PROJECT OF DISTRIBUTED INFORMATIONAL SYSTEM ON MOLECULAR SPECTROSCOPY

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The work on creation of information resources on atmospheric spectroscopy has been conducted at the Institute of Atmospheric Optics since the eighties. With the advent of personal computers at the beginning of the nineties, there appeared information systems operating at the client’s side. Appearance of the Internet technologies has allowed one more step in the development of the information system for molecular spectroscopy. The information resource available on the Internet (http://spectra.iao.ru) [1] was based on the known spectroscopic databases HITRAN and GEISA. The majority of the problems to be solved by means of the information-computational system (ICS) were related to database search. Scientific publications containing the *ab initio* calculation of the H_2O line position and intensities [2] have led to significant growth of the extensional domain. Data amount for water spectrum, for example, has risen a thousand times (about 3×10^8 spectral lines). Publication of calculation results on the Internet in files has promoted semantic analysis of the data accumulated on various Internet sites.

Some information systems nevertheless use the data format introduced in the HITRAN database. Restrictions imposed by the HITRAN data structure on the information systems being currently developed required modifications to the intensional domain (molecular spectroscopy). To solve this problem, we have chosen new data and information handling tools appeared in the late nineties and based on semantic web recommendations.

The information system for molecular spectroscopy that we have developed and are now implementing is a part of a web portal (http://atmos.iao.ru). While creating the information system, a series of problems were to be solved. This report is devoted to the description of three of them:

1. extension of traditional data format and its organization on the basis of spectral data input within the frames of metadata determined in the XML system.
2. creation of ontology on molecular spectroscopy.
3. metadata exchange in distributed information system on molecular spectroscopy.

[1]. Babikov Yu.L., et al., Internet-collection on molecular spectroscopy, Proceedings of the Third All-Russian Conference on Digital Libraries, Petrozavodsk, 2001, P. 183-187.
[2]. D.W. Schwenke and H. Partridge, Convergence testing of the analytic representation of an *ab initio* dipol moment function for water: Improved fitting yields improved intensities, J.Chem.Phys., Vol.113, No.16, P. 6592-6597, 2000.