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Sensitivity of microwave and FIR spectra to variation of fundamental constants

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Abstract. We estimate sensitivity coefficients to variation of the fine-structure constant α and electron-to-proton mass ratio μ for microwave Λ-type transitions in CH molecule and for inversion-rotational transitions in partly deuterated ammonia NH_2D. Sensitivity coefficients for these systems are large and strongly depend on the quantum numbers of the transition. This can be used for the search for possible variation of α and μ.

Key words. ISM: molecules – cosmological parameters

1. Introduction

Discrete microwave spectra of molecules are often used for astrophysical studies of possible variation of the fine structure constant $\alpha = e^2/(\hbar c)$, the electron-to-proton mass ratio $\mu = m_e/m_p$, and the nuclear g-factor g_n. Darling (2003) and Chengalur & Kanekar (2003) pointed out that 18 cm Λ-doublet line of OH molecule has high sensitivity to variation of α and μ. van Veldhoven et al. (2004) have shown that inversion transitions in fully deuterated ammonia $^{15}ND_3$ have high sensitivity to μ-variation, $Q_\mu = 5.6$. According to Flambaum & Kozlov (2007), the inversion transition in non-deuterated ammonia has a slightly smaller sensitivity, $Q_\mu = 4.5$. Note that molecular rotational lines have sensitivity $Q_\mu = 1.0$. Because of that, possible variation of constants would lead to apparent velocity offsets between Λ-doublet OH line, or ammonia inversion line on one hand and rotational molecular lines, originated from the same gas clouds, on the other hand. This method was used by Kanekar et al. (2005); Flambaum & Kozlov (2007); Murphy et al. (2008); Henkel et al. (2009) to establish very stringent limits on α- and μ-variation over cosmological timescale $\sim 10^{10}$ years.

Recently ammonia method was applied by Levshakov et al. (2008a) and Levshakov et al. (2009) to dense prestellar molecular clouds in the Milky Way. These observations provide a bound of a maximum velocity offset between ammonia and other molecules at the level of $|\Delta V| \leq 28$ m/s. This bound corresponds to $|\Delta\mu/\mu| \leq 3 \times 10^{-8}$, which is two orders of magnitude more sensitive than extragalactic constraints cited above. Taken at face value the measured ΔV shows positive shifts between the

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line centers of NH_3 and other molecules and suggests a real offset $\Delta\mu/\mu = (2.2 \pm 0.4_{\rm stat} \pm 0.3_{\rm sys}) \times 10^{-8}$, see Levshakov et al. (2009).

One of the main possible sources of the systematic errors in such observations is the Doppler noise, i.e. stochastic velocity offsets between different species caused by different spatial distributions of molecules in the gas clouds (see discussions by Kanekar et al. (2005) and Levshakov et al. (2008b)). Because of that it is preferable to use lines with different sensitivity to variation of fundamental constants of the same species. Kanekar & Chengalur (2004) and Kozlov (2009) showed that sensitivity coefficients for Λ-doublet spectra of OH molecule strongly depend on quantum numbers. In this paper we focus on the CH molecule and on partly deuterated ammonia NH_2D. The former is similar to OH and has Λ-doublet spectrum, which is highly sensitive to variation of α and μ. For the latter the rotational and inversion degrees of freedom are strongly mixed due to the broken symmetry. This leads to a significant variation of the sensitivity of different microwave transitions to μ-variarion. Note that microwave spectra of CH and NH_2D from the interstellar medium were detected by several groups (see, for example, Rydbeck et al. (1974); Ziurys & Turner (1985); Olberg et al. (1985); Roueff et al. (2005); Lis et al. (2008), and references therein).

2. Sensitivity coefficients

Let us define dimensionless sensitivity coefficients to the variation of fundamental constants so that:

$$\frac{\delta\omega}{\omega} = Q_\alpha\frac{\delta\alpha}{\alpha} + Q_\mu\frac{\delta\mu}{\mu} + Q_g\frac{\delta g_{\rm n}}{g_{\rm n}}\,. \quad (1)$$

