Astrochemistry in protoplanetary discs: disk shape and dust properties setting the stage

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and the DIANA team
Protoplanetary Disks

© Henning & Semenov (2013)
IS chemistry ≠ disk chemistry

- **larger densities** $\approx 10^4 \ldots 10^{16}$ cm$^{-3}$
- **higher temperatures** $\approx 10 \ldots 10000$ K ($T_{\text{gas}} \geq T_{\text{dust}}$)
- **central star** = strong UV and X-ray source
- **2D/3D structure**
  - → strongly irradiated and strongly shadowed regions
- **much larger dust grains** $\approx 0.1$ μm ... 1 mm (or even larger)
  - → reduction of UV dust opacity & total dust surface by factor $\sim 100$ (!)
  - → penetration depths: UV $\approx$ X-ray $\ll$ CR
  - → important for chemistry and heating/cooling balance
IS chemistry ≠ disk chemistry

UV field strength

densities, UV and X-ray radial optical depths

dust temperature

gas temperature
Analysis and Modelling of Multi-wavelength Observational Data from Protoplanetary Discs

<table>
<thead>
<tr>
<th>St Andrews</th>
<th>Vienna</th>
<th>Amsterdam</th>
<th>Grenoble</th>
<th>Groningen</th>
</tr>
</thead>
<tbody>
<tr>
<td>P. Woitke</td>
<td>M. Güdel</td>
<td>R. Waters</td>
<td>F. Ménard</td>
<td>I. Kamp</td>
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<tr>
<td>Greaves</td>
<td>Dionatos Rab Liebhart</td>
<td>Min Dominik</td>
<td>Thi Pinte Carmona Anthonioz</td>
<td>Antonellini</td>
</tr>
<tr>
<td>sub-mm to cm</td>
<td>X-rays</td>
<td>near-mid IR</td>
<td>near-far IR</td>
<td>near IR - mm</td>
</tr>
<tr>
<td>coordination</td>
<td>obs./mod.</td>
<td>mod./obs.</td>
<td>obs./mod.</td>
<td>mod./obs.</td>
</tr>
<tr>
<td>JCMT, eMERLIN</td>
<td>XMM, Herschel high energy</td>
<td>VLT, JWST dust mod.</td>
<td>HST, Herschel interferometry</td>
<td>Herschel, JWST gas mod.</td>
</tr>
</tbody>
</table>

**multi-λ data collection** X-ray to cm (archival and proprietary)

coherent, detailed modelling of gas & dust throughout the disc using disk modelling software ProDiMo, MCMX, MCFOST

**aim:** disc shape, temperatures, dust properties, chemistry in the birth-places of exoplanets
ProDiMo: a modular framework for your disc research

- select your chemical species
- compile your chemical rates (or use UMIST or OSU or KIDA)
- set stellar UV & X-rays properties
- grain material & size distribution
- column density & disc zones
- options:
  - parametric / hydrostatic vertical extension ?
  - dust settling ?
  - PAHs ? (RT / chemistry / heating)
  - X-ray radiative transfer ?
  - time-dependent chemistry ?
  - grain charges ? (in development)
  - surface chemistry ? (in development)

main papers: Woitke, Kamp, Thi (2009), Kamp et al. (2010), Thi et al. (2011), Woitke et al. (2016)
usage of UV and X-ray data

TW Hya

AB Aur
**X-ray radiative transfer**

→ Christian Rab, University of Vienna, Austria

**X-ray gas & dust opacities**

**X-ray ionisation rate [1/s]**

- absorption & scattering
- cosmic rays
- radioactive decay

**Diagram:**

- Cross-section vs. Energy [keV]
- Color map illustrating X-ray ionisation rate.
- Diagrams showing absorption and scattering.
Charged Grain Chemistry

\[
\begin{align*}
Z + \text{hv} & \rightarrow Z^+ + e^- \quad \text{photoelectric / photodetachment} \\
Z + e^- & \rightarrow Z^- \quad \text{electron attachment} \\
Z + A^+ & \rightarrow Z^+ + A \quad \text{charge exchange} \\
Z + AB^+ & \rightarrow Z^+ + A + B \quad \text{dissociative charge exchange} \\
Z & \rightarrow Z^+ + e^- \quad \text{thermionic emission} \\
Z + M & \rightarrow Z^+ + e^- + M \quad \text{collisional electron detachment}
\end{align*}
\]

