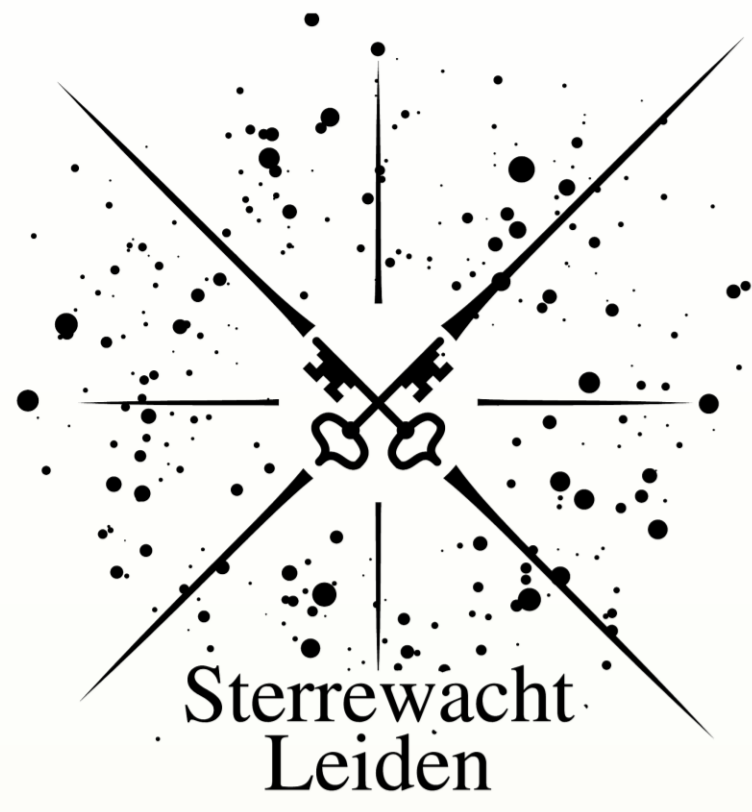


Modeling Polycyclic Aromatic Hydrocarbons in Circumstellar Disks: Chemistry and IR Emission



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Introduction

Polycyclic aromatic hydrocarbons (PAHs) are present in disks around T Tauri and Herbig Ae/Be stars.^{1,2} They show infrared (IR) emission features at 3.3, 6.2, 7.7, 8.6 and 11.3 μm . Depending on the position within the disk, and the physical conditions at that point, a PAH can be in different charge states (Z) and it can bear different numbers of peripheral hydrogen atoms (N_H). The IR emission properties are different for each charge/hydrogenation state. 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 more detailed treatment of the PAH chemistry⁵ and IR emission⁶ than has previously been done. In general terms, our model calculates the following:

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

Results

More than 90% of the PAHs throughout the disk are negatively charged and doubly hydrogenated (Table 1). However, the bulk of the emission originates from neutral and positively charged states and, for the smaller PAHs, from normally hydrogenated states. This is easily understood from the spatial distribution of both the individual charge/hydrogenation states and the PAH emission (Fig. 3): the emission comes from regions where the UV field is relatively strong. There, the extra hydrogen atoms are efficiently removed. Larger PAHs are more resistant to photodissociation, so they can sustain the extra hydrogen atoms everywhere.

The PAH emission extends across the entire disk (Fig. 1), with ~6% coming from the inner 1 AU and ~24% from the inner 10 AU. The 3.3 μm band, which is almost entirely due to neutrals and negative ions, is relatively strong in the inner region.

