2 \stackrel{L}{\hookrightarrow} R_2$ $R^2 \cdot R^2 \stackrel{L}{\hookrightarrow} R_2 \stackrel{L}{\hookrightarrow} R_2$ $R^2 \cdot R^2 \stackrel{L}{\hookrightarrow} R_2 \stackrel{L}{\hookrightarrow} R_2 \stackrel{L}{\hookrightarrow} R_2$ $R^2 \cdot R^2 \stackrel{L}{\hookrightarrow} R_2 \stackrel{L}{\hookrightarrow} R$		2.6			_		1	8.7				12 82	100							161 161 167 165	
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CO I MO - NO I M	2.5	2.3	2.7	2.6	20	24	14	E 12	100	1.1	10		2.0			1.5	1.7	1.5	12	100	
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about the asterisk:

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choice of 'p'

The most important reactions in astrochemistry

A. J. Markwick-Kemper

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O. Which reaction rate coefficient's is it most

Q. Which reaction rate coefficients in it much appearable to zero be confident of the medial absorbance of species X? A. The Basic charges have shown that the subset of various absorbance in the residual. For example, the top is active, rather up the description of the confidence of Collective species on the residual reaction of Collective species of principles of the confidence of the collective species of the confidence of the collective of Collective species of the collective s

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efficients are cardiomly valled within their uncertain-ties is a distribution around some mean value. This eanwalue's oftensione to the control value, but not

are concerning. William of fails of \$2.7 dts.?

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References



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Methodology

One control model: 'standard' parameters

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



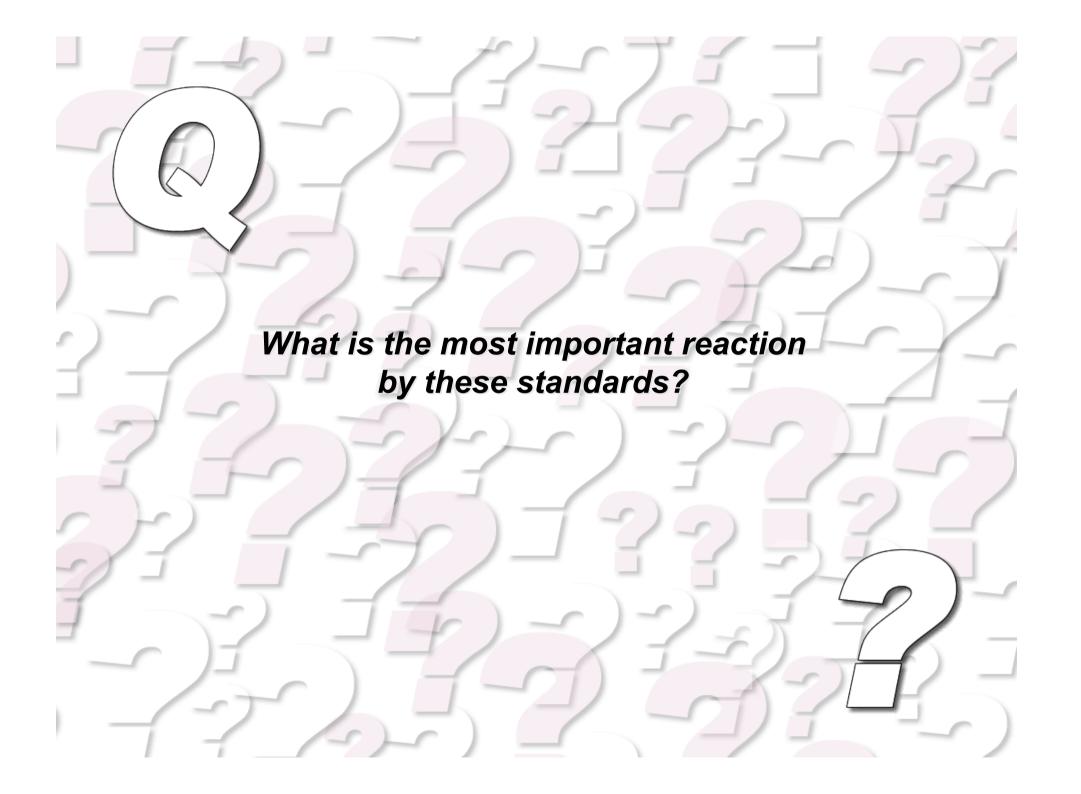
Compute the difference between the results so obtained as a percentage of the control value (= p), on a species by species basis.

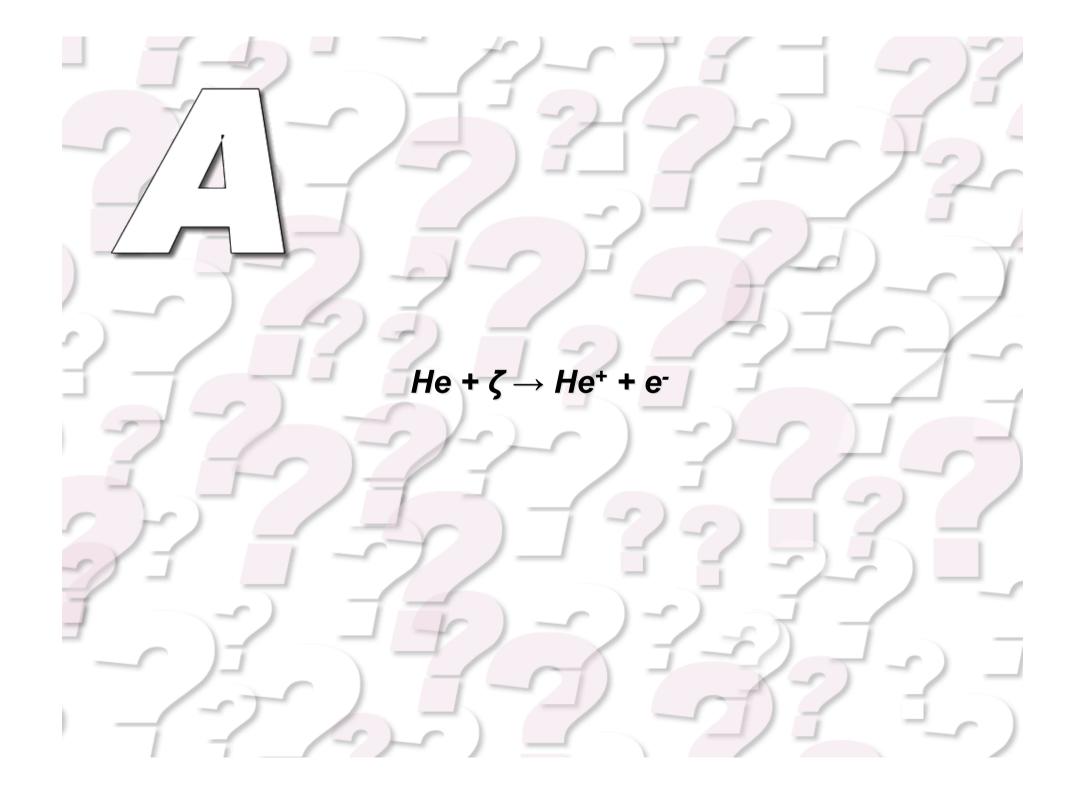
e.g. if p = 0, there was no effect on the species abundance by varying the reaction rate coefficient.

