

MOLECULES AS ABSOLUTE STANDARDS FOR OPTICAL TELECOMMUNICATION. REQUIREMENTS AND CHARACTERIZATION¹

Jan C. Petersen⁽¹⁾, Jes Henningsen⁽²⁾

⁽¹⁾*Danish Institute of Fundamental Metrology, Matematiktorvet 307, 2800 Lyngby, Denmark, jcp@dfm.dtu.dk*

⁽²⁾ *As ⁽¹⁾ above, but E-mail jh@dfm.dtu.dk*

ABSTRACT

A survey is given of molecules which are potential candidates for wavelength standards over the wavelength range 1510 nm to 1720 nm. Spectra are shown, and general considerations dictating the choice of molecules are outlined.

INTRODUCTION

In early days of coherent optical communication an optical fibre would carry a single communication channel with a carrier wavelength located somewhere in the C-band extending from 1530 to 1565 nm. The reason for choosing a wavelength in this range is that here damping in the fibre goes through a minimum, increasing in the direction of shorter wavelengths due to Rayleigh scattering from imperfections in the fibre, and towards longer wavelengths due to absorption from impurities, mainly OH⁻. With ever increasing demands for bandwidth, ways have been sought to increase the information carrying capacity of a single fibre. One solution is dense wavelength division multiplexing (DWDM) where the useful wavelength range is segmented into channels of fixed width of 100 GHz, corresponding to roughly 0.8 nm. Within the 1530 to 1565 nm range this will allow 44 channels, each of which can in principle transmit a carrier modulated at up to 100 Gbit/s without interfering with neighboring channels. The maximum bit rate used today is 40 Gbit/s, and it may prove advantageous to maximise the capacity by reducing the channel width to 50 GHz or even 25 GHz rather than by increasing the bit rate. However, quite independent of these considerations, a further dramatic increase in capacity is possible by extending the useful wavelength range to include the L-band extending from 1565 to 1625 nm, and instrumentation for this band is rapidly becoming available.

ABSOLUTE WAVELENGTH STANDARDS

In order to fully exploit the information carrying capacity of a DWDM system, it is mandatory that the laser dedicated to a given channel remains close to the channel center during the lifetime of the system. This can be ensured in a variety of ways, but in the end each of the possible solutions will always face the problem: how do we know for sure that the wavelength is what we believe it to be. This brings about the need for absolute wavelength standards [1]. These standards may be used directly for locking the individual lasers to the appropriate wavelengths, or they may be used indirectly by locking the lasers to secondary standards which are periodically checked with instruments calibrated against absolute standards [2,3].

An absolute wavelength standard is a standard which will always remain at the correct wavelength without any need for calibration, whose susceptibility to the environment is minimal and can be accurately quantified, and which can be reproduced anywhere in the world by following a well defined prescription. Wavelength standards in this sense are well known outside the realm of communication. In fact, any length measurement expressed in units of the SI system is ultimately linked to the wavelength of light from red Helium-Neon lasers whose frequencies are locked to hyperfine transitions of the iodine molecule, using saturated absorption in a thermal gas of molecules. From a very large number of international comparisons it is established that such standards have an absolute accuracy of better than about 10 kHz, corresponding to a relative accuracy of 2×10^{-11} . While this serves to illustrate the potential of molecules as the basis of absolute wavelength standards, it is obvious that the requirements in the context of optical communication are much less strict. An accuracy of the order of 0.2 GHz, corresponding to a relative accuracy of 10^{-6} , can probably be considered adequate in relation to channel widths down to 25 GHz.

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CHOICE OF MOLECULES

In Fig.1 we show the optical spectrum bands, designated according to ITU-T SG15, superimposed on Fourier transform spectra for some candidate molecules which together constitute a survey of important concepts of molecular spectroscopy. Also, the spectrum of water has been included for reference, since its strong lines and universal abundance makes it the potentially most important source of interference. However, it is seen that the optical communication bands are favorably located in a window where water absorption is essentially non-existent.

