#### Water in the Universe

Ewine F. van DishoeckLeiden Observatory / Max-Planck Inst. für Extraterrestrische PhysikWith thanks to many colleagues, i.p. WISH teamSee Euronews space magazineSee Euronews space magazine

## Outline

- Why water?
- How to observe water
- Water puzzles
  - External galaxies
  - Evolved stars
  - Shocks
  - Diffuse + translucent clouds
  - Molecular clouds, pre-stellar cores
  - YSOs
  - Disks: outer vs. inner disks
  - Comets and the solar system

See Cernicharo & Crovisier 2005, Bergin & Melnick 2005, Th. Encrenaz 2008 ARA&A for recent reviews

## Why interest in water?

- A dominant form of oxygen => affects all species
  - Oxygen budget puzzle
- Diagnostic for 'hot spots'
  - Large variation H<sub>2</sub>O gas abundance <10<sup>-8</sup> to 3.10<sup>-4</sup>
- Role in energy balance as coolant
  - Heating agent if IR pumped
- Origin of water on Earth (through HDO/H<sub>2</sub>O)
  - Water trail from clouds disks comets, planets
- Chemistry of life occurs in water



#### Oxygen budget in a cold dense cloud

Component	Fraction of solar O	Observations
<b>Refractory dust</b>	30%	<b>Optical/UV, IR</b>
Ices (H <sub>2</sub> O,CO <sub>2</sub> , CO)	26%	Mid-IR
Gas-phase CO	9%	Submm Mid-IR
Remainder (O? O <sub>2</sub> ? H <sub>2</sub> O?)	35%	Far-IR, Submm, Mid-IR

Taurus cloud

Q: where is missing oxygen?

### **Further motivation**

- Traces basic ice formation and desorption: test of gas-grain chemistry
- H<sub>2</sub>O as a dynamical probe of warm high density gas: infall, outflow, quiescent gas, mixing, ...
- H<sub>2</sub>O as a radiative transfer challenge: high/low optical depths, masers, ....

## H<sub>2</sub>O transitions (µm)



- Also 22 GHz maser, first detected in Orion by Cheung et al. 1969

#### H<sub>2</sub>O Herschel-HIFI lines



Lines with range of excitation conditions available, with orders of magnitude better sensitivity, spatial and spectral resolution

#### Infrared: absorption gas and solids



# H<sub>2</sub>O gas chemistry

- Cold ion-molecule chemistry:
  - O + H<sub>3</sub><sup>+</sup> OH<sup>+</sup> ... H<sub>3</sub>O<sup>+</sup> + e H<sub>2</sub>O Typical abundances ~10<sup>-7</sup>
- High-temperature chemistry (>230 K):
  O + H<sub>2</sub> OH H<sub>2</sub>O

Drives all gas-phase O into  $H_2O =>$  abundance  $>10^{-4}$ Back reactions with H drive  $H_2O$  back to OH and O

Photodissociation by UV radiation:
 H<sub>2</sub>O OH + H

Rates for most/all (?) reactions well known

## **Oxygen chemistry**



Pure gas phase chemistry at low T produces H<sub>2</sub>O abundance of ~10<sup>-7</sup>, and eventually drives all O into O<sub>2</sub>

#### X-ray destruction of water



- $H_2O$  destroyed close to X-ray source in 5x10<sup>4</sup> yr for  $L_X = 10^{27}$  erg s<sup>-1</sup>
  - $H_3^+$  and  $He^+$  more abundant
  - UV from secondary electrons with H<sub>2</sub>
- Faster destruction for higher fluxes

# H<sub>2</sub>O grain chemistry

- Three routes for producing H<sub>2</sub>O, through hydrogenation of O. O<sub>2</sub> and O<sub>3</sub>
  - Relative importance depends on rates, energy barriers, hopping, diffusion, ...
- Postulated >25 yr ago, only now being tested in laboratory
  - Miyauchi et al. 2008, Ioppolo et al. 2008
- Desorption mechanisms
  - Thermal desorption: Fraser et al.
  - Photodesorption: Öberg et al.
  - CR-induced desorption



Tielens & Hagen 1982

Q: can this model be tested observationally?

## Water ice formation

- Formation several monolayers of H<sub>2</sub>O and OH ice in translucent clouds
- Form thick ice layers in dense clouds
- Results depend sensitively on molecular data, grain morphology, ...
- Underproduce H<sub>2</sub>O ice compared with observations



Cuppen & Herbst 2007

### Water in O-rich evolved stars



Neufeld et al. 1996

- Major coolant of outflowing circumstellar gas
- Many lines detected by ISO-LWS and SWS
- Major differences in inferred *dM/dt* by different groups, related to different gas temperature structures?

#### Q: what does $H_2O$ tell us about physical structure ?

## Water in C-rich evolved stars

- Detection of H<sub>2</sub>O in C-rich envelope IRC+10216 came as a surprise
- Evaporating icy planetesimals?





Q: Origin O-rich species in C-rich stars? How common?

### Water in external galaxies



Arp 220 ISO-LWS

Gonzalez-Alfonso et al. 2004

- H<sub>2</sub>O 22 GHz megamasers; trace black hole mass; 183 GHz Arp 220
- H<sub>2</sub>O/OH~1 in nucleus, ~0.1 in extended region from ISO-FIR absorption
  - Gonzalez-Alfonso et al. 2004, 2008, Goicoechea et al. 2005
- $H_2O/H_2 < 10^{-8}$  from ODIN on kpc scale; increases to 10<sup>-7</sup> if 10% filling factor
  - Wilson et al. 2007
- H<sub>3</sub>O<sup>+</sup> detected ⇒ H<sub>2</sub>O/H<sub>2</sub>~2. 10<sup>-7</sup> on few hundred pc van der Tak et al. 2007
   Q: Are these abundances characteristic of general ISM?

