

An Accurate Secondary Frequency Standard from 515-815 nm : Improved Potentials for the B-X system in Molecular Iodine $^{127}\text{I}_2$.

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In a large part of the optical spectrum, extending from the green to the near infrared (500-900 nm), the Iodine Atlas [1] has become a useful tool for absolute frequency calibration. The accuracy of the Doppler-broadened lines is however limited to 30-60 MHz (1σ). In many applications there is a need for a more accurate standard. Indeed, in the past 30 years, approx. 130 hyperfine transitions have been measured with sub-MHz precision, using primary wavelength standards. But these reference lines are spread erratically over the visible spectrum. A more systematic approach was realized by Sansonetti [2], who measured the frequencies of hyperfine lines in a wavelength range from 560 to 656 nm and provided a grid of reference lines, but with gaps of about 2 nm.

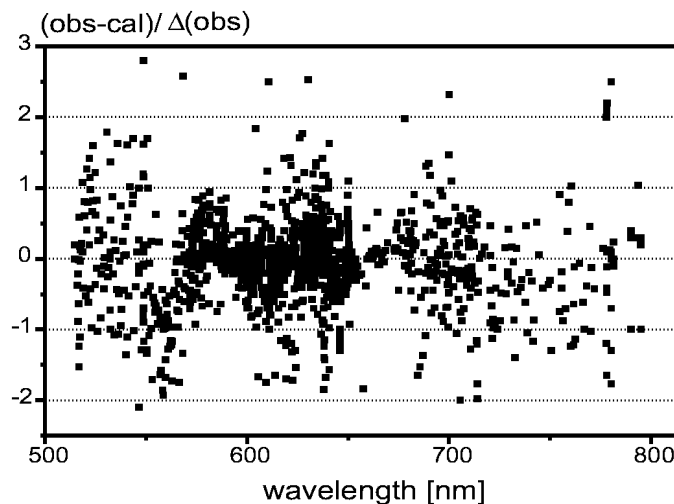
Here we present a substantially denser grid of high precision reference lines in the hyperfine structure of the B-X system of molecular iodine. The absolute frequency of hyperfine components of nearly 600 lines in the range 571 to 655 nm [3, 4] were measured relative to the standard provided by the work of ref. [2] and others. The data are distributed uniformly over 21 different rovibrational bands. The precision of the measured frequencies obtained is about 1 MHz (1σ) over the whole range. With these calibrations using a band by band description with fitted molecular parameters, unmeasured reference lines can be predicted, so that at least 1 transition falls in each interval of 1 cm^{-1} (30 GHz). The precision of this secondary frequency standard in the visible can be transferred to the (X)UV using frequency multiplication of the laser fields.

Moreover, we present a more global model description of the B-X spectrum of the iodine molecule, based on all precisely known hyperfine lines of the three molecular isotopes $^{127}\text{I}^{127}\text{I}$, $^{127}\text{I}^{129}\text{I}$ and $^{129}\text{I}^{129}\text{I}$ in the wavelength range from 515 to 815 nm.

The data on the hyperfine structure from the literature together with our own recent systematic measurements in the near infrared (NIR) [5, 6, 7] were used to establish precise model descriptions for the nuclear electric quadrupole, the nuclear spin-rotation and the nuclear spin-spin interactions, which are the relevant ones at the required level of accuracy.

Due to this systematic approach, it was possible to separate the hyperfine interactions of the ground and the excited state. This also allows to parametrize the quantum number dependencies in a more appropriate manner than was possible before.

All data on absolute frequency calibrations presently available from literature, our calibrations in the NIR ([8] and references therein) and the large body of lines discussed above were included in a model description of the rovibrational level structure of each electronic state based on fitted potentials and their eigenvalues. For the determination of the 'pure' rovibrational frequencies, the frequency shifts due to hyperfine structure were subtracted applying the aforementioned parametrizations of the hyperfine interaction parameters. A plot of the residuals (obs-cal) of the fit normalized by the uncertainty of the measurement $\Delta(\text{obs})$ is shown in the figure:



It will be shown that nonadiabatic contributions due to weak admixture of other electronic states are important for a good fit. This approach provides a high precision model description for the level energies.

A computer program [9] was set up combining the above results for the description of rovibrational and hyperfine structure. It is able to calculate and to display a requested spectral region of the iodine spectrum including the hyperfine structure and intensities. The improved level of accuracy of less than 12 MHz (1σ) for the range from 515 to 815 nm and of less than 5 MHz (1σ) for the range from 560 to 656 nm should make it a useful tool. Even better accuracy of 1 MHz (1σ) is achieved in the range from 571 to 655 nm using the band by band description [3, 4], and in the NIR from 776 to 815 nm a 150 kHz accuracy is available.

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