The fundamental absorption bands of infrared active molecules are located at wavelengths longer than about 3000 nm. At shorter wavelengths molecular absorption is associated with overtone or combination bands which owe their existence to anharmonicities in the interatomic potential, and which rapidly tend to become weaker with increasing order. An example of a molecule with very small anharmonicity is CO which has its fundamental and first two overtones located around 5000 nm, 2500 nm, and 1600 nm respectively. The decrease in line strength is almost a factor of 100 from one band to the next, and at a pressure of 100 mbar, this means that the absorption path length required in the three bands for attenuating the radiation by a factor of e^{-1} at the line center of one of the stronger lines will be approximately 0.2 mm, 20 mm, and 2000 mm respectively. At the other extreme we have molecules with large anharmonicities such as C_2H_2 where we find around 1530 nm strong combination bands with e^{-1} attenuation over a path length of just 10 mm.

Since it is not possible on the basis of the fundamental bands to deduce with sufficient accuracy the strength and location of the overtone or combination bands, candidate molecules have to be identified by studying the spectrum in each individual case. It is possible to narrow down the search somewhat by general considerations. The molecule should not have too many atoms. Since the number of normal vibrations for an N-atomic molecule is $3N-6$ ($3N-5$ if the molecule is linear), the number of possible combinations of modes increases dramatically with N. Although this increases the likelihood that there will be bands in the relevant wavelength range, it also means that the spectrum will tend to be very dense, and it may be difficult to ascertain the identity of the lines used for locking. Also, the molecule should not be too heavy. A large moment of inertia means that the rotational lines will be closely spaced, and this may lead to congested spectra which with increasing number of atoms will eventually become unresolved.

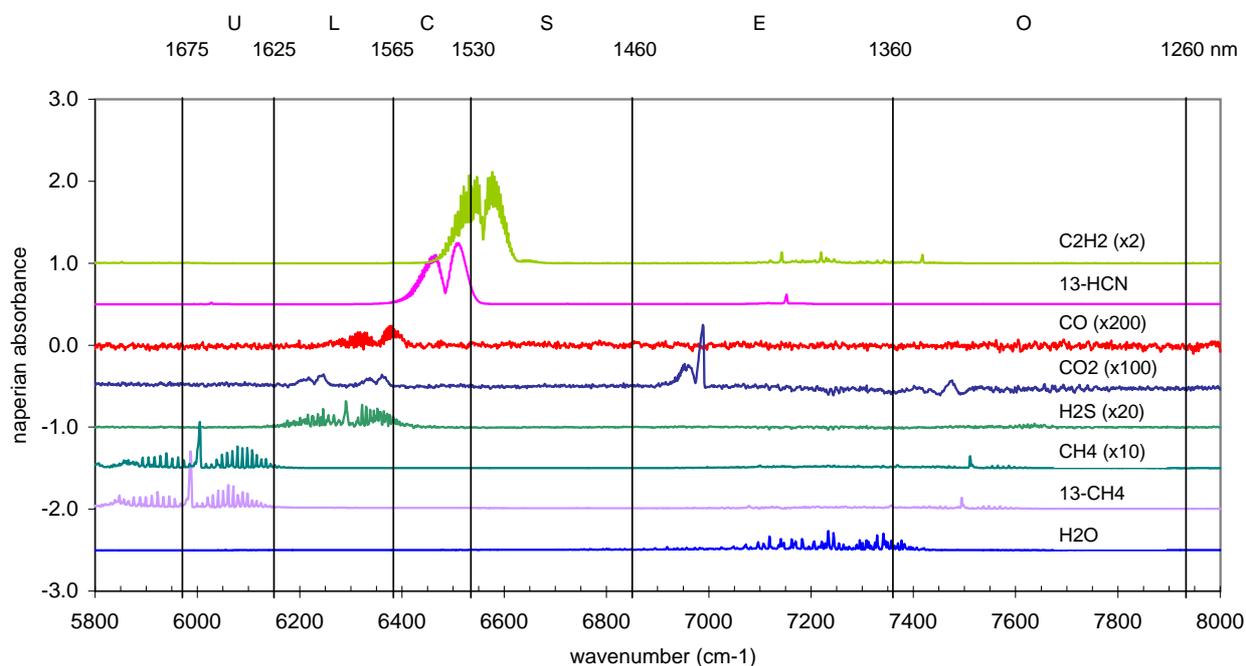


Fig.1 Band designations and Fourier transform spectra for some relevant molecules. All spectra are recorded in 15 cm cells at resolution 2 cm^{-1} . The pressure is 300 mbar except for HCN and H_2O , where it is not known

