Ontology-Based Content Trust Support of Expert Information Resources in Quantitative Spectroscopy

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Abstract. An approach to assessing the content trust of information resources based on a publishing criterion has been developed and applied to several tens of spectroscopic expert datasets. The results represented as an OWL-ontology are shown to be accessible to programmable agents. The assessments enable the amount of measured and calculated trusted and distrusted data for spectroscopic quantities and ranges of their change in expert datasets to be determined. Building knowledge bases of this kind at virtual data centers intended for data-intensive science will provide realization of an automatic selection of spectroscopic information resources exhibiting a high degree of trust.

Keywords: Trust, OWL Ontology, Quantitative Spectroscopy

1 Introduction

Spectral line parameters are used in different subject domains: remote sensing, climate studies, astronomy, etc. Data of this type are in great demand, and the number of expert data providers is increasing progressively [10, 5, 7, 4, 18, 17, 26]. More stringent requirements are imposed on data quality, including data accuracy, completeness, validity, trust and resource consistency. For a wide range of applied tasks, currently available expert data are shown to be inadequate to meet the requirements, because they contain outdated, distrusted or incomplete information [14].

Quantitative spectroscopy is a data-intensive science dealing with information collected over the course of ninety years, but it is in the last six years when semantic technologies have been used in this domain. Processing of long-term data, linking together results of investigations retrieved from different publications and aligning these data provide an adequate valid data exchange and access to trusted information resources. In quantitative spectroscopy, this implies a low threshold of the spectral knowledge transfer to applied sciences. The low threshold has its practical benefits because investigators engaged in applied sciences lack sufficient knowledge to understand all the relevant aspects of expert data. The choice made by researchers is most often based on trust rather than on checks of data for validity. This is why investigators need information on validity and trust criteria to be satisfied by expert data.

We have assessed expert data content trust and presented the results obtained as an OWL ontology. The ontology is intended for two types of users 1) researchers using the ontology to assess trust in expert resources for certain purposes and 2) programmable agents making decisions on the selection of the parts of similar expert data that deserve the highest degree of trust in this ontology. The assessment of trust is part of a solution to the task of assessment of trust in the content of expert information resources. This task is broken down into four subtasks: (1) building multisets of values of physical quantities available in primary data sources, (2) alignment of values of physical quantities, (3) definition of quantitative restrictions found in a publishing criterion in different ranges of change of physical quantities and (4) decomposition of expert data. Solutions to these subtasks are presented in W@DIS[1] in the form of trusted consistent information resources for programmable agents. A publishing criterion specifies ranges of change of the physical quantity under study and permissible difference in the values of this quantity between published primary and expert data in these ranges.

A rigorous solution to the task of assessment of trust in expert resources of an information system will take a complete set of valid aligned published values of physical quantities. As of now, datasets of this type have been published solely for the ground electron state of isotopologues of the water molecule [23–25], hydrogen sulfide [16] and carbon monoxide [22].

The ontology under consideration has been built using a standard methodological approach wherein existing models for data and metadata for the subject domains being studied are assimilated into newly developed ontologies. The models are examined and extended (or reduced) to provide the required granulation level inherent to the subject domain in question.

2 A simplified data model for quantitative spectroscopy

Before proceeding to a data model for quantitative spectroscopy, we emphasize the fact that the proposed model does not include all facts relating to this subject domain. However, this is a major part of data applied in different disciplines of interest. Data of this type were obtained both theoretically and experimentally. This division into theory and experiment makes it possible to classify data measurements and predictions.

[1] Information system W@DIS, `http://wadis.saga.iao.ru`

The data associated with measurements or computations from one publication are referred to as a primary data source. The primary experimental and theoretical data are interrelated. This is due to the fact that the values of properties of transitions and states are not all measured. Among these are quantum numbers whose values are found only in the framework of mathematical models of molecules. Composite data are also used in spectroscopy in addition to primary data. Two types of composite data are of importance from the standpoint of applications: reference and expert data. The former are calculated by means of a multiset of measured data, whereas the latter constitute a set of consistent calculated, measured and reference data. The data layer includes three types of datasets. Arrows pointing from applications to datasets indicate data-producing applications, whereas arrows pointing from datasets to applications imply applications using the data.

