Effects of the new rate constants on a dark cloud model

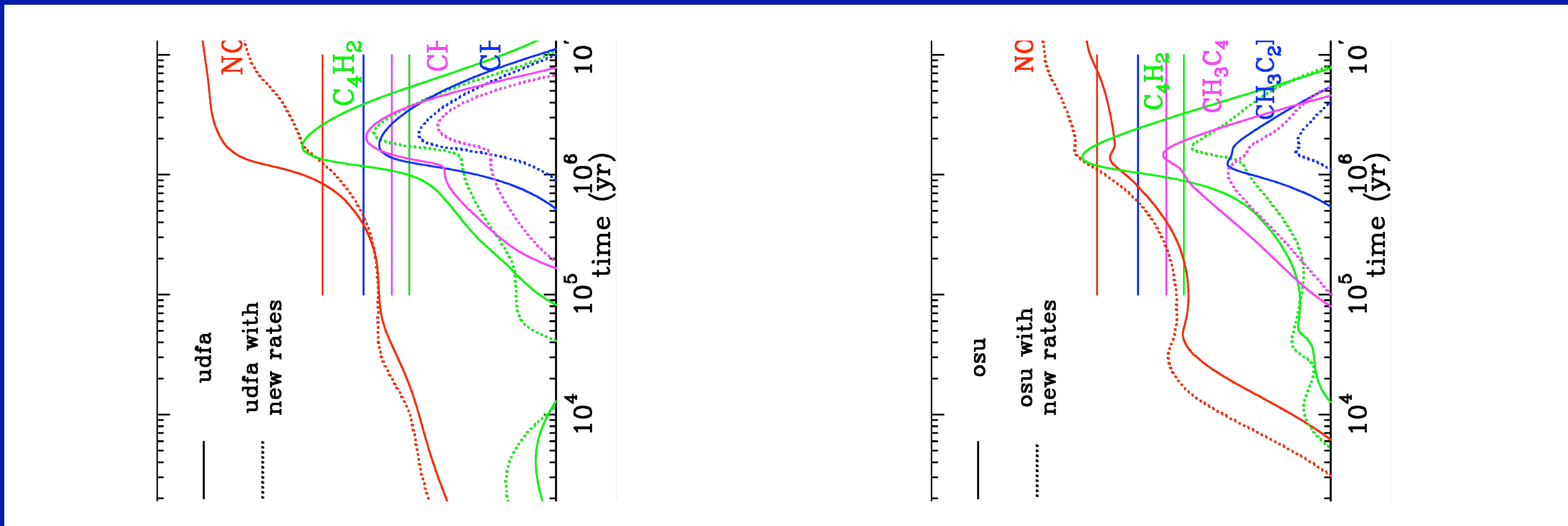
Dark cloud model

$k=3.75\times10^{-11}\exp(-26/T) \rightarrow 8\times10^{-11}$ ↑ $N + NO \rightarrow N_2 + O$ $k=3.0\times10^{-11}(T/300)^{-0.6} \rightarrow 8\times10^{-11}$ ↓

