Models of fractionation in disks

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Outline

➤ Static disk models
  • What processes affect isotope ratios in disks and can they change the ratios inherited from the interstellar medium?
    • Deuterium

➤ Mixing models (vertical mixing at 5 AU – near Jupiter’s orbit)
  • What effect does vertical mixing have on
    (a) Distribution of molecules between gas and ice
    (b) Isotope ratios
  • Deuterium
  • Carbon and oxygen
Star formation

M. Hogerheijde (1998), Shu et al. (1987)
Disk models

- Hydrostatic models (d’Alessio et al.) provide $n(R,z), T_{\text{grain}}(R,z)$
- $T_{\text{gas}}(R,z)$ from balancing heating and cooling processes (Kamp & Dullemond 2004, Kamp & van Zadelhoff 2001)
- Initial chemical abundances from molecular cloud model
- Basic reaction network from the UMIST database (RATE06: Woodall et al. 2007)
  - Gas phase reactions
  - Irradiation by UV, cosmic rays, X-rays
  - Freezeout and desorption
  - Grain surface reactions

\[ T_{\text{gas}} = T_{\text{grain}} \]

Photoelectric effect

\[ T_{\text{gas}} \gg T_{\text{grain}} \]
Disk chemistry

Bergin et al. 2007
Deuterium fractionation in static disks
What causes fractionation?

- **Deuterium**
  - Gas phase
    \[
    \text{H}_3^+ + \text{HD} \Leftrightarrow \text{H}_2\text{D}^+ + \text{H}_2 + \Delta E = 220K
    \]
    \[
    \text{CH}_3^+ + \text{HD} \Leftrightarrow \text{CH}_2\text{D}^+ + \text{H}_2 + \Delta E = 370K
    \]
    \[
    \text{C}_2\text{H}_2^+ + \text{HD} \Leftrightarrow \text{C}_2\text{HD}^+ + \text{H}_2 + \Delta E = 550K
    \]
  - Grain chemistry
    - Enhanced D/H atomic ratios on grains leads to high D/H in molecules formed on grains e.g. formaldehyde, water and methanol

- **Primordial D/H ratio \( \approx 10^{-5} \)**
  - Cold regions molecular D/H ratios can be as high as 0.1
Gas phase ratios

Fractionation

\[ \frac{\text{DCO}^+}{\text{HCO}^+} \]

\[ \frac{\text{H}_2^+}{\text{H}_3^+} \]

\[ \frac{\text{DCN}}{\text{HCN}} \]

\[ \frac{\text{HDCO}}{\text{H}_2\text{CO}} \]

\[ \frac{\text{HDO}}{\text{H}_2\text{O}} \]

Radius (AU)

Willacy (2007)
Deuterated ices

Model ratios:
DCN/HCN (ice) = 9.0 \times 10^{-3}
HDO/H_2O (ice) > 10^{-2}

Comet observations:
\frac{x(DCN)}{x(HCN)} = 2.3 \times 10^{-3}
\frac{x(HDO)}{x(H_2O)} = 5.0-6.6 \times 10^{-4} \text{ Oort cloud}
\frac{x(HDO)}{x(H_2O)} = 1.6 \times 10^{-4} \text{ Jupiter family}

Willacy & Woods (2009)

(Hartogh et al. 2011)
Mixing models
Mixing models

- Trace the vertical motion of a parcel of gas and dust in the disk at 5 AU using 3D MHD code.

- MHD shearing box calculation:
  - 600 particles
  - 300 orbits (Orbital period = $4 \times 10^8$ s)
  - take trajectories from 50 - 300 orbits
  - Concatenate trajectories together to make one path covering 1 Myrs

- MHD gives $n(t), T_{gr}(t)$

Inputs to chemical model
Selective photodissociation of CO

- Rates from Visser et al (2009)

![Graph showing interstellar photodissociation rates for different carbon isotopes.](image)
Photodissociation region
(hot gas)

$^{17}\text{O},^{18}\text{O},^{16}\text{O}$

Dissociation of $C^x\text{O}, \text{CO}_2$

CO, CO$_2$

Low $C^{16}\text{O}/C^x\text{O}$
Low $C^{16}\text{O}_2/C^x\text{O}_2$

Shielded region
(cooler gas)
Photodissociation region (hot gas)

17O, 18O, 16O

Dissociation of C^xO, CO₂

CO, CO₂

H₂O desorbed

High H₂¹⁶O/H₂^xO ice

Shielded region (cooler gas)

Low C¹⁶O/C^xO
Low C¹⁶O₂/C^xO₂
Photodissociation region (hot gas)

\[ 17\text{O}, 18\text{O}, 16\text{O} \]

Dissociation of \( C^{\text{xO}}, \text{CO}_2 \)

\[ \text{CO, CO}_2 \]

High \( \text{H}_2^{16}\text{O}/\text{H}_2^{\text{xO}} \) ice

\[ \text{H}_2\text{O desorbed} \]

Reform water and \( \text{O}_2 \)

\( \text{(OH} + \text{H} = \text{H}_2\text{O}) \)

\[ \text{Low C}^{16}\text{O}/C^{\text{xO}} \]

\[ \text{Low C}^{16}\text{O}_2/C^{\text{xO}_2} \]

Shielded region (cooler gas)
Photodissociation region (hot gas)

- Dissociation
- $\text{H}_2\text{O}$ desorbed
- High $\text{H}_2^{16}\text{O}/\text{H}_2^{x}\text{O}$ ice

Reform water and $\text{O}_2$

- $17\text{O}, 18\text{O}, 16\text{O}$
- Dissociation of $\text{C}^{x}\text{O}, \text{CO}_2$
- CO reforms

Grain reactions form water

- Low $\text{H}_2^{16}\text{O}/\text{H}_2^{x}\text{O}$ ice
- Low $16\text{O}/16\text{O}^{x}\text{O}$

Shielded region (cooler gas)

- Low $\text{C}^{16}\text{O}/\text{C}^{x}\text{O}$
- High $\text{C}^{16}\text{O}/\text{C}^{x}\text{O}_2$

- High $\text{C}^{16}\text{O}/\text{C}^{x}\text{O}$
- Low $\text{C}^{16}\text{O}_2/\text{C}^{x}\text{O}_2$

- Low $16\text{O}/16\text{O}^{x}\text{O}$
Mixing effects on CO and water fractionation

- **Gas phase CO fractionation**
  - CO, C^{17}O, C^{18}O
  - Fractionation vs. time (yrs)

- **Water ice fractionation**
  - H_2O/H_2^{17}O ice, H_2O/H_2^{18}O ice
  - Fractionation vs. time (yrs)

- **Grain temperature**
  - R = 5 AU
  - Temperature vs. time (yrs)

- **CO at 5 AU**
  - C^{16}O, C^{17}O, C^{18}O
  - Fractionation abundance vs. time (yrs)
Can mixing lead to a reduction in ice abundances at 5AU?
Summary

- Gas phase deuteration altered by reactions in disk
- Differential photodissociation at surface + mixing important for C and O bearing molecules
  - Explanation for anomalous oxygen isotope ratios in meteorites?
- Vertical mixing (5 AU)
  - Reduces HDO/H₂O ratio in ice by factor of 100
    => better agreement with comet observations
  - Alters oxygen isotope ratios in CO, CO₂ and H₂O
  - May lead to the loss of water ice at 5 AU
    => reduction in mass available for Jupiter formation