

Photochemistry in KROME

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Aims of this talk

- 1 Understand how energy binning works
- 2 How to include photochemical reactions in KROME
- 3 Get opacity from KROME

WARNING: non-local problem!

KROME Bootcamp 2021 - Main Equations

Photochemistry equations (thin)

$$k_{ph} = \frac{4\pi}{h} \int_{E_0}^{\infty} \frac{I(E)\sigma(E)}{E} dE \quad (1)$$

$$\Gamma_{ph} = \frac{4\pi}{h} \int_{E_0}^{\infty} \frac{I(E)\sigma(E)}{E} (E - E_0)\eta(E) dE \quad (2)$$

Units

$$k_{ph} = [s^{-1}] \quad (3)$$

$$\Gamma_{ph} = \left[\frac{\text{erg}}{\text{s}} \right] \quad (4)$$

$$E = [\text{eV}] \quad (5)$$

$$I(E) = \left[\frac{\text{eV}}{\text{cm}^2 \text{ s Hz sr}} \right] = \left[\frac{\text{eV}}{\text{cm}^2 \text{ sr}} \right] \quad (6)$$

$$\sigma(E) = [\text{cm}^2] \quad (7)$$

Photochemistry equations (thin)

$$k_{ph} = \frac{4\pi}{h} \int_{E_0}^{\infty} \frac{I(E)\sigma(E)}{E} dE \quad (8)$$

$$\Gamma_{ph} = \frac{4\pi}{h} \int_{E_0}^{\infty} \frac{I(E)\sigma(E)}{E} (E - E_0)\eta(E) dE \quad (9)$$

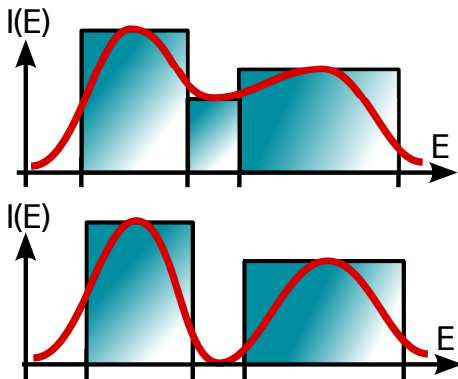
Bins in KROME

$$k_{ph} = \frac{4\pi}{h} \sum_{i=1}^{N_{bins}} \frac{I_i \sigma_i}{\langle E_i \rangle} (E_i^{right} - E_i^{left}) \quad \langle E_i \rangle > E_0 \quad (10)$$

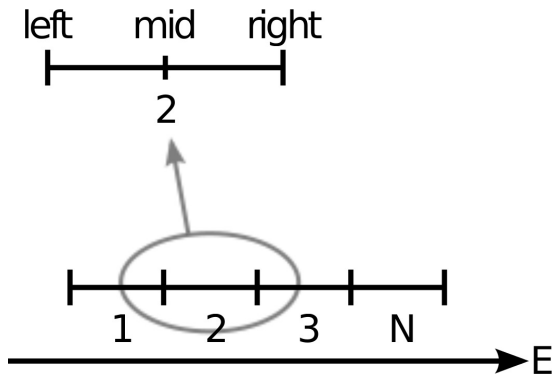
$$\Gamma_{ph} = \frac{4\pi}{h} \sum_{i=1}^{N_{bins}} \frac{I_i \sigma_i}{\langle E_i \rangle} (E_i^{right} - E_i^{left}) (\langle E_i \rangle - E_0) \quad (11)$$

$$\langle E_i \rangle = \frac{E_i^{right} + E_i^{left}}{2} \quad (12)$$

Energy binning: why and how



$$I(E) = \left[\frac{\text{eV}}{\text{cm}^2 \text{s Hz sr}} \right] = \left[\frac{\text{eV}}{\text{cm}^2 \text{sr}} \right]$$

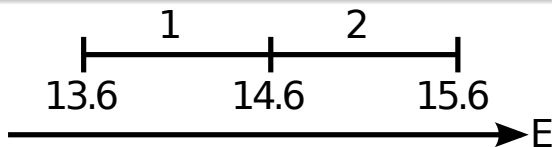


$$\langle E \rangle = E_{\text{mid}} = 0.5(E_{\text{left}} + E_{\text{right}})$$

```
use krome_user
call krome_set_photoBinE_lr(arrayL(:), arrayR(:))
```