\text{included species}

\[
Z^{+++}, Z^{++}, Z^{+}, Z^-, Z, \quad Z^+, Z^{++}, Z^{+++}, Z^{++++}
\]
ice abundances

→ impact of adsorption energies


Kamp et al. (2016, in prep.)
simulated observations

SED and line fluxes

emission line maps

continuum images

velocity profile

channel maps

new: high-res IR spectrum

13CO line @ 220.399 GHz from an edge-on disk
“Impactograms”

Impact of PAHs

→ Woitke et al. 2015, submitted to A&A
Impact of PAHs

Woitke et al. 2015, submitted to A&A

**HD 142666**

\[ \text{gen} = 2196, \chi = 1.51 \]

\[ f_{\text{PAH}} \approx 0.1-0.2 \]

**HD 169142**

\[ \text{gen} = 0500, \chi = 2.72 \]

\[ f_{\text{PAH}} \approx 0.2-0.4 \]
PAH and dust opacities

→ Woitke et al. (2016, A&A 586, 103)

\[ f_{\text{PAH}} = 1 \]
All results are public

google "DIANA SED-fit"

find the DIANA standard models here

access our public database DIOD here (complete data collection)

27 well-studied discs, host star = single star, spectral type M3 ... B9
All results are public

281 plots! (physico-chemical structure, dust properties, SED, images, line results ...)

detailed 2D model output

complete model setup: input parameter, observational data files, … → reproducible model (ProDiMo / MCFOST / MCMAX)

human-friendly model parameter

selection of derived properties (IR-excess, SED-fluxes, apparent sizes, mm-slope, line fluxes and FWHM vs. observations, predicted line fluxes, ...)

White dashed contour lines mark radial \( A_v = 0.1 \) and 1, black dashed contour lines mark vertical \( A_v = 1 \) and 10. For SED and comparison to continuum and line observations, click on TWHya_DIANAdat.ps.gz below.

TWHya_coldens.png
TWHya_dens.png
TWHya_DIANAdat.ps.gz
TWHya_ModelOutput.tar.gz
TWHya_ModelSel.tar.gz
TWHya_para
TWHya.properties
Conclusions

astrochemistry in protoplanetary disks ...

- at least 2D with wide range of conditions
  → densities
  → dust and gas temperatures
  → radiation fields
  → disc shape → shielding
  → different lines come from different disc regions
  → “nebula analysis” highly questionable (for example rot. diagrams)

- large grains need to be included to fit SED
  → reduction of UV dust opacity & total dust surface by factor ~100
  → deeper warm, chemically active disk surface layer
  → stronger emission lines (e.g. far-IR lines, CO ro-vib)
  → less ice
  → fewer charged grains, larger electron concentration in midplane
a word on lab chemistry ...

ProDiMo uses ~ 530 physical/chemical input data files (!)

- non-LTE data for atoms and molecules
  - energy states & degeneracies (rotational, vibrational, some electronic)
  - line data (level indices, wavelengths, Einstein coefficients)
  - collisional data (!), specific pumping processes, ...

- ice data
  - adsorption energies (!)
  - photodesorption efficiencies,
  - optical constants, ...

- dust data
  - optical constants
  - photoelectric effect efficiencies, threshold energies, ...

- cross sections, cross sections, cross sections ...
  - e.g. UV-photodissociation, X-ray processes, PAHs, ...