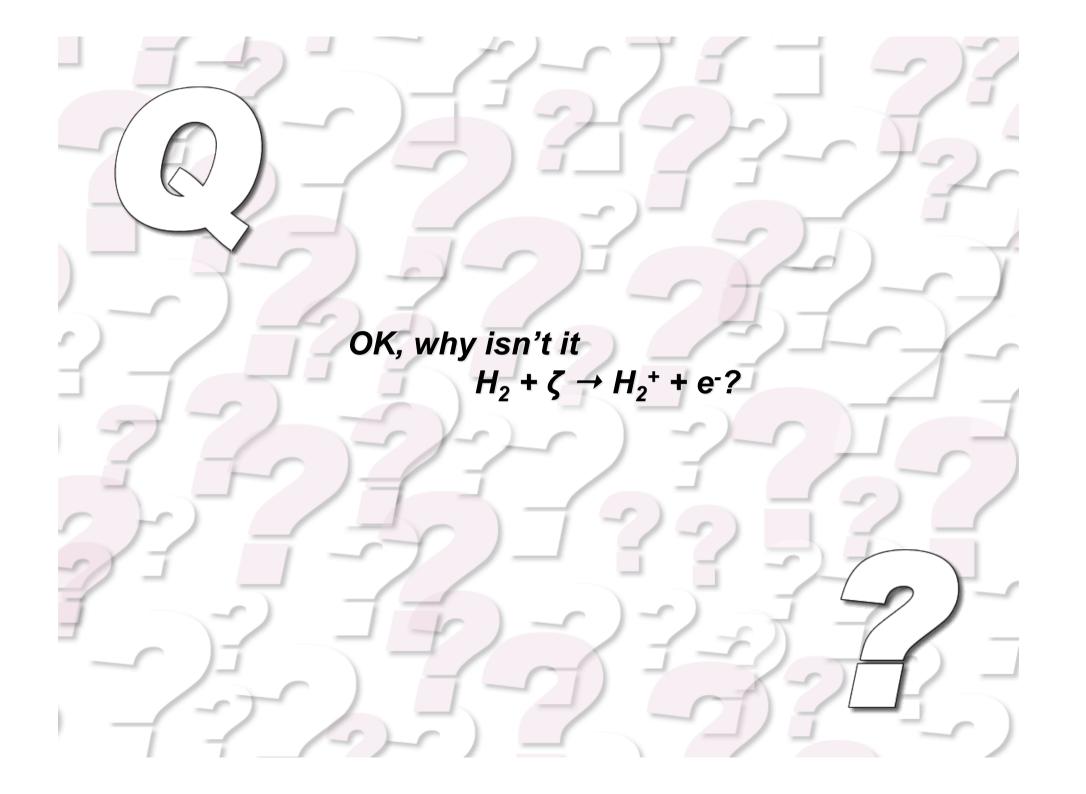
The bigger p is, the more significant the reaction is for that species

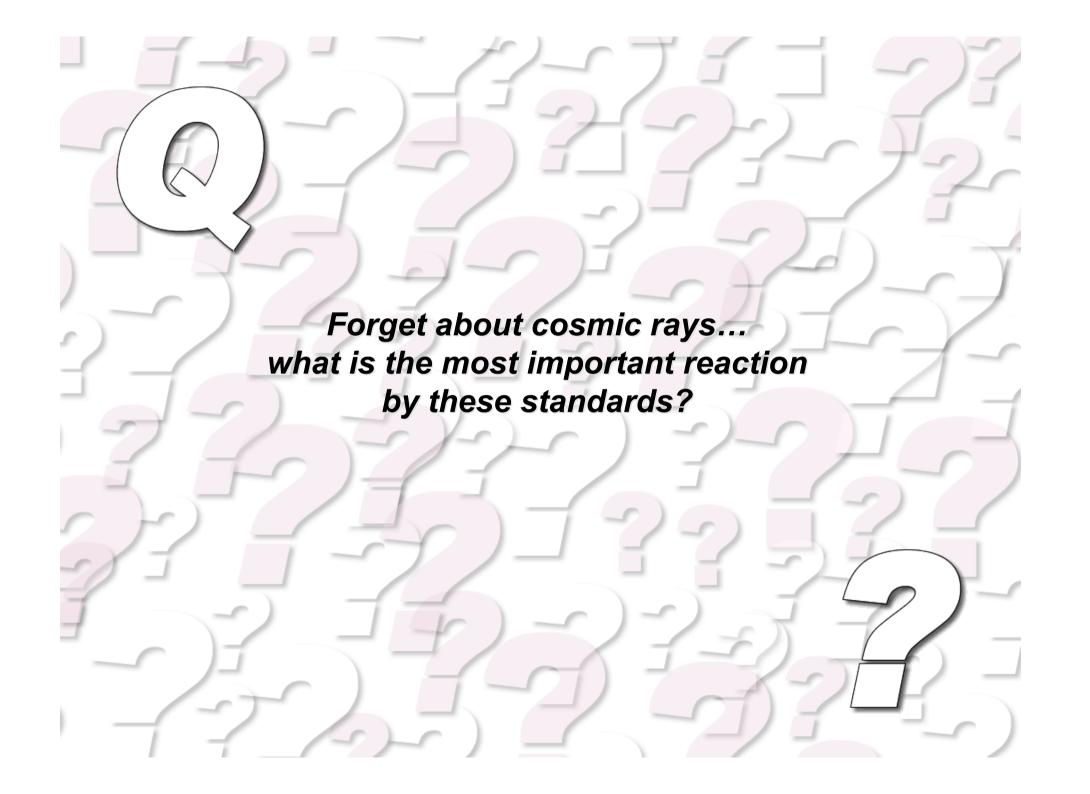
Summing p over all species, we can work out the 'most important reaction' * caveat caveat etc etc