↑ $O + C_2 \rightarrow CO + C$ ↑

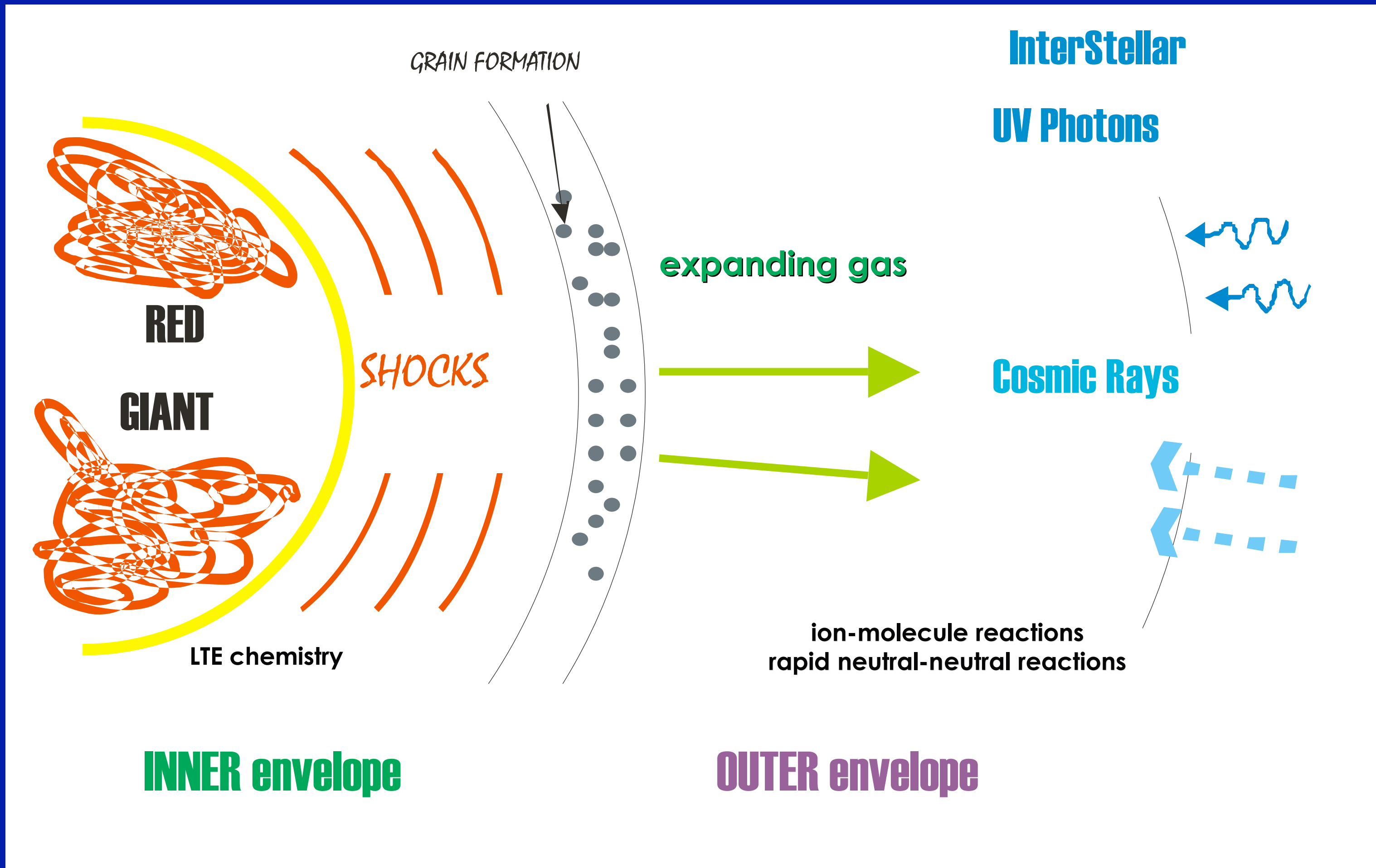
↑ $O + C_2H \rightarrow CO + CH$ ↑

↑ $O + C_3H \rightarrow CO + C_2H$ ↑



Effects of the new rate constants on a chemical model of IRC+10216

IRC+10216: a C-rich circumstellar envelope



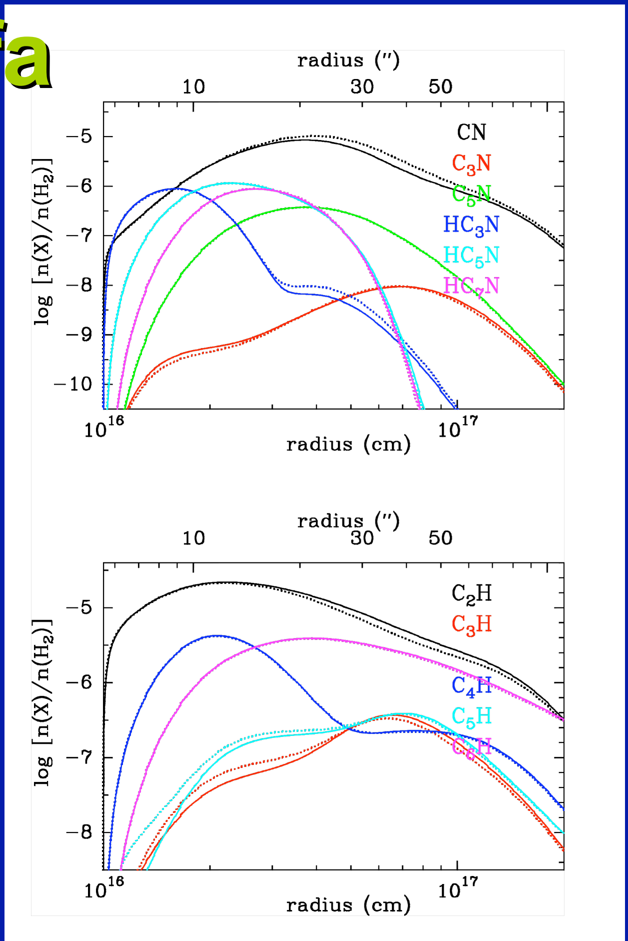
IRC+10216 model

There are not very big differences when including the new rate constants

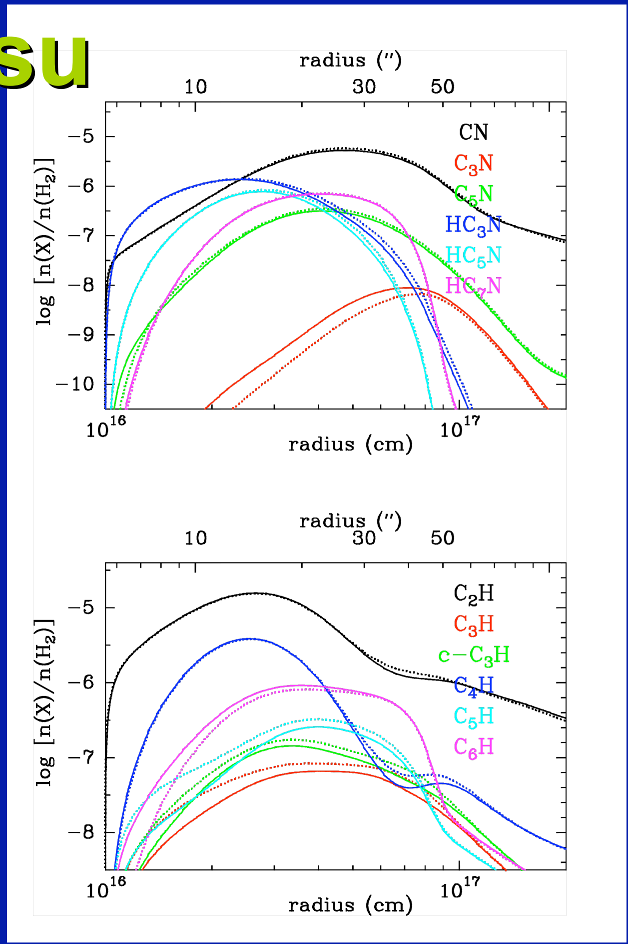
The reactions whose rate constants have been modified are critical in dark clouds but not in IRC+10216

