Chemistry in PDR

Chemical reactions and species

Chemistry in PDR: should we use the same of everything?

- Initial abundances → Probably YES
- Species set → YES for important species
- Rates → Probably NO

Initial Abundances

Sofia & Meyer 2001

He = 0.075

C = $1.79e^{-4}$

O = $4.45e^{-4}$

Na = $8.84e^{-7}$

Mg = $5.12e^{-6}$

S = $1.43e^{-5}$

Variations:

He = 0.14

S = $1.4e^{-7}$

C/O = 0.5-1?

Benchmarking:

He = 0.1

C = $1e^{-4}$

O = $3e^{-4}$

Important species: O, C (or C/O only?), He; but as you go more into the cloud, other species become important.

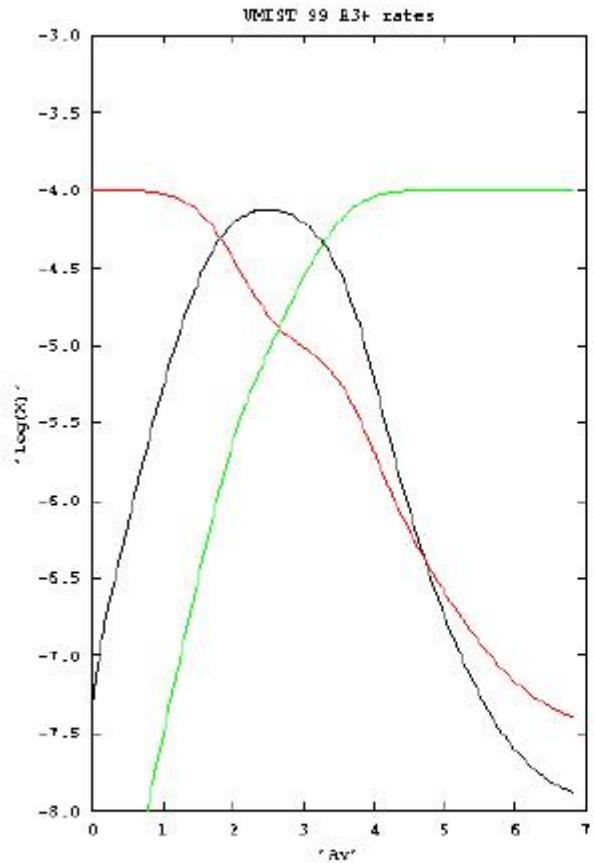
Species set

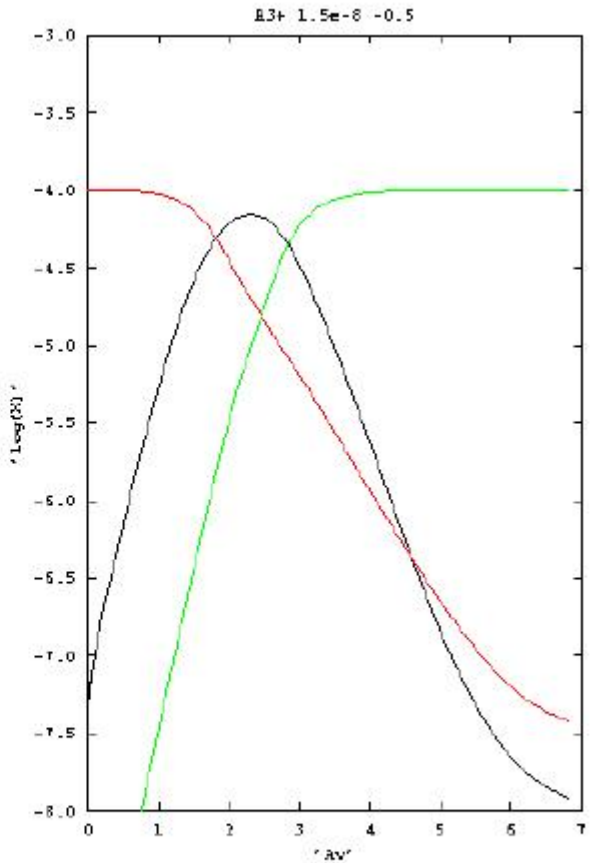
- Is the one we are using a good standard one for low Av PDR?
- Should we have a set of parameters within which the set is standard?
- Should we all include PAH?