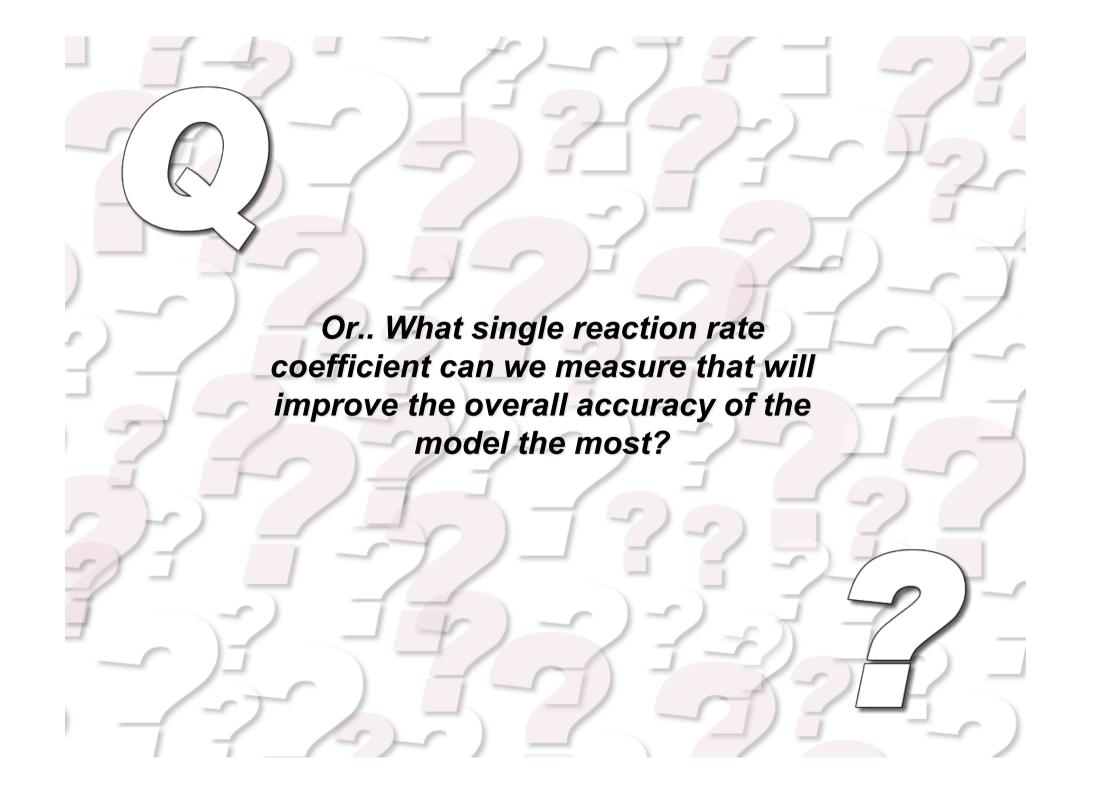


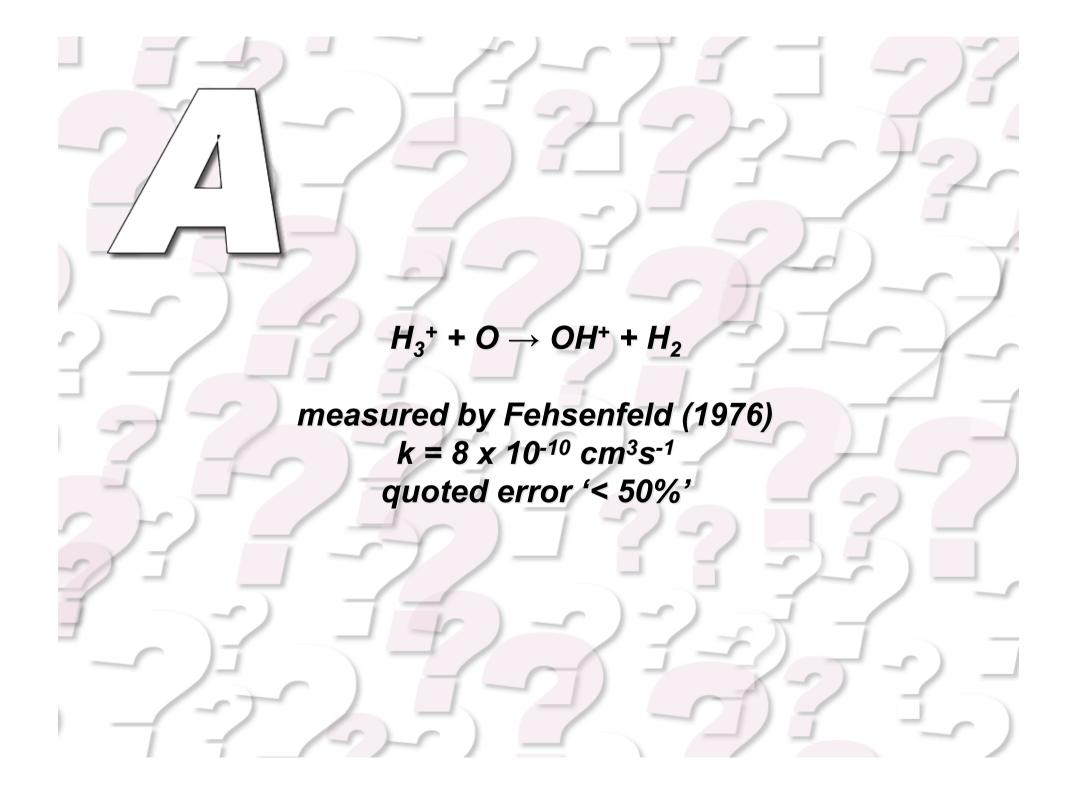


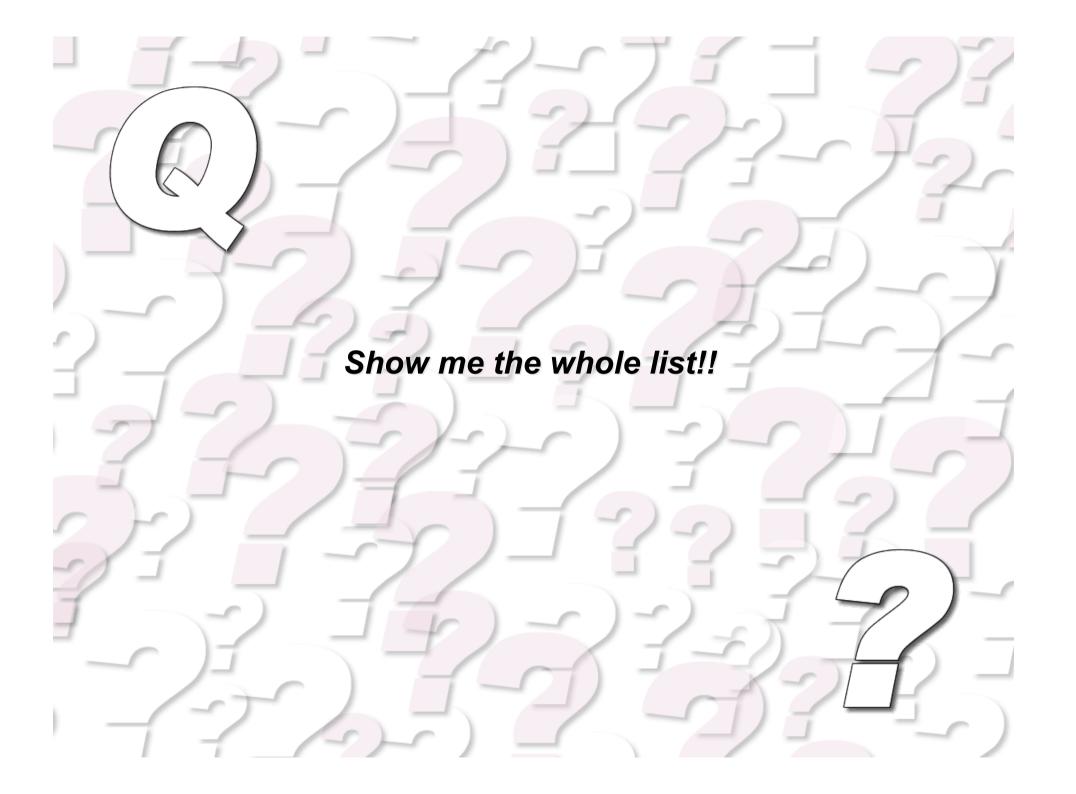




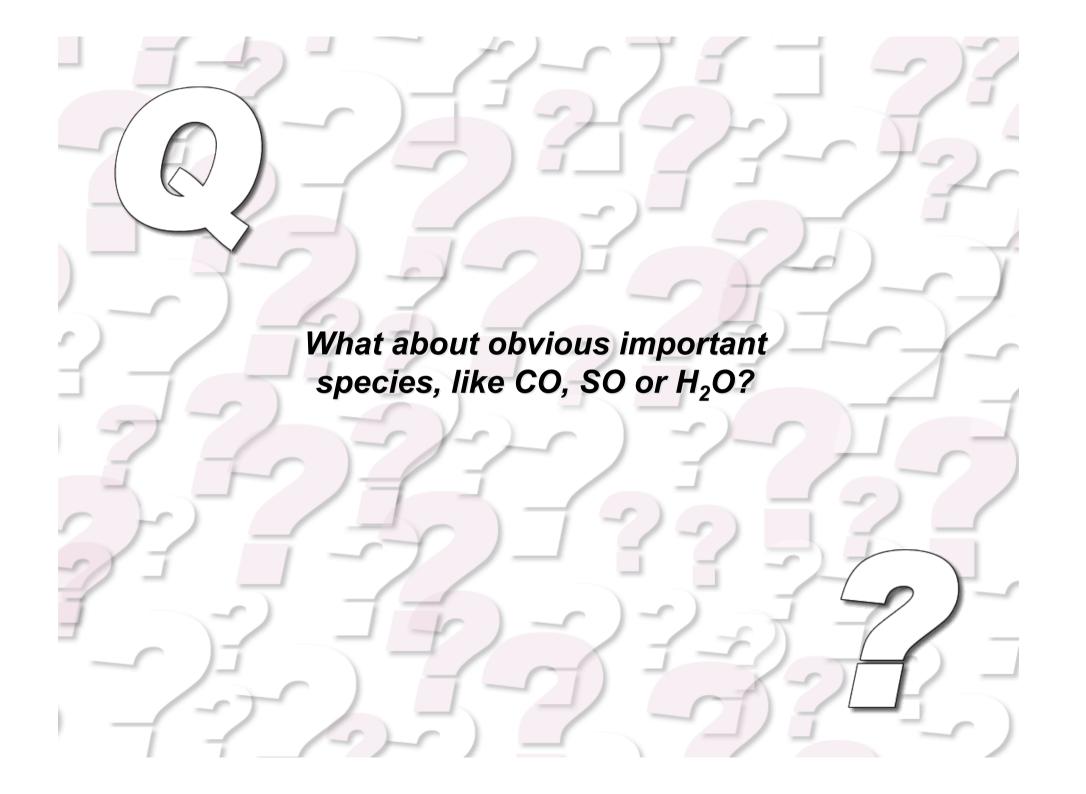


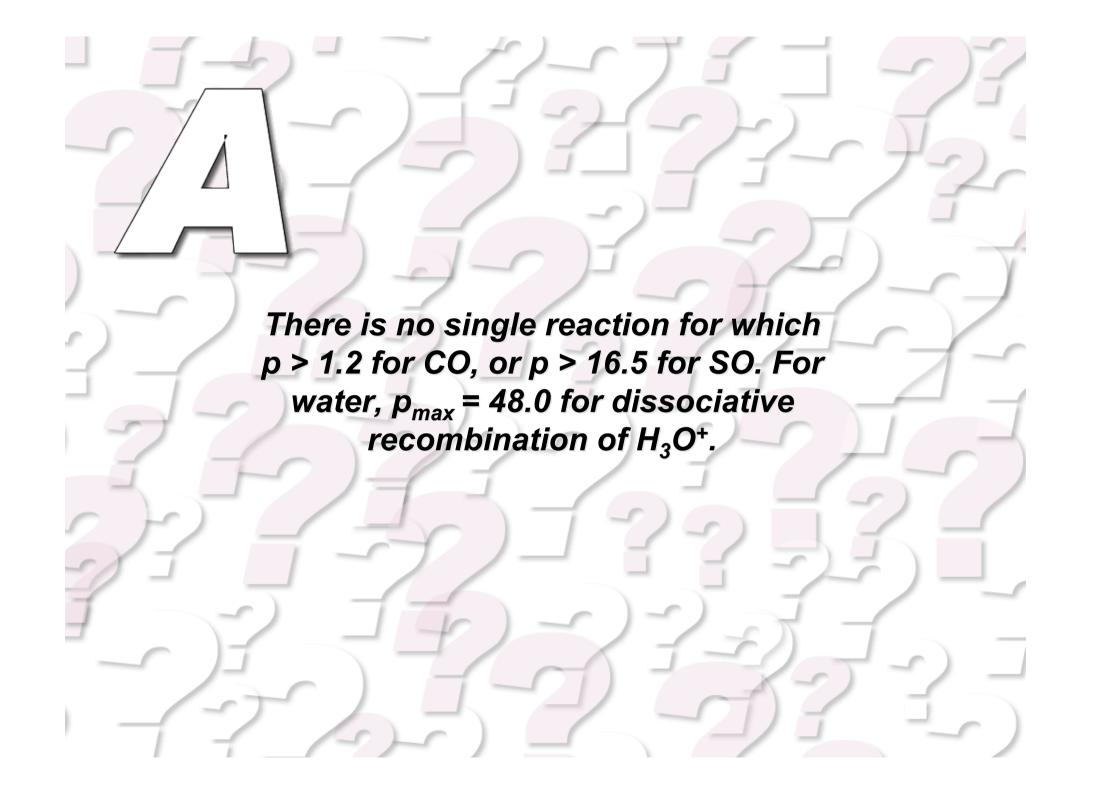


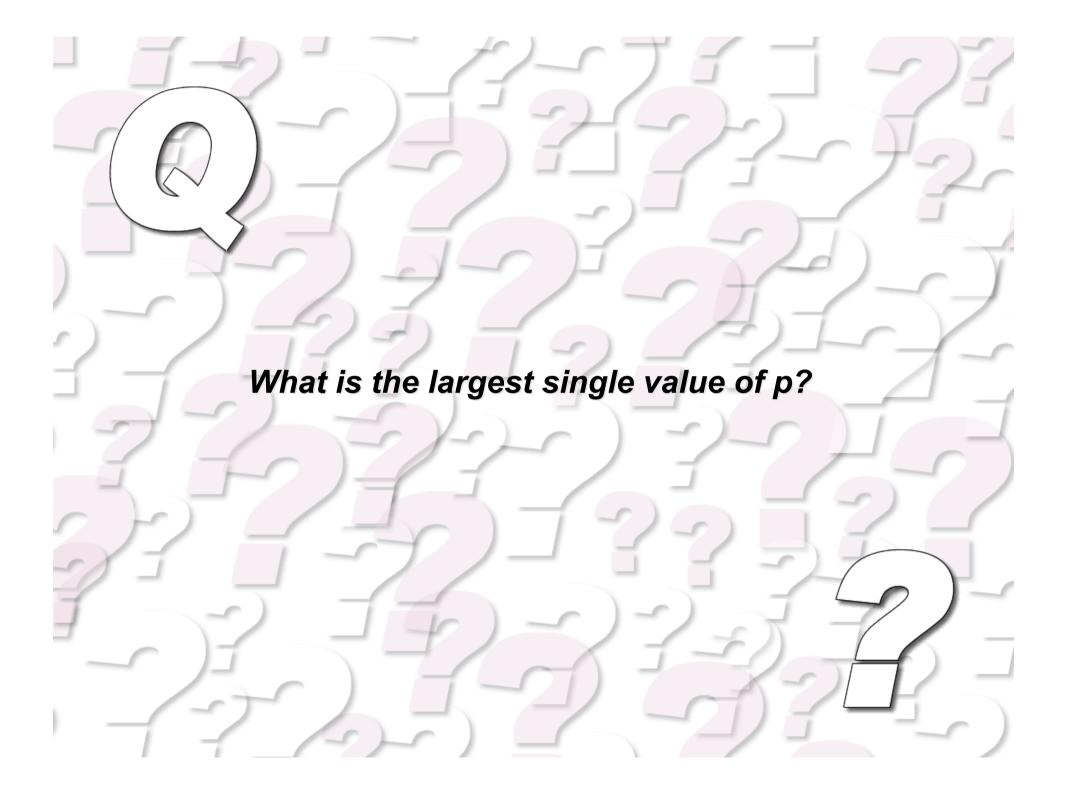


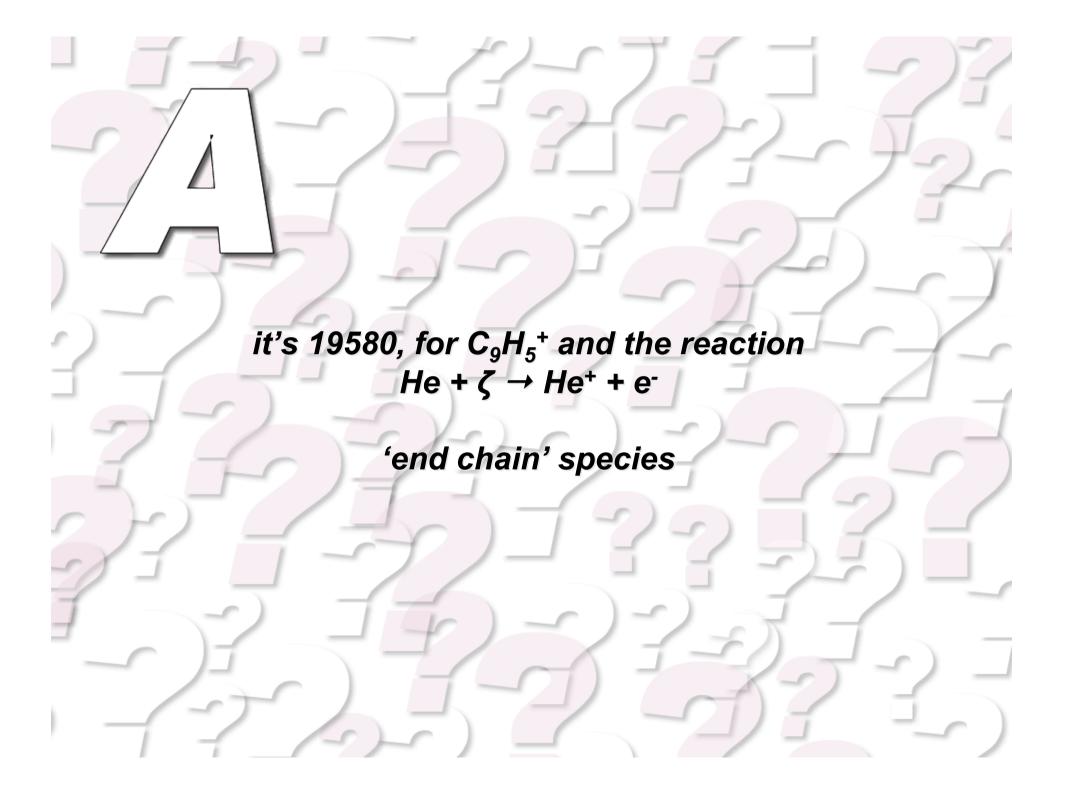


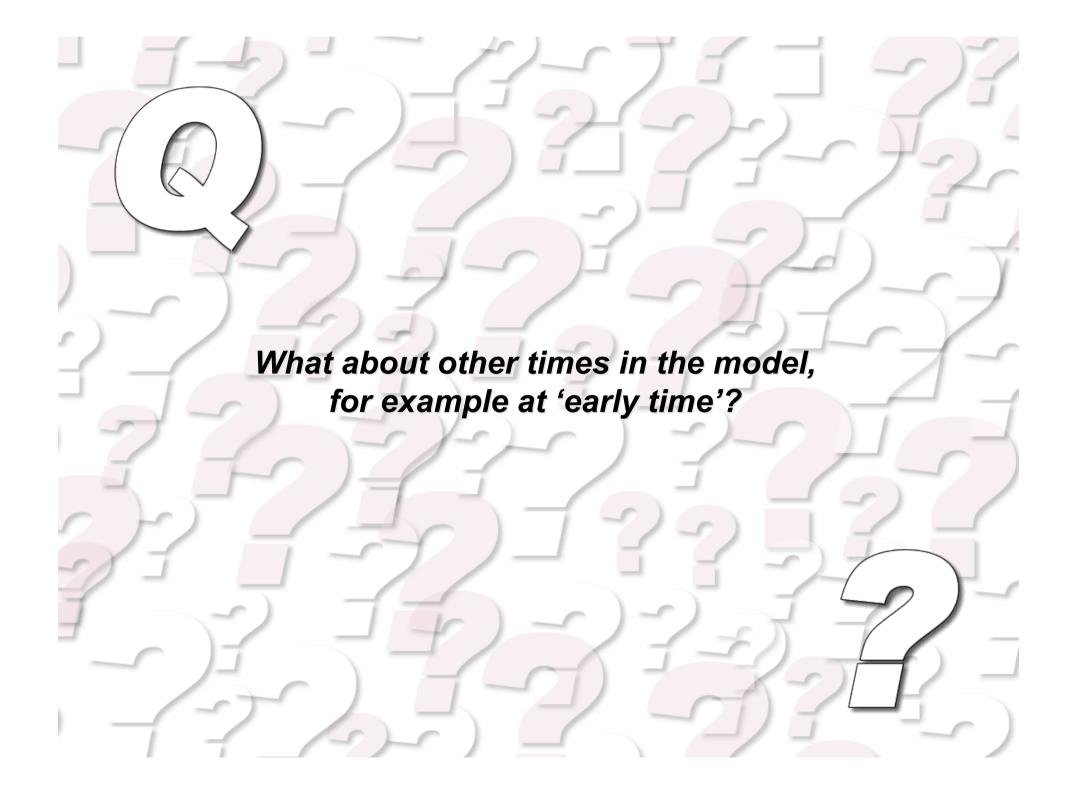
	(1)-5	75	(2)
p_X = the difference in Reaction C_2H C_2H_2 C_2H_5OH C_2S	in the steady state abundance of species X from runs with the reaction ${\sf C_3H_2}$ ${\sf CH_3CH}$ ${\sf CH_3CN}$ ${\sf CH_3OH}$ ${\sf CN}$ ${\sf CS}$ ${\sf H_2CO}$	rate at the extremes of its tabulated uncertainty, as a percen $H_2S = HC_3N = HC_7N = HCN = HCO^+ = HCS^+$	tage of the control value. HN_2^+ HNC NH_3 O_2 SO_2 $\mid p_{t\alpha,al}$
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
$H_2 \xrightarrow{\varsigma} H_2^+ + e^-$ 260.0 162.8 182.3 483.1 $H_3^+ + O \longrightarrow OH^+ + H_2$ 146.2 76.6 23.1 205.5	280.3 265.7 69.5 103.4 109.0 94.7 104.9 114.5 120.8 27.0 11.9 19.7 65.7 36.9	42.8 187.1 586.6 14.2 105.3 31.7 58.3 71.0 239.3 4.9 0.9 62.4	163.6 59.2 37.6 58.3 92.4 115364 9.4 28.9 0.7 37.7 65.9 38265
$R_3 + O \longrightarrow OR + R_2$ $C^+ + H_2 \longrightarrow CH_2^+ + hv$ 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		9.4 7.2 7.5 27.3 24.1 16801
