



Turbulent mixing, chemical disequilibrium and cloud formation in substellar atmospheres

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¹Zentrum für Astronomie Heidelberg, Landessternwarte ²CRAL/ENS de Lyon ³Uppsala Universitet Ultracool atmospheres (M dwarfs, brown dwarfs) are complex — planetary atmospheres are more complex Low Mass Star

Brown Dwarf

Jupiter

NASA

(Sub-) stellar atmosphere modelling

- independent Variables
 (minimal):
 - effective temperature

• surface gravity $g(r) = GM/r^2$

• mass *M* or radius *R* or luminosity $L = 4 \pi R^2 \sigma T_{eff}^4$

composition ("metallicity")



PHOENIX workflow (P. Hauschildt)

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- effective temperature T_{eff}
- surface gravity $g(r) = GM/r^2$
- mass *M* or radius *R* or luminosity $L = 4 \pi R^2 \sigma T_{eff}^4$
- composition ("metallicity")
- convection → (micro-) turbulence & mixing
- rotation
- chemical peculiarities



PHOENIX workflow (P. Hauschildt)

→ self-contained and internally consistent structure in 1D

(Ultra)cool Atmospheres — Molecular Bands

Importance of molecular bands dependent on

- Line strengths
 gf, Abundances
- Line shapes
- Line numbers
- Line distribution

Bands with complex spectra (polyatomic molecules) produce strongest blanketing effects.

Molecular Bands — Methane

10¹⁰ lines

ExoMol

Yurchenko et al. 2014



Fig. 2. Polyad energy-level structure for ¹²CH₄. Boudon et al. 2006

Molecular line blanketing: Methane

- 30 Mio. lines computed with the STDS program (Université de Bourgogne) — 2013 update: 80 Mio.
- Vibrational and rotational states up to ~ 8000 cm⁻¹
- Completeness: ~50% (mid-IR) 10% (H-band) 0% (Y/J)



Non-equilibrium Chemistry

- Nitrogen- and Carbon chemistry is inhibited by slow reaction steps breaking up the C=O and N=N bonds:
- $N_2 \leftrightarrow NH_3$: limited by $N_2 + H_2 \rightleftharpoons 2 NH$

 $K = 8.45 \times 10^{-8} \times e^{(-8151/7)}$ (Lewis & Prinn 1980)

• CO \leftrightarrow CH₄: limited by H₂ + CH₃O \Rightarrow CH₃OH + H

 $K = 1.77 \times 10^{-22} \times T^{-3.09} e^{(-3055/T)}$ (Visscher, Moses & Saslow 2010)

• $CO \leftrightarrow CO_2$: limited by $CO + H_2O \rightleftharpoons CO_2 + H_2$

 $K = 6.44 \times 10^3 \times T^{-3.09} e^{(33889/T)}$ (Graven & Long 1954)

Model atmospheres — molecular opacity



Turbulence & Mixing in Cool



• $\tau_{mix} = H_P/v$ or $D = v \cdot H_P$ to be compared to

• dust formation and sedimentation timescales



Freytag et al. 2010

Mixing and Diffusion - a closer Look



convective overshoot and gravity wave excitation dominant in brown dwarfs

Chemistry across the L-T transition



Chemistry across the L-T transition



Chemistry across the L-T transition



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Exoplanetary Atmospheres and Habitability Nice, 12 Oct. 2015

et al. 2010

Molecular Line Profiles

- Molecular line data for stellar atmosphere calculations:
 - Extensive data available from spectroscopy line lists (HITRAN and others)
 - Often damping widths and shifts included, sometimes temperature dependence





• Effects of dust and transition from CO- to CH₄-chemistry

Condensation



cloud opacity changes spectral energy distribution

King et al. 2010

Condensation



depletion and accurate broadening theory important

— Allard et al. in prep.

Exoplanets — Irradiation and Circulation

50x solar, 1.11 bar



Mixing and Diffusion - a closer Look







modelling mixing based on extrapolation of RHD simulations + GCM models (Parmentier et al. Kataria et al.)



Clouds in hot Neptunes and super-Earths



Clouds affect carbon/oxygen chemistry





Clouds in hot Neptunes and super-Earths

GJ 436b transit models and WFC3 observations (Knutson et al. 2014)



Conclusions

- Cloud modelling successful in brown dwarfs
- Impact also on measured gas phase composition and thermal structure (evolution boundary!)
- Peculiarities of planetary atmospheres (mixing, nucleation processes) yet to be consistently implemented
- For mature, irradiated planets connection to circulation models essential

Merci pour votre attention!

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