Deuterated H₃⁺ in Protoplanetary Disks

C. Dominik

and

University of Amsterdam

C. Ceccarelli

Abstract

In disks surrounding solar type protostars, the bulk of the disk mass resides in the outer midplane, which is cold (<20 K), dense (> 10^7 cm⁻³) and depleted of CO. Observing the disk midplane ist therefore a formidable challenge. Ceccarelli et al. (2004) detected H₂D⁺ emission in a proto-planetary disk and claimed that it probes the midplane gas. Indeed, since all heavy-elements bearing molecules condense out onto the grain mantles, the most abundant ions in the disk midplane are predicted to be H₃⁺ and its isotopomers. We present a theoretical study of the chemical structure of the outer midplane of proto-planetary disks. Using a self-consistent physical model for the flaring disk structure, we compute the abundances of H3+ and its deuterated forms across the disk. We also provide the average column densities across the disk of H₃+, H2D+, HD2+ and D3+, and the line intensities of the ground transitions of the ortho and para forms of H_2D^+ and HD_2^+ . A paper describing the model and results has been sumbitted to A&A.

Disk model

We are using a passive disk model with an inner hole (Dullemond, Dominik, Natta 2002, Dullemond et al 2002) to compute the density and temperature structure of a 400 AU radius disk with dust mass 2x10⁻⁴M_o around a solar-type pre-main-sequence star(L*=0.5 L_{o.} T*=3630K).

Chemistry of H₃⁺ deuteration

Following the work by Roberts et al (2003, 2004) and Walmsley et al (2004), we consider the chemistry in the midplane of a CS disk. Because of the high gas density and low temperature, most molecular species become depleted onto grains. The last two important molecules to disappear are CO and N₂ The chemistry is then dominated by cosmic ray ionization of H₂, which leads to the formation of H₃⁺, and, to a lesser degree, of H⁺. The negative charge is present as electrons and singly charged grains. Reactions with HD lead successively to H_2D^+ , HD_2^+ , and D_3^+ . The main destruction reaction for these molecules are recombinations with electrons, grains, or any remaining CO and N₂ molecules in the gas phase. The amount of these molecules is determined by an equilibrium between freeze-out onto grains and cosmic-ray driven liberation of single molecules from the ices. We solve the resulting chemical network by determining the steady state solution.

LAOG (Grenoble)



Chemical abundances in the disk. H₃⁺ it the most abundant ion close to the disk surface. Deep in the CO depleted disk the deuterated isotopes of H₃⁺ gain importance and dominate. D₃⁺ is about as abundant as H₂D⁺ and HD₂⁺, due to destruction by N₂.

Temperature and density structure of the disk model



Conclusions

- H3+ deuteration is significant in protoplanetary disks around low mass stars. Disks around intermediate and high mas stars are too warm
- H_2D^+ alone is **not** the dominating ion. H_3^+ , HD_2^+ and D_3^+ and are all equally important. H+ is only of minor relevance, in contrast to protostellar cores with densities below 107 cm-3.
- · With increasing depletion of CO and N2, D3+ eventually dominates as positive charge carrier.
- · Chemical structure and line intensities are a strong function of the local cosmic ionization rate.
- · The line intensities are also sensitive to the dust-to-gas ratio as long as depletion of heavy element bearing molecules is not complete.
- · The grain size has strong influence on column densities and line strengths. Small grains accelerate recombination and reduce the abundances of all positive ions

References

Dullemond C.P., Dominik C., Natta A. 2002, A&A 287, 313 Dullemond C., v. Zadelhoff G.-J., Natta, A. 2002, A&A 389, 464 Ceccarelli C; Dominik C, Lefloch B,Caselli P, Caux E, 2004, ApJ 607,L51 Walmsley C.M., Flower D.R., Pineau des Forêts G. 2004, A&A 418,1035 Roberts, H.; Herbst, E.; Millar, T. J. 2003, ApJ 591,L41 Roberts, H.; Herbst, E.; Millar, T. J. 2004, A&A 424, 905



Logarithm of the column density of the 3 deuterated isotopes of H3+, and the electrons, as a function of dust-to-gas ratio (i.e. changing gas mass while the dust mass is fixed) and cosmic ray ionization rate



v-integrated line intensities (mean beam temperature), of o-HD₂⁺ $1_{1,0}$ - $1_{1,1}$ (solid lines) and p-HD₂⁺ $1_{1,0}$ - $1_{0,1}$ (dashed lines) transitions, in mK for CSO and JCMT observations respectively. The three panels show the effect of different grain sizes.