How to Interpret Molecular Lines From Dense Gas in Galaxies

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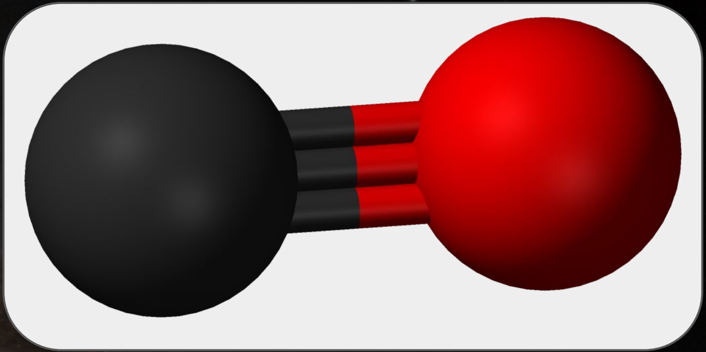
Motivation:

- **Understand the Physical Conditions of Molecular Gas in nearby galaxy:**
  - By analyzing **CO(2–1)** and **CO(3–2)** emission from **NGC 1068**, we aim to derive key physical parameters such as **gas temperature,** and **column density** in regions affected by both star formation and AGN activity.

Methodology:

- **Local Thermodynamic Equilibrium Methods:**
  - The project utilises the **LTE** approximations (like rotational diagrams) to determine gas temperature, and column density
- **Link Observational Results to Chemical Evolution:**
  - By incorporating **astrochemical modeling**, **UCLCHEM** **(Holdship+2017;** https://uclchem.github.io/), we explore how gas abundance gets affected by varied parameters (e.g. density, radiation field, cosmic ray ionisation rate and temperature).
  - Determine values of these parameters giving rise to the observed column densities of CO in this galaxy.

Carbon Monoxide (CO)



Wikipedia

- **Second most abundant** molecule in the Universe
- Used as **tracer** of **molecular gas**

Rotational transitions:

- J=1-0 through J=6-5 accessible in ALMA Bands 3-9 (ALMA Receiver Bands); critical densities n_{crit} ~10^3-10^6 cm^{-3} (Harris+1991).

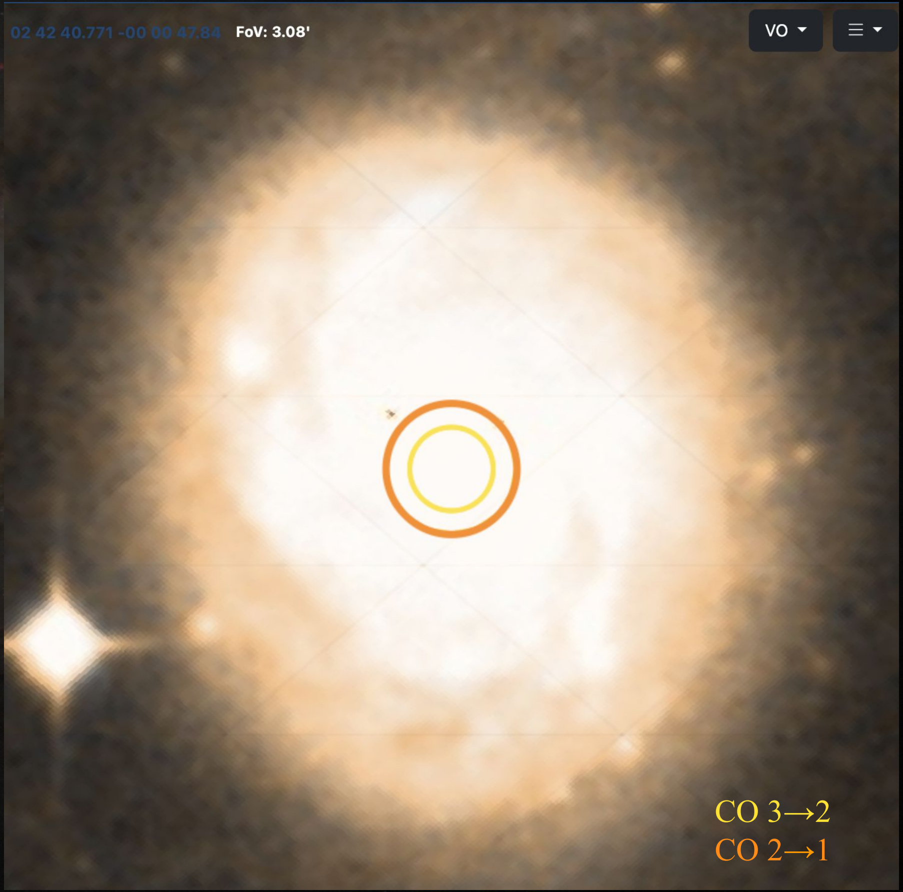
X_{co} calibration:

