Distributed information system on molecular spectroscopy

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First publications

Block of mathematical models. Programs library
- System of analytical calculations
- Formulas bank
- Molecular constants archive

Information synthesis and reliability evaluation
- Software for statistical analysis
- Inverse Problems Block

General management system, Interactive mode, management and diagnostics
- Graphical presentation analysis
- Serving programs

Recommended spectral line parameters database
- Spectroscopic constants archive
- Experimental spectral line parameters database
- Experiment descriptor archive
- Experimental data input system

Information systems for atmospheric molecular spectroscopy
Web approach

Molecular Constants Archive
Spectroscopic Constants Archive
Gas Mixtures Archive
Recommended Spectral line Parameters Database
Calculated Spectral line Parameters Database
Cross-sections Database
Energy Levels and Transitions of Ozone Database

Spectroscopy of Atmospheric Gases
http://spectra.iao.ru
Spectroscopy & Molecular Properties of Ozone
http://smpo.iao.ru

Disadvantages of the previous generation of information systems

1. There are data in these information systems, but there are no their properties. The absence of the properties does not allows one make decision on validity of the data. In fact user of these information systems has one criteria of data validity – his own faith.

2. These information systems have no information resources oriented on automatic semantic processing.

3. These information systems have no facilities for automatic exchange of their data with the other information systems.
Distributed Information System for Atmospheric Molecular Spectroscopy

Semantic Web approach

- Logical theory of molecular spectroscopy tasks’ solutions properties
- Inference engine
- Logical consistency check
- Protégé interface
  - Knowledge layer
  - Web-service for the formation of an ontology of molecular spectroscopy tasks’ solutions properties
- Data and computations layer
  - Web-service of publications data base synchronization
  - Web-service for the formation of a homogeneous set of inverse and direct tasks solutions properties in a distributed system
- Interfaces
  - Data Node Applications
  - Web-services
  - Distributed Information System for Atmospheric Molecular Spectroscopy
Horizontal Hierarchy of Domains

Climate and weather
TSU, Novosibirsk

Atmospheric Chemistry
Moscow

Atmospheric Radiation
Volgograd, Ekaterinburg

Atmospheric spectroscopy
Nizhnii Novgorod, Sankt Petersburg

DIS W@DIS (H₂O),
DIS CaD@DIS (CO₂),
green-house gases

Substance
Web-service of publications data base synchronization

Distributed ICS on molecular spectroscopy

Distributed ICS on atmospheric radiation

ICS on climate  (TSU, Institute of Computational Technologies SB RAS)
Web-service for the formation of a homogeneous set of inverse and direct problems solution’s properties in a distributed information system

Schema of molecular spectroscopy applied ontology relations