HIFI Spectroscopy of H$_2$O sub-millimeter Lines in Nuclei of Actively Star Forming Galaxies


Liu et al. 2017 submitted
The H$_2$O molecule

Angular momentum: $J_{K_a,K_c}$

ortho-H$_2$O
para-H$_2$O

Selection rules:
$\Delta J=0,+/-1$

Energy diagram
Why do we care about H$_2$O in galaxies?

- H$_2$O is one of the most abundant gas in molecular clouds (the 3rd most abundant species $\sim 10^{-5}$-$10^{-4}$ in warm regions).
- H$_2$O possesses a large number of sub-mm and FIR transitions. It can be an important coolant in dense molecular clouds.
- H$_2$O can be effectively excited by collision and IR pumping. The relative strengths of H$_2$O lines give us information of the ISM physical structure and FIR radiation density.

Van der Werf et al., 2014
Observations of Extragalactic Water So Far

Table 1. Important Telescopes for Water Observations

<table>
<thead>
<tr>
<th>telescope</th>
<th>wavelength/frequency</th>
<th>spectral resolving power $R$</th>
<th>spatial resolution $^a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>SWAS</td>
<td>557 GHz</td>
<td>$10^6$</td>
<td>$3.2' \times 4.0'$</td>
</tr>
<tr>
<td>Odin</td>
<td>557 GHz</td>
<td>$10^6$</td>
<td>2'</td>
</tr>
<tr>
<td>ground cm</td>
<td>22 GHz</td>
<td>$10^6$</td>
<td>0.001' to a few arcsec</td>
</tr>
<tr>
<td>ground mm</td>
<td>many, e.g., 183, 380 GHz, 203$^b$, 391$^b$, 692$^b$ GHz</td>
<td>$10^7$</td>
<td>0.2–20&quot;</td>
</tr>
<tr>
<td>Herschel-HIFI$^c$</td>
<td>480–1250 GHz</td>
<td>$10^7$</td>
<td>0.2–20&quot;</td>
</tr>
<tr>
<td></td>
<td>1410–1910 GHz</td>
<td>$10^7$</td>
<td>44&quot;–17&quot;</td>
</tr>
<tr>
<td>Herschel-PACS$^d$</td>
<td>55–210 μm</td>
<td>$(1 – 5) \times 10^3$</td>
<td>15&quot;–9&quot;</td>
</tr>
<tr>
<td>Herschel-SPIRE$^e$</td>
<td>200–670 μm</td>
<td>$\sim 10^3$</td>
<td>9.4&quot;</td>
</tr>
<tr>
<td>Spitzer</td>
<td>10–38 μm</td>
<td>600</td>
<td>17–42&quot;</td>
</tr>
<tr>
<td>ISO-SWS$^f$</td>
<td>2.5–45 μm</td>
<td>2000, 200000</td>
<td>10&quot;</td>
</tr>
<tr>
<td>ISO-LWS$^g$</td>
<td>45–197 μm</td>
<td>200, 100000</td>
<td>14&quot; × 20&quot; to 17 × 40&quot;</td>
</tr>
<tr>
<td>ground 4–10 m optical</td>
<td>2.8–3.3 μm</td>
<td>$\leq 10^5$</td>
<td>$\leq 1''$</td>
</tr>
<tr>
<td>ground 4–10 m infrared</td>
<td>11–14 μm</td>
<td>$10^8$</td>
<td>1&quot;</td>
</tr>
</tbody>
</table>

SWAS & ODIN, not sensitive enough
ISO & Spitzer, only high excitation lines
Herschel-PACS/SPiRE, coarse spectra/velocity resolution

Herschel-HIFI: allowed for the first systematic and comprehensive studies of multiple $H_2O$ lines in galaxies
The Herschel/HIFI EXtraGALactic (HEXGAL) Key Project

Sample: nine nearby galaxies:

- **M82** nuclear SB                    LIRG extended
- **NGC 253** nuclear SB                LIRG extended
- **NGC 4945** nuclear SB/AGN          LIRG extended
- **Centaurus A** nuclear SB/AGN       LIRG extended
- **Arp220** SB/AGN Major Merger       ULIRG compact
- **NGC 4038/39** SB Major Merger      LIRG extended
- **NGC1068** AGN/SB                   LIRG extended
- **Mrk 231** AGN/SB                    ULIRG compact
- **NGC6240** AGN/SB                   LIRG compact

Selected H₂O transitions:

- **o-H₂O**
  - 5_{23}
  - 2_{12}
  - 5_{14}
  - 3_{03}
  - 4_{22}
  - 2_{21}
  - 1_{10}

- **p-H₂O**
  - 5_{14}
  - 4_{31}
  - 3_{13}
  - 2_{02}
  - 4_{13}
  - 2_{01}
  - 2_{02}