$CH_4 \xrightarrow{\zeta} CH_3 + H$ 54.9 54.7 53.1 $C_2H_2 \xrightarrow{\zeta} C_2H + H$ 15.2 70.8 26.9 68.4	54.1 109.7 0.9 0.7 0.5 20.9 70.0 37.1 0.3 0.2 0.4	0.6 54.7 107.5 1.2 0.3 67.9 138.8 0.3	0.5 0.3 0.4 12932 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 $C^+ + O_2 \longrightarrow CO^+ + O$ 20.0 21.8 16.8 28.9	44.5 52.2 0.2 0.4 27.9 32.1 20.8 10.5 12.8 7.8 9.8	0.2 42.6 1.9 30.8 56.2 8.6 1.3 8.0	0.5 8.2 2.3 1.9 1.2 7.652
$CH_3^+ + H_2 \longrightarrow CH_5^+ + hv$ 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
$CH_4 \xrightarrow{\circ} CH_2 + H_2$ 30.1 30.2 30.5 29.1 $He^{+} + H_2 \longrightarrow H_2^+ + He$ 21.4 19.3 19.9 30.3	30.2 59.1 3.5 2.1 0.3 0.5 17.8 24.8 28.3 16.4 13.3 6.1 9.4 8.9	30.5 59.0 0.6 0.3 4.3 20.5 41.0 5.6 1.3 9.1	0.5 0.4 7233 2.1 8.2 1.6 1.9 5.2 6662
$H_1^+ \stackrel{e^-}{\longrightarrow} H_1^+ H_1^+ H_2^-$ 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
$N_2 \xrightarrow{\xi} N + N$ 6.4 6.1 28.1 26.8 $C^+ + CH_4 \longrightarrow C_2H_3^+ + H$ 31.5 29.0 8.6 28.6	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 $He^+ + O_2 \longrightarrow O^+ + O_2 + He$ 15.6 14.5 9.8 23.1	28.7 29.6 0.4 0.2 2.2 19.4 21.4 13.7 4.2 6.1 8.3 6.7	0.1 28.7 57.3 0.3 4.4 16.6 33.1 6.2 8.0	0.5 5839 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
