**Tutorial 2** February 12, 2024

## Exercise 1: Rotational diagram for methanol ($CH_3OH$)

The molecule methanol has been detected in the young low-mass (Class 0) protostar IRAS 16293–2422. In the datafile you can find parameters associated to each detected transition, such as

1. frequencies ($\nu$ in GHz)
2. energies of the upper level ($E_u$ in K)
3. Einstein-A coefficients ($A_{ul}$ in $s^{-1}$)
4. degeneracies ($g_u$)
5. integrated intensities ($W = \int T_{mb}\, d\nu$ in K km $s^{-1}$)
6. 1σ error associated to $W$

The column density of the upper level, $N_u$, is

$$\frac{N_u}{g_u} = C\frac{(\nu[\mathrm{GHz}])^2\ W[\mathrm{K\ km\ s^{-1}}]}{A_{ul}[\mathrm{s^{-1}}]\ g_u},$$

where C=1942.75.

**Q1:** Write a small program (per example in Python), to plot a diagram of $\ln(N_u/g_u)$ as a function of $E_u$.

**Q2:** Fit a linear function to the data and obtain the values for a and b such that $\ln(N_u/g_u) = a + b\, E_u$.

**Q3:** If we consider LTE, we can write

$$\frac{N_u}{g_u} = \frac{N}{Q(T_{\mathrm{rot}})}e^{-E_u/T_{\mathrm{rot}}},$$

where $Q(T_{rot})$ is the partition function. Derive the relation between the parameter b and $T_{rot}$ and calculate $T_{rot}$ using your results from **Q2.**

**Q4:** Derive the relation between the parameter a (from Q2) and $N$. Use the information given in the table below to find the partition function at the rotational temperature found in Q3, $Q(T_{rot})$. Finally derive the total column density $N$.

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| T(K) | 300.0 | 225.0 | 150.0 | 75.0 | 37.5 | 18.75 | 9.375 |
| Q(T) | 6413.573 | 4165.815 | 2267.776 | 801.678 | 283.465 | 100.207 | 35.432 |

## Exercise 2: Making $ArH^+$ in the ISM

$ArH^+$ was the first molecule containing a noble gas element detected in the ISM (Barlow et al. 2013, Science, 342, 134) and it is considered a good tracer of neutral gas.
The most important reactions involved in the formation of $ArH^+$ are

$$\mathrm{Ar} + \mathrm{CR} \xrightarrow{k_1} \mathrm{Ar}^+ + \mathrm{e}^- \tag{1}$$

$$\mathrm{Ar} + \mathrm{H}_2^+ \xrightarrow{k_2} \mathrm{Ar}^+ + \mathrm{H}_2 \tag{2}$$

$$\mathrm{Ar} + \mathrm{H}_3^+ \xrightarrow{k_3} \mathrm{ArH}^+ + \mathrm{H}_2 \tag{3}$$

$$\mathrm{Ar}^+ + \mathrm{e}^- \xrightarrow{k_4} \mathrm{Ar}^+ h\nu \tag{4}$$

$$\mathrm{Ar}^+ + \mathrm{H}_2 \xrightarrow{k_5} \mathrm{ArH}^+ + \mathrm{H} \tag{5}$$

$$\mathrm{ArH}^+ + \mathrm{H}_2 \xrightarrow{k_6} \mathrm{Ar} + \mathrm{H}_3^+ \tag{6}$$

$$\mathrm{ArH}^+ + \mathrm{CO} \xrightarrow{k_7} \mathrm{Ar} + \mathrm{HCO}^+ \tag{7}$$

$$\mathrm{ArH}^+ + \mathrm{O} \xrightarrow{k_8} \mathrm{Ar} + \mathrm{OH}^+ \tag{8}$$

$$\mathrm{ArH}^+ + \mathrm{C} \xrightarrow{k_9} \mathrm{Ar} + \mathrm{CH}^+ \tag{9}$$

$$\mathrm{ArH}^+ + \mathrm{e}^- \xrightarrow{k_{10}} \mathrm{Ar} + \mathrm{H} \tag{10}$$

$$\mathrm{ArH}^+ + h\nu \xrightarrow{k_{11}} \mathrm{Ar}^+ + \mathrm{H} \tag{11}$$

**Q1:** Classify each type of reactions above.

**Q2:** Write the ordinary differential equation (ODE) that describes the evolution of $[ArH^+]$ as function of time. (**TIP:** consider only the reactions that create and destroy $ArH^+$)

**Q3:** Among the reactions related to $ArH^+$, the most important according to Schilke et al ( A&A, 566, A29) are the following

$$\mathrm{Ar} + \mathrm{CR} \xrightarrow{k_1} \mathrm{Ar}^+ + \mathrm{e}^-$$

$$\mathrm{Ar}^+ + \mathrm{H}_2 \xrightarrow{k_5} \mathrm{ArH}^+ + \mathrm{H}$$

$$\mathrm{ArH}^+ + \mathrm{H}_2 \xrightarrow{k_6} \mathrm{Ar} + \mathrm{H}_3^+$$

$$\mathrm{ArH}^+ + \mathrm{O} \xrightarrow{k_8} \mathrm{Ar} + \mathrm{OH}^+$$

$$\mathrm{ArH}^+ + h\nu \xrightarrow{k_{11}} \mathrm{Ar}^+ + \mathrm{H}$$

Assuming conditions of steady state (*dn/dt=0)*, derive the following expression for the abundance ratio of $ArH^+$ and Ar in the diffuse ISM,

$$\frac{n(\mathrm{ArH}^+)}{n(\mathrm{Ar})} = \frac{\zeta(Ar)}{k_6 n(\mathrm{H}_2) + k_8 n(\mathrm{O})}$$

where $\zeta(\mathrm{Ar})=k_1$ is the cosmic-ray ionization rate of Ar. (**TIP:** You need the expressions describing the steady-state abundances of both $ArH^+$ and $Ar^+$)

**Q4:** Consider now a diffuse clouds with the following properties

$$\begin{aligned}
k_1 &= 11.4\,\zeta_p(\mathrm{H})\,\mathrm{s}^{-1} \\
k_6 &= 8.0 \times 10^{-10}\,\mathrm{cm}^3\,\mathrm{s}^{-1} \\
k_8 &= 8.0 \times 10^{-10}\,\mathrm{cm}^3\,\mathrm{s}^{-1} \\
\zeta_p(\mathrm{H}) &= 2.0 \times 10^{-16}\,\mathrm{s}^{-1} \\
n(\mathrm{O}) &= 2.9 \times 10^{-4}\,n_\mathrm{H} \\
n(\mathrm{Ar}) &= 3.2 \times 10^{-6}\,n_\mathrm{H}
\end{aligned}$$

a) Write an expression that tells how the abundance of $ArH^+$ changes as a function of the logarithmic molecular abundance of $H_2$ that is $[H_2]=\log_{10}(2n(H_2)/nH)$.
b) Evaluate how $[ArH^+]$ changes for the following values of $\log_{10}(2n(H_2)/nH)$ => -1.0, -2.5, -2.5, -4.0.
c) Make a plot of how $[ArH^+]$ changes as function of $\log_{10}(2n(H_2)/nH)$. How can we conclude that $ArH^+$ is a good tracer of atomic gas? (**TIP:** density is key)