- chemical rates
  - Arrhenius parameters
  - self-shielding factors
  - special processes (H₂-formation on grains, excited H₂, surface chemistry, ...)
standard model  CY Tau

CTTS, $M_1$, $A_V = 0.1$, $T_{\text{eff}} = 3640$ K, $L_* = 0.36 L_{\odot}$, $M_* = 0.42 M_{\odot}$, $M_{\text{acc}} \sim 7 \times 10^{-9} M_{\odot}/\text{yr}$, age $\sim 2.2$ Myr

Diagram showing gas density and column density. The SED plot includes various models and data points.
standard model  CY Tau

12CO J=2-1

12CO v=1-0 R(3)

13CO J=2-1

12CO v=1-0 P(26)

also [OI] 63μm, [OI] 6300A
The R-branch CO fundamental with FLiTs ...

*model with high densities in inner disk*

*model with low densities in inner disk*
standard model HD 163296
A massive outer disc in the shadow of a tall tenuous inner disc?

- HD 142666*
- HD 163296
- CY Tau*
- BP Tau*
- DM Tau
- MWC 480*
- RECX 15
- HD 169142*
- GM Aur*
- AB Aur*
- TW Hya*

*: CO ro-vib lines fit
*: CO ro-vib lines do not fit
“holistic” modelling approach

**MCFOST** or **MCMMax**
- dust physics
- radiative transfer

**ProDiMo**
- gas & ice chemistry
- UV & X-ray physics
- heating & cooling
- non-LTE physics

**FLiTs**
- high-res. spectra
- line profiles
- line maps
- channel maps

**SED**
- cont. images
- visibilities

**chemical structure**
- line flux estimations
- where do the lines form?

**element abundances**
- species & reactions
- non-LTE rates

**stellar properties**
- density structure
- dust parameters
- PAH parameters
- dust settling

**dust opacities**
- $J_\nu(r,z)$
- $T_{\text{dust}}(r,z)$
- $T_{\text{PAH}}(r,z)$

**MCFOST**
- $T_{\text{gas}}(r,z)$
- $n_i(r,z)$
- $\text{pop}_i^k(r,z)$

**or**
- MCMax
- dust physics
- radiative transfer

**discAnalysis**
Opacities of aggregates

- DDA, 100 dipoles/GRF, up to 8000 GRFs (4 μm)
- results include phase function, polarisation, ...

Fit with “simple” methods

(Effective medium, porosity, DHS)

DIANA dust opacity standard

- Effective mixture of
  - ~60% laboratory amorphous silicates
    (Mg_{0.7}Fe_{0.3}SiO_3, Dorschner+1995)
  - ~15% amorphous carbon
    (Zubko 1996, BE-sample)
  - ~25% porosity
- Powerlaw size distribution $f(a) \sim a^{-\text{pow}}$
  ($a_{\text{min}} \sim 0.05 \mu m$, $a_{\text{max}} \sim 3 \text{ mm}$, $a_{\text{pow}} \sim 3.5$)
- Distribution of hollow spheres
  (hollow volume ratio 0.8)
“Standard” dust opacities for disks

→ Min et al. 2015, University of Amsterdam, NL, A&A submitted
“Standard” dust opacities for disks

→ Min et al. 2015, University of Amsterdam, NL, A&A submitted

Download Fortran-90 code to compute dust standard opacities for pp discs from

http://www.diana-project.com/data-results-downloads
impact on gas modelling  
→ Woitke et al. 2015, submitted to A&A
Table 3. Unsettled dust properties in the reference model in comparison to a MRN size distribution and uniform $a=0.1 \mu m$ dust particles.