$$N(H_2) = X_{CO} W(^{12}C^{16}O: J=1 \rightarrow 0)$$

- Milky Way average: Xco~2×10^{20} cm^{-2} (K km s^{-1}) (Bolatto+2013).
- Central molecular zones in galaxies: Xco~1.9×10^{19} cm^{-2} (K km s^{-1}) (Israel 2020).
- ➡ Estimates the **molecular gas mass** and **column density** in that region.

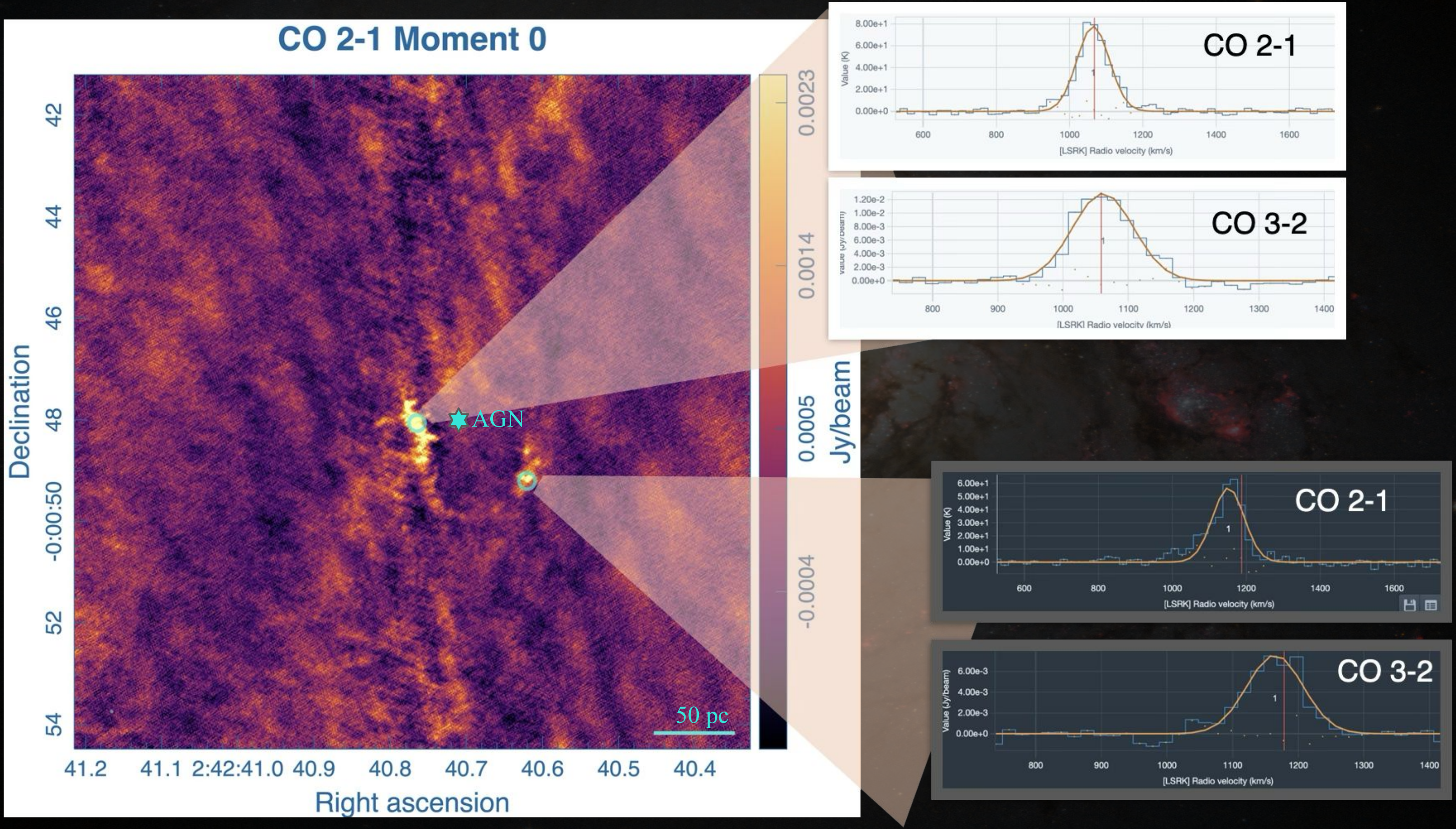
NGC 1068 ALMA Data (PI Santiago Garcia-Burillo, 2016.1.00232.S)

