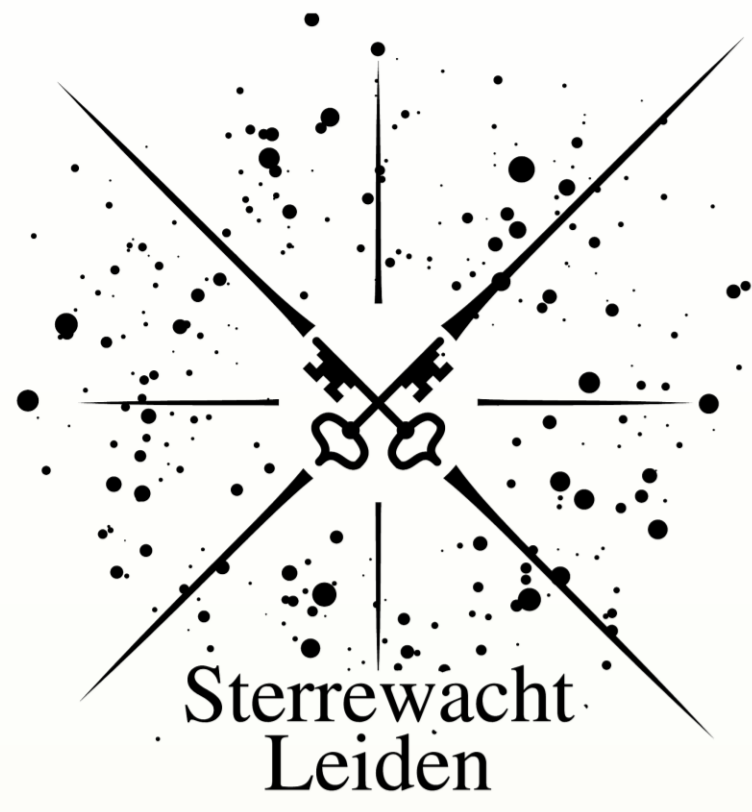


Modeling Polycyclic Aromatic Hydrocarbons in Circumstellar Disks: Chemistry and IR Emission

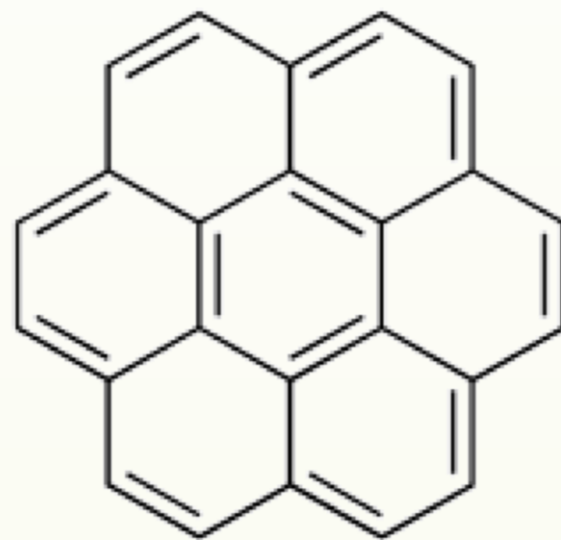


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Introduction

Polycyclic aromatic hydrocarbons (PAHs) have been detected in the mid-infrared (IR) spectra of disks around T Tauri and Herbig Ae/Be stars.^{1,2} The details of their spectral features (primarily at 3.3, 6.2, 7.7, 8.6 and 11.3 μm) depend on the size and shape of the PAHs, the charge (Z) and the number of peripheral hydrogen atoms (N_H). Hence, in order to understand observed spectra, it is important to understand the chemical behaviour of PAHs in disks.