$C + O_2 \longrightarrow CO + O$ 1.4 0.2 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 $C_4H_7^+ \xrightarrow{e^-} C_4H + H$ 0.7 1.1 0.4 1.4	13.2 11.3 9.3 46.1 5.3 2.1 4.9 7.0	2.1 11.6 23.0 5.6 2.6 2.1 2.9 40.5	3.6 6.3 1.1 1.9 1.2 3968 3872
$C_4H_2 \longrightarrow C_4H + H$ $C + C_4H \longrightarrow C_5 + H$ 1.6 0.9 0.8 11.2	3.1 0.6 0.2	1.6 53.9 0.3	0.5
$CO \xrightarrow{\zeta} C + O$ 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
$C+C_2H_2 \longrightarrow C_3H+H$ 2.1 3.2 0.8 10.9 $C^++CH_4 \longrightarrow C_2H_2^++H_2$ 10.6 13.2 22.7 13.1	30.2 1.3 0.2 12.4 7.5 0.2 0.9	0.1 5.8 46.6 0.3 13.2 25.8	0.5 0.5 2844
$H_3^+ + C_3 H_2 \longrightarrow C_3 H_3^+ + H_2$ 1.8 3.2 0.8 11.2	33.3	5.8 29.8	0.5 2775
$NH_4^+ \xrightarrow{e^-} NH_2 + H + H$ 3.7 4.3 27.3	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 $NH_4^+ \xrightarrow{e^-} NH_3 + H$ 3.7 4.3 26.9 22.9	10.8 22.6 3.6 5.4 2.5 36.3 1.4 26.1 15.2 0.4	0.1 11.1 21.9	0.5 2627 2.6 34.2 39.6 1.6 2551
$NH_{4}^{+} \xrightarrow{e^{-}} NH_{3} + H$	0.9	4.8 14.5 11.2 36.4 0.9 8.5 130.6 1.1	2.6 34.2 39.6 1.6 2551 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
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	8.5 3.8 0.9 13.9 0.6	8.2 16.3 8.9 36.0	0.5 2342 0.5 2339
$CH_5^+ + CO \longrightarrow HCO^+ + CH_4$ 9.9 9.8 9.8	10.1 20.1	0.1 10.0 19.7	0.5