- Distance: 14.4 Mpc
- Seyfert 2 active galaxy
- ALMA archival data
- Observations of the circumnuclear disk
- From r~100pc to central
  7-10pc-diameter torus



https://almascience.nrao.edu

Data Used



CO 2-1 Moment 0
Declination
Right ascension
Jy/beam
AGN
50 pc
CO 2-1
CO 3-2
CO 2-1
CO 3-2
[LSRK] Radio velocity (km/s)

Data Analysis: Observations

$$\ln(\gamma_u W/g_u) = \ln(N) - \ln(Z) - (E_u/kT)$$

Eq.(23) from Goldsmith and Langer 1999.

$$\gamma_u = (8\pi k_B \nu^2) / (h c^3 A_{ul})$$

Eq.(11) from Goldsmith and Langer 1999.

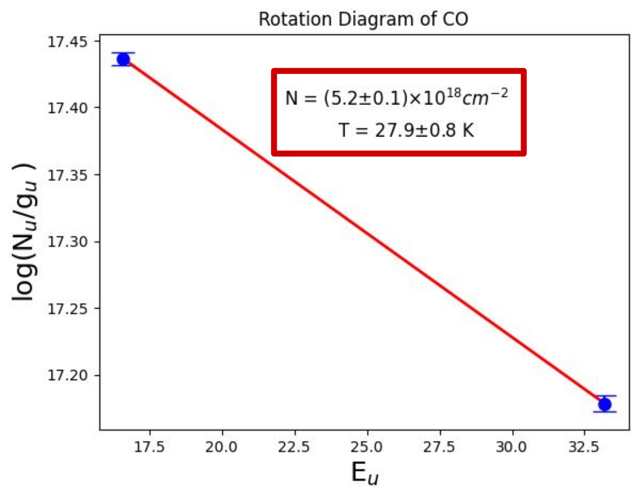
$Z \sim (k T_{ex}) / (h B_0) e^{hB0/3kTex}$ approximation

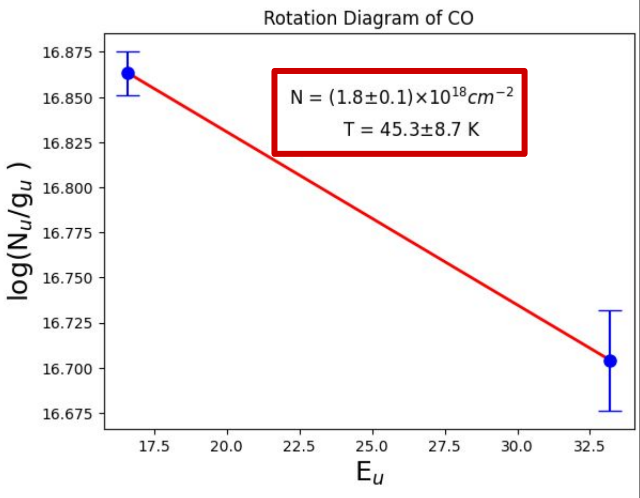
Eq.(D.3) from Santa-Maria et al. 2023.