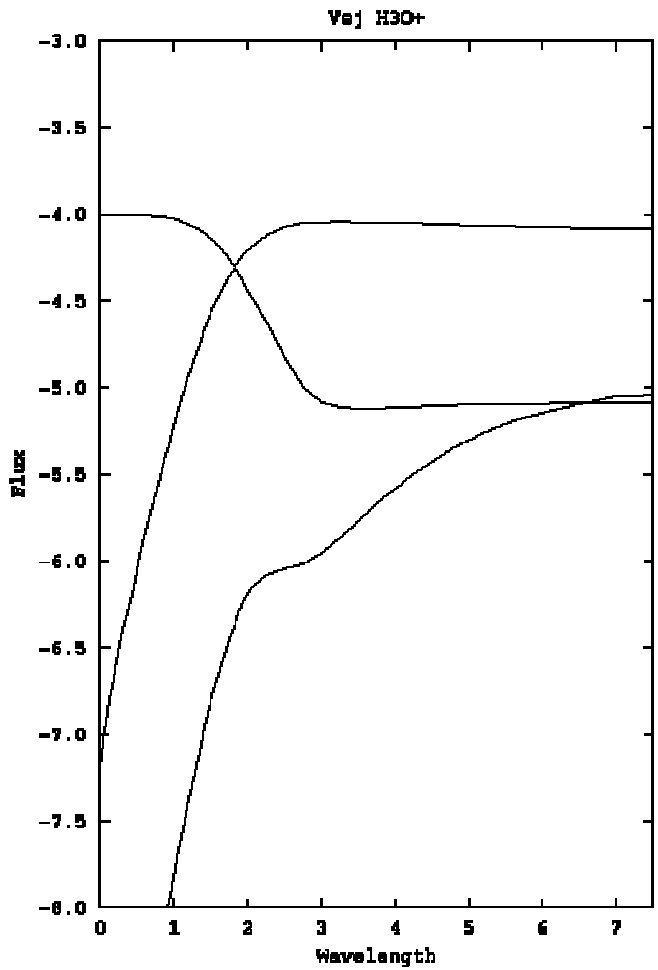
Rate files

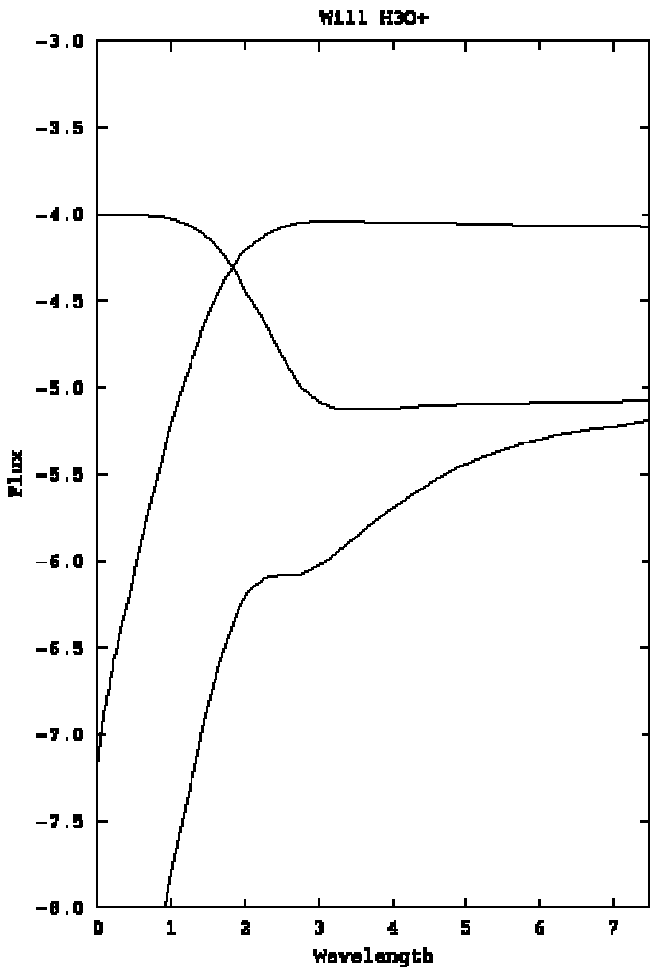
- Ohio, UMIST, Personal, Mixtures
- List of relevant rates? Please list
  - $H_3^+ + e$
  - $H_3O^+ + e$
  - $CH_5^+ + e$?
  - PAH?
  - ……please add

- Next 2 plots shows effect of different rates for $H_3^+ + e$ and $H_3O^+ + e$ respectively.
- H_3^+ rates are from UMIST 99 (left plot) and old UMIST 96 (right)
- H_3O^+ are from Vejby-Christensen et al. 1997 (left plot) and Williams et al 1996 (right plot).


UMIST 99 A3+ rates
-3.0
-3.5
-4.0
-4.5
-5.0
-5.5
-6.0
-6.5
-7.0
-7.5
-8.0
'Log(X)'
0
1
2
3
4
5
6
7
'Av'


A3+ 1.5e-8 -0.5
-3.0
-3.5
-4.0
-4.5
-5.0
-5.5
-6.0
-6.5
-7.0
-7.5
-8.0
'Log(X)'
0
1
2
3
4
5
6
7
'Av'


Vaj H3O+
Flux
Wavelength
-3.0
-3.5
-4.0
-4.5
-5.0
-5.5
-6.0
-6.5
-7.0
-7.5
-8.0
0
1
2
3
4
5
6
7


Will H3O+
Flux
Wavelength
-3.0
-3.5
-4.0
-4.5
-5.0
-5.5
-6.0
-6.5
-7.0
-7.5
-8.0
0
1
2
3
4
5
6
7