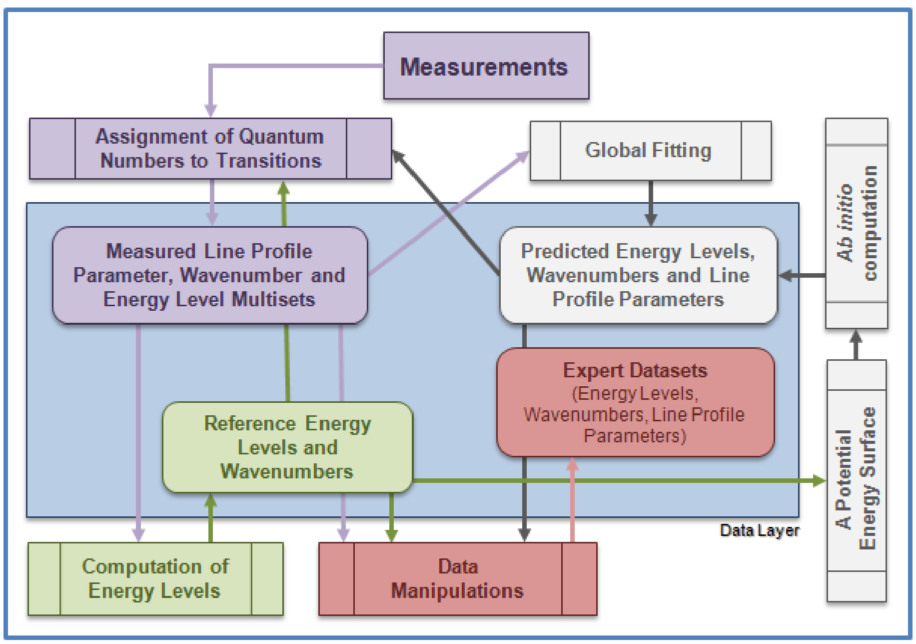

Fig. 1. Schematic representation of the relationship between applications and their associated input and output data

Figure 1 demonstrates four groups of data and their association with experiment and calculations. These groups are related to six tasks of quantitative spectroscopy and a task of building expert datasets. The quality of data included in three datasets (a multiset of measured transitions and predicted and reference transitions) can be assessed by formal criteria alone (validity), whereas expert datasets should be tested according to trust criteria, because formal methods for building such datasets remain to be developed. The computational method used to formalize data manipulation for construction of expert datasets was described in [13]. Since spectral information resources in the form of expert datasets are in great demand, it is the expert data which are the focus of attention in this paper. There are two reasons for that. First, expert data are acquired for applied subject domains the number of which is over several tens. Notably, the data intended for one or another subject domain must satisfy certain requirements on their quality. Second, expert data are acquired from informal manipulations in which case professional skills and preferences of experts play an important role. This is why different forms of publishing criteria appear to be a useful tool for assessing the expert data quality.

3 Content quality of information resources for quantitative spectroscopy

According to the Semantic Web (SW) approach, the content of information resources involves data, information and knowledge. These terms are treated in the literature in an apparently contradictory way. We will follow the terminology being created within the SW approach and employ the terms “data”, “linked data” and “ontology” to mean data, information and knowledge, respectively. In the SW approach, the terminological interpretation of data, information and knowledge is closely related to the semantics of formal languages (XML, RDF and OWL). Moreover, the terms “data layer”, “information layer” and “knowledge layer” were introduced in e-Science [20] to describe the infrastructure of information resources. In particular, W@DIS whose information resources are dealt with in this work has a three-layer architecture of this type [1].

The object of this paper is to assess the data extension quality. The emphasis is on the data extension trust and validity. Validity is taken to mean that the data satisfy formal constraints derived from mathematical molecular models and conditions for consistency of identical canonical parts of spectral data sources. The publishing criterion is applied to canonical parts of data sources to identify distrusted values of physical quantities. These may be unpublished data or data unaligned with primary data. Students of applied subject domains using expert spectral data would have to check distrusted data according to criteria employed in the relevant subject domain.