Use spectral databases for CO properties

Solve for temperature, partition function, and column density

Transition	Frequency (GHz)	E_u(K)	$\log(A_{ul})$
CO 2-1	230.538	16.60	-6.16
CO 3-2	345.796	33.19	-5.60





UCLCHEM (Holdship+2017)

What is UCLCHEM?:

- Time-dependent gas-grain **chemical code** for astrochemical modelling

How it works:

- Modules for **molecular clouds, hot cores, C-shocks**, and the post-processing of **hydrodynamic simulations**
- Evolves **chemical abundances** under user-specified physical conditions (e.g. density, temperature, radiation field, cosmic-ray ionization)
- Simultaneously treats **gas-phase reactions and grain-surface chemistry**

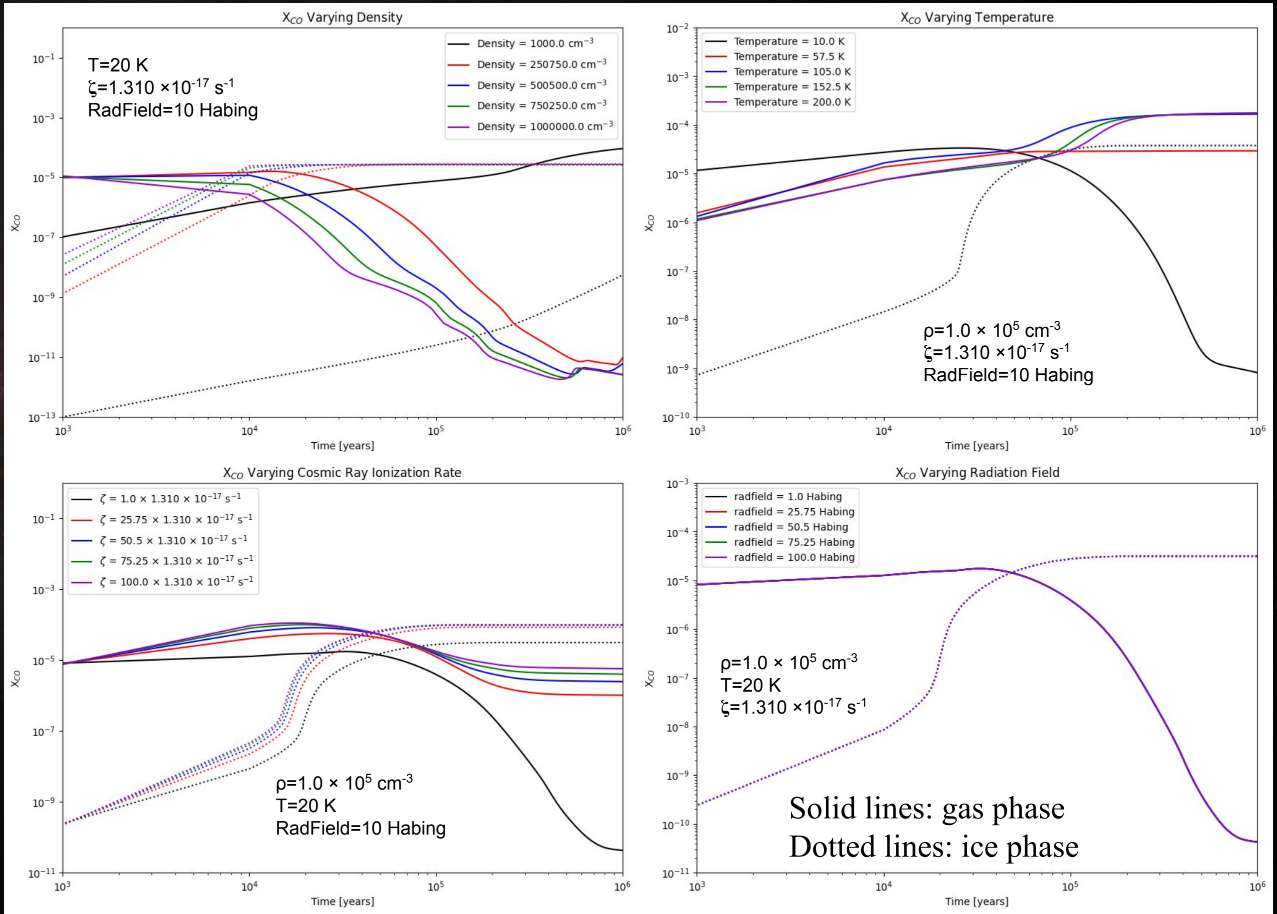
Why use it?:

- Integrates **gas and ice chemistry** in a single framework
- **Proven** applications from star-forming cores to AGN environments

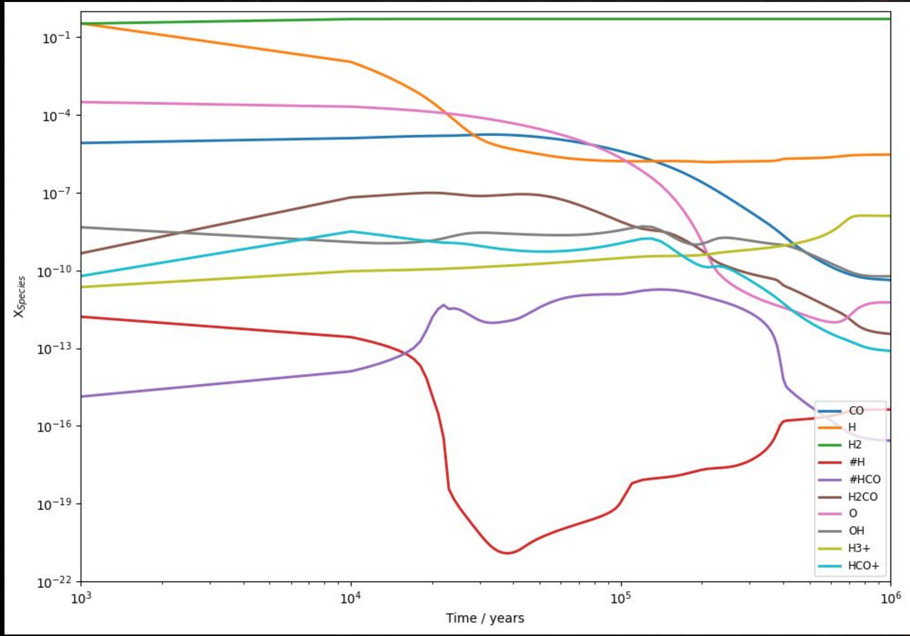
Data Analysis: UCLCHEM

Model inputs:

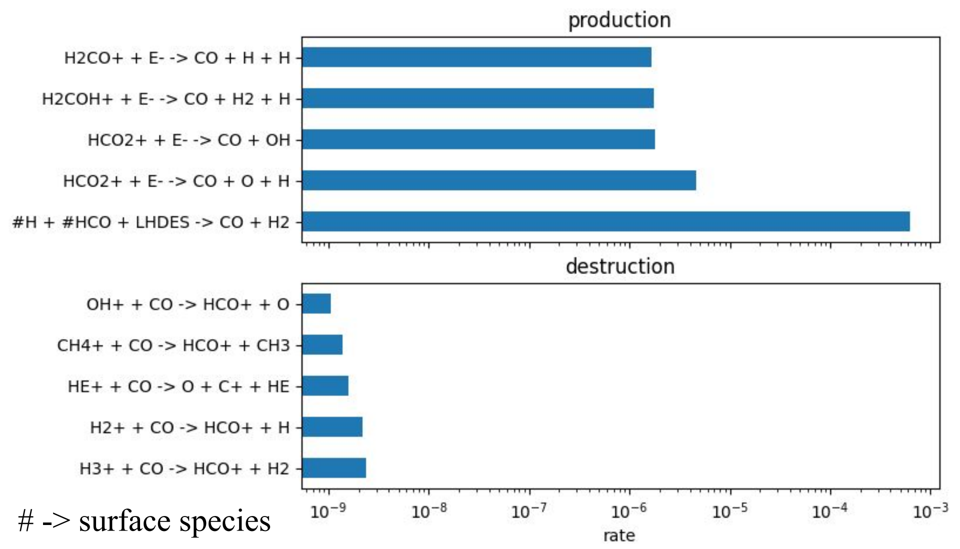
- Static Density: 1×10^{5} H/cm^{3}
- Temperature: 20 K
- Extinction A_V: 2090
- Cosmic Ray Ionization Rate: 1.310×10^{-17} s^{-1}
- Radiation Field: 10 Habing
- Observed region radius: 11 pc