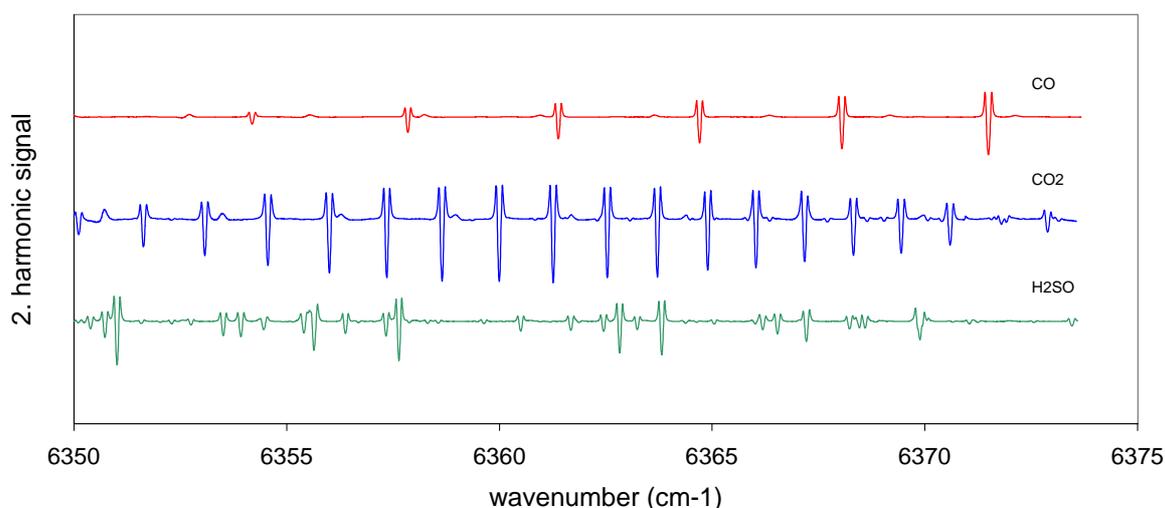


Fig.2 Second derivative spectrum of small segment of Fig.1, recorded with a diode laser spectrometer

The selection rules for electric dipole transitions depend on the structure of the molecule. Linear molecules such as CO, CO₂ and HCN have particularly simple spectra composed of a P-branch and an R-branch where the angular momentum quantum number J decreases or increases by 1 in absorption. The Q-branch corresponding to unchanged J is absent due to the linearity, but appears for nonlinear molecules such as the spherical top molecule CH₄. For asymmetric top molecules such as H₂S and H₂O the selection rules are liberal, leading to a much more complex spectrum. Although the overall band shapes still displays the PQR structure, the details are much more confusing with no apparent regularity as seen in Fig.2. While it is certainly possible to use such molecules, particular attention must be paid to the problem of identifying the lines used for locking.

To increase the probability of finding absorptions at the relevant wavelengths, one may include isotopomers with less abundant isotopes. Fig.1 includes spectra of ¹²CH₄ as well as of ¹³CH₄, and the isotope shift of about 18 cm⁻¹ is clearly visible. At the pressures required it is straightforward to produce permanently sealed absorption cells which will work for many years. Thus, even relatively expensive isotopomers will only represent a modest cost.