These coefficients Q_i are most relevant in astrophysics, where lines are Doppler broadened and linewidth $\Gamma \approx \Gamma_D = \omega \times \delta V/c$, where δV is the velocity distribution width and c is the speed of light. Frequency shift (1) leads to the change in the apparent redshifts of individual lines. The difference in the redshifts of two lines is given by:

$$\frac{z_i - z_j}{1+z} = -\frac{\delta\mathcal{F}}{\mathcal{F}}\,, \quad \mathcal{F} \equiv \alpha^{\Delta Q_\alpha}\mu^{\Delta Q_\mu}g_{\rm n}^{\Delta Q_g}\,. \quad (2)$$

where z is the average redshift of both lines and $\Delta Q_\alpha = Q_{\alpha,i} - Q_{\alpha,j}$, etc. The typical values of δV for extragalactic spectra are about few km/s. This determines the accuracy of the redshift measurements on the order of $\delta z = 10^{-5} - 10^{-6}$, practically independent on the transition frequency. For gas clouds in the Milky Way the accuracy can be two orders of magnitude higher, $\delta z = 10^{-7} - 10^{-8}$. In both cases *the sensitivity of astrophysical spectra to variations of fundamental constants directly depends on* ΔQ_i.

In the optical range the sensitivity coefficients are typically on the order of $10^{-2} - 10^{-3}$, while in the microwave and far infrared frequency regions $Q_i \sim 1$. However, Eq. (2) shows, that we need lines with *different* sensitivities. It is well known that for rotational transitions $Q_\mu = 1.0$, whereas for vibrational transitions $Q_\mu = 0.5$. For both of them $|Q_\alpha| \ll 1$ and $|Q_g| \ll 1$. Inversion transition in NH_3 has $Q_\mu = 4.5$. In the microwave region one can also observe hyperfine transitions ($Q_\alpha = 2$, $Q_\mu = 1$, $Q_g = 1$) and Λ-doublet transitions, where Q_α and Q_μ strongly depend on quantum numbers and can be very large. This makes observations in microwave and far infrared wavelength regions potentially more sensitive to variations of fundamental constants, as compared to optical observations. Because of the lower sensitivity, systematic effects in the optical region are significantly larger Griest et al. (2009).

Λ-doublet transitions in CH In light diatomic molecules, like CH and OH, the electron spin **S** is weekly coupled to the molecular axis due to the spin-orbit interaction, which scales as α^2. As rotational energy (which scales as μ) grows with rotational quantum number J, the spin **S** gradually decouples from the axis. This decoupling strongly affects frequencies of the Λ-doublet transitions and respective coefficients Q_α and Q_μ.

Quantitatively this effect can be described by the effective Hamiltonian suggested by

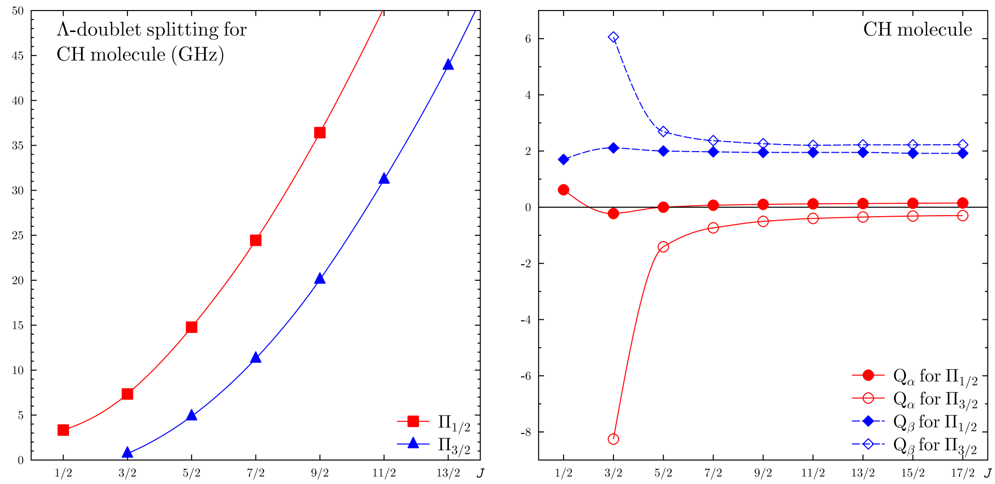

Fig. 1. Frequencies (left panel) and sensitivity coefficients (right panel) of the Λ-transitions for the ground multiplet $^2\Pi_{1/2}$ and $^2\Pi_{3/2}$ in CH molecule.

Meerts & Dymanus (1972). Results of the diagonalization of this Hamiltonian for CH molecule are presented in Fig. 1. We see that first line of the $^2\Pi_{3/2}$ state (Λ = 42 cm) has highest sensitivities Q_α and Q_μ, while the first line of the $^2\Pi_{1/2}$ state (Λ = 9.0 cm) has much smaller sensitivities. Both these lines were observed in the interstellar medium by Rydbeck et al. (1974) and Ziurys & Turner (1985).