Reactions involving O atoms and O-bearing species are not important in IRC+10216

udfa

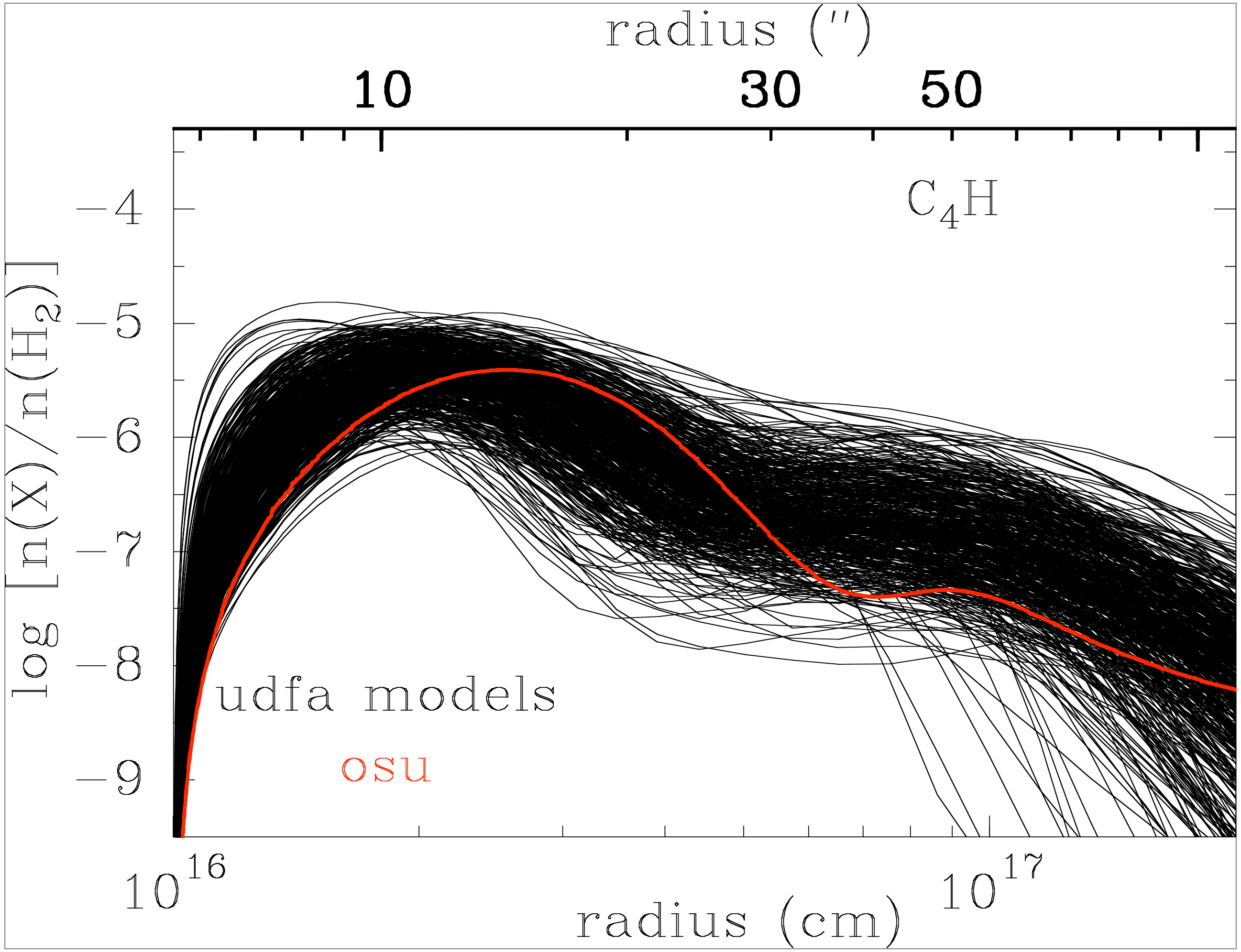


osu

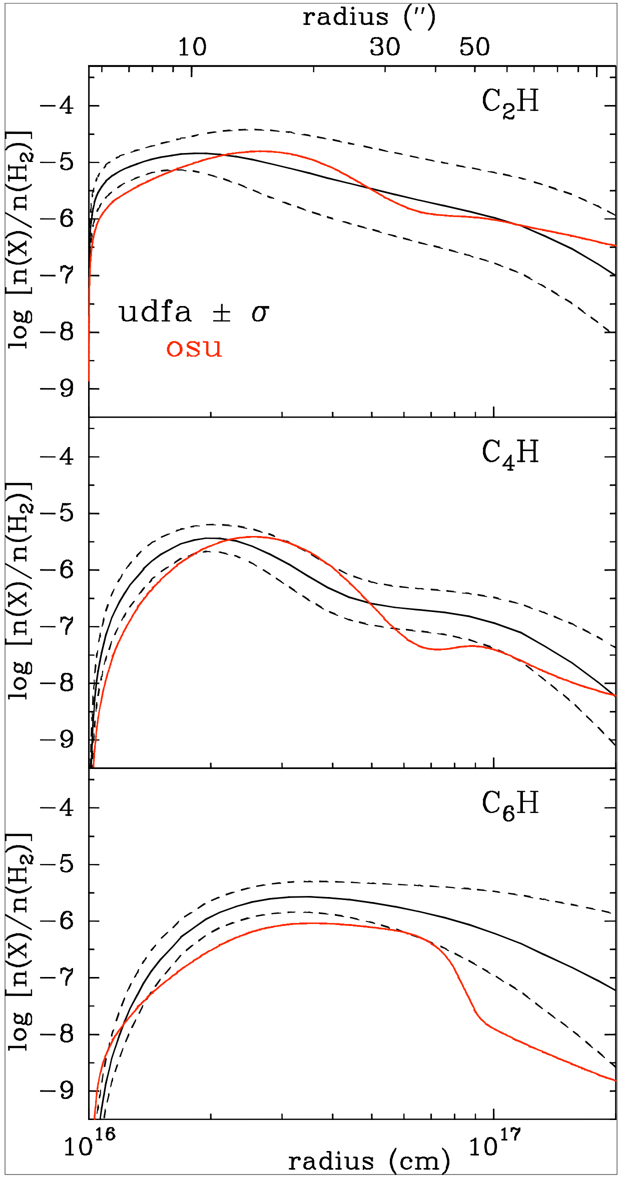


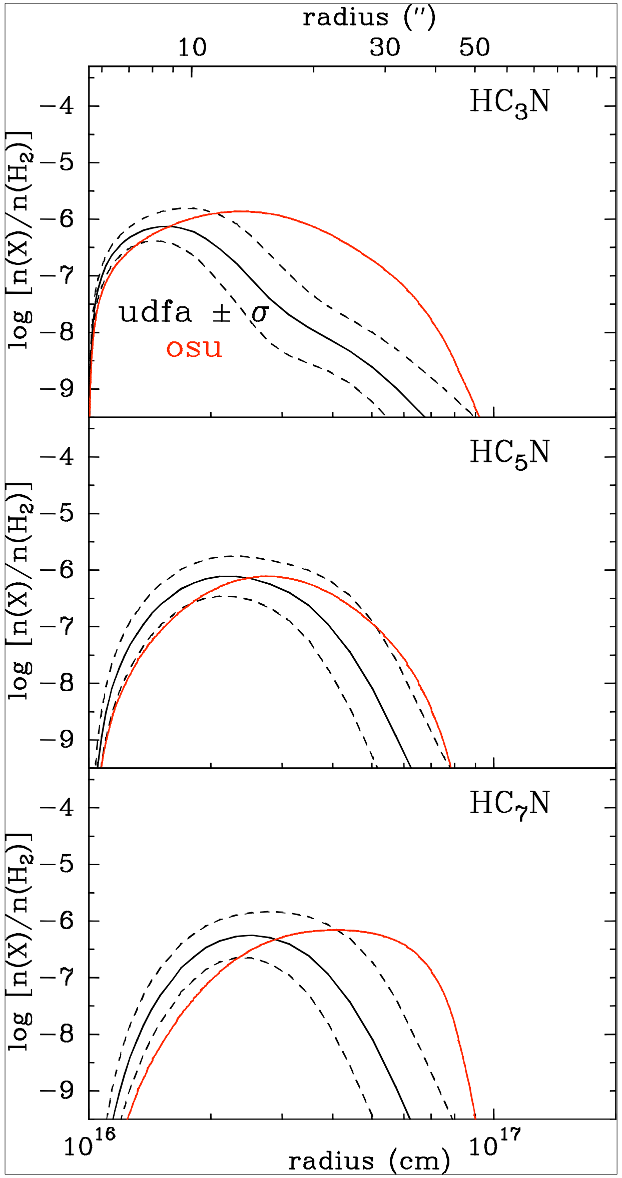
Uncertainties in IRC+10216

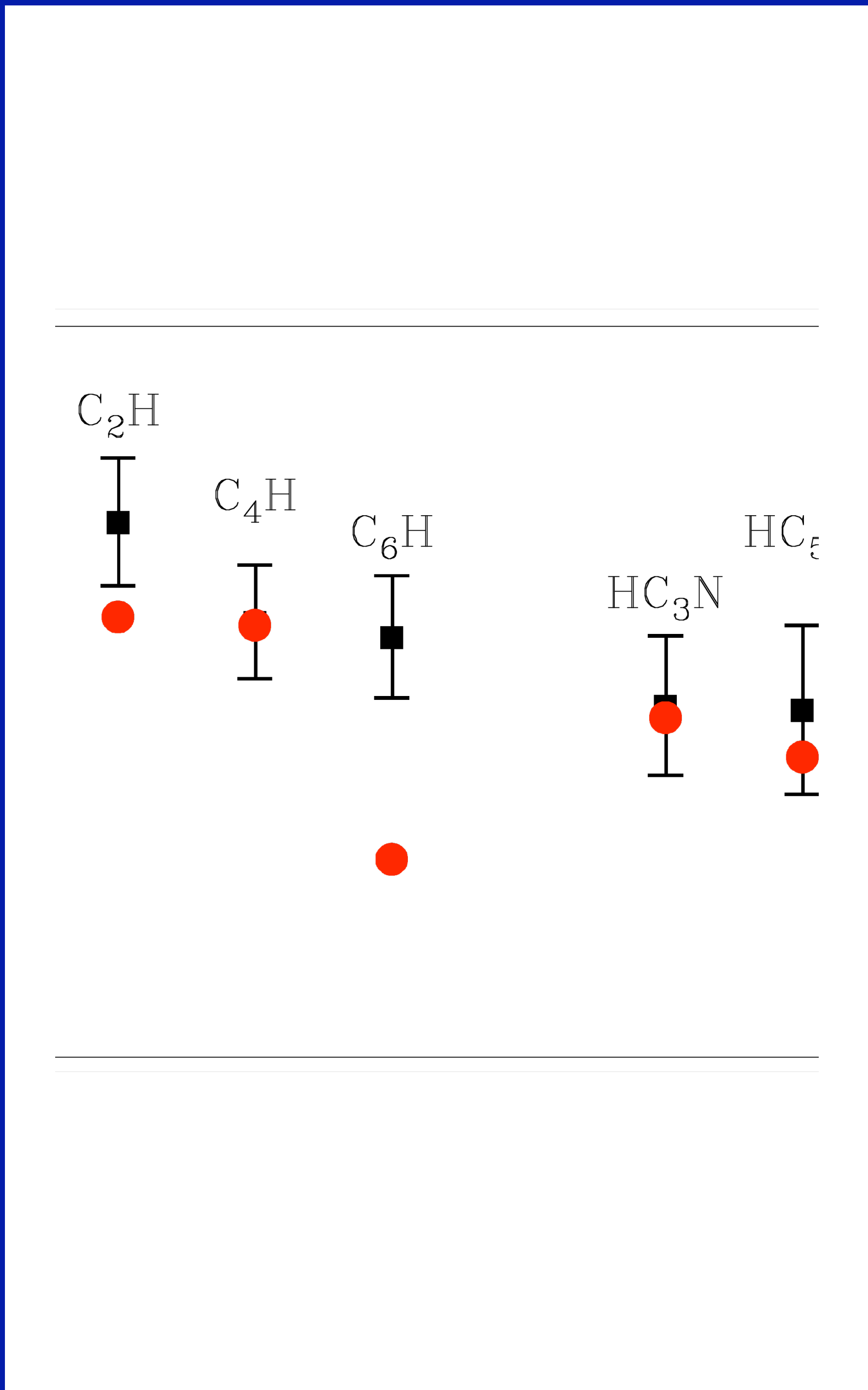
500 runs



radius (″)
10
30
50
C4H
−4
−5
−6
−7
−8
−9
log [n(X)/n(H2)]
udfa models
osu
10^16
10^17
radius (cm)


radius (″)
10
30
50
log [n(X)/n(H2)]
−4
