Project B2:

Astrochemistry in the atmosphere and winds of photoevaporating discs

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Requested positions: 1 Postdoc

Abstract:
Protoplanetary discs lose mass via a slow disc wind, probably driven by photoevaporation from the central star, which eventually creates a cavity, leading to the formation of a Type 1 TD (see discussion in the Introduction to the Research Unit). The strength and profile of these winds remains, however, unconstrained from the models, as so suitable diagnostic is known to directly determine the wind properties from observations. This is due to the fact that a thermochemical study of this important component of evolved discs does not exist to date. The study of the chemistry in disc winds however relies on a knowledge of the opacities, which are largely dominated by small dust grains which are entrained in the wind from the underlying disc at the launch point. In this project we plan to develop a reduced chemical network appropriate for photoevaporative wind conditions and couple our chemical codes to space and time-varying dust distribution obtained in project C2. Using state-of-the-art radiation-hydrodynamic models of photoevaporating primordial and TDs, we will for the first time be able to draw detailed chemical profiles of these winds and provide predictions by using radiative transfer codes. This is of fundamental importance to identify and interpret new spectral line diagnostics in existing and upcoming observations.

1. State of the art and preliminary work

1.1 Models of Disc Dispersal

Disc dispersal models, like photoevaporation, have been motivated by the observation that the dispersal of protoplanetary disc is not a continuous process. In particular the detection of transition discs i.e. discs with an evacuated inner dust and/or gas gap/cavity, and their frequency with respect to full discs has encouraged models which could match dispersal timescales about 10 times faster than the global disc lifetimes, and inside-out dispersal (e.g. Ercolano, Clarke & Hall 2011; Koepferl, Ercolano et al. 2013).

Recent reviews (e.g. Alexander et al. 2014, Armitage 2011) describe the available photoevaporation models in detail, and they point out that the predictions from these differ, sometimes by order of magnitudes in critical wind properties like mass loss rates and profiles (see Introduction to the Research Unit and project B1). Current photoevaporation models differ substantially in the approach to the complex problem of driving a thermal wind from the surface of a disc.

The different models can be grouped, depending on the type of stellar radiation supposed to be driving the wind. They include basically 3 categories':

1. FUV-driven models (e.g. Gorti, Dullemond & Hollenbach 2009). Photons just below 13.6 eV,

mass loss rates vary strongly with input, but up to $10^{-8} M_{\odot}/yr$, mass loss profile extending from $\sim$1 AU to $>\sim$100 AU a solar. Main model limitations: no hydrodynamics.

2. EUV-driven models (e.g. Alexander et al. 2006). Photons at roughly 13.6 eV, mass loss rate approx $10^{-10} M_{\odot}/yr$, mass loss concentrated at the gravitational radius (around 1AU for a solar mass star). Main model limitations: isothermal calculation, input flux unknown.

3. X-ray-driven models (e.g. Owen, Ercolano et al. 2010). Photons with 13.6 $<$ E $<$ a few 100 eV, mass loss rate approx $10^{-8} M_{\odot}/yr$, mass loss profile broader extending from $\sim$1 AU to $\sim$70 AU a solar type star. Main model limitations: no chemistry.

The consequences of these large differences in the dispersal model on the formation and evolution of planets have been often demonstrated (e.g. Ercolano & Clarke 2009; Ercolano & Rosotti, 2015; Alexander & Pascucci 2012), but still no quantitative dispersal model exists The fundamental reason why the theoretical models still wildly disagree with each other is because until now they could not be directly tested with observations. The B2 project aims at enabling the construction of a detailed chemical model of disc winds and atmospheres to directly compare with observations and provide a quantitative picture of the wind properties.

As well as thermal winds driven by irradiation from the central star, the idea of magnetically driven winds has also been recently proposed. The classical magnetically supported/driven winds were developed to explain outflows from young stars, particularly in the class I phase. One set of these models were based on disc/magnetosphere interactions and mostly deal with the ideal MHD region of the disc (e.g. Shu et al. 2006, Ferreira et al. 2006). More recently, Bai et al. (2016), based on an extrapolation of the local calculations of Bai & Stone (2013) have suggested, however that non-ideal MHD effects, may also cause a disc wind which may be launched from a much extended region of the disc, overlapping/supporting/competing with photoevaporation to the dispersal of the disc. These authors suggest that these magnetically-launched disc winds, if they exist, may be so vigorous as to compete with photoevaporation for the dispersal of the disc. The magnetic driving models are, however, highly uncertain as they are based on a number of assumptions that still need to be verified. In particular, the models require a minimum level of ionisation for the gas to be coupled to the magnetic field and assume that this may be delivered from far ultra-violet (FUV: 122-200nm) radiation ionising the atmosphere of a disc. The level of ionisation in the upper layer is currently estimated rather crudely as a fixed ionisation fraction of f = 2×10^{-5} in the form of carbon in the FUV layer, whose column density is chosen by default as Σ_{FUV} = $0.03 gcm^{-2}$. This is based on results from Perez-Becker & Chiang (2011), who however also consider a simplified disc model. Crucially, these models do not include the contribution of the wind which itself may shield the disc atmosphere from the more energetic FUV photons, meaning that the currently used ionisation fractions may be overestimated. The models developed in this project will be able for the first time to provide a case-specific assessment of the level of coupling of the gas to the magnetic fields in the class II phase, taking into account the opacity provided by the wind itself. This is a fundamental ingredient to assess the possible role played by magnetic winds.

1.2 Chemical models of discs

Chemical models of gas in the protoplanetary and transition discs (TDs) are essential to pin down the initial conditions of the gas and dust from which planets form. Several sophisticated models have been and are continuously being developed to interpret the recent (e.g.) Herschel and ALMA observations of discs (e.g. Bruderer et al. 2015; Thi et al. 2013; Aresu et al. 2012; Meijerink et al. 2012; Woitke et al. 2010). These models however deal with with the dense parts of the discs, in rare cases extending to the bound disc atmospheres. Panoglou et al. (2012) have followed ionisation, chemical and thermal evolution within a steady state magneto-hydrodynamic disc wind solution and investigated various stages of young stellar objects (from Class 0 to Class II). No chemical model of a photoeveaporative

TD wind as well as no time-dependent chemical model coupled with the dynamical evolution of a disc exist to date. This is a serious shortcoming for the identification of suitable wind tracers and more importantly wind diagnostics, to guide new observations and constrain disc dispersal models (see discussion in the introduction to the Research Unit and in project B1).

The physical conditions valid for material in the bound disc itself are not appropriate at all for a disc wind. First of all winds are much less dense than the material in the bound discs. Even in the case of vigorous X-ray driven winds, the densities at the base of the wind are rarely above ten million hydrogen atoms per cubic centimetre, and they decrease roughly with the square of the distance (i.e. they behave roughly like Parker winds, see e.g. Owen et al. 2010; Font et al. 2004). The opacity in the wind is further reduced because of the decrease in dust content, as only a fraction of the grains contained in the underlying disc are entrained in the wind (see Owen et al. 2011b, Hutschison et al. 2016ab and discussion in project C2). For these reasons molecules may have a much shorter lifetime and indeed parts of the gas in the wind will be completely photodissociated. For such physical conditions processes like surface chemistry, freeze-out etc. are not important, yielding a simpler problem, which bears less uncertainties compared with chemical models for colder and more opaque material in the bulk of the disc.