We have adapted an existing radiative transfer and ray-tracing model^{3,4} to include a detailed treatment of the PAH chemistry⁵ and IR emission⁶. Our model calculates:

1. The disk structure and radiation field.
2. At each point in the disk, the destruction rate of the PAHs.
3. At each point in the disk, the equilibrium (steady state) distribution of the PAHs over all possible charge/hydrogenation states.
4. Emission from all charge/hydrogenation states.
5. Spectrum as observed through telescope.

Template model

The template model is a Herbig Ae/Be star ($R=2.8R_\odot$, $M=2.9M_\odot$, $T_{\text{eff}}=10,000$ K) with a $0.01M_\odot$ disk stretching out from 0.83 to 300 AU. The disk has a puffed-up inner rim ($H/R_{\text{in}}=0.02$) and is slightly flaring ($H/R_{\text{disk}}=0.14$). $C_{50}H_y$ is added as a prototypical PAH at a constant abundance.

Photodestruction of PAHs

The radiation field in the disk can be as high as $G_0=10^{10}$ (Fig. 1), so destruction of PAHs in multi-photon absorption events has to be taken into account. $C_{50}H_y$ is destroyed within the disk lifetime for $G_0'>1.2\cdot 10^5$. Some 75% of the emission comes from such regions, so this has to be removed from the calculated spectrum. Larger PAHs are less easily destroyed. For instance, $C_{100}H_y$ survives until $G_0'=2.2\cdot 10^7$, which is only reached in a very small part of the emitting region (Fig. 1).