The spectra included in Fig.1 are all recorded in 15 cm cells and cover an absorbance range of almost three orders of magnitude. The usefulness of even the weaker bands is evident from Fig.2, where the spectra for CO and CO₂ are recorded in a 125 cm cell. In this context it should be noted that the absorbance as measured in Fourier transform spectroscopy with low resolution does not relate in a simple way to the line strengths of the individual lines. In our case the resolution is 2 cm⁻¹, and from Fig.2 it is evident that for CO₂ and H₂S, where the line separation is smaller than 2 cm⁻¹, the absorbance will always include contributions from a range of lines.

REQUIREMENTS

In a generic setup for a wavelength standard, part of the radiation from the oscillator is transmitted through an absorption cell containing a gas with suitable absorption lines, and the frequency is locked by deriving an error signal from the absorption feature. Radiation transmitted through a cell of length L is attenuated according to the Beer-Lambert law as

$$I(L) = I(0) \exp(-\alpha L)$$

$$\alpha = NSg(\nu-\nu_0)$$

The quantity αL is denoted the naperian absorbance, and the absorption coefficient α is related the line strength S of the selected absorption line, centered at the frequency ν_0 , and the area normalized line shape function $g(\nu-\nu_0)$. N is the number density of molecules in the cell, and may be expressed as $N=p/kT$ where p is the partial pressure of the

absorbing molecular species, k is Boltzmann's constant, and T is the absolute temperature. In principle, the partial pressure becomes identical to the total pressure if the cell contains an isotopically pure molecular species. However, it should be noted that databases such as HITRAN [4], which are structured to facilitate calculations of atmospheric transmission, have chosen to include the natural abundance in the definition of the line strength. Thus, a calculated absorption coefficient based on a line strength from HITRAN will apply to the line as observed in a cell with all isotopomers present in their natural abundance.

For practical purposes, the minimum detectable absorbance may be taken as 10^{-4} , and requiring a signal-to-noise ratio of 100 in order to produce a reliable lock, the absorbance should be larger than 10^{-2} . The maximum cell length L is dictated by practical considerations, and although it is relatively straightforward to achieve many metres of path length in multipass configurations, we shall here assume a maximum practical path length of 1 m. For typical absorption lines this then leads to the requirement that the line strength should be larger than about $5 \cdot 10^{-24}$ cm/mol, the precise value depending on the details of the line profile.

An absorption line used as wavelength standard should have a line width as small as possible. The width of an absorption line is determined by the combined effect of Doppler broadening due to the random thermal motion of the molecules, and collision broadening due to the finite time of flight between their mutual collisions. Collision broadening is proportional to the pressure with coefficients of typically 2-10 MHz/mbar, while Doppler broadening in the 1550 nm range is independent of pressure and in the range 100 to 300 MHz, depending mainly on the mass of the molecule. The area under the absorption profile is proportional to the number density N . With decreasing pressure the amplitude of the line will remain constant while the line width will decrease until it meets the Doppler limit at typically around 100 mbar. Further reduction of the pressure will lead to reduced amplitude at constant width. For optimum performance as wavelength standard the cell should thus be operated slightly above the Doppler limit where collisions do not produce appreciable excess broadening. Since it is straightforward to lock to the line center with an accuracy of 10% of the line width, the required accuracy of better than 0.2 GHz can easily be achieved without resorting to Doppler free techniques at very low pressure.

In general, the line center position will show some dependence on the pressure, and this effect has to be taken into account if maximum accuracy is desired. Very little information is available in the literature, but for the cases studied, the shifts have been linear in pressure with coefficients in the range -0.2 to -0.5 MHz/mbar, usually tending to increase with the angular momentum quantum number of the transition. If the pressure of a sealed cell is assumed to change by less than 10 mbar over its lifetime, the maximum change in wavelength due to pressure shifts will be less than 5 MHz, and hence insignificant.

Conclusion

Molecules are ideally suited as a basis for wavelength standards required in DWDM systems. A number of them have absorption bands which coincide with the communication C- and L-bands, and which are strong enough to enable wavelength locking of laser sources without the use of sophisticated techniques. We present Fourier transform spectra for some of them and state some general considerations which will assist in the search for further candidates.

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