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ASTROCHEMISTRY

# Detection of two interstellar polycyclic aromatic hydrocarbons via spectral matched filtering

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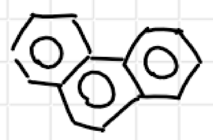
Unidentified infrared emission bands are ubiquitous in many astronomical sources. These bands are widely, if not unanimously, attributed to collective emissions from polycyclic aromatic hydrocarbon (PAH) molecules, yet no single species of this class has been identified in space. Using spectral matched filtering of radio data from the Green Bank Telescope, we detected two nitrile-group–functionalized PAHs, 1- and 2-cyanonaphthalene, in the interstellar medium. Both bicyclic ring molecules were observed in the TMC-1 molecular cloud. In this paper, we discuss potential in situ gas-phase PAH formation pathways from smaller organic precursor molecules.

## Background



多環式芳香族炭化水素 (PAHs) → 未同定赤外線バンド放射 (UIR band) のキャリアとして有力

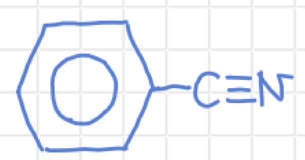
→ 星間空間にある炭素の 10–25 % 近くが PAH として存在している可能性

※ 小質量星の進化末期の星周環境で形成: gas phase reaction (bottom-up) v.s. dust origin (top-down)

※ サイズの小さい PAHs は UV で破壊されやすく星間空間では寿命が短い ($10^4$–$10^6$ yr)

※ ほぼ無極性なこともあって分子として同定されることはほとんどなかった

分子雲 TMC-1 で **benzonitrile** の検出 (McGuire et al., Science, 2018)



⇒ PAH 分子の宇宙空間での初の同定 & 分子雲内部で PAHs が合成された可能性を示唆 (= bottom-up)

(McGuire et al. 2018)

