Solutions 3: CH_3OH rotation diagram

If you have problems writing the code necessary to solve the exercises, I can provide you with an example *Python* script.

a. You should obtain a plot similar to Fig. 1.

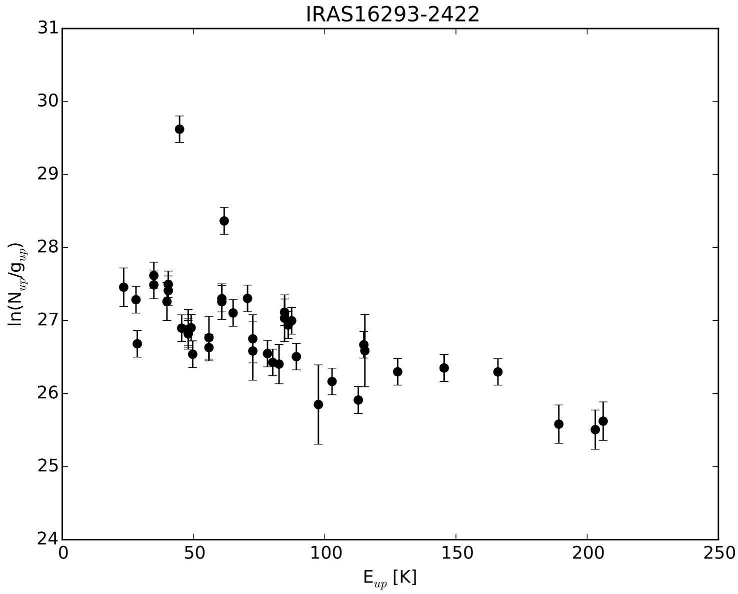

Figure 1: Rotation diagram for CH_3OH in IRAS16293–2422

b. `curve fit` yields: $a = 27.7253 \pm 0.07077$ and $b = -0.0105 \pm 0.00079$.

c.

$$\frac{N_u}{g_u} = \frac{N}{Q(T_{\rm rot})} e^{-E_u/T_{\rm rot}} \tag{1}$$

$$\Rightarrow \ln\left(\frac{N_u}{g_u}\right) = \ln\left(\frac{N}{Q(T_{\rm rot})} e^{-E_u/T_{\rm rot}}\right) \tag{2}$$

$$= \ln\left(\frac{N}{Q(T_{\rm rot})}\right) - \frac{E_u}{T_{\rm rot}} \tag{3}$$

Now set: $\ln\left(\frac{N_u}{g_u}\right) = a + b\ E_u$

Then $b = -\frac{1}{T_{\rm rot}} \Rightarrow T_{\rm rot} = -\frac{1}{b}$
From (b), $b = -0.0105 \pm 0.00079$, hence $T_{\rm rot} = 95 \pm 7$ K.

d. Similarly, $a = \ln\left(\frac{N}{Q(T_{\rm rot})}\right) \Rightarrow N = Q(T_{\rm rot})\ e^a$.
Interpolating the data for Q at 95 K using `interp1d` in log space yields $Q(T_{\rm rot}) = 1057.86$. Hence $N = 1057.86 \times e^{27.7253} = 1.16 \times 10^{15}$ cm^{-2}, and $\Delta N = 1057.86 \times e^{27.7253} \times 0.07077 = 0.08 \times 10^{15}$ cm^{-2}. So $N = 1.16 \pm 0.08 \times 10^{15}$ cm^{-2}.