The chemical structure of the underlying bound disc is however still important, as it provides the initial conditions for the chemistry in the wind. Furthermore, the ionisation level in the upper layers as well as in the deep layers of the disc has recently been shown to be of outmost importance to the evolution and perhaps dispersal of discs, due to the role it plays in coupling the gas to magnetic fields. A minimum amount of coupling is indeed necessary for magnetic turbulence to take hold.

1.3 Disc Wind diagnostics

A number of disc wind tracers have been studied to date, both observationally and theoretically. To date however no diagnostic could be identified to directly measure the wind properties. Figure **??**, taken from an upcoming review on transition discs by Ercolano & Pascucci (2017, to appear in Royal Society Open Science) shows an example of possible wind diagnostics, which are summarised in the caption.

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We will divide our discussion on wind diagnostics into two parts, ionic and atomic species on the one hand and molecular species on the other.

Ionic and atomic species

The presence of disc winds has been confirmed via the observation of a few km/sec blue-shift in the line profiles of a number of tracers like [NeII] 12.8μm and [OI] 6300 (e.g. Pascucci et al 2007, Rigliaco et al. 2013) and a number of collisionally excited lines in the optical region (Natta et al. 2014).

We have demonstrated, however, that the [NeII] 12.8μm and the optical forbidden lines cannot be used to infer the underlying mass-loss-rates (e.g. Ercolano & Owen 2010, Ercolano & Owen 2016). For example, the intensity and the profile of the [NeII] 12.8μm line can be equally well fitted using an EUV (Alexander 2008) or an X-ray photoevaporation model (Ercolano & Owen 2010), as shown in Figure 2. The problem with the [NeII] line is that the Ne+ formation route can occur both via the removal of a valence electron in the fully-ionised winds driven by EUV radiation, but also by charge exchange of Ne++ with neutral H which is abundant in the quasi-neutral winds driven by X-ray. The problem with the [OI] 6300 line and all other optical collisionally excited lines considered to date is the strong temperature dependence imposed by the Boltzmann term in the emissivity. This means that these lines are mostly just tracing the hot layer of the wind heated by the EUV radiation and not actually tracing the bulk of the wind where it matters (Ercolano & Owen 2016), hence they cannot be used to infer mass-loss-rates or to constrain the wind driving mechanism.

This picture was further complicated by the recent high spectral resolution observations of Simon et al. (2016) who found that low velocity emission in [OI] forbidden lines, classically attributed to a slow-

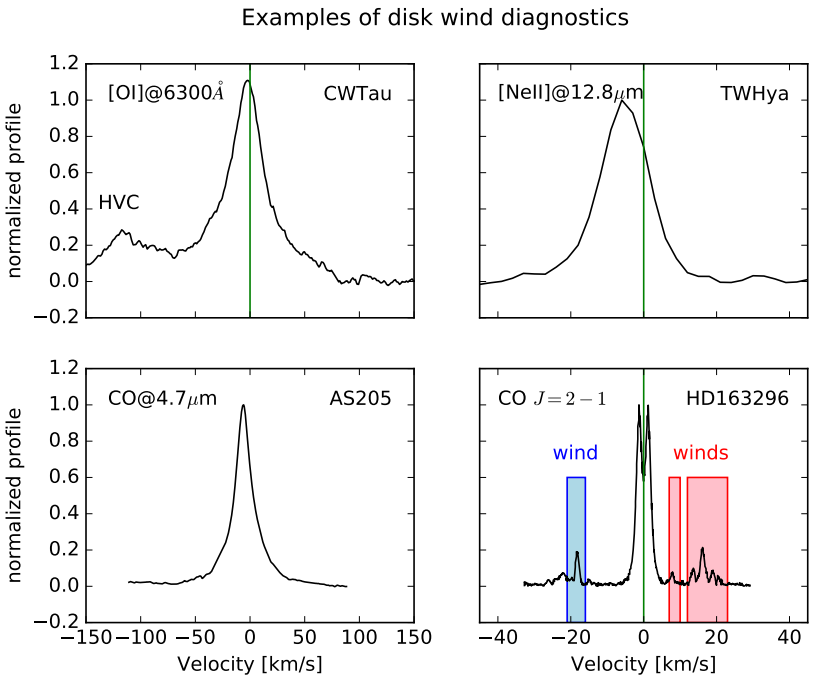

Figure 1: Examples of wind diagnostics. The [OI] 6300 Å profile of CW Tau is from Simon et al. (2016), note that the highvelocity component (HVC) is associated with fast jets. The [OI] 5577 Å transition is weaker than the 6300Å but shows a very similar low-velocity profile (Simon et al. 2016). The CO-M band profile of AS205 is from stacked CO rovibrational lines around 4.7μm (Banzatti & Pontopidan 2015). The [NeII] 12.8μm profile is the mean profile from Pascucci et al. (2011) and the CO J=2-1 profile of HD163296 is from Klaassen et al. (2013). All profiles, except that of AS205, are in the stellocentrc reference frame. Emission shifted in velocity with respect to the stellar velocity is indicative of unbound gas. M-band CO profiles do not have an absolute velocity calibration, indication of a slow wind in AS205 comes from spectro-astrometry (Pontoppidan et al. 2011). This figure is from Ercolano & Pascucci 2017.

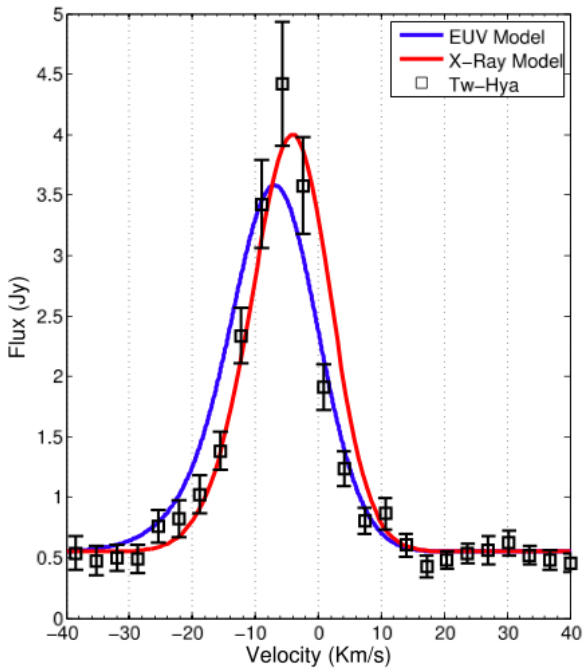

Figure 2: NeII 12.8μm line profile as predicted by the X-ray models of Ercolano & Owen (2010), red line, and by the EUV-only model of Alexander (2008), blue line, compared to the observation of TW-Hya by Pascucci et al. (2009), black line.

moving disc wind, is present in all T-Tauri stars with dust disks, even those classified as WTTs, but it is best fit by a superposition of a broad and a narrow component. Most of the broad component emission arises within 0.5AU and Simon et al. (2016) interpret it as being produced in a magnetically driven wind, given that the emitting region is well inside the gravitational potential well of the central star. The narrow component, which, unlike the broad component, is always present in also in transition discs, traces gas further away (0.5-5 AU) and is probably associated with photoevaporative winds.

The interpretation of the broad component as a tracer of a magnetic wind is however problematic for a number of reasons. The main problem is that one would need a very large scale height to overcome the fact that the emitting volume dominates as one goes to larger radius. Presumably a very large magnetic pressure would be needed to achieve this. Furthermore, if an hypothetical magnetic wind would have enough density to match the observed broad component, it may also absorb out all UV flux, which would then not be available to irradiate the wind at larger radii, which is clearly indicated in the observations.

