measurements, single-photon timing, streak camera measurements, fluorescence upconversion, and optical Kerr gating). The paper starts with a brief description of the basic principles for time and frequency domain fluorescence spectroscopy. The fundamental equations are given, and recommendations for adequate use are emphasized. The up-to-date, commonly-employed excitation sources and photodetectors are described in detail. The analysis of time-resolved fluorescence data is discussed. Attention is paid to possible artifacts and remedies are presented on how to avoid them or to account for them. Finally, fluorescence lifetime standards for the nanosecond and picosecond timescales are collected. This report was prepared in the framework of IUPAC project 2004-021-1-300. 

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The NPU format for clinical laboratory science reports regarding properties, units, and symbols


The terminology of NPU (nomenclature for properties and units) aims at describing properties examined in clinical laboratories for a patient. It was originally jointly approved in 1966 by IUPAC and by the International Federation of Clinical Chemistry (IFCC) and covers multiple disciplines in the field of clinical laboratory sciences, including clinical allergology, clinical chemistry, clinical haematology, clinical immunology and blood banking, clinical microbiology, clinical pharmacology, molecular biology and genetics, reproduction and fertility, thrombosis and haemostasis, and toxicology. The NPU terminology adheres to international standards of metrology and of terminology, in particular the International System of Quantities (ISQ) and International System of Units (SI), the International Vocabulary of Metrology (VIM), and also to ‘An outline for a vocabulary of nominal properties and examinations – basic and general concepts and associated terms,’ recently prepared on behalf of the IFCC-IUPAC Committee-Subcommittee on Nomenclature for Properties and Units.

The present document recalls the definitions of the concepts used to express a property of a patient, regarded as a system. The aim is to promote by this comprehensive summary the proper NPU terminology for reliable exchange of patient examination data. The use of this syntax and of SI units enables the translation of these descriptions into other languages without loss of meaning or accuracy. The NPU format is also well adapted for comparative and epidemiological studies.

More information will be found in the upcoming 2nd edition of the Compendium of Terminology and Nomenclature of Properties in Clinical Laboratory Sciences, the IUPAC and IFCC ‘Silver Book’, and in the recently published ‘Properties and units in the clinical...
Spectroscopy of Water

reviewed by Jonathan Tennyson and Attila G. Császár

Scientific questions demand scientific explanations. Our understanding of the greenhouse effect on earth and of the radiation balance on planets raises a number of complex scientific questions. These questions and the answers are often discussed in the public media as if the background knowledge was complete, while this is not the case. Most significantly, many of the questions lead to unexplored or at least understudied territories of high-resolution molecular spectroscopy. In order to move beyond the state-of-the-art in our understanding of the greenhouse effect and the radiative balance of atmospheres of planets, the way the water molecule absorbs and emits light must be understood all the way from the microwave to the visible and ultraviolet regions. This important challenge led the IUPAC Physical and Biophysical Chemistry Division to sponsor the activities of two task groups: first, “A database of water transitions from experiment and theory,” (project 2004-035-1-100) and then, “Intensities and line shapes in high-resolution spectra of water isotopologues from experiment and theory,” (project 2011-022-2-100). The two task groups have recently completed their work and reported their results and recommendations [1,2], some of which are reviewed briefly below.

Water vapor is both the major absorber of incoming sunlight in a clear sky and also the dominant greenhouse gas in our atmosphere. As a result, a trace species, isotopically-substituted water, H$_2$O, is already the fifth biggest absorber of sunlight in the Earth’s atmosphere.

From the theoretical point of view, water is also an interesting molecule. It is a rather non-rigid system meaning that its vibrational modes can absorb light and be excited by multiple quanta. It is also a light, asymmetric rotor which means that the vibrational bands have a very open structure. The result of this is that strong absorption by water bands is found throughout the infrared and, increasingly weakly, throughout the visible region of the electromagnetic spectrum. Indeed, recent atmospheric studies are focusing on vibration-rotation absorption in the near-ultraviolet which means transitions involving the jumps of 8 or 9 vibrational quanta.

The first task group used a methodology co-developed by the two co-authors to create an information system of refined empirical rotation-vibration energy levels, and hence transition frequencies, for altogether nine water isotopologues. The MARVEL (measured active rotation-vibration energy levels) procedure for doing this was refined significantly during the course of the IUPAC-sponsored research efforts. The resulting MARVEL procedure is both robust and computationally efficient; it is now being applied to a number of other molecules of scientific and practical interest.

The energy levels and the comprehensive sets of transition frequencies generated by the TG for the water isotopologues are being used for a variety of applications. For example, a complete set of lines has been generated for H$_2$^{18}O and H$_2$^{17}O by combining MARVEL-based transition frequencies with transition probabilities computed using high-accuracy, first-principles quantum chemistry. These results are incorporated in the latest edition of the canonical HITRAN database, which is extensively used for atmospheric modeling. The energy levels are also being used to update the so-called steam tables, which tabulate the temperature-dependent thermochemical properties of water.

The second task group was formed to answer the question of how to represent the precise shape of a spectroscopic line observed under high resolution, a property which depends considerably on the environment in which the system is being observed. The so-called Voigt profile, a convolution of the Doppler profile, to represent thermal motions, and a Lorentzian, to model collisional effects, has been widely used. But the Voigt profile is known to be inadequate for precise modeling work, leading, for example, to W-shaped systematic residues in atmospheric water spectra. Going beyond the Voigt profile requires the inclusion of a variety of rather subtle collisional effects. Consideration of these effects has led to the proposal of a whole zoo of different possible models and functional forms to represent the line shape. It was clear that databases and modelers require a clear recommendation of a single beyond-Voigt line profile. The TG-recommended profile, which we named the Hartmann-Tran Profile (HTP), has the advantage that it captures the complex physics involved in collisional line-broadening with a functional form that can easily, and rapidly, be evaluated. Furthermore, the HTP profile reduces to other, simpler profiles including Voigt in the absence of a full parameter set.