There are different interpretations of trust in the literature [6, 3, 15, 21, 2, 9] and, accordingly, a rich variety of trust criteria are suggested. Common to the majority of interpretations is the fact that trust criteria are partially formalized constraints. The publishing criterion formulated in [14] refers to a set of criteria for assessing the content trust of information resources [2, 9]. The publishing criterion enables the distributed part of the content to be identified. The use of the publishing criterion assumes that a check is made of values of identical spectral line parameters in the expert dataset for a fit to published primary data within a specified accuracy.

Early in the development of the SW approach, the notion of trust has come to occupy the central place. Trust implies that Internet users will get access to valid information sources characterized by a high degree of trust. Dealing with information resources, researchers can check the resources of interest for validity within their competence. Moreover, their professional skills and experience allow for making decisions in the case where partially formalized trust criteria are available, whereas the trust assessment is based on resources characterized by an uncertainty. The SW approach is intended not only for a scientific community but for programmable agents capable of solving tasks of this type as well. "In a Semantic Web where content will be reflected in ontologies and axioms, how will a computer decide what sources to trust when they offer contradictory information?" [2]. The question refers to programmable agents.

Along with papers on methods of assessing trust in information resources on the basis of knowledge about providers, developers of agents and relevant technologies, there have been recent publications pertaining to the content trust of resources [2, 9], where 19 factors influencing the content trust were described. The factors can be divided into two groups. One group includes factors independent of social relations or outlook of the researcher: topic (resource trusted within certain domains may be distrusted within others), content trust, alternative resources available, provenance, limited or biased resources, specificity, likelihood, age, deception and regency. The other group includes popularity, authority, recommendations, direct experience, user expertise and ability to make decisions.

Expert data in quantitative spectroscopy satisfy a number of trust factors. These are popularity, authority, recommendations for applied subject domains, several expert groups of providers and absence of deceptive intentions. However, there are factors that cast some doubt upon the correctness (adequacy) of part of the data. The fraction of distrusted data depends to a large extent on a rigorous definition of the area of application of expert data. In most popular resources [10, 18, 17], a small number of physical quantities (vacuum wavenumbers in the case at hand) is not valid, the origin of part of data is not known (as a rule, they are not published), some of distrusted data are of fairly old age, and the user-expert feedback mechanism is not available. The above-listed disadvantages of expert data point to the importance of assessing the expert data trust in quantitative spectroscopy.

4 Content trust of expert resources

The task of assessment of trust in expert resources is as follows. Let a physical quantity PQ describe a state or a transition in a physical system and uniqueness of states or transitions be determined by a factor qn_i. Let there be a set of expert values of the physical quantity $A = \{PQ(p_i, qn_i)\}$, such as an energy level, vacuum wavenumbers or line intensity, where p_i are values of the physical quantity and all values of qn_i are unique. Let $M(p^i_j, qn_j)$ be a multiset of all published measured values of PQ which contains only *valid* values, whereas

$T(p_j^i, qn_j)$ is a multiset of *all published* calculated values of PQ. Here j numbers all pairs (p_j^i, qn_j) of values of physical quantities and their associated quantum numbers. The index i is the number of publication from which the value of the pair (p_j^i, qn_j) was retrieved. The value of $p_j^i (i = 1, \ldots, n)$ for a fixed value of j may vary. Let D_k be a maximum permissible difference between the expert value of a physical quantity and the value of the physical quantity given in a primary data source. Let D_k vary in the range of change of PQ from A by virtue of the fact that measuring instruments operate on different principles. There may be other reasons for specifying part of the range of change of PQ to determine a permissible deviation of expert values of PQ from identical values of PQ from $M(p_j^i, qn_j)$ and $T(p_j^i, qn_j)$ according to the publishing criterion. The task is to find the number of values of PQ from A that satisfy or fail to satisfy the publishing criterion ($E(p_j^i, qn_j)$ and $F(p_j^i, qn_j)$, respectively) and determine the ranges of change of (E) and (F) in each of the ranges of change of PQ characterized by D_k with the proviso that the procedure used to obtain expert values is implicit and uncontrollable.