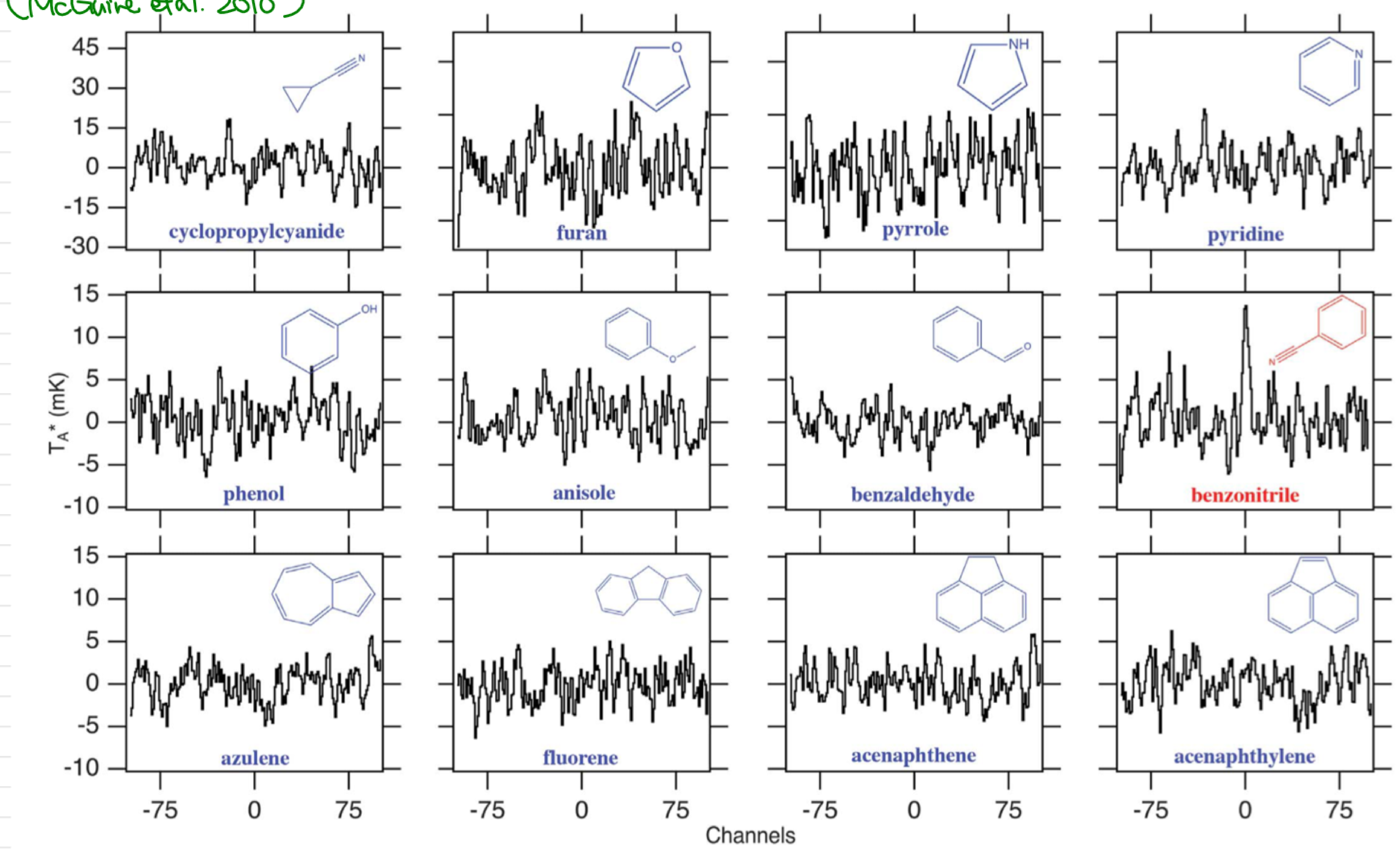



**Fig. 1. Composite averages of molecules toward TMC-1.** Velocity-stacked composite averages of all transitions of a given molecule with upper state energy ($E_U$) < 70 K constructed from the entire survey (8.8 to 50 GHz) of TMC-1 (19) are shown. The channel spacing is 20 kHz. If a molecule is present, signal in antenna temperature ($T_A$*) would be expected at channel 0. A detectable signal was present only for benzonitrile (red).

## Point

TMC-1 でより大きな PAH である 1- & 2-cyanonaphthalene を検出

分子雲内部での PAH 形成 (gas phase) を示唆するが今の化学進化モデルでは桁で abundance が足りない

## Observation/Data

100-m Robert C. Byrd Green Bank Telescope (GBT) による TMC-1 の line survey プロジェクト

GBT Observations of TMC-1: Hunting Aromatic Molecules (GOTHAM)

DR1: 2018.02 — 2019.05

DR2: 2019.05 — 2020.06

8–11.6 & 18–30 GHz with a 1.4 kHz resolution

## Results

DR1 では どの輝線も検出限界以下

⇒ 輝線が出るはずの周波数を切り出して stacking

⇒ 1-CNN, 2-CNN ともに存在を確認

DR2 は SN がいいので個別の輝線が検出可能

⇒ matched filtering (≈ template fitting) を用いてパラメタ ($T_{ex}$, $N_T$, $\Delta V$, $\theta$, $V_{LSR}$) を推定

測定した abundance と化学進化モデルと比較

1. top-down ⇒ 星間空間を生き残れない
2. fiducial bottom-up ⇒ $10^6$ 倍足りない
3. naphthalene マシマシ ⇒ ~$10^5$ yr しか保たない