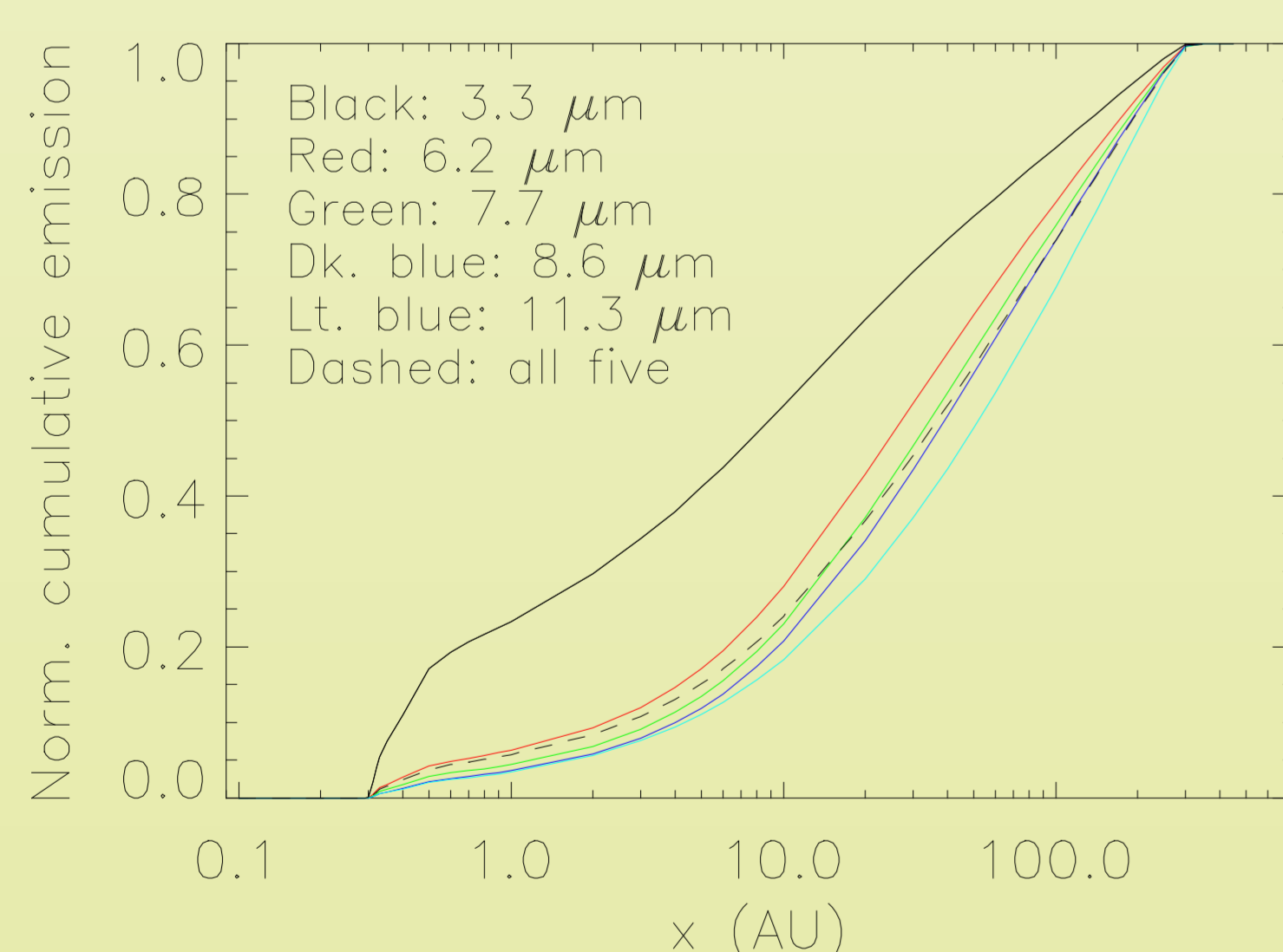


Fig. 1 Spatial extent of the five major PAH features for $N_C=50$. The disk's inner rim lies at 0.3 AU and its radius is 300 AU.