An alternative explanation could be that the broad component is not produced in the wind, but is emitted by bound material in the disc itself. The broad component, if coming from the inner disc, cannot have however a thermal origin. We have tested that with a new higher resolution set of hydrodynamical calculations, similar to those presented by Ercolano & Owen (2016), which extend further into the inner disc, to $r_{\rm in}$=0.04 AU. The line profiles for the high resolution hydrodynamical calculations are shown in Figure 3 for R=25000, which represent the resolution of the Rigliaco et al (2013) data, when the two component had not been resolved yet, and R=50000, which is more representative of the work of Simon et al. (2016). The R=50000 line profiles in our simulations do show broad wings at high disc inclinations. The wings are due to bound material in the inner disc. However the wings from our high resolution models are still much smaller (i.e. do not carry enough flux) than those detected by Simon et al. (2016). In fact in our calculations the line flux is completely dominated by the (unbound) emission at larger radii. This is easy to understand as the flux is proportional to

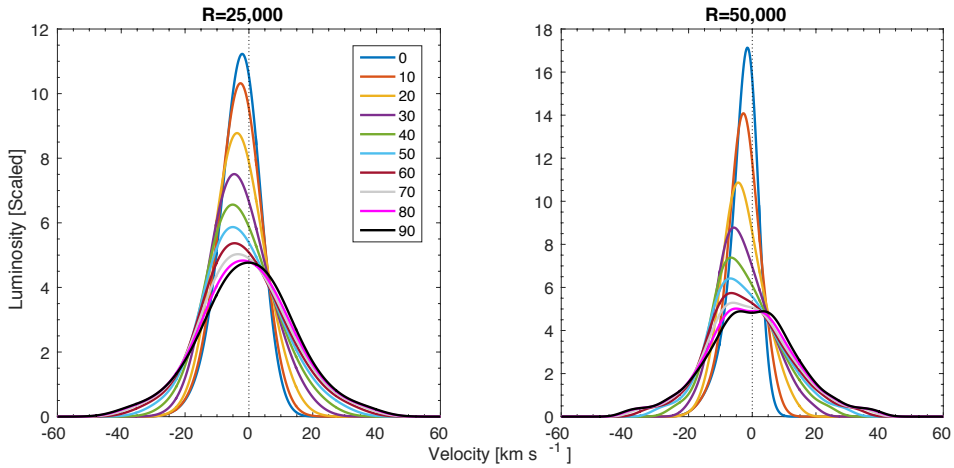

Figure 3: [OI] 6300 line profiles for the high resolution hydrodynamical calculations of Ercolano & Owen (2016) for R=25000 (**left panel**), which represent the resolution of the Rigliaco et al (2013) data, when the two component had not been resolved yet, and R=50000 (**right panel**, which is more representative of the work of Simon et al. (2016). In the left panel wings due to the bound material are clearly seen, but they are much smaller than those presented by Simon et al. (2016).

density squared times the volume and the volume for an isothermal region in the disc scales like $R^{7/2}$ ($R^2 \times H$). Given that the density does not fall off steeply enough in the heated region then the emission at larger radii dominates. For example a density profile set by the absorption of photons to a fixed column - indicative of our case - would fall of approximately as $n \propto 1/R$, provided the absorption is dominated at large radius.

Our calculation show nevertheless that bound material in the very inner disc can indeed produce broad wings. If the column of emitting bound material were larger then stronger wings would be produced. A non-thermal process acting at higher columns in the inner disc, as for example dissociation of the OH molecule, could indeed produce the missing flux in the wings. This could also be blue-shifted if the OH-layer extends to the base of the wind (see e.g. Gorti et al. 2011). As our codes currently lack chemistry we have been unable to test a non thermal origin of the broad component. This is however an important task, as if confirmed, there would be no need to invoke magnetic disc winds to explain the observations.

While a number of chemical models exist of the deeper, denser regions of discs, no model is currently available for the optically thinner disc winds. The work of Gorti, Dullemond & Hollenbach (2009), while carrying out detailed chemical calculations extending to the disc atmosphere, used a hydro*static* disc model which was analysed in a 1+1D fashion. Without hydro*dynamics* no predictions on line profiles can be made.

Studying the kinematic of the emitting gas is the only way to constrain the origin and intensity of the disc wind and hence shed light on the driving mechanism behind the dispersal of discs and the formation of Type 1 transition discs.

Molecular species

Mid-infrared observations of molecular lines (e.g. CO) provide a new promising alternative to directly measure disc winds. Indeed recent observations suggest that these lines may be tracing a disc wind which is slow and partially molecular (e.g. Pontoppidan et al. 2011; Brown et al. 2013). The spectro-astrometric survey of molecular gas in the inner regions of protoplanetary discs using CRIRES, the high-resolution infrared imaging spectrometer on the Very Large Telescope (Pontoppidan et al. 2011), showed that for several sources the astrometric signatures are dominated by gas with strong non-Keplerian (radial) motions. These authors concluded that the non-Keplerian spectro-astrometric

signatures are likely indicative of the presence of wide-angle disc winds. More observations of this type are planned after the update of the CRIRES instrument, which is expected to be completed by 2019. Observations with ALMA in molecular lines like e.g. CO J = 2-1 and J = 3-2 emission are also able to trace the presence of a wind (e.g.Klaassen et al. 2013, 2016). Molecular lines are sensitive to the mass loss rates since they sample a significant area of the wind launching regions. However the exploitation of molecular tracers is currently severely hampered by the lack of a suitable hydrodynamic wind model coupled to chemistry and to dust evolution models (which dominate the opacity in the wind) to interpret the observations.

Molecular tracers of outflow activity are common in the protostellar phase, they also probe a low velocity ($<$10 km/s) component whose intensity decreases while the opening angle increases going from the Class 0 through to the Class II phase (e.g. Frank et al. 2014 for a recent review). This slow wide-angle component, around a much faster jet, is naturally produced in MHD disc winds launched out to several AU (e.g. Pudritz et al. 2007, Panoglou et al. 2012). ALMA maps of outflow activity are corroborating this picture by providing the sensitivity to study in detail the faint Class II sources, see e.g. the CO disk wind surrounding the fast jet from the $\sim$4 Myr-old Herbig Ae star HD 163296 (Klaassen et al. 2013). Interestingly, the rough mass loss rate from the molecular wind is inferred to be similar to the mass accretion rate onto HD 163296 suggesting that winds contribute significantly to disc dispersal. Like optical forbidden lines, M-band CO ro-vibrational lines also show a broad and a narrow line emitting region (e.g. Banzatti et al. 2015) with FWHMs typically larger than the [OI] 6300 Å lines suggesting emitting gas closer to the central star (Simon et al. 2016). Blueshifts of $\sim$5 km/s are reported in 4 out of 7 single-peaked CO lines (Bast et al. 2011) while clear evidence of non-Keplerian motion is found in 2 out of the 16 sources observed with the spectro-astrometry technique (RU Lup and AS 205N, Pontoppidan et al. 2011). In the case of AS 205N, followup high-resolution ALMA observations also show deviations from Keplerian rotation in mm CO emission which could be due to a low velocity disk wind or tidal stripping by its companion AS 205S.