## **Shocks**

- H<sub>2</sub>O clearly detected in shocks associated with supernova remnants and YSOs
- Abundance ~10<sup>-7</sup>-10<sup>-6</sup> ⇒ not all O driven into H<sub>2</sub>O, except in densest regions and highest velocities
- UV photodissociation of pre-shock and shocked gas? Freeze-out behind shock? Shock physics?

#### Supernova remnant IC443



Snell et al, 2005; Franklin et al. 2008

#### **Q**: why not all oxygen driven into $H_2O$ at high T?

#### **Orion outflow**



- Wealth of ISO-LWS and SWS lines, including absorption and P-Cygni profiles
- H<sub>2</sub>O/H<sub>2</sub>~(2-3).10<sup>-5</sup>

### **Orion-KL H<sub>2</sub>O and H<sub>2</sub><sup>18</sup>O profiles**



- H<sub>2</sub>O abundance in extended cloud may be as low as 10<sup>-8</sup>, but still controversial

Water in diffuse and translucent clouds



- H<sub>2</sub>O/H<sub>2</sub><10<sup>-8</sup> from UV absorption
- H<sub>2</sub>O/H<sub>2</sub>~10<sup>-8</sup>-few.10<sup>-7</sup> from 557 GHz absorption
  - Neufeld et al. 2000, 2002; Plume et al. 2004

H<sub>2</sub>O/H<sub>2</sub>~3.10<sup>-7</sup> from IR absorption toward Galactic Center

Moneti & Cernicharo 2000

Q: are results consistent with pure gas-phase chemistry?

### General molecular clouds

o-H<sub>2</sub>O 557 GHz 1<sub>10</sub>-1<sub>01</sub>

Snell et al. 2000 Wilson et al. 2003



#### -SWAS and ODIN (~3'):

Water emission is weak => most water frozen out on grains in cold clouds

Q: how low is water abundance in cold clouds? is this consistent with ice abundances?

## Summary (o-)H<sub>2</sub>O abundances



Bergin & Melnick 2005

#### Low-Mass: Pre-stellar cores



## **Model B68 water profile**



- Q: Where does onset for  $H_2O$  ice formation and freeze-out occur?
- Q: How effective are non-thermal desorption mechanisms?
- Q: What is para-H<sub>2</sub>O abundance?

Hollenach et al. 2008

#### Ice abundances in cold clouds



-Q: why is most, but not all, oxygen in ices? Atomic O?

Pontoppidan et al. 2004

## High-mass pre-stellar cores

#### MSX

**SCUBA** 



-Q: do high-mass pre-stellar cores have similarly low H<sub>2</sub>O gas abundances?

Johnstone et al. 2003

#### Hot, steaming water near protostars

**ISO-SWS mid-IR absorption for high-mass YSOs** 



Combine with SWAS and ISO-LWS data to constrain abundance profile

Helmich et al. 1996 Boonman et al. 2003

#### **Inferred abundance profile**



### Low-Mass: Class 0 sources



-Q: What is origin of strong H<sub>2</sub>O emission? Quiescent warm envelope or outflow?

Nisini et al. 1999, 2000 Ceccarelli et al. 1998

### Try to link H<sub>2</sub>O with mm continuum and SiO



- Q: Are these real correlations or not?

Ceccarelli et al. 1999

#### Low-Mass: Class I sources



Class 0: H<sub>2</sub>O

**Class I: OH** 

-Why do Class I sources have lower H<sub>2</sub>O abundances and larger OH/H<sub>2</sub>O ratio? Enhanced photodissociation? Longer timescale for freeze-out?

Nisini, Giannini et al. 2002

#### Hot water from disk accretion shock?







Deeply embedded Class 0 protostar

Q: Chemical signatures of accretion disks? How is material modified as it is incorporated into disk?

Watson et al. 2007

#### Where is water in protoplanetary disks?



# Q: use water as tracer of radial and vertical mixing? Probe snow line?

JWST + Herschel

#### **Surface layer**

**Intermediate layer** 

#### Midplane



## H<sub>2</sub>O ice in disks





Terada et al. 2007, Pontoppidan et al. 2005

#### Q: how much water gas is in outer disk?

### Water and organics in inner disk



#### Hot water and organics in inner disk



NASA / JPL-Caltech / J. Carr (Naval Research Laboratory)

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Carr & Najita 2008 Salyk, Pontoppidan et al. 2008

#### Near-IR H<sub>2</sub>O and OH in disks from ground



 $\Rightarrow$  H<sub>2</sub>O and OH come from inner 0.5-1 AU!

## Implications

- Water gas is found well inside the 'snow' line (estimated at ~3 AU)
- Water is expected to disappear in ~10<sup>5</sup> yr
   ⇒ replenishment needed
- Inward radial migration or upward mixing of icy grains and planetesimals, followed by evaporation?

#### Water in comets



Q: - Formation temperature and history (from o/p ratio)? - Source of water on Earth (from HDO/H<sub>2</sub>O)?

### Conclusions

- H<sub>2</sub>O found throughout universe: 'waterworld'
- H<sub>2</sub>O abundance varies greatly from region to region
- Model scenarios available, but many questions remain
- Herschel HIFI and PACS will provide our best chance for decades to 'nail down' gaseous H<sub>2</sub>O and OH in galaxies, evolved stars, clouds, YSOs, outer disks
- Need SOFIA for spectrally resolved [O I]
- Need JWST, SOFIA, ELTs for hot gas in inner disk
- Need JWST, ground for ice mapping
- Need complementary laboratory data, theoretical studies of collision rates, and good radiative transfer codes!