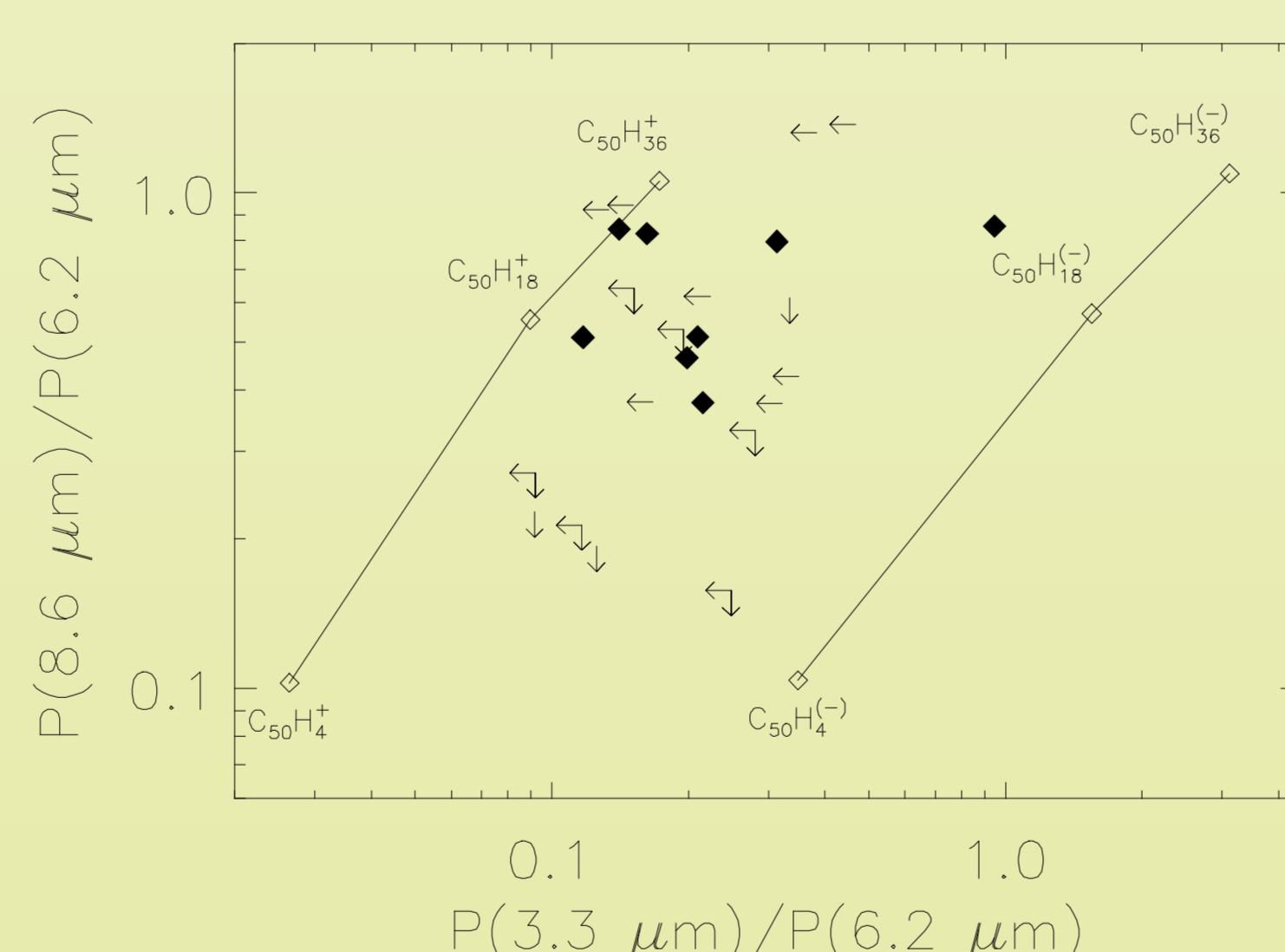


Fig. 2 Peak flux ratios: 8.6/6.2 versus 3.3/6.2. Observations (filled dots) and upper limits (arrows) from Herbig Ae/Be disks² are located between the model values for neutral and positively charged PAHs.