It is thus of outmost importance to understand how to distinguish the outflow signatures of a photoevaporating wind from those of a wide angle magnetically driven wind. Spectral line profiles are in this case helpful to determine the spatial location of the outflow, or of the region where the line originates. Comparison of profiles from transition discs and primordial discs are very helpful to shed light of the wind driving mechanism at different times. Indeed Ercolano & Owen (2010, 2016) and Simon et al. (2016) both discuss the expected and observed differences in the two cases. In general, a profile which shows a large component coming from unbound material at small disc radii ($<$ 0.5AU), for example is difficult to explain in terms of photoevaporation, where mass loss is only expected outside the so-called gravitational radius ($>$0.5AU), while, classically, magnetically driven wide angle winds are expected to come from the regions closer to the star.

1.4 Contributions of the team to the study of disc chemistry and ionisation

The study of chemistry in disc winds self-consistently with their atmospheres is pretty much uncharted territory, this also contributes to the fact that the determination of the ionisation level in discs is still based on simple models (e.g. Perez-Becker & Chiang, 2011). The team members have collectively large expertise in chemical and ionisation calculations of various environments including discs interiors as well as expertise in the development of photoevaporation models. This puts them in a prime position to be able to pioneer this work. The contributions of the PI Ercolano to the field of photoevapor-oratve winds can be appreciated from the work described in the previous section. In what follows, we briefly describe the state-of-the-art in the field of disc chemistry and ionisation, where the other team members of Project B2 have played a crucial role.

Chemical models of protoplanetary discs

Gas and solid chemistry play a key role in the evolution of planet-forming discs and in planet formation theories, and determine the original composition of (exo)-planets (Henning & Semenov 2013). Planets

are formed in protoplanetary discs that evolve over typical lifetimes of a few millions years (Fedele et al. 2010) by viscous spreading (e.g., Hueso & Guillot 2005; Baillié & Charnoz 2014) combined with photoevaporation (Alexander et al. 2013). During that time, the dust grains coagulate to each other to reach the size of meter- then kilometre- sized bodies (Birnstiel et al. 2010, 2012). Those bodies can agglomerate into planets or participate to the late episodes of heavy bombardments, bringing material onto planetary atmospheres and surfaces. Detection of the main belt asteroids reinforces the idea that asteroids may have brought most of the water on Earth (Jewitt 2012). Another key role played by chemistry is to set the location of the disc region where water is frozen onto solids, the so-called ice zone. Beyond the water ice zone, giant gas planets like Jupiter can form after the rapid accumulation of solid cores of 10 Earth masses by the core-accretion model (Helled et al. 2014, Öberg et al. 2015a, Helling et al. 2014).

Contrary to their young counterpart 'hot-corinos' (Cazaux et al. 2003), a much limited amount of molecules have been detected in protoplanetary discs. The outer disc molecular inventory includes CO, CN, HCN, formaldehyde, C_2H, CS, CH_3CN, HCO^+ and after a lot of effort CH_3OH (e.g. Dutrey et al. 2014; Öberg et al. 2015b; Walsh et al. 2016). The low abundance of many of the molecules has been ascribed to a combination of photodissociation at the disc surfaces and freeze-out onto grain surfaces towards the disc mid-plane. Simple molecules such as H_2, HD, CO, CO_2, H_2O, C_2H_2, HCN, N_2H^+, and potentially CH_3OH, have been detected from the terrestrial planet-forming region of protoplanetary discs by high-resolution spectrometers from ground-telescopes and by the Spitzer Space Telescopes (Pontoppidan et al. 2014). The gas is sufficiently warm such that many molecules are formed by neutral-neutral reactions with activation barrier. The ro-vibrational transitions in the mid-infrared have the advantage that homonuclear species such as CO_2 or C_2H_2 can emit contrary to pure rotational transitions. In addition to those small species, Polycyclic Aromatic Hydrocarbons (PAHs) infrared emissions are prominently seen from discs around the UV-luminous Herbig Ae stars.

Carbonaceous compounds such as tholins may have been detected in an evolved disc (Debes et al. 2008, Köhler et al. 2008). The detected lines in both the inner and outer disc are emitted well above the mid-plane. Although the amount of detected species may be low, the chemical paths are not because of the large range of density, temperature, and UV field strength. Thermo-chemical disc models use a common unique network to model the entire disc. Many questions remain on the origin and survivability of complex organic molecules in protoplanetary discs in general and in the Solar Nebula in particular. We expect that grain surface thermal- and photoreactions (UV and X-ray) and high-energy particles play an important role in the formation of complex species in the disc regions where water can be frozen onto grains (Throop 2011, Ciesla & Sandford 2012, Walsh et al. 2014). The energetic radiation break molecular bonds producing reactive radicals and ions but stellar wind can inhibit the propagation of cosmic rays (Cleeves et al. 2013). Grain surfaces enhance considerably the probability for two species to meet and form other species. Throop (2011) and Ciesla & Sandford (2012) models do quantify neither the specific species that are synthesised nor their amount, but have demonstrated that complex organics can indeed form on the Solar Nebula grain surfaces. In addition Ciesla & Sandford (2012) results suggest that gas and dust transport in the Solar Nebula (and in discs) will interconnect disc regions with dissimilar physical and chemical environments.

Members of the PI group are active collaborators within the ProDiMo[1] consortium (see e.g. Thi et al. 2014; Woitke et al. 2016). ProDiMo is a software package to model static protoplanetary discs including gas phase, X-ray and UV-photo-chemistry, gas heating and cooling balance, disk structure and (dust & line) radiative transfer. Surface chemistry has been recently included (Thi et al., in preparation).

Ionisation in discs

An accurate calculation of ionisation-recombination balance in dense protoplanetary conditions is essential for understanding various fundamental problems, such as coupling of the gas with magnetic field (Li et al. 2014), accretion processes (Turner et al. 2014), chemistry (Semenov et al. 2004;

[1] http://homepage.univie.ac.at/peter.woitke/ProDiMo.html

Larsson et al. 2012) and dust evolution (Okuzumi et al. 2011b; Akimkin 2015). The charging of grains in such environments affects their interaction of surrounding ions and electrons (Okuzumi 2009; Weingartner & Draine 1999) and hence modifies the chemistry at the grain surface.

Both the ionisation and recombination processes can arise from several sources. Primary agents of ionisation in dense gas (at visual extinctions above $A_V \sim 10 - 30$ mag, where interstellar UV photons are absorbed) are X-rays, cosmic-rays (CRs), and the decay of radionuclides, leading to the ionisation fraction that decreases with density (Oppenheimer & Dalgarno 1974; Caselli et al. 2002; Maret et al. 2006). In discs around young, active stars the situation is complicated due to the presence of stellar X-rays (Glassgold et al. 1997) and the possible exclusion of low-energy CRs by protostellar winds (Cleeves et al. 2013b). Efficiency of stellar X-rays to ionize the circumstellar gas depends on the total fluxes and the hardness of the spectra (Igea & Glassgold 1999; Ercolano & Glassold 2013). Near the disc midplane, where X-rays and CRs are strongly attenuated, radioactive elements may substantially contribute to the electron fraction. In this case the ionisation rate is proportional to the abundance of the radioactive element and its decay rate (Umebayashi & Nakano 2009; Cleeves et al. 2013a): Short-lived radionuclides (SLR, mostly ^{26}Al with half-life 7.4×10^5 yr) contribute comparatively more than long-lived radionuclides (LLR, mostly ^{40}K with half-life 1.3×10^9 yr), but decay faster.