−5
−6
−7
−8
−9
C2H
C4H
C6H
udfa ± σ
osu
10^{16}
10^{17}
radius (cm)


radius (″)
10
30
50
log [n(X)/n(H2)]
−4
−5
−6
−7
−8
−9
HC3N
HC5N
HC7N
udfa ± σ
osu
10^{16}
10^{17}
radius (cm)


C_2H
C_4H
C_6H
HC_3N
HC_5

The most critical reactions in IRC+10216

1	C_2H + photon → C_2 + H	Err=10	C_3H_3, H_2C_3, C_2N, C_4H_3
2	^{13}CO + photon → O + ^{13}C	Err=10	NO, HNO, H_2CO, ^{13}C, CNC+
3	N_2 + photon → N + N	Err=10	C_3N, C_2N, C_4N, C_7H, N
4	C_2H + C_4H_2 → C_6H_2 + H	Err=2	C_6H_2, HC_7N, C_6H, C_7N, C_5N
5	C_2H_2 + photon → C_2H + H	Err=2	HC_3N, C_8H_2, C_5H_2
6	^{13}C + photon → ^{13}C+ + e-	Err=10	^{13}C, CNC+
7	HCN + photon → CN + H	Err=50%	CNC+, HC_3N, HC_5N, C_5N
8	C_4H_2 + photon → C_2H + C_2H	Err=2	C_5N, C_4N, C_5H, C_4H_2+, HC_5N
9	C_2H + C_6H_2 → C_8H_2 + H	Err=2	C_8H_2, C_7N, C_8H, HC_7N, C_6H
10	C_2 + photon → C_2+ + e-	Err=2	C_2H_2+, C_2H_3, C_2H_3+, CH, H_2C_3