KROME Bootcamp 2021 - Get / Set

```
./krome -n network.ntw -usePhotoBins=2
```

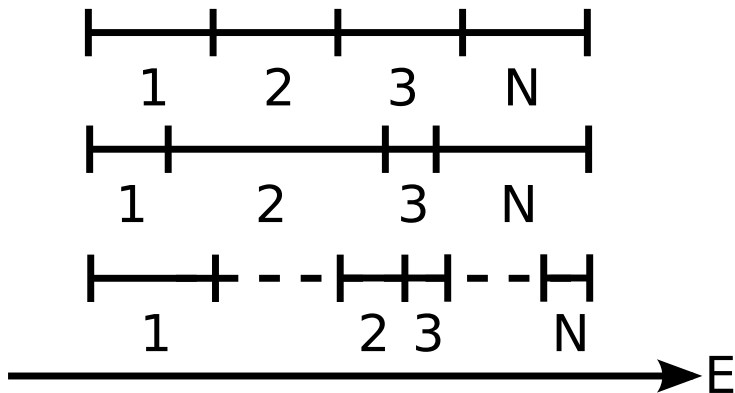


```
use krome_user
real*8::arrayL(krome_nPhotoBins)
real*8::arrayR(krome_nPhotoBins)
arrayL(:) = (/13.6d0, 14.6d0/) !eV
arrayR(:) = (/14.6d0, 15.6d0/) !eV
call krome_set_photobinE_lr(arrayL(:), arrayR(:))
arrayR(:) = krome_get_photoBinE_right()
print *,arrayR(:)
```

```
14.6000000 15.6000000
```

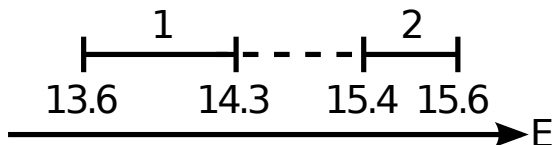
Why left and right?

Left / Right allow to customize intervals (including empty)



KROME Bootcamp 2021 - Custom bins (example)

```
./krome -n network.ntw -usePhotoBins=2
```



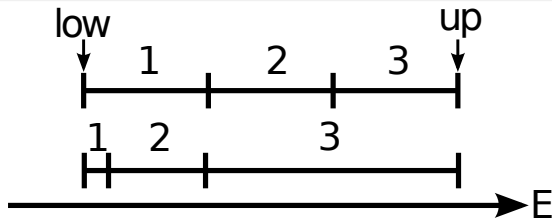
```
real*8::arrayL(krome_nPhotoBins)
real*8::arrayR(krome_nPhotoBins)
arrayL(:) = (/13.6d0, 15.4d0/) !eV
arrayR(:) = (/14.3d0, 15.6d0/) !eV
call krome_set_photobinE_lr(arrayL(:), arrayR(:))
mid(:) = krome_get_photoBinE_mid()
print *,mid(:)
```

13.95000000000000

15.50000000000000

KROME Bootcamp 2021 - Automatic bins (example)

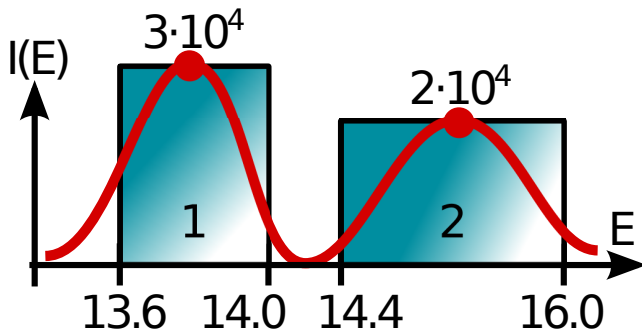
```
./krome -n network.ntw -usePhotoBins=3
```