While the treatment of ionisation, despite the variety of ionisation sources, could be reduced to a single (total) ionisation rate, the description of recombination is less straightforward. At sufficiently high densities, where the dominant sink of free electrons and ions are dust grains, the recombination rate non-trivially depends on properties of the grains (Okuzumi et al. 2011a,b; Ivlev et al. 2016).

The grain charges are determined by different mechanisms operating in different regions of discs: In the disc atmosphere, the photoelectric emission from grains is a prominent charging mechanism, leading to positive charges (Weingartner & Draine 2001; Weingartner et al. 2006; Akimkin 2015). Not only stellar radiation, but also H_2 fluorescence induced by CRs can contribute to this (Ivlev et al. 2015). In the inner, midplane disc regions the photoemission becomes negligible, and the grain charges are determined by collection of electrons and ions from the surrounding weakly ionized gas, leading on average to negative grain charges.

Depletion of electrons in dense disc regions, caused by the presence of negatively charged grains, significantly reduces the degree of ionisation (Umebayashi 1983; Umebayashi & Nakano 1990; Nishi et al. 1991). As the ionisation controls the coupling of the gas to the magnetic field, and hence the development of the magnetorotational instability (MRI, e.g. Velikhov 1959, Balbus & Hawley 1991; Armitage 2015), dust is the essential ingredient for any MRI model. It has been shown that the grain size critically affects the size of a disc's "dead zone" (Sano et al. 2000; Salmeron & Wardle 2008; Bai 2011a,b; Dudorov & Khaibrakhmanov 2014).

Recently we have developed an exact analytical model which describes ionisation and dust charging in dense disc conditions, for arbitrary grain-size distribution (Ivlev et al. 2016). Unlike previously developed approaches (Ilgner & Nelson 2006; Okuzumi 2009; Fujii et al. 2011; Dzyurkevich et al. 2013; Mori & Okuzumi 2016), our model does not make assumptions on the form of the grain charge distribution, and enables convenient analysis of results in a general form, in terms of a few dimensionless numbers, which allows us to identify universality in the behavior of the charged species.

1.5 Project-related publications

Kees to Paola/Barbara: Please add some text in each of the 10 publications below to argue what their relevance is to this project.

Carmona, A. et al. 2014, A&A, 567, 51 **Kees: This is strange, because this paper does not have any of the PIs on it**

Caselli, P., Walmsley, C.M., Terzieva, R., & Herbst, E. *The Ionization Fraction in Dense Cloud Cores*, 1998, ApJ, 499, 234.

Caselli, P., Walmsley, C.M., Zucconi, A., Tafalla, M., Dore, L. & Myers, P.C. *Molecular Ions in L1544. II. The Ionization Degree*, 2002, ApJ, 565, 344.

Ercolano, B. & Glassgold, A.E. *X-ray ionization rates in protoplanetary discs*, 2013, MNRAS, 436, 3446.

Ercolano et al. 2009 **Kees to Barbara: Cannot figure out which one**

Ivlev, A.V., Padovani, M., Galli, D. & Caselli, P. *Interstellar Dust Charging in Dense Molecular Clouds: Cosmic Ray Effects*, 2015, ApJ,

812, 135.
Ivlev, A.V., Akimkin, V.V. & Caselli, P. *Ionization and Dust Charging in Protoplanetary Disks*, 2016, ApJ, 833, 92.
Keto, E., Caselli, P. & Rawlings, J. *The dynamics of collapsing cores and star formation*, 2015, MNRAS, 446, 3731.
Thi, W.-F. et al. 2014, A&A, 561, 50 **Kees: This is strange, because this paper does not have any of the PIs on it**
Woitke, P. et al. 2016, A&A, 586, 103 **Kees: This is strange, because this paper does not have any of the PIs on it**

2. Objectives and work programme

2.1 Anticipated total duration of the project

36 months

2.2 Objectives

The overarching aim of this project is together with projects B1 and C2 to quantitatively characterise the dispersal mechanism of protoplanetary discs, leading to the formation of Type 1 Transition Discs. This will constrain the physical and chemical properties in the disc at the time of planet formation and provide case-specific limits to the timescales of formation and migration of gas giants, which must occur in a gaseous discs.

The intermediate goals that will lead to the achievement of the project main aim are:

1. Devise a chemical model appropriate for photoevaporative wind conditions which takes into account of the varying dust properties in the wind.
2. Directly measure the wind mass-loss-rates and profiles by comparing synthetic line profiles from the models to existing and upcoming observations.
3. Devise a chemical/ionisation model appropriate for protoplanetary disc atmospheres that self-consistently accounts for the shielding of stellar radiation from the wind. This will allow to assess the role of magnetic fields for launching a wind.

2.3 Work programme including proposed research methods

As will be detailed in what follows, a number of steps are required to further develop our methods to be able to deal with the problem at hand. Nevertheless as an example we have applied our chemical model to the standard wind solution from Owen et al. (2010). Figure 4 shows maps of the CO and of the electrons resulting from our toy model.

Some interesting features are already visible from this toy calculation, most notably that CO survives in the atmosphere of the disc and at the base of the wind, where it can be launched.

We use now the simple calculation above to describe the limitations of the current methods, which we aim to lift in this project.

1. The model makes simple assumptions for the irradiating spectrum of the central star (we assume here a radius and effective temperature of 2.076 R_s and 3862 K for the central star, which are appropriate for a $0.7 M_{\odot}$ star at 1 Myr age, Baraffe et al. 1997, 2002).
2. Only thermal effects of X-rays on the gas temperature are taken into account (i.e. the X-ray ionisation rate to 0) and the current chemical network does not include specific X-ray chemistry.
3. A standard dust opacity model was used to attenuate the FUV (Ossenkopf & Henning, **???**). As the models depend strongly on this a tailored dust model is necessary.

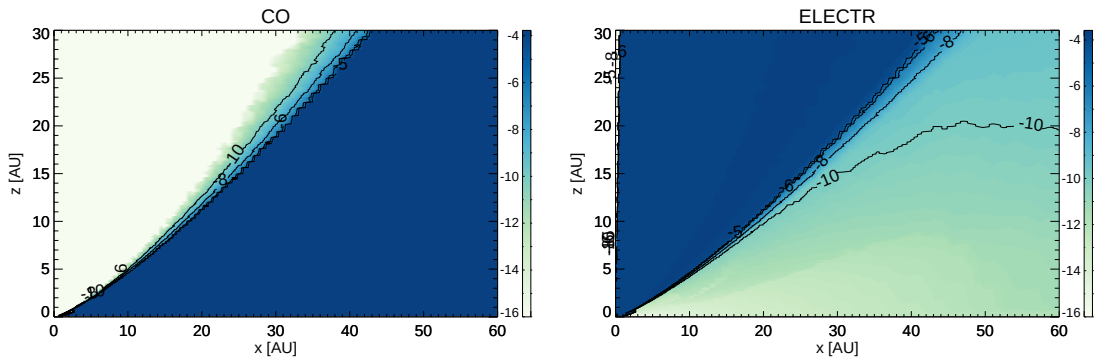

Figure 4: CO (left) and e^- maps from our toy chemical model applied to the Owen et al. (2010) wind solutions. See text for details

4. The H_2 and CO self-shielding calculation assumed constant 0.5 and 1e-4 abundances. This overestimates the true shielding, so a more realistic model would need to iterate the chemical model with updated shielding coefficient from the previous iteration.