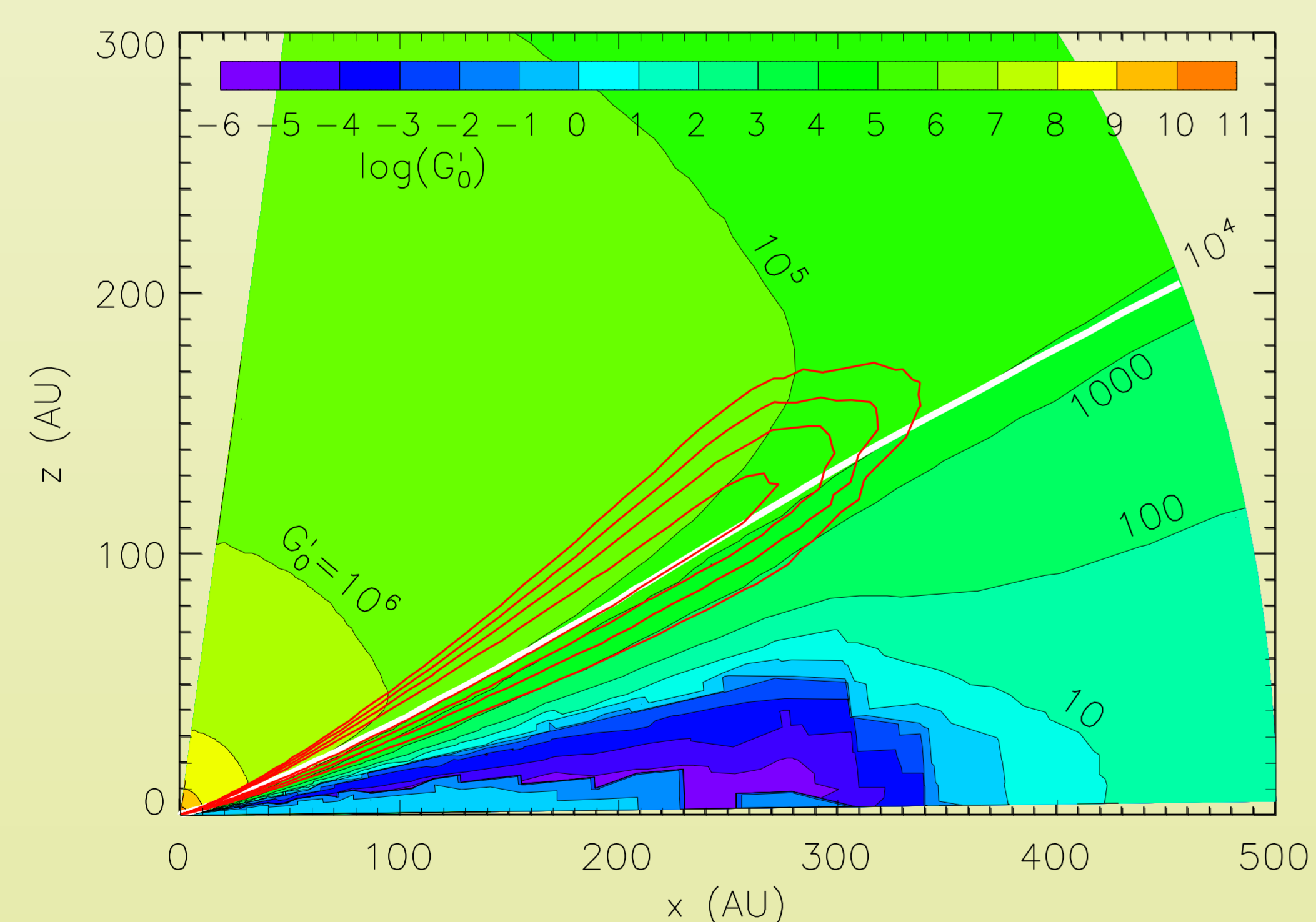


Fig. 1 Disk structure and radiation field

Radiation field in the disk around a 10,000 K star, characterized by G_0 in the colour scale. The red contour lines denote the region responsible for most of the PAH emission before photodestruction of PAHs is taken into account; from the outside inward, the contours contain 93, 87, 73 and 49% of the total mid-IR emission. The solid white line denotes the $\tau_{\text{vis}}=1$ surface.

Conclusions

1. Many charge/hydrogenation states contribute to the emission.
2. Observations are in agreement with a mix of charge states.
3. PAH emission originates from all disk radii and mostly from the surface layer.

Results: Chemistry

This table shows the emission and abundance of the eight most important charge/hydrogenation states, after photodestruction has been taken into account. The spatial distribution of six of these is plotted in Fig. 2.

Species	Emission (% of total PAH em.)	Abundance (% of total PAH abun.)
$C_{50}H_{17}$	18	0.18
$C_{50}H_{17}^+$	24	0.026
$C_{50}H_{18}^-$	— ^a	31
$C_{50}H_{18}$	32	21
$C_{50}H_{18}^+$	20	0.025
$C_{50}H_{36}^-$	— ^a	45

^a Negatively charged species (PAH anions) are assumed not to contribute to the emission because of the high probability of photodetachment upon UV absorption.