Species Evolution



Major Reaction Routes



-> surface species

Matching Observations

Fractional abundance f_{CO} ⟶ Column density N_{CO} (optically thin):

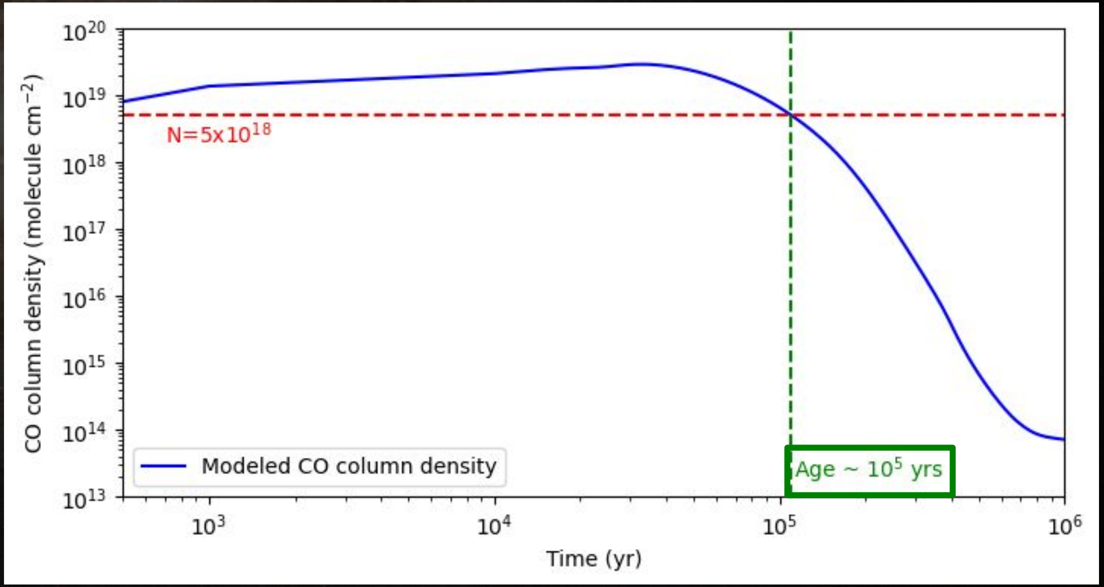
$N_{CO} \sim f_{CO} \times A_V \times 2.2 \times 10^{21}$

A_V calculation:

$A_V \sim$ n(H) × radius of region

n(H): Input in model

radius of region: From observation



Room for Improvement

Assumptions:

- Size of gas cloud
- Density of hydrogen
- Static condition (constant hydrogen density)
- LTE
- No calibration errors

Need to include error propagation

Need more CO transitions for better temperature estimate

Obtain the temperature and density distribution of NGC 1068 with CO transitions

Need more molecules for gas dynamic/chemical constraints

Summary

- ALMA archival CO data of circumnuclear disk of **NGC 1068**
  - CO v=0, 2 - 1
  - CO v=0, 3 - 2
- Calculated **temperature and column density** of CO using **rotational diagram**
- Tested a range of temperatures, densities, cosmic ray ionization rates, and radiation fields on chemical model **UCLCHEM**
- Calculated column density of **CO over time**
- Studied the **time-evolution** of fractional abundance of CO and related molecules
- **Calculated extinction value** to match our observations to directly compare to model results
- Estimated **age** of the observed gas cloud

Thank You...

Citations

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- Molecular catalogs: https://splatalogue.online/#/advanced & https://cdms.astro.uni-koeln.de/cdms/portal/catalog/83/#
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- Harris, A. I., et al. "First observations of the CO J= 6-5 transition in starburst galaxies." Astrophysical Journal, Part 2-Letters (ISSN 0004-637X), vol. 382, Dec. 1, 1991, p. L75-L79. 382 (1991): L75-L79.