5. The chemical model is the KIDA 2015 release, which is a gas-phase chemical network, but it takes the formation of H_2 on grain surface and charge exchange with grains into account. The network however does not include double or higher ionisation states, which would be produced by X-rays. Freeze-out of gas phase species are also not considered, while this is not a problem in the warm atmosphere and wind of the disc, it produces unrealistically high CO abundance in the mid-plane.

6. The chemical network is solved time-dependently, and evolved to 1 Myr, which is longer than most of the chemical timescales at typical disc densities (although this is not always true in the atmosphere). The abundances shown are then roughly equilibrium abundances (especially since no grains surface chemistry is considered). Time-dependence is likely to play a role in the modeling of the tenuous disc atmospheres and winds.

2.3.1 Research tools and inputs

This project will make use of a newly developed code, MOCASSIN+KROME, to solve the geometry independent radiative transfer through gas and dust, including photoionisation and chemical calculation including X-rays. PI Ercolano has been working on coupling her 3D Monte Carlo photoionisation and dust radiative transfer code MOCASSIN (Ercolano et al. 2003, 2005, 2008b) to the KROME package (Grassi et al. 2014), to perform arbitrary chemical calculations (Ercolano & Grassi, 2017, in preparation). Simple photoionisation benchmarks from the set of Pequignot et al. (2001) have already been successfully performed with the new coupled version, and a toy network has also been introduced, which is however inadequate for any realistic modelling of disc chemistry. The development of an appropriate chemical network to be included into MOCASSIN+KROME is indeed one of the first tasks of the work program described below.

The advantage of using this new code compared to existing chemical codes for discs, is that it allows a fully self-consistent treatment of the radiative transfer and hence radiation field attenuation through dust and gas. The code is fully 3D (but can work in 2D) and it can handle complex, multi-component and space-varying dust grain models.

MOCASSIN (without KROME) has already been used to post-process hydrodynamical calculations of photoevaporating discs (e.g. Ercolano & Owen 2010, 2016) to produce synthetic spectral line profiles of atomic and ionised species in the wind and atmosphere.

The abundances calculated with MOCASSIN+KROME will then be further post-processed using the popular RADMC-3D code, developed and mantained by Prof. Dullemond (PI of project D1) or the LIME code (Brinch & Hogerheijde 2010), which has also already been used by members of our B2 team for other projects.

2.3.2 Work Program

The project will develop along a path of growing complexity. It is possible that some of the tasks in the last stage (time-dependance) may be carried over to the next funding period. While this complex project will be led by the postdoc, the PIs and collaborators who will take an active part in the work. One of the PIs of this project has extensive experience in devising efficient and reliable reduced networks (see e.g. Keto & Caselli 2008, 2010; Keto, Rawlings & Caselli 2014), while one of the collaborators and the other PI are leading effort in the ionisation structure and radiative transfer of discs (e.g. Ivlev et al. 2016, Glassgold & Ercolano 2013, Ercolano et al. 2008,2009).

2.3.2.1 Months 1-12

The reduced network. A first task for this project is to simplify the gas-grain chemistry by reducing the chemical network to the minimum number of reactions needed to properly follow the formation/destruction of important species (in particular Hydrogen, Carbon, Oxygen as well as simple C-, O-bearing molecules) and the electron abundance or ionisation fraction. The reduced chemical network will be benchmarked against comprehensive chemical networks to make sure that the abundances of important (diagnostic) species such as C^+, C, O, CO are well reproduced in the range of conditions appropriate for evolved and transitions discs. This will imply running the comprehensive and reduced networks in a grid of physical conditions by varying temperature, density, and UV/X-ray fluxes. As lines of Ne ([NeII], [NeIII]) and Ar ([ArII]) are good tracers of disc winds (e.g. Pascucci 2007, Szulágyi et al. 2012), Ne and Ar will be included in the chemical code.

Particular attention will be dedicated to the inclusion of X-rays and the identification of the regions within the disc where X-rays, FUV photons and cosmic-rays (CRs) dominate the chemical and thermal properties. Typical assumption is that the X-ray spectrum is given by the bremsstrahlung spectrum ($I_\nu \simeq 1/E \times exp(-E/kT)$ on the 0.1 - 10 keV energy range (e.g. Glassgold et al. 2007, Aresu et al. 2011, Meijerink et al. 2012). The observed luminosity ranges are $L_X = 10^{29} - 10^{31}$ erg/s (based on the Taurus survey, Güdel et al. 2007). The X-rays heat up the gas with 10-40% efficiency (UV heating has only a few per cent efficiency).

Impinging X-rays may ionise the disk or wind material via primary or secondary ionisation. Primary ionisation may produce a single or multiple electrons due to the Auger effect. Their energy range depends on the shell from which the Auger electron originates. The rate coefficient is given by the integral of the product of the X-ray energy spectrum and the ionisation cross section of the element (see e.g. Meijerink 2012, equation A.13). Secondary electrons might have keV energies, capable of $\sim$20-30 hydrogen ionisation. In fact the secondary electron ionisation rate per H nucleus is higher than the primary by an order of a magnitude, thus often only the secondary ionisations are considered in chemical models (e.g. Ádámkovics et al. 2011, Bruderer 2012). The exact expressions and the peak electronic ionisation cross sections are given in Ádámkovics et al. (2011).

Chemical models in the literature deal differently with X-ray reactions. The Semenov et al. (2010) and associated papers (Akimkin et al. 2013) model these reactions as an additional contribution to cosmic ray ionisation reactions (i.e. the rate is given by $R = \alpha \times (\zeta_{CR} + \zeta_X)$). Bruderer et al. (2012) accounts for only the secondary ionisation. Finally, Meijerink et al. (2012) take both the primary and secondary ionisation into account, as described above (see also Table 3 in Henning & Semenov 2013).

X-rays affect the chemistry in various ways: (i) X-rays might directly ionise H (while FUV radiation does not), initiating H_2 formation via the H-path. In high temperature regions, where the grain surface H_2 formation is less efficient, this reaction might contribute significantly to the total H_2 formation rate.

(ii) Secondary electrons interacting with H_2 produce H_2^+ that quickly reacts with a further H_2 to form H_3^+ or reforms H_2 via charge transfer with neutral H. This can lead to H_3^+ abundances as high as 10^{-8}. This then initiates efficient ion-neutral reactions which e.g. result in efficient H_2O production (see e.g. Meijerink et al. 2012). Furthermore, the heating effect might also increase the rate of neutral-neutral reactions with reaction barriers. (iii) H_3^+ initiates ion-molecular reactions which keep molecular abundances high even at high temperatures (if X-rays are present, compares to only FUV). (iv) Ne, Ne+, Ar and Ar+ have ionisation potentials 21.56, 40.96, 15.76 and 27.63 eV respectively. They are only ionised due to X-rays or X-ray induced fast electrons. Therefore, their ionisation is an indicator for X-rays and, as already mentioned, these species will be included in our chemical models. (v) Enhanced CO destruction through reaction with He^+, which has an ionisation energy of 24.6 eV (CRs can also ionize it). (vi) Other observational tracers (suggested by Meijerink 2012) are: H_2O, Ne^+, C/C^+ ratio,O^+.

Finally, while X-rays are unlikely to interact at the low column densities of the wind they are crucial for the chemistry in the underlying disc material, which feeds the wind.