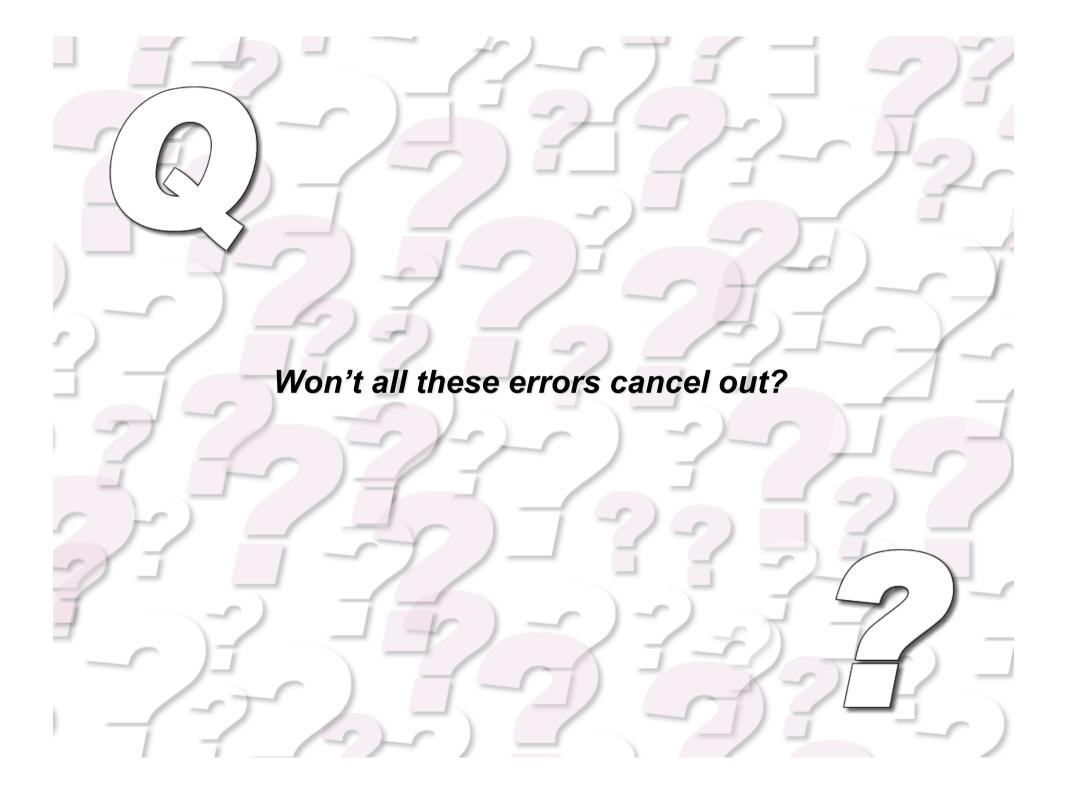


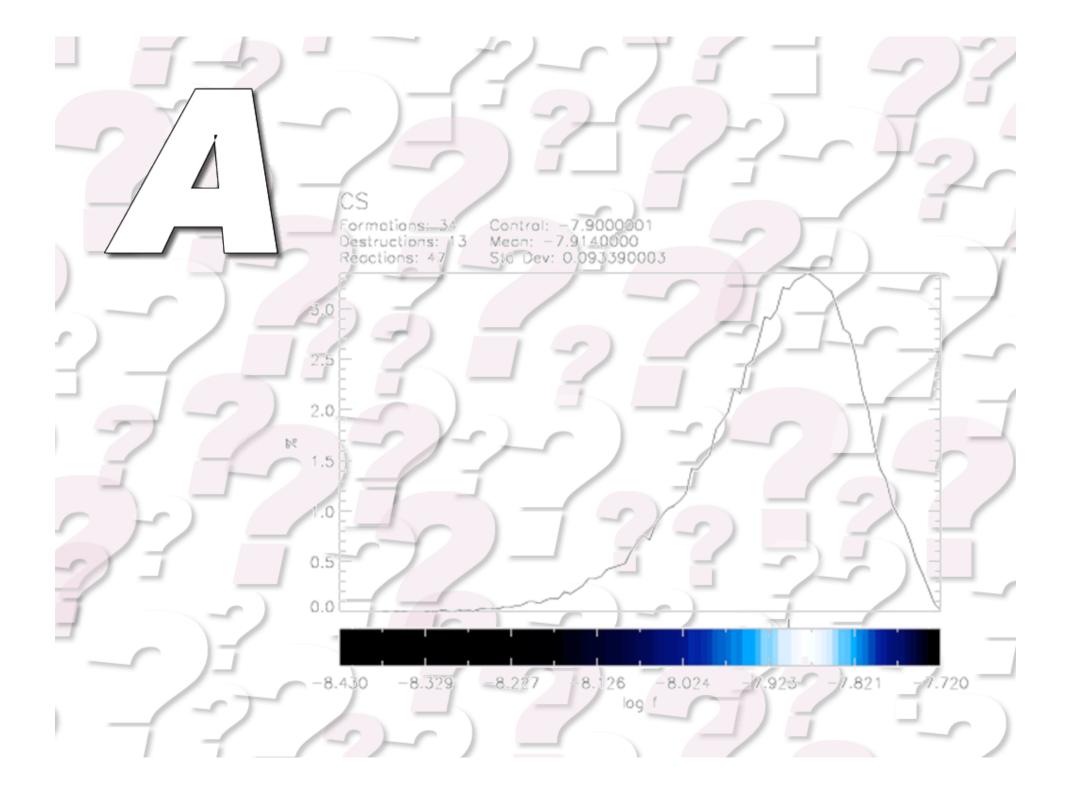
The results are similar.

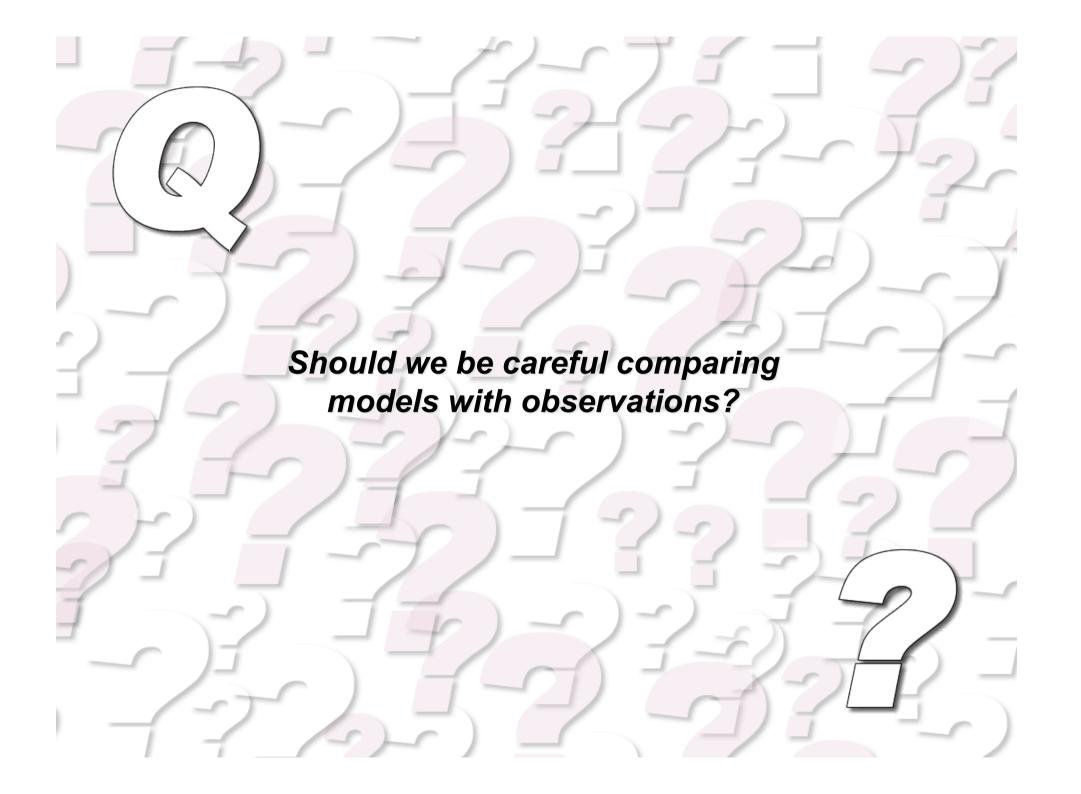
The uncertainties are always less than at steady state.

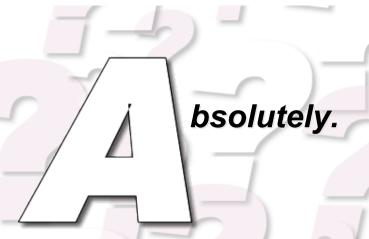
The cri reactions for H₂ and He switch places.

The top non cr reactions are still $H_3^+ + O \rightarrow OH^+ + H_2$ and $C^+ + H_2 \rightarrow CH_2^+ + hv$