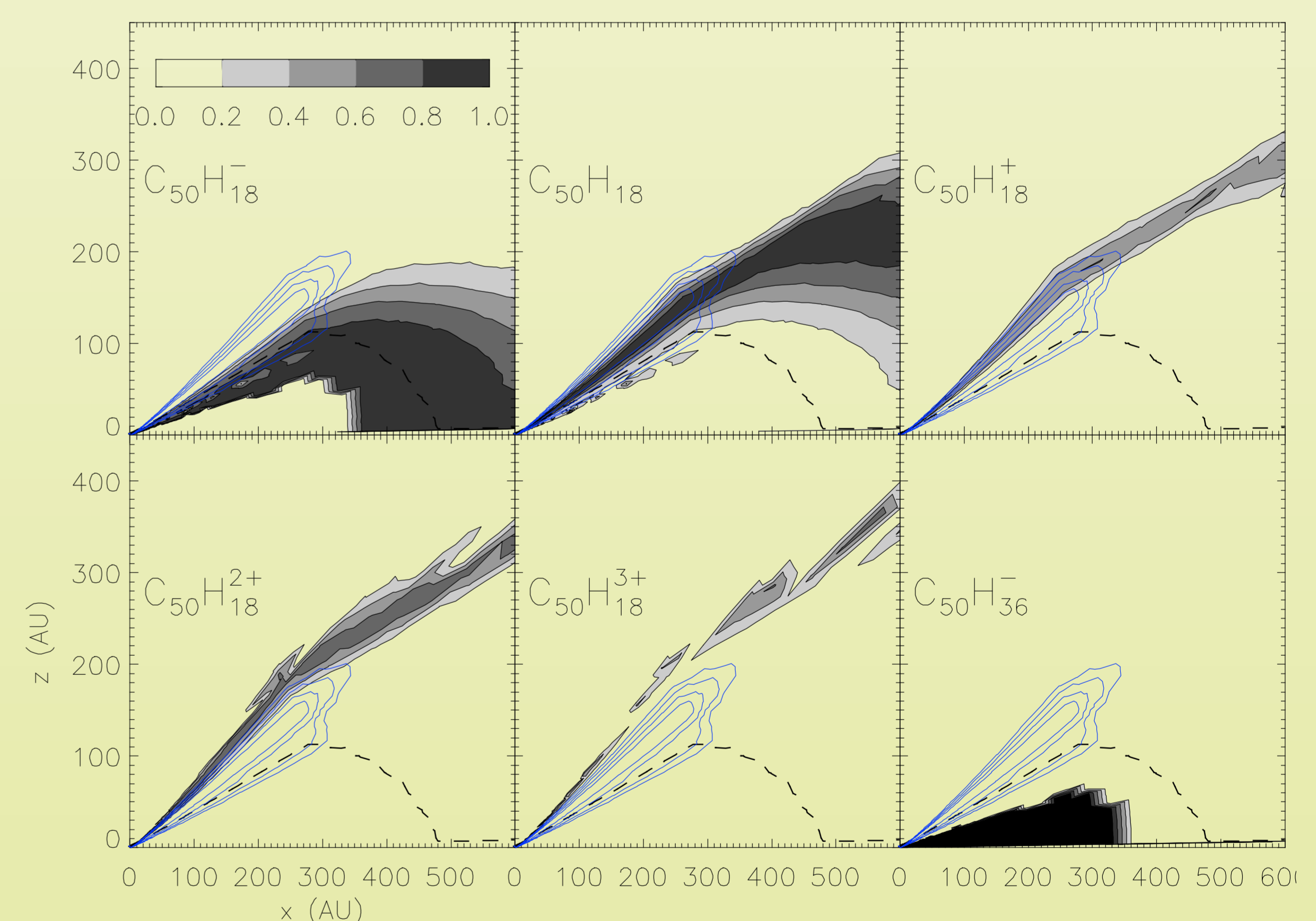


Fig. 3 Spatial distribution of six charge/hydrogenation states for $N_C=50$. They grey scale shows the abundance of each state w.r.t. the total PAH abundance. The dashed line is the $\tau=1$ surface. The blue contour lines trace the strength of the PAH emission; they are spaced in intervals of $10^{1/3} \approx 2.15$.

Conclusions

1. Larger PAHs are more strongly hydrogenated.
2. Negatively charged PAHs contribute to the spectrum as well as neutral and positively charged PAHs.
3. Observations are in agreement with a mix of charge states.
4. PAH emission originates from all disk radii and mostly from the surface layer.

Table 1 Relative abundance and emission per charge/hydrogenation state for four PAH sizes.

N_C	Abundance ^a	Emission ^b	N_H, Z
24			12, -1 12, 0 24, -1
50			18, -1 18, 0 18, +1 18, +2 36, -1 19, +1
72			42, -1 42, 0 42, +1 42, +2 42, +3
96			48, -1 48, 0 48, +1 48, +2 48, +3 48, +4

^a In the entire disk

^b Between 2.5 and 13.5 μm

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