1-CNN, 2-CNN を検出したが, 形成パスに謎が残った

DR1 での stacked spectra

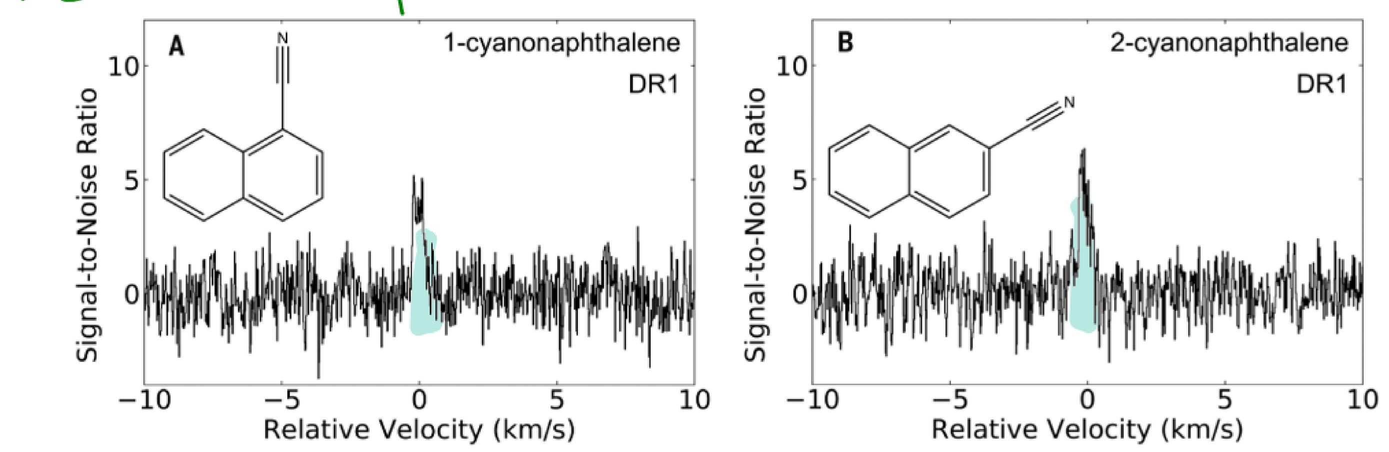



**Fig. 1. Molecular structures and spectral stacks of 1-CNN and 2-CNN in the GOTHAM DR1 data.** These molecules are derivatives of naphthalene, substituting a nitrile (–CN) group for a hydrogen atom. This substitution produces two distinct isomers, both of which are highly polar, with dipole moments (μ) along the *a* and *b* principal axes: (**A**) 1-CNN: $\mu_a$ = 3.6 debye, $\mu_b$ = 3.0 debye and (**B**) 2-CNN: $\mu_a$ = 5.1 debye, $\mu_b$ = 1.0 debye (6). The spectral stacks are shown relative to the TMC-1 systemic velocity of 5.8 km $s^{-1}$. The weighting process assumed an excitation temperature of $T_{ex}$ = 7 K.

DR2 のデータに matched filtering を適用

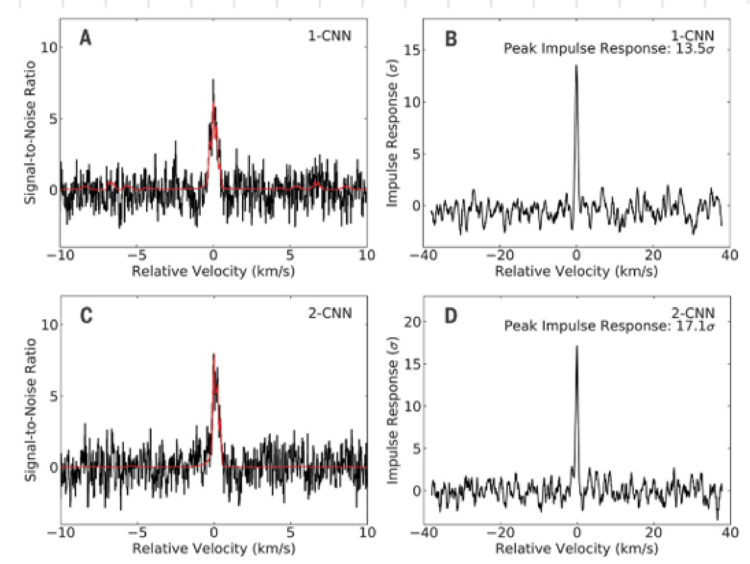



**Fig. 3. Stacked spectra and impulse responses for the matched filtering analyses of 1-CNN and 2-CNN.** The stacked spectra of (**A**) 1-CNN and (**C**) 2-CNN from the GOTHAM DR2 data are shown in black overlaid with the line profile in red from the MCMC analysis of the DR2 data. The SNR is shown on a per-channel basis. Impulse response functions of the stacked spectra of (**B**) 1-CNN and (**D**) 2-CNN are shown, using the simulated line profiles as matched filters. The peak of the impulse response functions provides a minimum significance for the detections of 13.5σ and 17.1σ, respectively.