Examined below are two tasks: (1) formulation of quantitative restrictions found in the publishing criteria in different ranges of change of physical quantities and (2) decomposition of expert data.

4.1 Restrictions on physical quantities in a publishing criterion

A publishing criterion is based on the inequality $|p_{i,expert} - p_{i,primary}| < D_k$, where $p_{i,expert}$ and $p_{i,primary}$ are the expert and primary values of physical quantities, respectively, and D_k is the deviation satisfying the publishing criterion in the spectral range of interest. In view of the fact that the operation of measuring instruments used in quantitative spectroscopy is based on different physical principles, the permissible deviation will be different for different ranges of change of the physical quantities under consideration.

Decomposition is performed in three ways: decomposition into experimental primary data, into theoretical primary data and into experimental and theoretical primary data. This principle is independent of the physical quantity used in the decomposition. A comparison of expert data with primary data according to the publishing criterion performed here for vacuum wavenumbers makes use of division of the range of change of wavenumbers (from 0 to 100,000 cm^{-1}) into twelve subranges. The limiting accuracy that determines the areas of application of the publishing criterion in checking an expert dataset for conformity to the criterion is related to each of the subranges. In the microwave region, the limiting accuracy is 0.00001 cm^{-1}, in the far, long-wave, middle, near infrared and visible regions, it is 0.005 cm^{-1}, whereas in the short-wave infrared, it is 0.01 cm^{-1}.

4.2 A decomposition task

A representation of the results (E, F) obtained from decomposition that allows for the breakdown of expert data into computed and measured values provides a quantitative characterization of trust. In the overwhelming majority of cases, trust in measured characteristics of transitions in quantitative spectroscopy is much higher than trust in computed values.

Table 1 gives the number of distrusted transitions $F(p^i_j, qn_j)$ in the expert data from [10–12, 17, 19] for water and carbon dioxide isotopologues and hydrogen sulfide. Using the main water isotopologue as an example, we show the way the number of distrusted transitions changed, as new versions of information resources were created by two expert groups in 2005–2011. Trust in vacuum wavenumbers in the visible is seen to increase dramatically. Column "All Regions" comprises a complete number of distrusted transitions in the expert data examined.

The following abbreviated forms were used in the table for decomposition ranges: L.W.IR for long-wave infrared and S.W.IR for short-wave infrared. The blue rows of the table show the number of distrusted transitions in the region of interest. The numbers opposite chemical formulas of molecular isotopologues correspond to the number of transitions available in the publication containing associated expert data.

Assessment of trust in information resources for carbon dioxide is indicative of a high degree of trust in resources for the $^{12}C^{16}O_2$, $^{12}C^{16}O^{18}O$ and $^{13}C^{16}O_2$ isotopologues [17].

Accordingly, this is evidence that resources based on a considerable body of measured data evoke a higher degree of trust.

Assessment of trust in resources for the hydrogen sulfide molecule has shown that about 40% of transitions are distrusted for the values of D_i given in Section 4.1. The ranges of change of distrusted vacuum wavenumbers are specified along with distrusted transitions for hydrogen sulfide.

5 An ontological representation of assessment of trust

The OWL ontology of assessment of trust in expert data comprises taxonomies of classes and properties and a set of individuals. The taxonomy of classes and the structure of individuals are described below. Here no consideration is given to the properties. However, certain properties are shown in Fig. 3 to describe the structure of an individual. A description of the properties and classes is available in the code of the ontology (see `http://wadis.saga.iao.ru`).

5.1 The structure of individuals

The structure of an individual $\mathbf{A_1}$ describing a complete assessment of trust in an expert data source is shown in Fig. 2 where the trust is assessed for expert data from [17] as an example for the hydrogen sulphide molecule. Notably, the structure is the same for all molecules. The minimum cardinality of property *hasVacuumWavenumberDescriptionClassifiedByPrimaryInformationSource* is 1, whereas its maximum cardinality is 3. The value of this property is an individual **B** describing one of three expert data decomposition techniques. Figure 2 shows