Mostly photo-reactions and neutral-neutral reactions

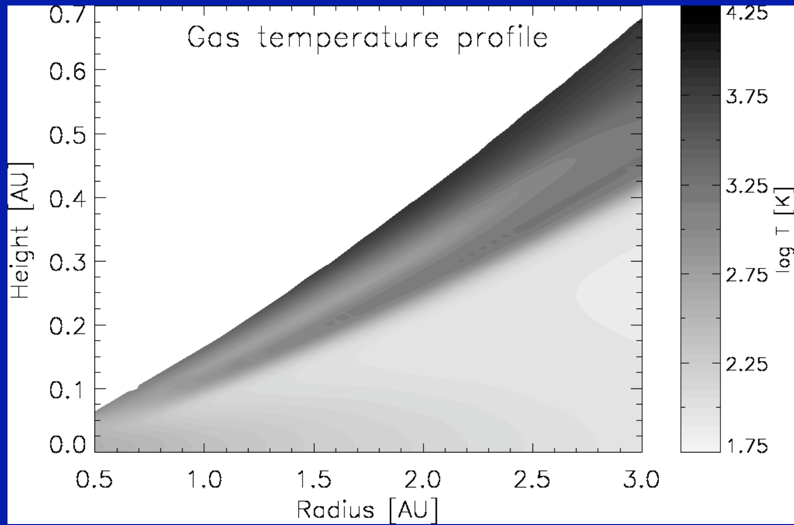
… perhaps, instead of $k_{ph}=A\exp(-C^*A_V)$, $k_{ph} = A\exp(-B^*A_V - C^*A_V^2)$

Some issues concerning chemical networks for use in molecular astrophysics

1) Need for rate constant expressions throughout a *as wide as possible* temperature range (e.g. 10 K - 4,000 K)

Dark cloud: T=10 K

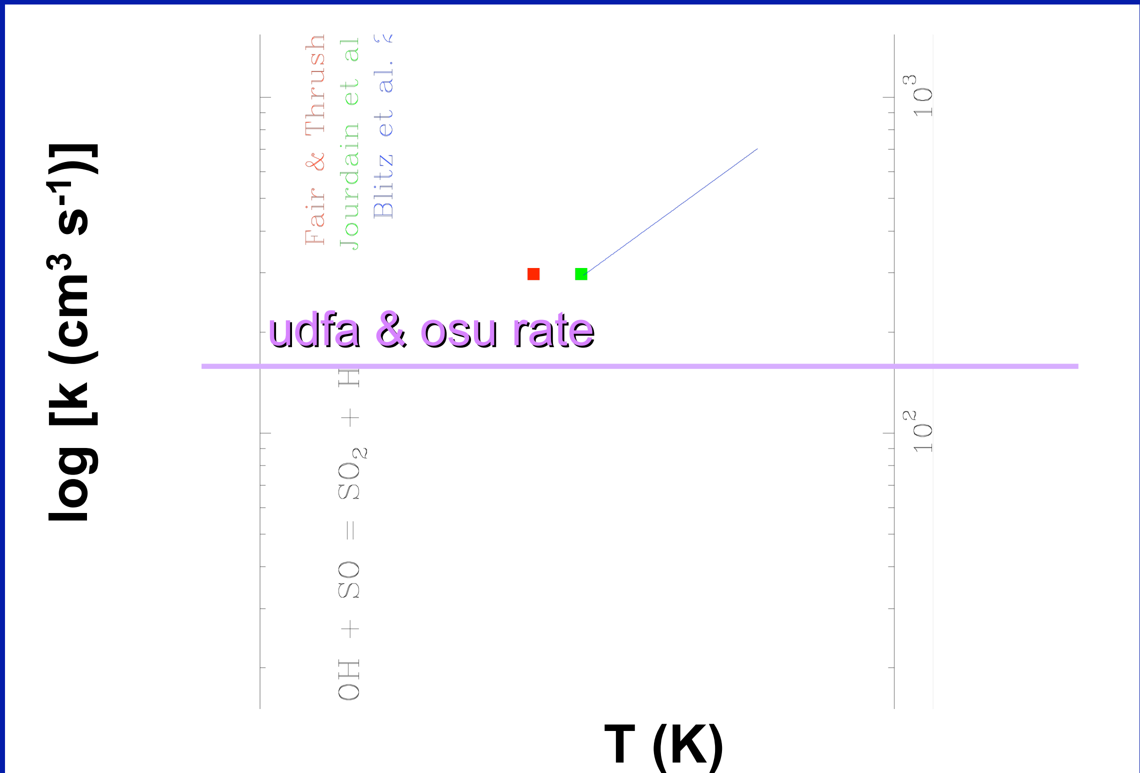
… but, e.g. in the inner regions of protoplanetary disks: T~4,000 K



