Systematization of Published Spectral Data on N_2O and OCS molecules and Isotopologues

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The goal of this work is to collect publications on N_2O and OCS and their isotopologues, provide spectral data import describing results obtained from measured and calculated data processing, develop software for data alignment relating to solutions to four spectroscopic tasks and automatically build information resources and ontologies for quantitative spectroscopy.

The work was performed in 3 stages. In the first place, more than 420 publications on N_2O and OCS and their isotopologues were collected and systematized for 1931-2012, and quantum number notation was selected for building a relational database. In the second place, data import in W@DIS was performed and an ontology was built automatically to assess the imported data quality. Associated with each of 287 imported datasets are the data properties of these sets generated automatically in accordance with a given metadata set. The metadata are intended for solving the task of search for information resources in accordance with a number of criteria. A key criterion is the validity of collected values of physical quantities. Imported data and generated properties of these data form an information source pertaining to the solution of one or another spectroscopic task. In the third place, work is underway to align the data.

The collected data enable trust in expert data containing 33074 transitions to be assessed in accordance with a publishing criterion [1]. Published transitions of N_2O and OCS molecules and their associated knowledge base are available in the W@DIS via Internet (http://wadis.saga.iao.ru/n2o).