Decomposition Group	Vacuum Wavenumbers, cm^{-1}									
	RF	Microwave	Far IR	L.W. IR	Middle IR	S.W. IR	Near IR	Visible	Near UV	All Regions
H_2O	2011_JaCrArBo [1] (**41147**), 2008_JaScChCr [26] (**41148**)									
Distrusted Data		16	616	426	1242	1909	1335	359	2	5905
	2009_RoGoBaBe [6] (**37432**)									
Distrusted Data	1	6	612	462	1131	1343	521	3	0	4079
	2005_RoJaBaBe [25] (**32365**)									
Distrusted Data	1	6	612	462	1131	1343	605	520	2	4682
	2005_JaScChGa [24] (**36701**)									
Distrusted Data		16	619	420	1337	2691	2221	516	2	7822
$H_2{}^{17}O$	2009_RoGoBaBe (**6992**)									
			117	45	171	377	412	64		1186
$H_2{}^{18}O$	2009_RoGoBaBe (**9753**)									
	1	28	139	66	130	153	936	3		1456
HDO	2009_RoGoBaBe (**13238**)									
	3	24	523	84	204	620	59	76		1603
$^{12}C^{16}O_2$	2009_RoGoBaBe [6] (**128170**)									
			13	53	84	26	27			202
$^{12}C^{16}O^{17}O$	2009_RoGoBaBe (**19264**)									
			38	187	29	926	0			1180
$^{12}C^{16}O^{18}O$	2009_RoGoBaBe (**79958**)									
		7	79	944	214	433	0			1677
$^{13}C^{16}O_2$	2009_RoGoBaBe (**49777**)									
			0	0	81	41	1			123
$^{13}C^{16}O^{17}O$	2009_RoGoBaBe (**2953**)									
			127	364	590	0	127			
$H_2{}^{32}S$	2009_RoGoBaBe (**12330**)									
		2.985	15.683	994.127	1250.024	3303.930				2.985
		7.624	609.328	1249.221	3033.307	4256.547				4256.547
		8	969	62	1446	2504				4989

Table 1. Results of decomposition of expert data for four water and five carbon dioxide isotopologues and hydrogen sulfide