2.3.2.2 Months 13-18

Line diagnostics from chemical models. Once the reduced network is benchmarked and tested, it will be included in the MOCASSIN-KROME code by the co-PI Ercolano. The MOCASSIN-KROME code will be used to obtain the chemical abundances, while, radiative transfer codes available at the PI Institute (RADMC-3D[2] and LIME[3]) will be used to obtain fluxes in dust continuum and lines to then perform simulated observations and compare with available data and/or make predictions for future observations. We note that at this stage the chemical models will still use an unrealisticly simple dust model. However this step is important to guide us towards interesting diagnostics and to help us refine our chemical model. This step to obtain synthetic observations will be repeated every time a significant update is performed on the model.

At this point we will already be able to further investigate the nature of the broad-component of the neutral hydrogen emission, for which we have suggested a non-thermal origin coming from OH dissociation in the bound inner disc regions. Even if our models our not final, they can already be used to assess the plausibility of our proposed scenario.

In this second part of the project, we will also explore the effect of varying initial conditions, taking into account effects of accretion, vertical mixing and magnetic disk wind on chemistry following prescriptions by Heinzeller et al. (2011). Often low metal elemental abundances are assumed (H_2 molecular, C^+ ionised) or the chemical network is initially evolved to simulate the conditions of the parent cloud. Depending on what kind of disk wind model is considered, the wind starts to dominate the mass loss rate at different times. For example, EUV winds tend to be efficient at late times, thus the initial chemical composition might not matter, while the X-ray winds might dominate the mass loss over accretion in early times, and thus the initial chemical abundances might matter (see review of Alexander et al. 2014, page 483 end of section 2.3). Furthermore, several papers shows that the radial movement of material and the vertical mixing affect the chemistry in disks, i.e. by lowering concentration gradients and enhancing abundances of NH_3, CH_3OH, C_2H_2 and sulphur-containing species (e.g. Ilger et al. 2004, Semenov et al. 2010, Heinzeller et al. 2011). If the chemical timescales are long compared to the disk wind dynamic time, then the disk composition will affect the wind as well. Thus, we will model the effects of the radial accretion flow and vertical mixing (although the later is more important, see Semenov 2010) on the disk chemistry (even if these motions are not included in the original simulation). As the MOCASSIN simulations start from an alpha-disk model, we will take this disc structure to model the vertical mixing and accretion similarly as was done by Heinzeller et al. (2011).

[2]http://www.ita.uni-heidelberg.de/ dullemond/software/radmc-3d/
[3]http://www.nbi.dk/ brinch/index.php?page=lime

2.3.2.3 Months 19-24

Dust evolution. The chemical model assumes initially that dust grains can be approximated by one-size particles of 0.1μm in diameter and that the dust-to-gas mass ratio is fixed. However, this assumption is completely inappropriate for disc winds. Indeed as explained in detail in project C2 of this proposal, the maximum grain size that can be entrained in the wind at a given radial distance from the star results from the local force balance between the drag force, gravity and the centrifugal force. A further complication is that the underlying distribution of grains is also not constant and varies as a function of disc radius and vertical distance from the mid-plane, due to the effects of grain growth, fragmentation, settling and drift. A detailed model of the spatially and time-varying grain abundances and size distributions in the wind is however essential for the chemical model, since grains provide the bulk of the opacity in the FUV. The third task of the Postdoc employed for this project will be to include spatially-varying grain abundances and size distributions provided by project C2 into the chemical code, at different evolutionary times, to properly account for dust opacities in the wind. Also the effects of different dust grain properties on the chemical composition will be explored at this point. At MPE, we are already studying the effect of varying grain-size distribution on the ionisation structure of discs (Ivlev et al. 2016).

This step will be further decomposed into levels of increasing complexity. We will begin with decoupling the time and space evolution of the grains. We will then compare the timescales involved and asses whether the time-evolution of the dust must be treated self-consistently or if we can work with snapshots.

An important **milestone** at the end of this step will be a case specific assessment of the ionisation level in the atmospheres of discs We will make this immediately available to the international community as this is a crucial ingredient for the development of MHD calculations. This will also help us assess under what conditions, if any, one can expect that a significant component of observed outflow emission may be indeed magnetically driven.

2.3.2.4 Months 25-36

Time-dependent chemistry. It is unclear at this stage if equilibrium chemistry is an appropriate approximation for disc winds. The material flows at a few km/sec and as it moves along the wind streamlines it is subject to changes in density and radiation field. It is possible that time dependent calculations will be necessary for this problem, where the dust properties in the chemical code will be provided by the time-dependent calculation of the dust evolution described in C1. This will be the final task of the Postdoc employed for this project, who will first study the time scales of the various physical/chemical processes (e.g. photochemistry, accretion, mixing, wind) and quantify the validity of equilibrium chemistry.

After this, the whole team will work together with the B1 and the C2 teams to couple time-dependent gas-grain chemistry and dust evolution. Depending on the level of complexity required, part of this final step may be carried out in the second funding period.

2.3.2.5 Summary of the Work Program

The Gannt chart below summarises the approximate time-line of the B2 project:

Year 1: (i) focus on the chemical network update, to make sure that all the most recent reaction rates will be included. This will be done by comparing our code with KIDA[4], the kinematic database for astrochemistry, as well as with comprehensive literature research. (ii) Include detailed ionisation processes, taking into account the effects of ionisation-recombination from FUV and CRs. (iii) Include X-ray chemistry based on the extensive literature work available as well work done within the ProDiMo code. (iv) Finalise the reduced chemical network, including Ne and Ar, and test/benchmark it.

[4] http://kida.obs.u-bordeaux1.fr

TASK NAME	Year 1	Year 2	Year 3
The reduced network	- update chemical model - include detailed ionisation processes - insert X-ray chemistry - finalise reduced network		
Line diagnostics from chemical models		- inclusion of chemical code in MOCASSIN by B1 - radiative transfer - comparison with observations	
Dust evolution		- from mono-disperse to grain-size distribution - grain-size from C2 - radiative transfer - comparison with observations	
Disc ionisation		- case-specific ionisation rate	
Time-Dependent chemistry			- study of time scales of various processes - benchmark of time-dependent chemical code - inclusion of time-dependent chemistry in dynamical model - radiative transfer - comparison with observations

Figure 5: Gannt chart for B2. More details have been outlined in the previous section.

Year 2: (i) inclusion of reduced chemical network in MOCASSIN-KROME. (ii) Calculation of the chemical-physical model, which will then be used as input in radiative transfer code to produce dust continuum emission and line fluxes. (iii) Comparison with observations and further update of chemical code based on observational constraints. (iv) Study of the effect of changing the grain size from mono-disperse (0.1 μm) to MRN grain-size distribution (Mathis et al. 1977) or evolved-MRN distributions (e.g. Zhao et al. 2016; Ivlev et al. 2016). (v) ionisation level calculations. (vi) Calculation of an updated chemical-physical model, which will then be used as input in radiative transfer code to produce dust continuum emission and line fluxes. Comparison with observations.

Year 3: (i) study of time scales of various processes in chemical and dynamical model. (ii) Benchmark of time-dependent reduced chemical code. (iii) Inclusion of time-dependent chemistry in dynamical model. (iv) Calculation of an updated chemical-physical model, which will then be used as input in radiative transfer code to produce dust continuum emission and line fluxes. Comparison with observations.

Continuous Assessment of New Diagnostics Jointly with the B1, C2 and A1 team members as well as with our external collaborators Prof. Henning and Prof. van Dishoeck, we will regularly compare our models to the observations via the production of synthetic spectra. This will allow us to promptly identify and characterise new wind diagnostics and allow us to use the observations to measure the crucial wind properties of mass loss rate and wind profile, which have a large impact on the formation and evolution of planetary systems.