Woods & Willacy 2007

It occurs that the same astrochemical network is used in both situations

e.g. the OH + SO → SO_2 + H reaction



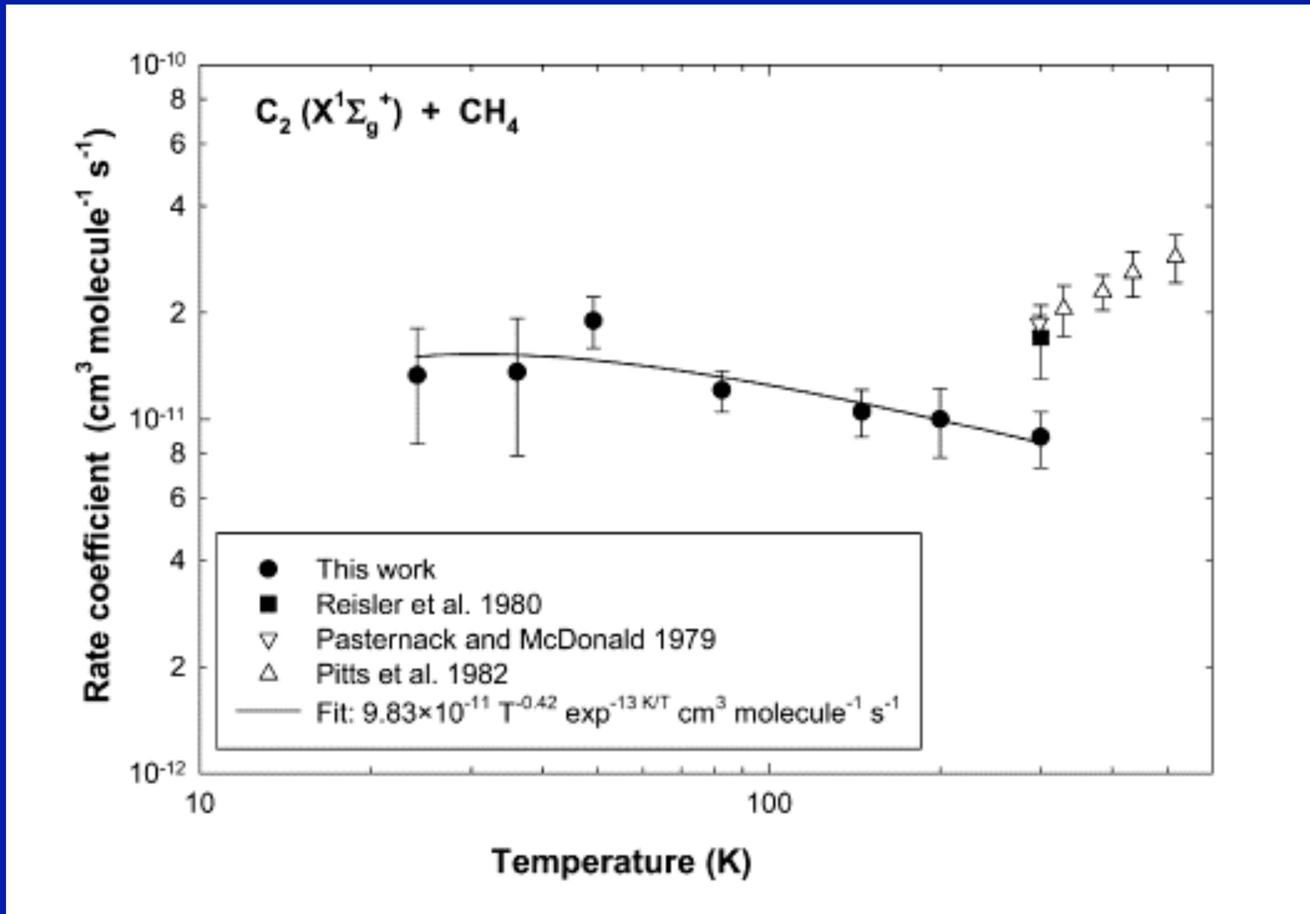
Fair & Thrush (1969) and Jourdain et al. (1979) measure the rate at room temperature.

Then Blitz et al. (2000) measure the rate in the 295-703 K range and find a negative activation barrier.

WHICH EXPRESSION SHOULD ONE CHOOSE ?

	Blitz et al. (2000) expression $k=8.1\times10^{-11}\ (T/300)^{-1.35}$ cm^3 s^{-1}	udfa & osu expressions $k=8.6\times10^{-11}$ cm^3 s^{-1}	difference
T=10 K	$k=8.0\times10^{-9}$ cm^3 s^{-1} propably too large	$k=8.6\times10^{-11}$ cm^3 s^{-1}	a factor 100
T=4000 K	$k=2.5\times10^{-12}$ cm^3 s^{-1}	$k=8.6\times10^{-11}$ cm^3 s^{-1} perhaps too large	a factor 30

another example: $C_2 + CH_4$ reaction



WHICH EXPRESSION SHOULD ONE CHOOSE ?

1) Need for rate constant expressions throughout a *as wide as possible* temperature range (e.g. 10 K - 4,000 K)

2) Thermochemistry in chemical networks

- Useful to check for eothermicity of reactions.
- Applying detailed balance it is possible to include the direct and reverse reactions.

In high temperatre and high density environments (inner regions of CSEs, planetary atmospheres,…) chemical kinetics should recover chemicalequilibrium.

Problems:

- not all species have known thermodynamic data

Sources of thermodynamic data:
JANAF, NIST, therm files (Alexander Burcat webpage, NASA)

1) Need for rate constant expressions throughout a *__as wide as possible__* temperature range (e.g. 10 K - 4,000 K)