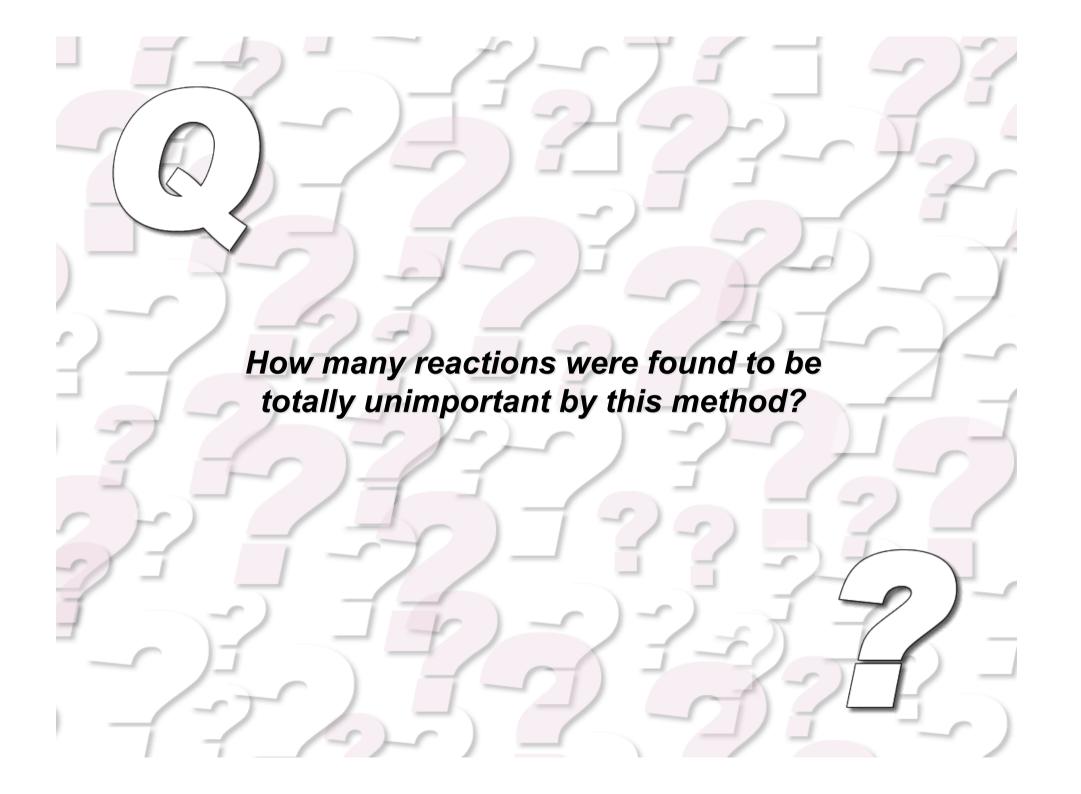


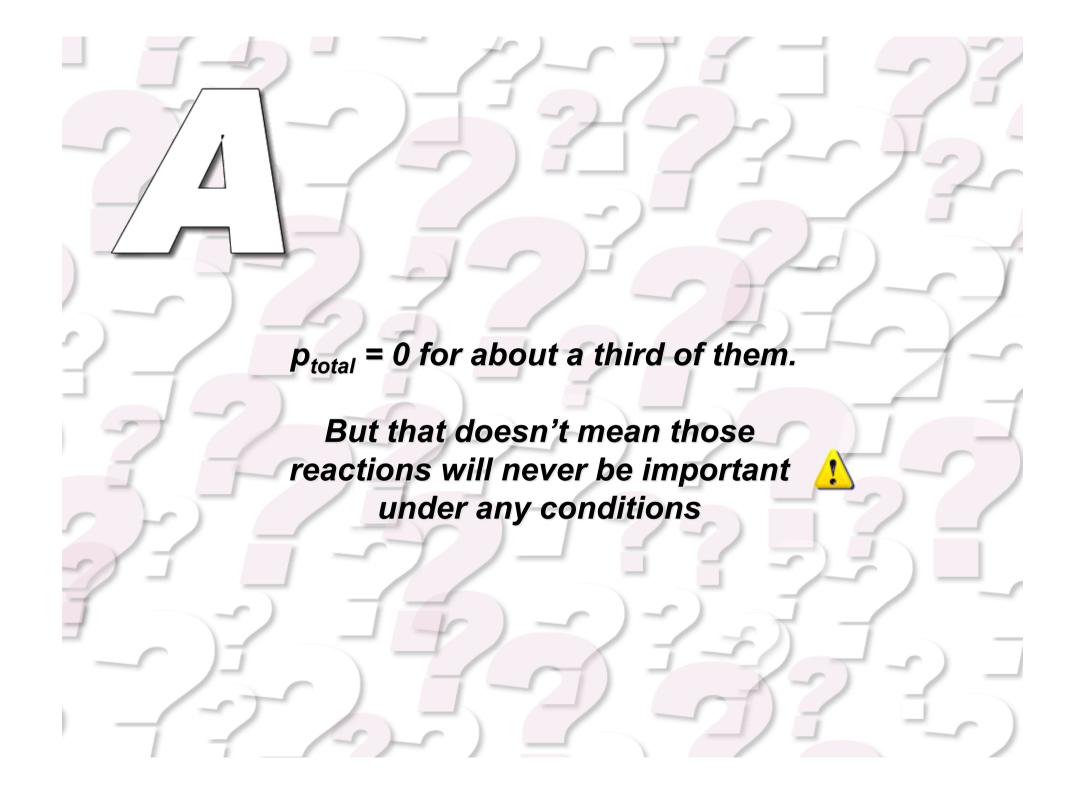
Simple species are OK but bigger molecules are definitely not

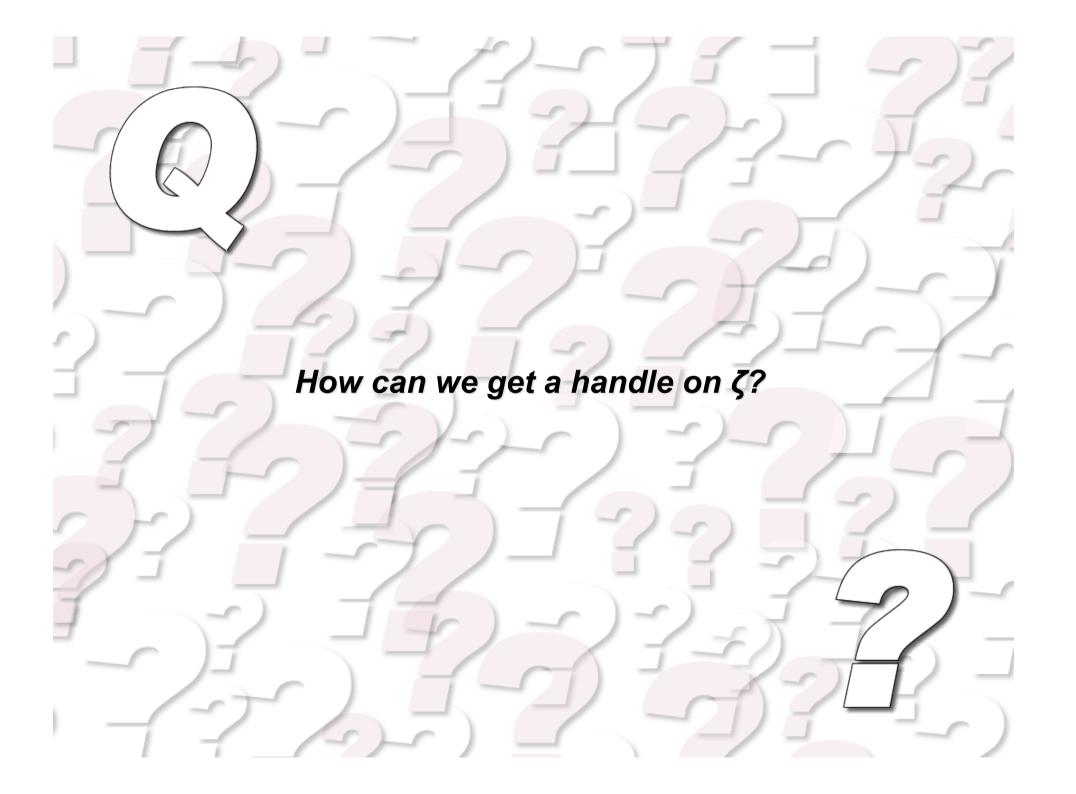
e.g. HC₇N abundance uncertain to an order of magnitude because of a single rate!

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

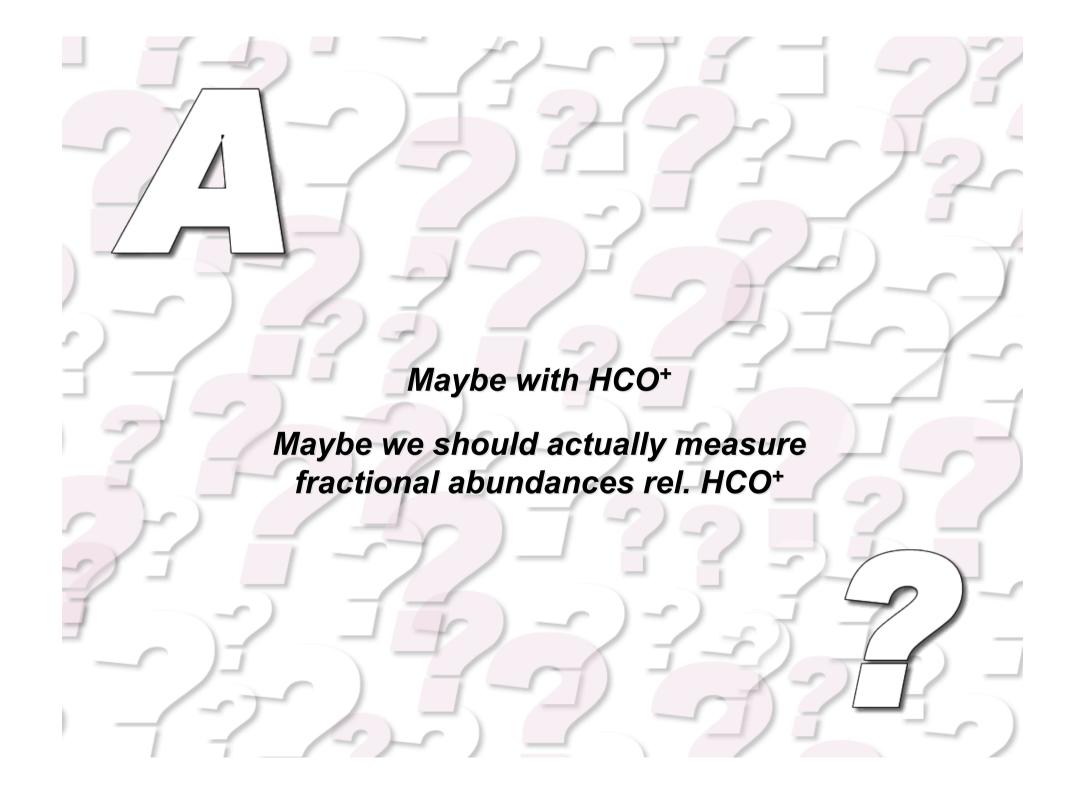
For most species with $n_c > 2$, $p_{max} \sim 500$