2.4 Data handling

We will make the sets of line profiles for the different wind and disc characteristics publicly available in electronic format on the public partition of the Research Unit server. The reduced and full networks will also be made available at the end of the first funding period, when they will have reach their final form.

2.5 Other information

Not Applicable

2.6 Information on scientific and financial involvement of international cooperation partners

Not applicable

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4. Requested modules/funds

4.1 Basic Module

4.1.1 Funding for Staff

We require funding for one Postdoc to work jointly at the MPE with Prof. Caselli and at the LMU in the group of Prof. Ercolano. A Postdoc with at least some experience of astrochemistry would be certainly desirable to work on this complex project. The Postdoc will receive scientific support form the PIs, but also from experienced astrochemists and plasma physicists (e.g. Dr. Ivlev, Dr. Thi) at the Centre for Astrochemical Studies led by Prof. Caselli at the MPE.

In case of an award Dr. Szücs, currently working at the MPE in the group of PI Caselli, has expressed interest in taking on the position. His expertise in this field would be very beneficial to the achievement of the aims of this project.

4.1.2 Direct Project Costs

4.1.2.1 Equipment up to EUR 10,000, Software and Consumables

Will be provided by the host institution

4.1.2.2 Travel Expenses

Total: 9900 € Justification : Each year one national trip (meeting of Astronomical Society, national meetings) and one international trip (conference, visit collaborators). During the course of the postdoc one week long visits to our main international collaborator, Dr. Grassi.
Cost estimate:

- National trip: 5 overnight stays, train/airfare, conference fee; 1000 € (3000 over 3 years).
- International trip: 6 overnight stays, airfare, conference fee; 1500 € (4500 over 3 years).
- Visit to/from T. Grassi: airfare, 6 overnight stay 1200 € (2400 for 2 visits)

4.1.2.3 Visiting Researchers (excluding Mercator Fellows)

Not Relevant

4.1.2.4 Other Costs

None

4.1.2.5 Project-related publication expenses

We request 770 €/year (total 2250 €) for publication expenses.

4.1.3 Instrumentation

None

4.1.3.1 Equipment exceeding EUR 10,000

None

4.1.3.2 Major Instrumentation exceeding EUR 100,000

None

5. Project requirements

5.1 Employment status information

Paola Caselli, Director at the Max Planck Institute for Extraterrestrial Physics (MPE) – permanent
Barbara Ercolano, Professor at the Ludwig-Maximilians-Universität München – permanent

5.2 First-time proposal data

Not Relevant

5.3 Composition of the project group

Alexei Ivlev, Dr, permanent scientist at the MPE Wing Fai, Thi, Dr, postdoctoral assistant at the MPE

5.4 Cooperation with other researchers

5.4.1 Planned cooperation on this project

5.4.1.1 Collaborating researchers for this project within the Research Unit

This project is intimately linked to project B1 (PI Ercolano) and to project C2 (PI Ercolano). It requires the input from the radiation-hydrodynamic models from B1 as well as the MOCASSIN-KROME code which is developed by the PI Ercolano for B1 and B2 (with different immediate objectives). It also requires input from project C2 (PI Ercolano) and will work closely with T. Birnstiel (C1, C2) for help in the implementation of the dust models. The synthetic spectra will be compared with observations with the help of the A1 team (PI Testi) and our external collaborators Prof. Henning and Prof. van Dishoeck.

Kees to Paola/Barbara: Maybe this project B2 can also provide a "service" to the projects D1 and D2 in terms of providing the chemical basis for the abundance of molecules used for line transfer for probing the gas and the kinematics of Type 2 TDs?

5.4.1.2 Collaborating researchers for this project outside of the Research Unit

Dr. Grassi, the author of the KROME package has already helped Prof. Ercolano with the implementation of KROME into MOCASSIN and is expected to help further in implementing the new networks and optimising the chemistry routine (inclusion, for example, of a better equilibrium chemistry option. It is envisioned that Dr. Grassi will play regular visits to our group.

5.4.2 Researchers with whom you have collaborated scientifically within the past three years

Maite Bertran (INAF-Osservatorio Astrofisico di Arcetri), Aaron Boley (University of British Columbia), Sandra Brünken (University of Cologne), Stephanie Cazaux (University of Groningen), Cecilia Ceccarelli (Univ. Grenoble Alpes), Francesco Fontani (INAF-Osservatorio Astrofisico di Arcetri), Thomas Hartquist (University of Leeds), Izaskun Jimenez-Serra (Queen Mary University London), Eric Keto (Harvard-Smithsonian Center for Astrophysics), Marco Spaans (University of Groningen), Jonathan Tan (University of Florida), Stephan Schlemmer (University of Cologne), Charlotte Vastel (Université de Tulouse), Malcolm Walmsley (INAF-Osservatorio Astrofisico di Arcetri) Niederhofer (STSci, USA); M. Hilker (ESO, Garching); N. Bastian (U. Liverpool, UK); M. Guarcello (U. Palermo, Italy); M. Tazzari (U. Cambridge, UK); A. Natta (Florence, Italy); R. Alexander (U. Leicester); D. Hubber (LMU); J. Dale (U. Hertfordshire, UK); C. Koepferl (LMU); I. Bonnell (U. St. Andrews, UK); A. McLeod (ESO, Garching); D. Boneberg (U. Cambridge, UK); R. Parker (U. Liverpool, UK); R. Wesson (UCL, London, UK); M. Barlow (UCL, London, UK); A. Glassgold (u. Berkeley, USA); C. Manara (ESA, Noordwjik, Netherlands); A. Danekhar (CfA, Harward, USA); Q. Parker (Sidney, Australia); S. Casassus (U. de Chile, Santiago, Chile); I. Pascucci (U. Arizona, USA); A. Bevan (UCL, London, UK).

5.5 Scientific equipment

The CAS centre led by Prof. Caselli has available computer facilities for visiting scientists and students. CAS has its own cluster: an HPC cluster comprising of 25 nodes with 20 cores and 128 GB memory each; 4 nodes with 20 cores and 256 GB memory each (Infiniband, 50 TB storage, Login-Node, Batch-System; 2 Compute nodes, i.e. 2 nodes with 20 cores and 512 GB (10 TB storage).

The group of Prof. Ercolano has two own computer clusters comprising

- 2 CPU Intel Xeon X5650 (Westmere, beginning 2010, 2.66 GHz) 6 cores each 12 cores total (24 virtual) 74 GB ram.
- 4 CPU Intel Xeon E7-4850 (Ivy Bridge, beginning 2014, 2.30 GHz) 12 cores each 48 cores total (96 virtual) 660 GB ram.

Further computational power is provided through the C2PAP facility of the Excellence Cluster to which the group has guaranteed time. This comprises 126 nodes, each node with 2 CPU Intel Xeon E5-2680 (Sandy Bridge, beginning 2012, 2.7 GHz) 8 cores each 16 cores total (32 virtual) 64 GB ram. Note that while the future of the Excellence Cluster Universe is uncertain, the C2PAP facilities will be in any case supported by the LMU.

The facilities at the Leibniz Rechenzentrum (LRZ) , with the iDataPlex HPC System HYDRA with Intel Ivy Bridge processors (3500 nodes with 20 cores at 2.8 GHz each are also available to us.

5.6 Project-relevant interests in commercial enterprises

Not Relevant

5.7 Additional information

Not Relevant