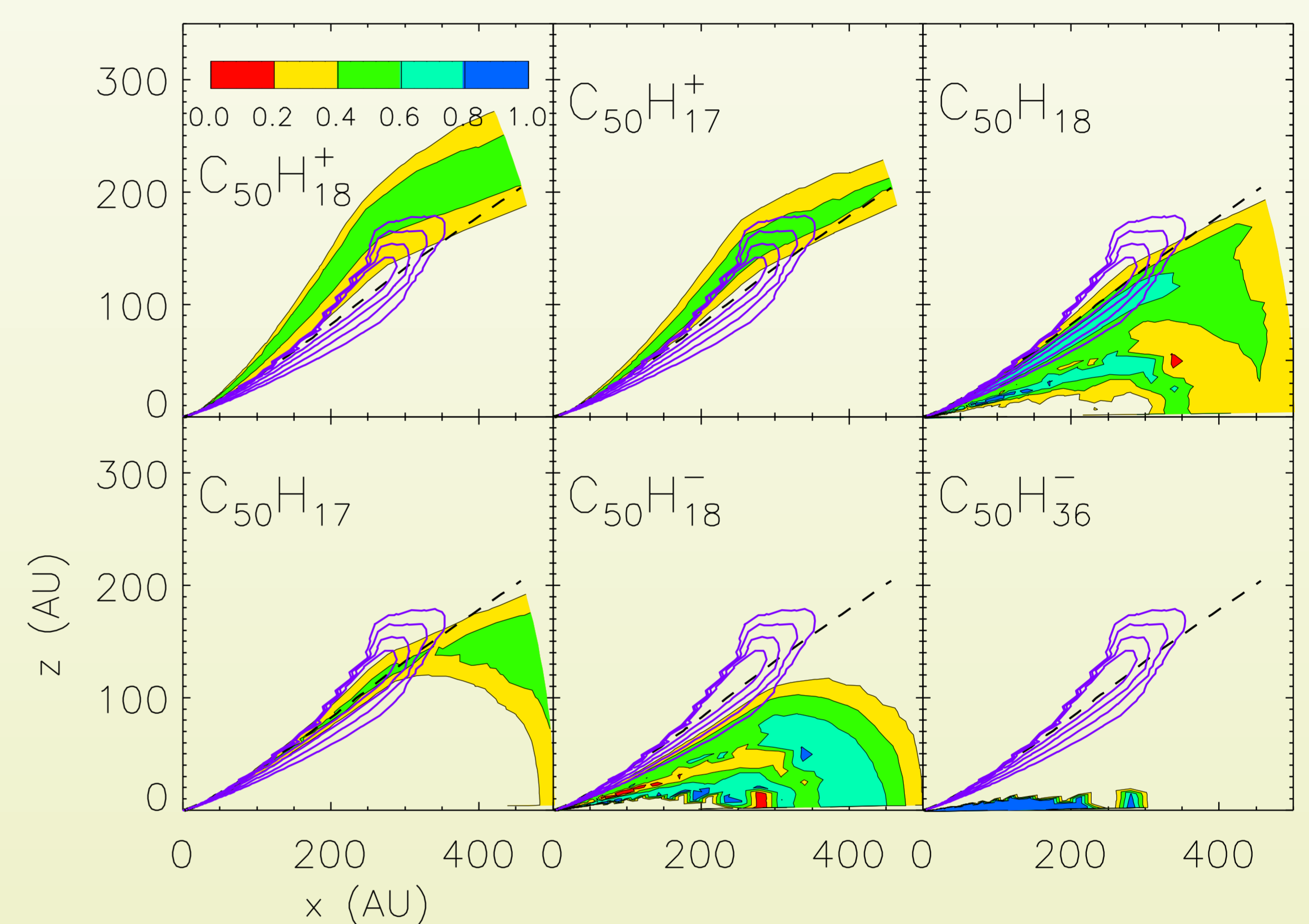


Fig. 2 Spatial distribution of charge states

Spatial distribution of six charge/hydrogenation states for $N_C=50$. The colour scale shows the abundance of each state w.r.t. the total PAH abundance. The purple contour lines contain 93, 87, 73 and 49% of the mid-IR PAH emission after photodestruction of PAHs was taken into account. The dashed line is the $\tau_{\text{vis}}=1$ surface.