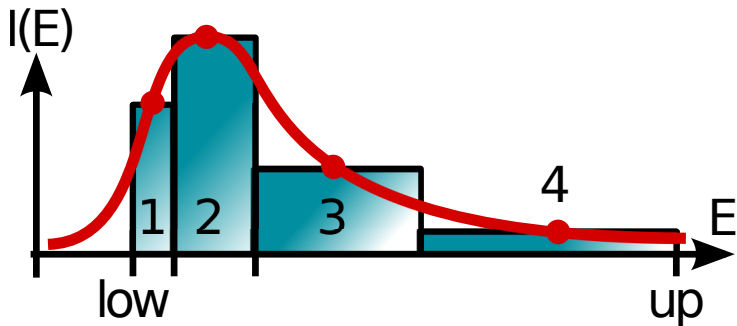
```
low = 1d0, up = 1d3 !eV  
call krome_set_photobinE_lin(low, up)  
call print *, krome_get_photoBinE_mid()  
call krome_set_photobinE_log(low, up)  
call print *, krome_get_photoBinE_mid()
```

```
167.5000000    500.5000000    833.5000000  
5.500000000    55.00000000    550.0000000
```

KROME Bootcamp 2021 - I(E) bins (example)



```
arrayL(:) = (/13.6d0, 14.4d0/) !eV
arrayR(:) = (/14.0d0, 16.0d0/) !eV
arrayJ(:) = (/3d4, 2d4/) !eV/cm2/sr
call krome_set_photoBinE_lr(arrayL(:), arrayR(:))
call krome_set_photoBinJ(arrayJ(:))
```



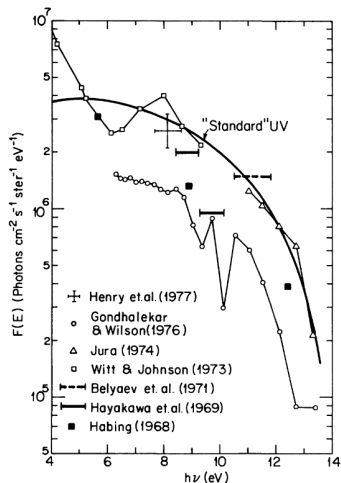
```
low = 5d0 !eV
```

```
up = 2d1 !eV
```

```
Tbb = 3d4 !K
```

```
call krome_set_photoBin_BBlog(low, up, Tbb)
```

KROME Bootcamp 2021 - Automatic I(E)/2

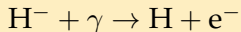


```
low = 5d0 !eV
```

```
up = 12d0 !eV
```

```
call krome_set_photoBin_draineLog(low, up)
```

How to add a photoreaction to a network file



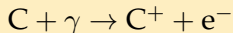
```
@format:idx,R,P,P,Tmin,Tmax,rate
```

```
@photo_begin
```

```
42,H-,H,E,0.755,1d3,2.11d-16*(energy_eV-.755)**(1.5)  
*energy_eV**(-3)
```

```
@photo_end
```

Automatic $\sigma(E)$



```
@photo_begin
```

```
11,C,C+,E,auto
```

```
@photo_end
```

NOTE: KROME is not a reaction database (GIGO)!



PHOTO IONIZATION/DISSOCIATION RATES

HOME Photon Spectra How to Use this Website References Contact

Photo Cross Sections Blackbody Radiation Field Interstellar Radiation Field Solar Radiation Field

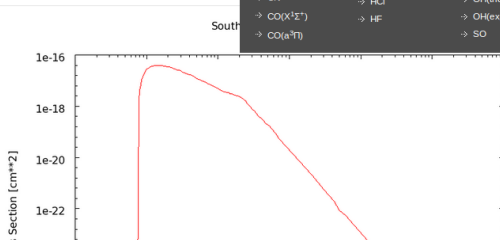
Photo Cross Sections

TOTAL AND PARTIAL CROSS SECTIONS

X Axis Value: Wavelength Energy

Cross Sections of H⁺

Total



Molecule Selection

Atomic Neutrals

Atomic Ions

Diatomics

Triatomics

Tetratomics

Pentatomics

> 5 Atoms

- BrO
- C₂
- CH
- CN
- CO(X¹Σ⁺)
- CO(a³Π)
- Cl₂
- F₂
- H₂
- HCl
- HF
- N₂
- NO
- O₂
- OH(theor)
- OH(exp)
- SO

External cross section (network)

```
@photo_start  
  1, H-, H, E, @xsecFile=SWRI  
@photo_end
```

```
data/database/swri_xsecs/H-.dat
```