<table>
<thead>
<tr>
<th></th>
<th>ref. model</th>
<th>MRN</th>
<th>0.1 (\mu m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>dust material density $\rho_d$ [g/cm$^3$]</td>
<td>2.09</td>
<td>3.0</td>
<td>3.0</td>
</tr>
<tr>
<td>mean dust size $\langle a \rangle$ [(\mu m)]</td>
<td>0.083</td>
<td>0.0083</td>
<td>0.1</td>
</tr>
<tr>
<td>mean dust size $\langle a^2 \rangle^{1/2}$ [(\mu m)]</td>
<td>0.11</td>
<td>0.010</td>
<td>0.1</td>
</tr>
<tr>
<td>mean dust size $\langle a^3 \rangle^{1/3}$ [(\mu m)]</td>
<td>0.53</td>
<td>0.016</td>
<td>0.1</td>
</tr>
<tr>
<td>particle density $n_d/n(H)$</td>
<td>1.7(-14)</td>
<td>4.9(-10)</td>
<td>1.9(-12)</td>
</tr>
<tr>
<td>surface $n_d 4\pi\langle a^2 \rangle/n(H)$ [cm$^2$]</td>
<td>2.7(-23)</td>
<td>6.6(-21)</td>
<td>2.3(-21)</td>
</tr>
<tr>
<td>FUV extinct. $\kappa_{912\AA}^{\text{ext}}/n(H)$ [cm$^2$]</td>
<td>2.5(-23)</td>
<td>2.8(-21)</td>
<td>1.2(-21)</td>
</tr>
<tr>
<td>FUV dust albedo</td>
<td>64%</td>
<td>33%</td>
<td>47%</td>
</tr>
<tr>
<td>mm opacity $\kappa_{1.3\text{mm}}^{\text{abs}}/\rho$ [cm$^2$/g]</td>
<td>0.038</td>
<td>0.0018</td>
<td>0.0018</td>
</tr>
</tbody>
</table>
Spitzer molecular emission lines

→ Antonellini et al. 2015, A&A accepted

![Spitzer IRS (R=600) data from Rigliaco et al. (2015)](image)

Disk model (continuum subtracted)
Spitzer IRS (R=600) data from Rigliaco et al. (2015)

Spitzer molecular emission lines

→ Antonellini et al. 2015, A&A accepted
10/20μm silicate features, IR interferometry

sub-mm interferometry (e.g. ALMA)

PAHs mid-IR

μm grains

mm-grains

migration?

ice

gas

CO ro-vib (e.g. CRIRES)

H₂O, OH, CO₂, HCN ...

(Spitzer, JWST)

high-J CO, H₂O

(Herschel)

[OI] 63μm

(Herschel, Sofia?)

(sub-)mm HCO⁺, CN, HCN, H₂CO, N₂H⁺, ...

scattered light images
The PAH UV-shield

→ Woitke et al. 2015, submitted to A&A

dust grain

UV

IR
The PAH UV-shield

→ Woitke et al. 2015, submitted to A&A
The PAH UV-shield

→ Woitke et al. 2015, submitted to A&A
Gas Heating & Cooling

heating

cooling

- heating by coll. de-excitation of H2exc
- heating by formation of H2 on dust
- heating by thermal accomodation on grains
- heating by C photo-ionisation
- cosmic ray heating
- PAH heating
- IR background heating by H2O rot-vib
- X-ray Coulomb heating
- chemical heating
- background heating by CH4 rovib (pseudo-NLTE)

- cooling by thermal accomodation on grains
- Ly-alpha line cooling
- OI line cooling
- CO rot & ro-vib cooling
- H2O rot and rovib cooling
- NH3 rot cooling
- OIII line cooling
- HCN rovib cooling (pseudo-NLTE)
Dust settling

**gas (assumed):** exponential tapering-off

**dust (calculated):** Dubrulle-settling $\alpha = 10^{-3}$
some modelling results

gas density

H$_2$O concentration

dust temperature

gas temperature
Density Structure

(1+1d) - hydrostatic

(1+1d) – hydrostatic, $T_{\text{gas}} = T_{\text{dust}}$ assumed

Woitke, Kamp & Thi (2009, A&A 501, 383);