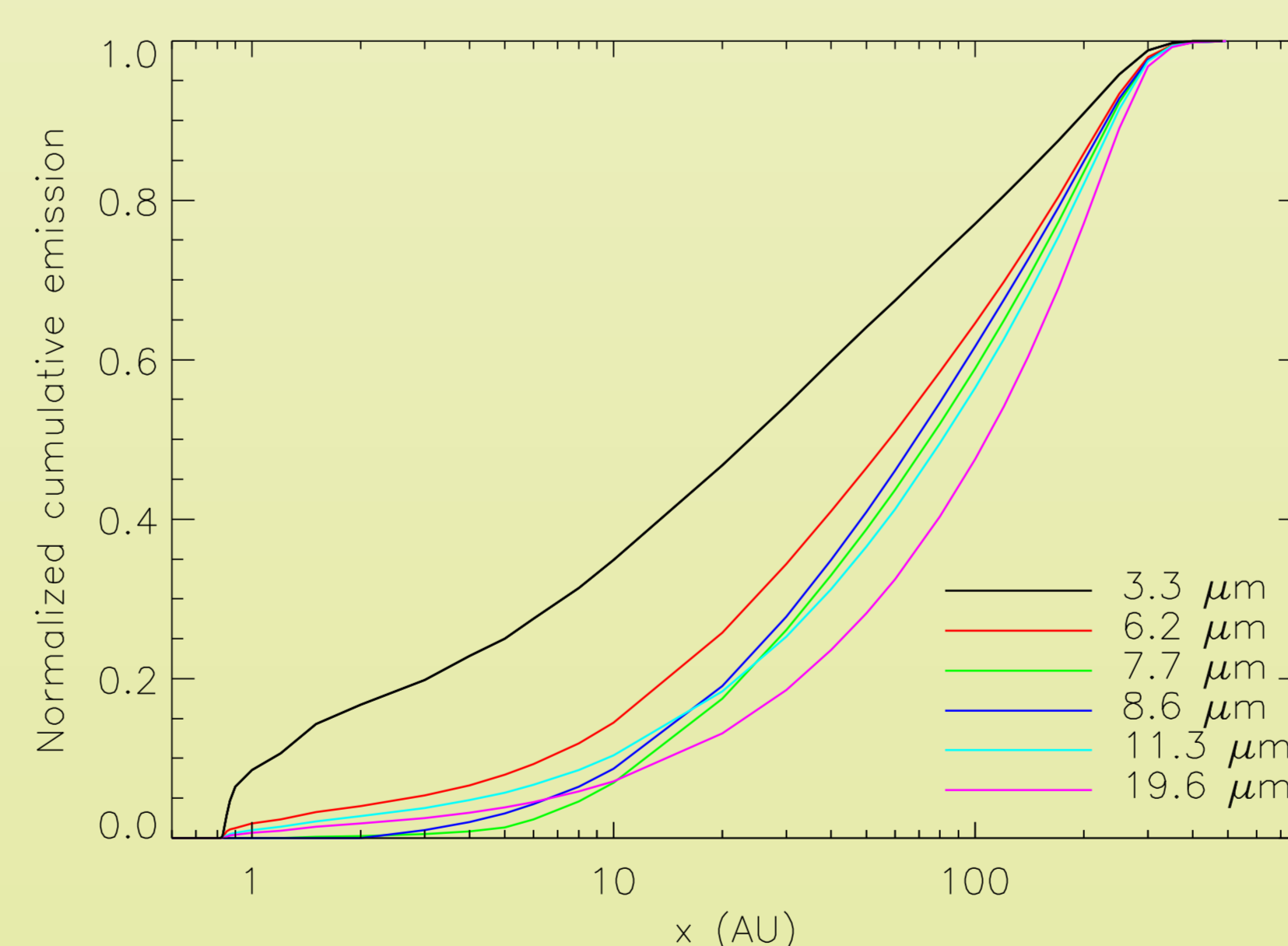


Fig. 3 Spatial extent of emission

Spatial extent of the five major PAH features and the 20- μm continuum for $N_C=50$. Some 10% of the emission comes from the inner 10 AU. The 3.3- μm feature is less extended than the other features, which in turn are less extended than the 20- μm continuum. These results are in good agreement with the model by Habart et al. (2004).⁷