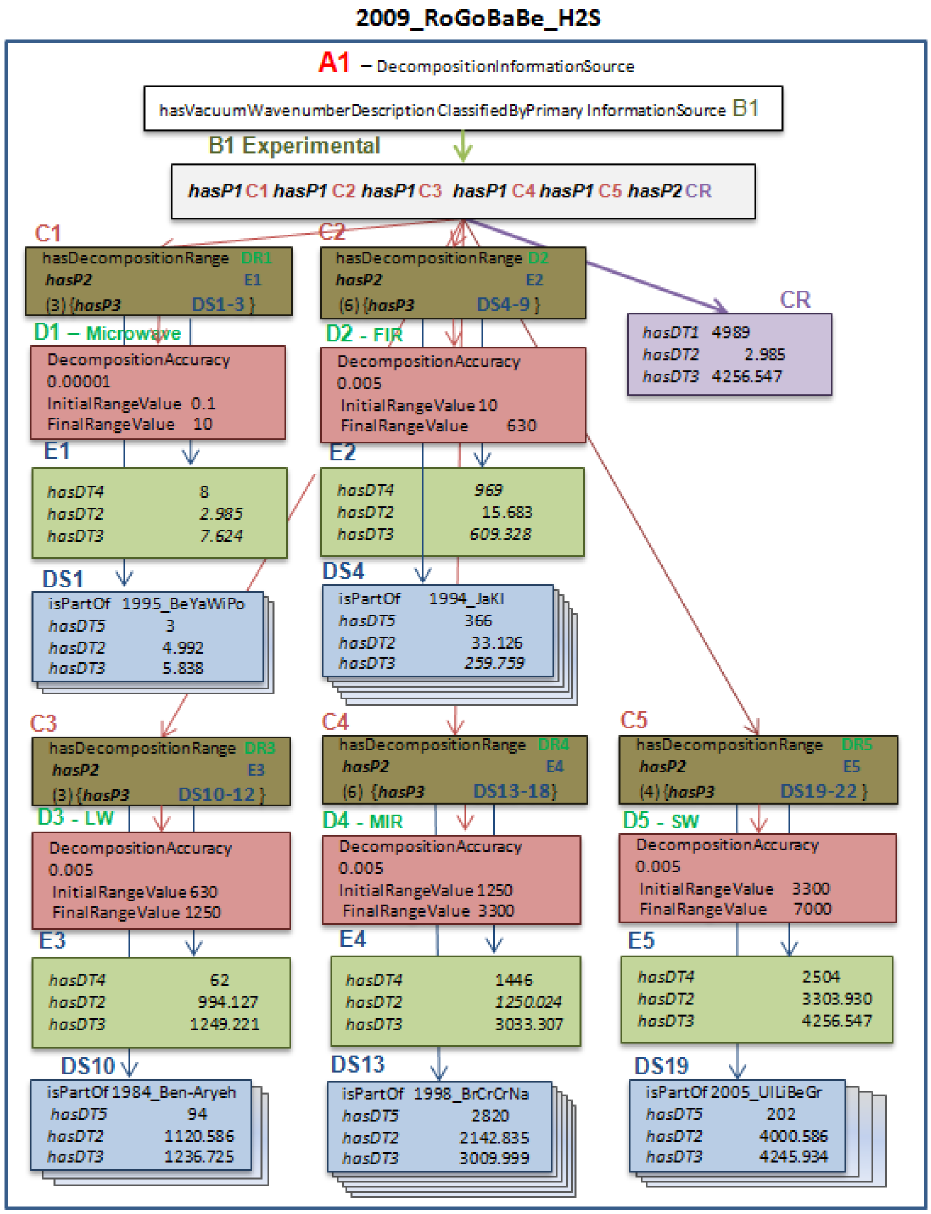

Fig. 2. Subject-predicate structure of an individual describing the assessment of trust in the expert data on vacuum wavenumbers for the H_2S molecule

one value of this property (namely, $\mathbf{B_1}$) describing results obtained from decomposition into primary measured data. This example has no other individuals related to this property, because calculated published data for this molecule are lacking. The maximum cardinality of property *hasVacuumWavenumberDecompositionDescriptionClassifiedByRange* corresponding to *hasP1* in Fig. 2 is 12, whereas its minimum cardinality is 1. The values of this property are individuals ($\mathbf{C_n}$) describing the assessment of trust in a certain range of change of vacuum wavenumbers. The values of property *hasDistrustedTransitionDescription* corresponding to *hasP2* in Fig. 2 are individuals **CR** and $\mathbf{E_n}$ specifying the entire range of change of vacuum wavenumbers or typical regions (microwave, visible, etc.) where the wavenumbers available in the expert data are found, respectively. Individuals **CR** and $\mathbf{E_n}$ represent the number of values of distrusted physical quantities and ranges of their change. Finally, the value of property *hasTrustedTransitionDescription* (corresponding to *hasP3* in Fig. 2) is an individual **DS** specifying the number of trusted transitions and range of their change.

Figure 3 shows a fragment of Fig. 2 describing the structure of an individual $\mathbf{C_5}$ of class DecompositionInShortWaveInfraredRangeDescription. This individual has three properties whose values are individuals $\mathbf{DR_n}$, $\mathbf{DS_n}$ and $\mathbf{E_n}$ specifying the decomposition range and trusted and distrusted transitions in the expert data in this range, respectively. Trusted characteristics refer to each of the primary data sources that contain identical transitions with expert data. The wavenumbers of these transitions satisfy the restrictions imposed by the publishing criterion for this range.

Figure 3 demonstrates properties of one of the individuals ($\mathbf{DS_n}$). The properties of an individual **2005_UlLiBeGr** are not shown. The latter individual **2005_UlLiBeGr** is an information source describing the solution to task $T6$ published in [27] and includes about 100 axioms.

Considering the other individuals characterizing trusted transitions of expert data and similar individuals corresponding to other decomposition ranges and decompositions into different combinations of primary datasets, we will arrive at a detailed description of the trusted part of transitions for decomposition into vacuum wavenumbers.