DR2 でカバーしている輝線

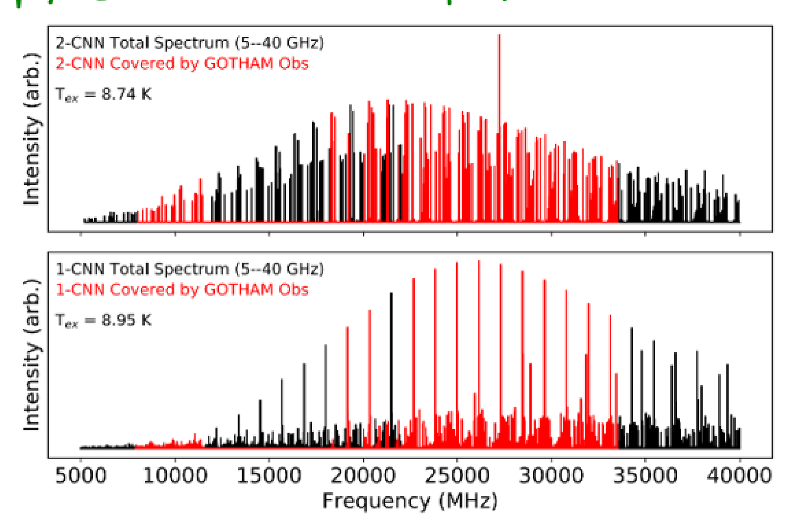



**Figure S3. Coverage of CNN spectra in GOTHAM DR2 data.** Simulations of the spectra of 1-CNN (bottom) and 2-CNN (top) between 5–40 GHz at the derived excitation temperatures in the GOTHAM data, and accounting for beam dilution effects. The lines which are covered by GOTHAM data are shown in red. The line of 2-CNN near 27 GHz is particularly intense due to a fortuitous overlap of individual transitions at that frequency. Detection of that individual signal at 5σ with the GBT would take ∼350–400 hours of dedicated integration time.