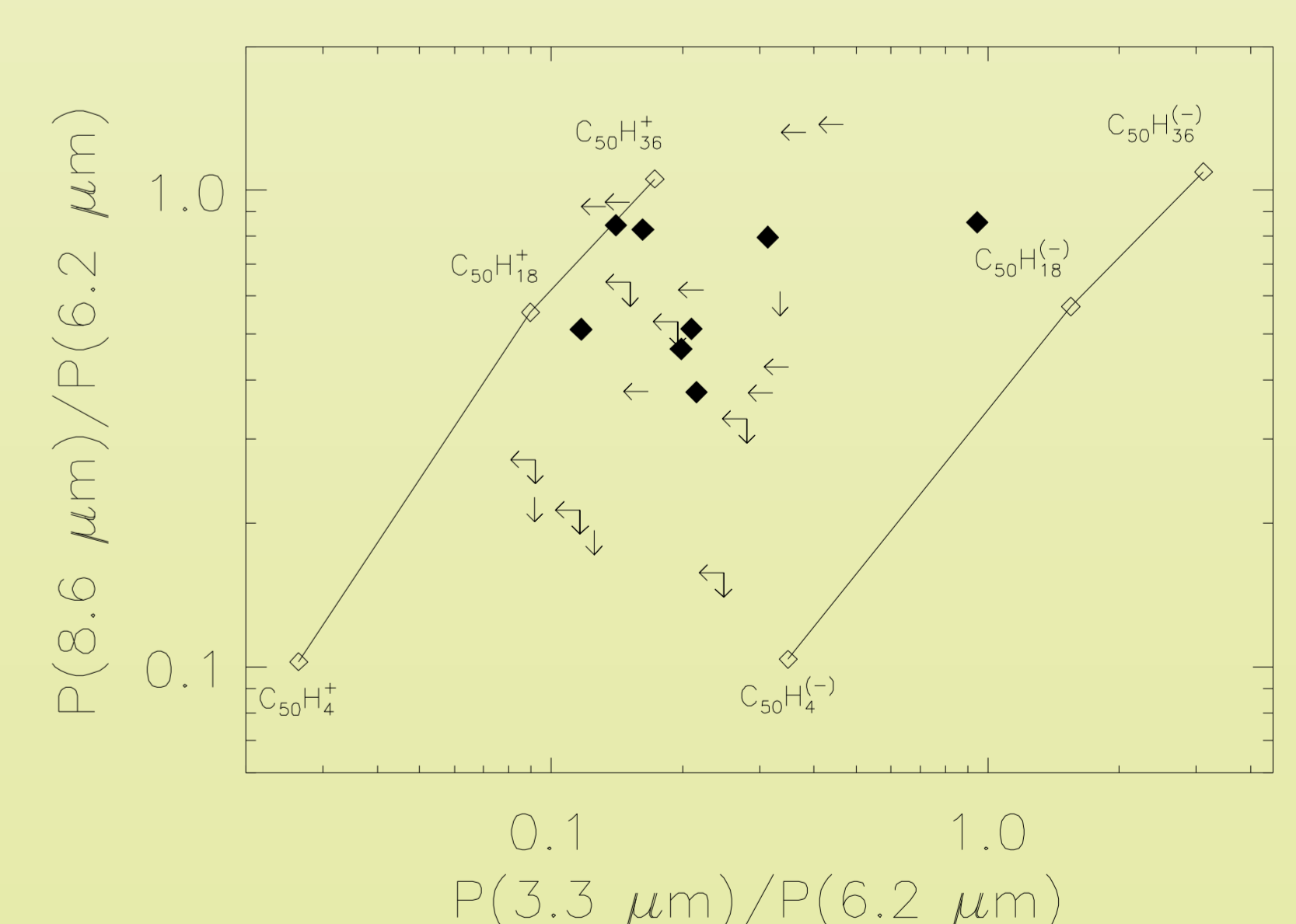


Fig. 4 Feature-to-feature ratios

Peak flux ratios: 8.6/6.2 versus 3.3/6.2. Observations (filled dots) and upper limits (arrows) from Herbig Ae/Be disks² are located between the model values for neutral and positively charged PAHs, confirming that the observed emission comes from a variety of charge and hydrogenation states.

For a practical application of the model, see the poster by V.C. Geers et al.

References

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- ⁵ Le Page et al. 2001, ApJS, 132, 233; 2003, ApJ, 584, 316
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