5.2 Taxonomy and an instance of a class definition

Results obtained from an analysis of trust in information resources in the ontology of information resources are individuals of class DecompositionInformationSource (here the terminology of ontology version 6 is used). Four classes are associated with decomposition techniques (e.g., DescriptionUnderExperimentalPrimaryInformationSourceDecomposition), and thirteen classes are associated with decomposition ranges (e.g., DecompositionVisibleRangeDescription). Two classes (TrustedTransitionDescription and DistrustedTransitionDescription) contain elements specifying the number of trusted and distrusted vacuum wavenumbers and ranges of change of the wavenumbers.

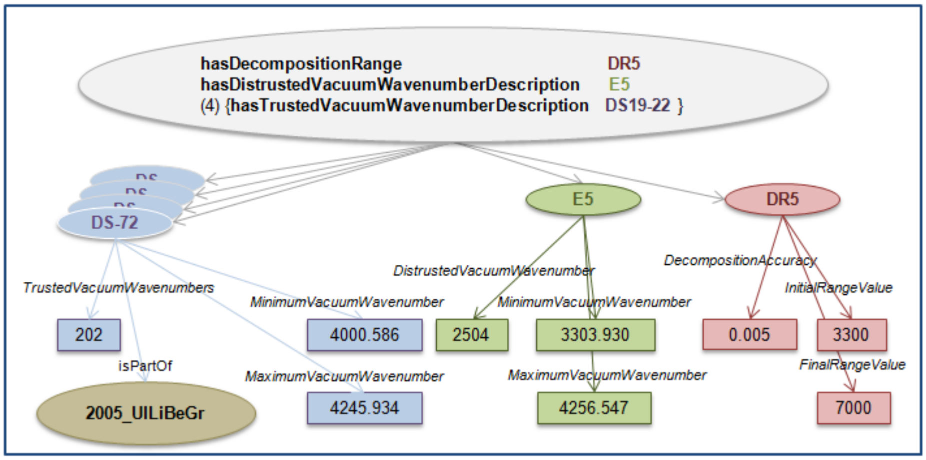

Fig. 3. Fragment of Fig. 2 with a detailed subject-predicate structure of an individual $\mathbf{C_5}$ of class DecompositionShortWaveInfraredRangeDescription

For the most part the classes are defined by a set of restrictions on the property values. Restrictions for class DecompositionVisibleRangeDescription using the Manchester syntax can be exemplified in the following way:

(*hasTrustedDescription* **some** TrustedVacuumWavenumberDescription **or** *hasUntrustedDescription* **some** UntrustedVacuumWavenumberDescription) **and** (*hasDecompositionRange* **value** VisibleDecompositionRange)

This class includes individuals each of which specifies the number of trusted and distrusted transitions, associated ranges of change of trusted and distrusted transitions in the visible for one molecule and one expert data source.

The ontology of assessment trust in expert resources for quantitative spectroscopy comprises 19 classes, 14 properties and 9 types of structure of an individual describing the assessment of trust depending on the molecule under study, spectral range of expert data relating to this molecule and number of primary sources which may vary between 20 and 150.

6 Summary

The quality of expert resources in quantitative spectroscopy has been assessed. Use was made of primary data sources retrieved from more than 2000 publications. The primary data sources were uploaded to information system W@DIS and provided with semantic annotations [8]. The annotations contain information on the validity and degree of consistency of spectral data and are available for users in tabular form and OWL ontology.

To assess trust in expert resources, we applied a publishing criterion whose quantitative values vary in twelve ranges of vacuum wavenumbers. The structure of an individual characterizing the assessment of trust in expert resources is described. The former contains information for trusted and distrusted vacuum wavenumbers. Examples of assessment of trust in expert resources are expert values of vacuum wavenumbers.

Work is under way to apply the computed ontological knowledge base to development of an expert system for an assessment of and a semantic search for information resources in quantitative spectroscopy and to the Virtual Atomic and Molecular Data Centre [7]. A knowledge base of this type makes it possible to perform an analysis of data obtained by other experts for a number of molecules, on the one hand, and to form expert data aligned with published expert data, on the other. Thus experts will have quantitative assessments of validity of and trust in resources of this type at their disposal.

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