2) Thermochemistry in chemical networks

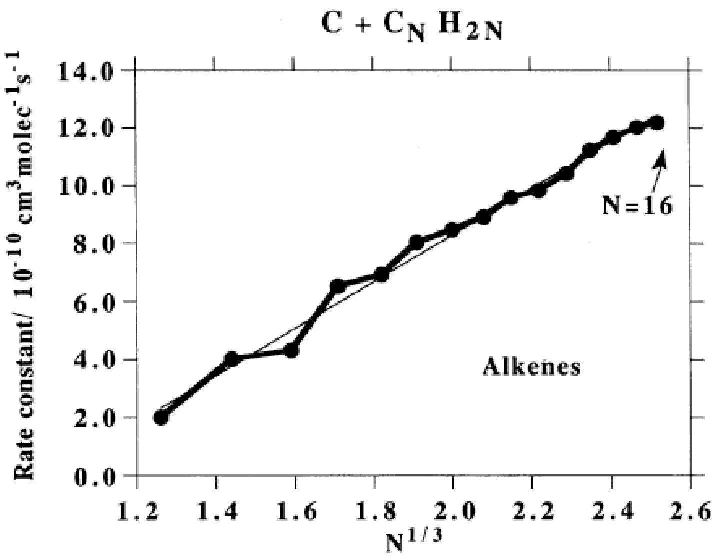
3) Extrapolation for analog reactions with larger species

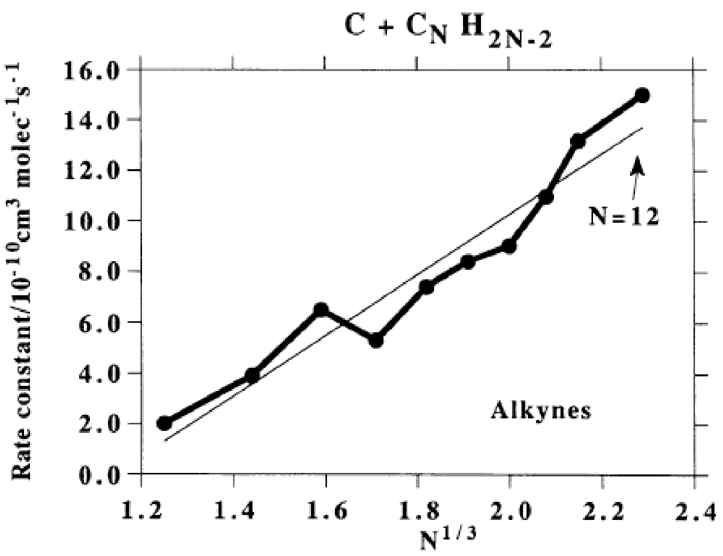
C + 1-alkenes

$K=8.0xN^{1/3}$ -7.8

C + 1-alkynes

$K=11.9xN^{1/3}$ -13.6





Clary et al. 1994

1) Need for rate constant expressions throughout a *as wide as possible* temperature range (e.g. 10 K - 4,000 K)

2) Thermochemistry in chemical networks

3) Extrapolation for analog reactions with larger species

e.g.

$C + C_2H_2 \rightarrow \ldots$

$C + C_4H_2 \rightarrow \ldots$

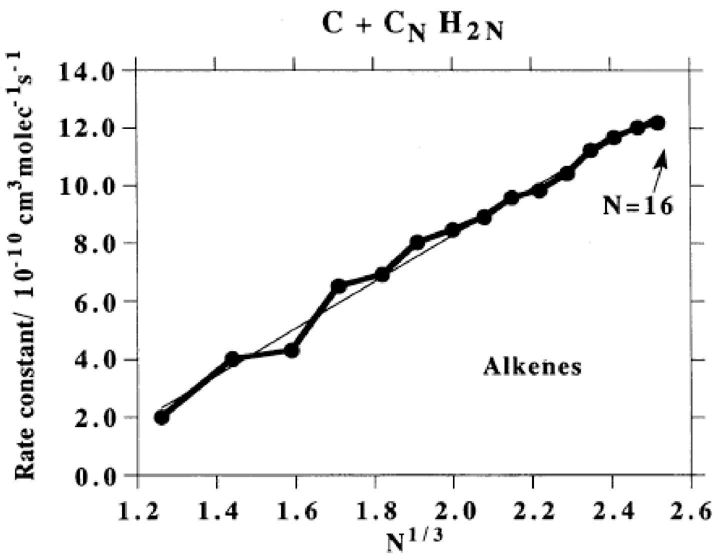
…

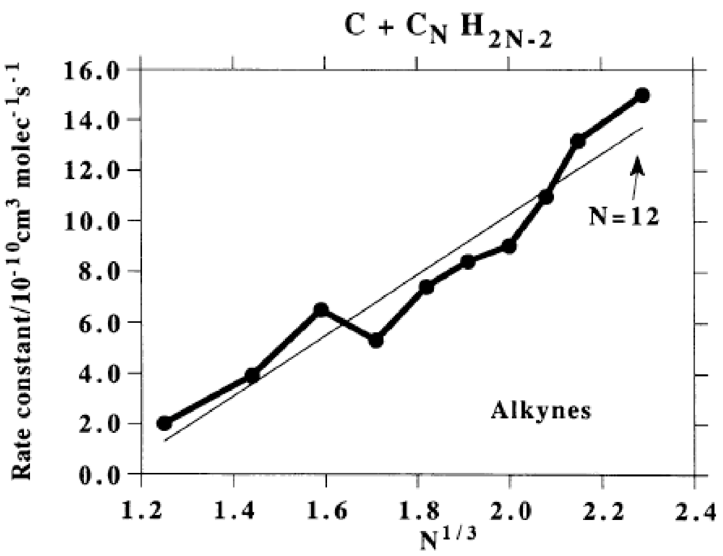
C + 1-alkenes

$K = 8.0 \times N^{1/3} - 7.8$

C + 1-alkynes

$K = 11.9 \times N^{1/3} - 13.6$





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