Aims to study the physical and chemical composition of the ISM in galactic nuclei using HIFI spectroscopy:

- ISM in the galactic center region
  - detailed investigation of the GC region
- Gas excitation in starbursts and ULIRGs
  - CO & fine structure line excitation
  - The extragalactic water trail
- Chemical complexity of extragalactic nuclei
  - Line surveys of selected sources
  - Absorption line study in selected source
HIFI H$_2$O Line Shape

**H$_2$O Emission Lines & CO Line**

- CO 3-2
- o-H$_2$O ($3_{12}$-$3_{21}$) x 2.1
- p-H$_2$O ($2_{02}$-$1_{11}$) x 1.2
- p-H$_2$O ($2_{12}$-$2_{21}$) x 1.5
- o-H$_2$O ($3_{21}$-$3_{12}$) x 1.1

NGC4945

- CO 3-2
- o-H$_2$O ($3_{12}$-$3_{21}$) x 1.8
- p-H$_2$O ($2_{02}$-$1_{11}$) x 1.4
- p-H$_2$O ($2_{12}$-$2_{21}$) x 1.9
- p-H$_2$O ($2_{12}$-$2_{21}$) x 1.7
- p-H$_2$O ($2_{02}$-$1_{11}$) x 1.5

NGC253

- CO 3-2
- p-H$_2$O ($2_{02}$-$1_{11}$) x 2.3
- p-H$_2$O ($1_{10}$-0$_{0}$) x 2.7
- p-H$_2$O ($2_{12}$-$2_{21}$) x 2.9
- o-H$_2$O ($1_{10}$-1$_{01}$) x 7.9

NGC1068

- CO 3-2
- p-H$_2$O ($4_{02}$-$3_{12}$) x 0.5
- p-H$_2$O ($2_{12}$-$2_{21}$) x 0.3
- o-H$_2$O ($3_{21}$-$3_{12}$) x 0.3
- p-H$_2$O ($2_{02}$-$1_{11}$) x 0.4

Arp220

**H$_2$O Absorption Lines**

- NGC4945
- o-H$_2$O ($1_{10}$-1$_{01}$)

- NGC253
- o-H$_2$O ($1_{10}$-1$_{01}$)

- Arp220
- o-H$_2$O ($1_{10}$-1$_{01}$)
Step 1: Spectra Gaussian Decomposition
Method: fit full water spectra into several gaussian components with almost fixed velocity centers ($\Delta v \leq 5 \text{ km s}^{-1}$) and line width ($\Delta \text{FWHM} \leq 10\%\text{FWHM}$).

Step 2: IR and (sub)mm Photometry & Dust SED Fitting
IR maps: Spitzer, WISE, IRAS, Herschel PACS/SPIRE and ISO
(sub)mm maps: APEX SABOCA/LABOCA
Method: measure the fluxes within apertures of various HIFI beams, and use the derived fluxes to fit dust SED and perform aperture corrections required by resolved sources.

Step 3: CO SLED (1 \leq \text{Jup} \leq 14)
CO fluxes: SPIRE, HIFI, ground telescopes

Step 4: Radiative Transfer Calculation
Method: $\beta3D$
Advantages of β3D:

(1) its dimensionality: a unique temperature, density, abundance value and, more importantly, 3D velocity vector can be attributed to every position in the model.

(2) its high speed of convergence: due to the extended escape probability method implemented.

(3) its ability to account for the effects of dust: the effect of dust emission and absorption (i.e., IR-pumping) on the excitation of molecules was also considered.

(4) its output of channel maps: a new line tracing approach where both line and continuum emission are calculated across the full velocity range (i.e., line profile) over a projected surface along an arbitrary viewing angle.
<table>
<thead>
<tr>
<th>Models for Individual Galaxies</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>NGC 4945 center</strong></td>
</tr>
<tr>
<td><img src="image1.png" alt="Diagram" /></td>
</tr>
<tr>
<td><strong>NGC 253 center</strong></td>
</tr>
<tr>
<td><img src="image2.png" alt="Diagram" /></td>
</tr>
<tr>
<td><strong>M82 center</strong></td>
</tr>
<tr>
<td><img src="image3.png" alt="Diagram" /></td>
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<tr>
<td><strong>NGC 1068 center</strong></td>
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<tr>
<td><img src="image4.png" alt="Diagram" /></td>
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<tr>
<td><strong>Mrk 231</strong></td>
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<tr>
<td><img src="image5.png" alt="Diagram" /></td>
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<tr>
<td><strong>NGC 6240</strong></td>
</tr>
<tr>
<td><img src="image6.png" alt="Diagram" /></td>
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<tr>
<td><strong>Arp 220</strong></td>
</tr>
<tr>
<td><img src="image7.png" alt="Diagram" /></td>
</tr>
<tr>
<td><strong>Cen A center</strong></td>
</tr>
<tr>
<td><img src="image8.png" alt="Diagram" /></td>
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</tbody>
</table>
General Modelling Results: warm + cold ER