	(1)-5	75	(2)
p_X = the difference in Reaction C_2H C_2H_2 C_2H_5OH C_2S	in the steady state abundance of species X from runs with the reaction ${\sf C_3H_2}$ ${\sf CH_3CH}$ ${\sf CH_3CN}$ ${\sf CH_3OH}$ ${\sf CN}$ ${\sf CS}$ ${\sf H_2CO}$	rate at the extremes of its tabulated uncertainty, as a percen $H_2S = HC_3N = HC_7N = HCN = HCO^+ = HCS^+$	tage of the control value. HN_2^+ HNC NH_3 O_2 SO_2 $\mid p_{t\alpha,al}$
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
$H_2 \xrightarrow{\varsigma} H_2^+ + e^-$ 260.0 162.8 182.3 483.1 $H_3^+ + O \longrightarrow OH^+ + H_2$ 146.2 76.6 23.1 205.5	280.3 265.7 69.5 103.4 109.0 94.7 104.9 114.5 120.8 27.0 11.9 19.7 65.7 36.9	42.8 187.1 586.6 14.2 105.3 31.7 58.3 71.0 239.3 4.9 0.9 62.4	163.6 59.2 37.6 58.3 92.4 115364 9.4 28.9 0.7 37.7 65.9 38265
$R_3 + O \longrightarrow OR + R_2$ $C^+ + H_2 \longrightarrow CH_2^+ + hv$ 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		9.4 7.2 7.5 27.3 24.1 16801
$CH_4 \xrightarrow{\zeta} CH_3 + H$ 54.9 54.7 53.1 $C_2H_2 \xrightarrow{\zeta} C_2H + H$ 15.2 70.8 26.9 68.4	54.1 109.7 0.9 0.7 0.5 20.9 70.0 37.1 0.3 0.2 0.4	0.6 54.7 107.5 1.2 0.3 67.9 138.8 0.3	0.5 0.3 0.4 12932 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 $C^+ + O_2 \longrightarrow CO^+ + O$ 20.0 21.8 16.8 28.9	44.5 52.2 0.2 0.4 27.9 32.1 20.8 10.5 12.8 7.8 9.8	0.2 42.6 1.9 30.8 56.2 8.6 1.3 8.0	0.5 8.2 2.3 1.9 1.2 7.652
$CH_3^+ + H_2 \longrightarrow CH_5^+ + hv$ 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
$CH_4 \xrightarrow{\circ} CH_2 + H_2$ 30.1 30.2 30.5 29.1 $He^{+} + H_2 \longrightarrow H_2^+ + He$ 21.4 19.3 19.9 30.3	30.2 59.1 3.5 2.1 0.3 0.5 17.8 24.8 28.3 16.4 13.3 6.1 9.4 8.9	30.5 59.0 0.6 0.3 4.3 20.5 41.0 5.6 1.3 9.1	0.5 0.4 7233 2.1 8.2 1.6 1.9 5.2 6662
$H_1^+ \stackrel{e^-}{\longrightarrow} H_1^+ H_1^+ H_2^-$ 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
$N_2 \xrightarrow{\xi} N + N$ 6.4 6.1 28.1 26.8 $C^+ + CH_4 \longrightarrow C_2H_3^+ + H$ 31.5 29.0 8.6 28.6	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 $He^+ + O_2 \longrightarrow O^+ + O_2 + He$ 15.6 14.5 9.8 23.1	28.7 29.6 0.4 0.2 2.2 19.4 21.4 13.7 4.2 6.1 8.3 6.7	0.1 28.7 57.3 0.3 4.4 16.6 33.1 6.2 8.0	0.5 5839 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
$C + O_2 \longrightarrow CO + O$ 1.4 0.2 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 $C_4H_7^+ \xrightarrow{e^-} C_4H + H$ 0.7 1.1 0.4 1.4	13.2 11.3 9.3 46.1 5.3 2.1 4.9 7.0	2.1 11.6 23.0 5.6 2.6 2.1 2.9 40.5	3.6 6.3 1.1 1.9 1.2 3968 3872
$C_4H_2 \longrightarrow C_4H + H$ $C + C_4H \longrightarrow C_5 + H$ 1.6 0.9 0.8 11.2	3.1 0.6 0.2	1.6 53.9 0.3	0.5
$CO \xrightarrow{\zeta} C + O$ 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
$C+C_2H_2 \longrightarrow C_3H+H$ 2.1 3.2 0.8 10.9 $C^++CH_4 \longrightarrow C_2H_2^++H_2$ 10.6 13.2 22.7 13.1	30.2 1.3 0.2 12.4 7.5 0.2 0.9	0.1 5.8 46.6 0.3 13.2 25.8	0.5 0.5 2844
$H_3^+ + C_3 H_2 \longrightarrow C_3 H_3^+ + H_2$ 1.8 3.2 0.8 11.2	33.3	5.8 29.8	0.5 2775
$NH_4^+ \xrightarrow{e^-} NH_2 + H + H$ 3.7 4.3 27.3	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 $NH_4^+ \xrightarrow{e^-} NH_3 + H$ 3.7 4.3 26.9 22.9	10.8 22.6 3.6 5.4 2.5 36.3 1.4 26.1 15.2 0.4	0.1 11.1 21.9	0.5 2627 2.6 34.2 39.6 1.6 2551
$NH_{4}^{+} \xrightarrow{e^{-}} NH_{3} + H$	0.9	4.8 14.5 11.2 36.4 0.9 8.5 130.6 1.1	2.6 34.2 39.6 1.6 2551 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
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	8.5 3.8 0.9 13.9 0.6	8.2 16.3 8.9 36.0	0.5 2342 0.5 2339
$CH_5^+ + CO \longrightarrow HCO^+ + CH_4$ 9.9 9.8 9.8	10.1 20.1	0.1 10.0 19.7	0.5





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⁻

H₂ $\xrightarrow{\zeta}$ H₂⁺ + e⁻

H₃ + O \longrightarrow OH⁺ + H₂

C⁺ + H₂ \longrightarrow CH₂⁺ + hv

C⁺ + O₂ \longrightarrow O + C

O₂ $\xrightarrow{\zeta}$ O + O

CH₄ $\xrightarrow{\zeta}$ CH₃ + H

C₂H₂ $\xrightarrow{\zeta}$ C₂H + H

He⁺ + CO \longrightarrow C⁺ + O + He

H₃ + N \longrightarrow NH₂ + H

C₂H₃ $\xrightarrow{e^-}$ C₂H + H₂

C⁺ + O₂ \longrightarrow CO⁺ + O

CH₃ + H₂ \longrightarrow CH₅ + hv

H₂ $\xrightarrow{\zeta}$ H⁺ + e⁻ + H

CH₄ $\xrightarrow{\zeta}$ CH₂ + H₂

He⁺ + H₂ \longrightarrow H₂ + He

H₃ $\xrightarrow{e^-}$ H + H + H

H₃ + CO \longrightarrow HCO⁺ + H₂

N₂ $\xrightarrow{\zeta}$ N + N

C⁺ + CH₄ \longrightarrow C₂H₃ + H

He⁺ + O₂ \longrightarrow O⁺ + O + He

CH₅ $\xrightarrow{e^-}$ CH₃ + H₂

C + O₂ \longrightarrow CO + O

H₃O⁺ $\xrightarrow{e^-}$ OH + H + H