Partly deuterated ammonia For non-symmetric molecules NH_2D and ND_2H the selection rules are such that purely inversion transitions are not observable. Still, it is useful to estimate sensitivity coefficients for the inversion transitions and after that consider mixed inversion-rotation transitions.

In the WKB approximation the inversion transition frequency is given by the expression Landau & Lifshitz (1977):

$$\omega_{\rm inv} = \frac{\omega_{\rm v}}{\pi} {\rm e}^{-S}\,, \tag{3}$$

where $\omega_{\rm v}$ is the vibrational frequency for the inversion mode and S is the action in the classically forbidden region. Differentiating this expression in respect to the mass ratio μ Flambaum & Kozlov (2007) obtained following expression for sensitivity coefficient:

$$Q_\mu = \frac{1}{2}\left(1 + S + \frac{S}{2}\frac{\omega_{\rm v}}{\Delta U - \frac{1}{2}\omega_{\rm v}}\right), \tag{4}$$

where $\Delta U \equiv U_{\rm max} - U_{\rm min} \approx 2020$ cm^{-1}is the hight of the potential barrier for ammonia.

Now we can use experimental frequencies $\omega_{\rm v}$ and $\omega_{\rm inv}$ for different isotopic variants of ammonia to find S from (3) and estimate Q_μ using (4). This way we get:

$$Q_\mu({\rm NH_2D}) = 4.7, \quad Q_\mu({\rm ND_2H}) = 5.1. \tag{5}$$

For partly deuterated ammonia inversion levels have different ortho-para symmetry. Because of that inversion transitions can be observed only in combination with rotational transitions $\omega_{\rm r}$ with $\Delta J = 1$, $\Delta K_c = 0$. For such a mixed transition,

$$\omega = \omega_{\rm r} \pm \omega_{\rm inv}\,, \tag{6}$$

where the minus sign correspond to the ortho molecule. Then, the sensitivity coefficient is equal to:

$$Q_\mu = \frac{\omega_{\rm r}}{\omega} Q_{{\rm r},\mu} \pm \frac{\omega_{\rm inv}}{\omega} Q_{{\rm inv},\mu}\,, \tag{7}$$

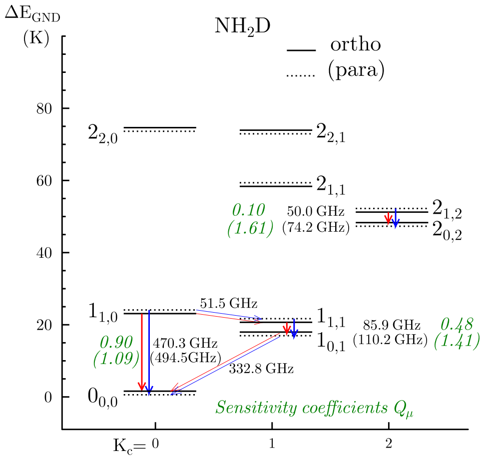

Fig. 2. Lower rotational levels of the molecule NH_2D. Sensitivity coefficients Q_μ are given in italic. For para molecule values are in brackets.

where $Q_{r,\mu} = 1$ and $Q_{inv,\mu}$ is given by Eq. (5). This expression shows that the sensitivity coefficient of the mixed transition is simply a weighted average of those of constituents.

Results of application of Eq. (7) to NH_2D are presented in Fig. 2. Vertical transitions on the plot are mixed and have different sensitivities Q_μ, while inclined transitions with $\Delta K_c = 1$ are purely rotational and have $Q_\mu = 1$. Note that $Q_\alpha = 0$ for all transitions, considered here.

We see that for levels with $J \leq 1$ and excitation energy $\Delta E_{GND} \lesssim 20$ K, we have four vertical and four inclined transitions with maximum $\Delta Q_\mu = 0.93$. The next two vertical transitions for $J = 2$ have even larger sensitivity, $\Delta Q_\mu = 1.51$. Unfortunately, they correspond to excitation energy about 50 K and are difficult to detect.

3. Conclusions

We have shown that there are several new microwave lines with high sensitivity to possible variation of the fundamental constants, which have been observed in the interstellar medium. Moreover, one can use the lines of the same species with different sensitivities and significantly reduce the Doppler noise.

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