External cross section (data file)

```
Branching ratio for H-      Total      2 branches  
Lambda      Total          H+/2e          H/e  
  1.0      2.00E-27      0.00E+00      2.00E-27  
  5.2      6.11E-25      4.58E-28      6.11E-25  
 10.0      5.60E-24      9.00E-27      5.59E-24  
 15.5      2.40E-23      6.22E-26      2.39E-23  
 20.0      5.53E-23      1.87E-25      5.51E-23  
  . . .
```


<http://home.strw.leidenuniv.nl/~ewine/photo/>

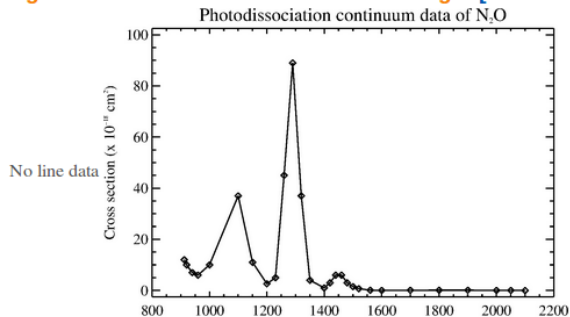
N₂O cross sections [\[download\]](#)

Tabulated photorates [\[download\]](#)

Tabulated photorates in units per second (s^{-1}).

	Draine Field	4000 K	6000 K	10000 K	20000 K
Continuum processes	1.9 (-09)	2.0 (-11)	7.9 (-11)	4.8 (-10)	1.5 (-09)

Figures of cross section versus wavelength [\[download\]](#)



External cross section (network)

```
@photo_start  
  1,N2O,N2,O,@xsecFile=Leiden  
@photo_end
```

```
data/database/leiden_xsecs/N2O__N2_O.dat
```

External cross section (data file)

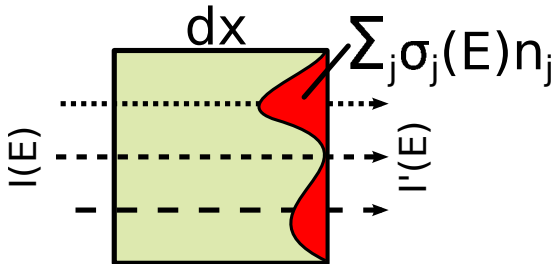
```
N2O P.D. CF. ZELIKOFF ET AL. ('53)  
  0  
 28  
-1.  
  1   912.0   0.120E-16  
  2   920.0   0.100E-16  
  3   940.0   0.700E-17  
...
```

External cross section (network)

```
@photo_start  
  1, C, C+, E, @xsecFile=photoC.dat  
@photo_end
```

External cross section (data file)

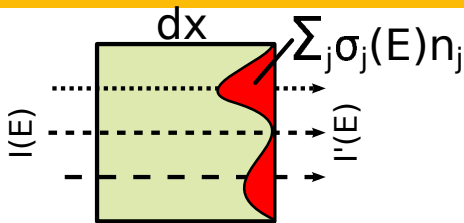
#LEFT (eV)	RIGHT (eV)	XSEC (cm ²)
14.6	14.8	1.3d-18
20.2	20.5	7.3d-19
...		



Opacity

$$I'(E) = I(E) e^{-\tau(E, \mathbf{n})}$$

$$\begin{aligned} \tau(E, \mathbf{n}) \rightarrow \tau_i &= \sum_{j \in \text{react}} \sigma_{ij} n_j \Delta x \\ &+ \pi \sum_{j \in \text{dust}} Q_{ij} a_j^2 n_j^d \Delta x \end{aligned}$$



No size information (assumes geometry)

```
./krome -n mynetwork.ntw -columnDensityMethod JEANS  
krome_get_opacity(n(:), Tgas)
```

Use table for dust opacity (size-based)

```
krome_load_opacity_table(fileName)  
krome_get_opacity_size_d2g(n(:), Tgas, dx, dust2gas)
```

Fully-consistent (size-based)

```
krome_get_opacity_size(n(:), Tgas, dx)
```

What you learned

- 1 KROME photobinning
- 2 Include photochemical reactions in KROME (cross sections)
- 3 How to get opacity from KROME

(Thank you for your attention!)