DR2 の Spectrum with 1-CNN model spectrum

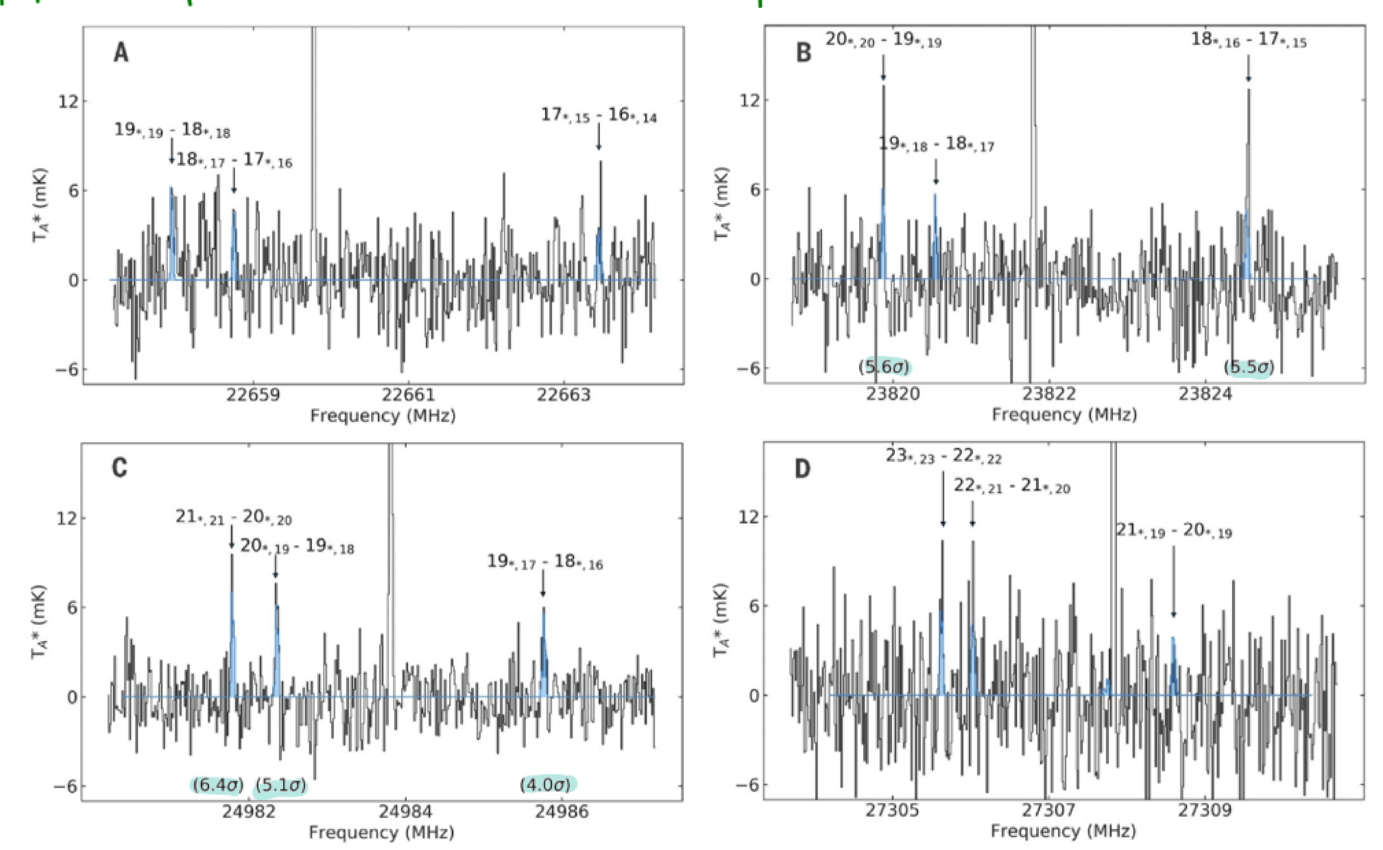



**Fig. 2. GOTHAM DR2 spectra in the vicinity of the strongest predicted 1-CNN transitions.** (**A** to **D**) Observations are shown in black, with simulated spectra of 1-CNN using the parameters derived from our MCMC analysis (table S5) overlaid in blue. The *y* axis is the atmosphere-corrected antenna temperature scale ($T_A$*). The observations have not been adjusted for the systemic velocity of TMC-1 (5.8 km $s^{-1}$). The spectra have been smoothed with a Hanning window to a resolution of 14 kHz for display. The quantum numbers of the transitions, ignoring hyperfine structure, are labeled at the predicted position of each line (arrows). Multiple closely spaced *K*-components of each transition contribute to each line and are denoted by asterisks. Transitions with SNRs ≥4σ are labeled in parentheses beneath the spectra.

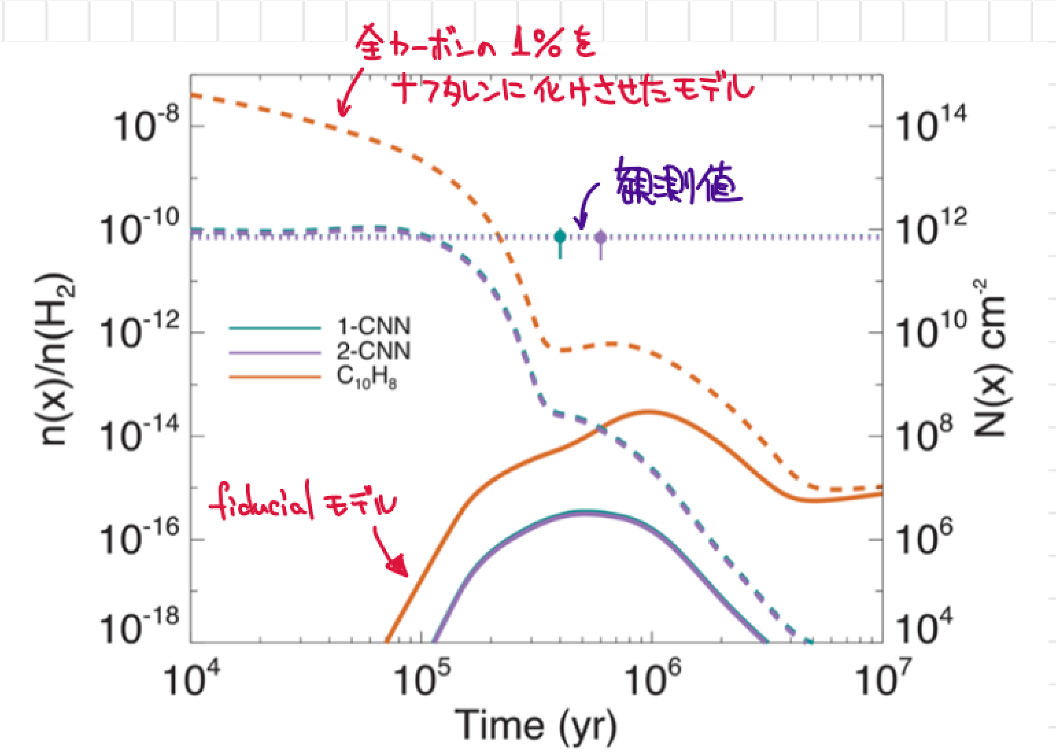



**Fig. 4. Results of the astro-chemical models.** Calculated abundances of naphthalene (orange), 1-CNN (purple), and 2-CNN (teal) under TMC-1 conditions. Data for 1-CNN and 2-CNN overlap. Results are shown for our fiducial model (solid lines) and a model that assumes an initial naphthalene abundance of $n(C_{10}H_8)/n(H_2)$ = $1.0 \times 10^{-7}$ [where $n(x)$ is the volume density of molecule $x$] (dashed lines). The right $y$ axis shows equivalent column densities, assuming $n(H_2) = 10^{22}$ $cm^{-2}$. The circles indicate the values for these species derived from our DR2 observations, with 1σ error bars, at arbitrary times. The dotted horizontal lines show these values extended over the range of the $x$ axis for display.