Two Typical Components

Typical Parameter Values

<table>
<thead>
<tr>
<th>Component</th>
<th>WARM</th>
<th>COLD ER</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho$ [H/cm$^3$]</td>
<td>$10^5 - 10^6$</td>
<td>$10^3 - 10^4$</td>
</tr>
<tr>
<td>$T_k$ [K]</td>
<td>40 - 70</td>
<td>20 - 30</td>
</tr>
<tr>
<td>$x$($H_2O$)</td>
<td>$10^{-8} - 10^{-7}$</td>
<td>$10^{-9} - 10^{-8}$</td>
</tr>
<tr>
<td>$T_{dust}$ [K]</td>
<td>40 - 70</td>
<td>20 - 30</td>
</tr>
<tr>
<td>$N_H$ [H/cm$^2$]</td>
<td>$1 - 4 \times 10^{24}$</td>
<td>$1 - 6 \times 10^{23}$</td>
</tr>
</tbody>
</table>
General Modelling Results: warm + cold ER

Two Typical Components

Fraction of Level Populations

Line Features from Cold and Warm Components
General Modelling Results: warm + cold ER

Dust SED

CO SLED

Friday, May 12, 17
General Modelling Results: absorbing gas

No absorbing gas in NGC 1068: $i < 40$ deg

Absorbing gas arise from part of ER

Absorbing gas is not part of ER

Friday, May 12, 17
**General Modelling Results: hot component**

<table>
<thead>
<tr>
<th>Component</th>
<th>Hot</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \rho ) [H/cm(^3)]</td>
<td>(~ 10^6)</td>
</tr>
<tr>
<td>( T_k ) [K]</td>
<td>100 - 200</td>
</tr>
<tr>
<td>( x(H_2O) )</td>
<td>(10^{-6} - 10^{-5})</td>
</tr>
<tr>
<td>( T_{dust} ) [K]</td>
<td>100 - 200</td>
</tr>
<tr>
<td>( N_H ) [H/cm(^2)]</td>
<td>(10^{24} - 10^{25})</td>
</tr>
</tbody>
</table>

**Line Features from Warm and Hot Components**

**Fraction of Level Populations**

- Cold
- Warm
- Hot

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General Modelling Results: hot component

Dust SED

CO SLED

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Water Excitation: collision vs. IR-pumping

- **Cold ER**: water gas is mainly collisionally excited
- **Warm Component**:
  levels with $E_{up} \leq 300 - 400$: collisionally exited
  levels with $E_{up} \geq 300 - 400$: IR-pumping exited
- **Hot Component**:
  levels with $E_{up} \leq 800 - 1000$: collisionally exited
  levels with $E_{up} \geq 800 - 1000$: IR-pumping exited
Cold ER:
- \( \frac{2_{12}-1_{01}}{1_{10}-1_{01}} \) line ratios is a good indicator of “shock condition”

Warm Component:
- H2O SLED seen in middle-lying lines (\( 2_{12}-2_{02} \) to \( 3_{22}-3_{13} \)) are nearly flat;
- The \( 3_{21}-3_{12} \) line has higher \( T_{ex} \) and stronger line intensity

Absorbing gas:
- The absorption line ratio depends on mainly the dust optical depth of absorbing gas;
- The \( 1_{11}-0_{00}/1_{10}-1_{01} \) (1113/557 GHz) and \( 2_{12}-1_{01}/1_{10}-1_{01} \) (1670/557 GHz) absorption line ratio > 1, if background is dust continuum; and < 1, if background is radio source

Hot component:
- Strong detections in high-lying lines (including both emission and absorption)

Friday, May 12, 17
Summary

‣ Our work has led to the first complete view of a number of water lines including ground transitions in a variety of active nuclear environments with spectral resolution

‣ The water spectra show a diversity of line shapes. The middle-lying lines are always seen in emission, while the low-lying lines tend to appear in absorption

‣ Line modelling with 3D radiative transfer code β3D suggests that water line profiles provide a powerful diagnostic tool, by:
(1) revealing the geometry and dynamics structure of ISM (gas and dust) through the various line shapes
(2) revealing the physical and chemical conditions of ISM
(3) constraining dust continuum model and local conditions of infrared-opaque sources (even without spatially resolving them), since IR-pumping is found to play an important role in warm regions

‣ The luminous IR galaxies (nuclei) contain three typical components:
(1) a widespread cold component, where only the lowest few energy levels of H2O are excited mainly by collision
(2) a warm region, a main contributor to the middle-lying H2O lines, dust SED and middle/high-J CO emissions
(3) a hot core (usually appears in ULIRGs), where high-lying water, mid-IR and high-J CO lines arise from