Quality control of scientific plot collections

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The article considers the problem of quality control of scientific plots on the example of published plots characterizing continuum radiation absorption, properties of weakly bound molecular complexes and absorption cross sections used in atmospheric chemistry. The tasks of systematization of graphical resources are formulated, the functionality of the GrafOnto information system containing graphical resources is described, statistical samples characterizing, in particular, the quality of graphical resources in the collection are presented. The analysis of the quality of citing plots and proximity estimates for pairwise comparisons of all plots in the collection is presented as well as the applied ontology of graphical resources.

1. Introduction

Scientific information resources can be divided into three parts, depending on the presentation of research results in publications in analytical, tabular or graphical forms. Professional training of researchers for the acquisition of such resources requires a significant amount of hidden knowledge, which is often outside of their scientific interests. Computer processing of data, information and knowledge contained in information resources greatly facilitates the acquisition of large amounts of information presented in graphic form.

This paper formulates the task of systematization of information graphic resources and gives an analysis of their quality. The relevance of this work is due to the presence of some domains that predominantly use graphic resources, in particular, one such domain is spectroscopy.

The creation of information systems (IS) for the systematization of plots in spectroscopy began with the work [1] in 2013. In [1], the subject of systematization was the absorption cross sections used in atmospheric chemistry to calculate the rates of photolysis reactions. Earlier, the absorption cross sections were used in the information system "Atmospheric Chemistry" that we created [2], when performing work on the ATMOS information portal [3]. In 2016-2023, a number of publications [5-8] were published on collections of plots characterizing continuum water absorption [7] and atmospheric dimer properties [5,6,8]. Information aspects of these collections were discussed in papers [9-10] that provided classification of scientific plots, plot related metadata, ontology of plot resources, virtual plots, statistics of scientific plots in collections on the three sections of spectroscopy, and problems of scientific plots citation. An article [11] described the search facilities of the GrafOnto information system. Finally, the paper [12] proposed a method of quantitative comparison of citing and cited plots, which allowed us to analyze the quality of plots in the GrafOnto collection.

This report presents the statement of the problem of graphical resources systematization, gives a brief description of the development of means for searching the closest plot to arbitrary user plots and characterizes the functionality of GrafOnto information system, presents a new version of the ontology of plot resources, which includes the results of analysis of the citation quality, statistics of IS information resources by type of plot or by different groups of substances, and similarity analysis of all pairs of plots in the collection, using the methane molecule as an example.

2. Problems of scientific graphics systematization

The main task of scientific graphics is to represent the properties of subjects defined by discrete functions for their comparison and visual assessment of the qualitative behavior of the studied values. For the researcher, the advantage of graphical representation in comparison with tabular or analytical representations is obvious, especially in the case of a significant number of function values being compared. It is worth noting that tabular representation in the IS is stored in a database; analytical functions are generalized by libraries of computing programs, plots are linked to generating software, and all three ways of representation are provided by the ontological description of the subject area. Building an IS of this structure is a step in the direction of using information systems in agent-based technologies.
In the GrafOnto IS, the systematization of scientific graphics is in two stages: analysis of the use of scientific graphics in publications and recommendations for creating software and structuring data and metadata.
The results of an analysis of published scientific plots in spectroscopy are discussed below, one part of the analysis relates to many different domains, and the other part reflects the features specific to the plots used in spectroscopy. The general features are for coordinate systems, functions and arguments, classification of plots, and quality control of plots. Most of the collection of scientific plots contains numerical arrays defining functions derived from the recognition of figures extracted from publications that contain sets of primitive plots described in the publications. There are two aspects to the quality of plots: technical (how accurately the plot is constructed by researchers, graphically represented by publishers, and how accurately the published plot is digitized) and semantic (the extent to which the citing plot corresponds to the cited plot). In complex domains problems with functions and arguments stem from the use of their synonyms in publications and their different units of measurement. The problem of synonyms can be solved in the following way: the names of functions most frequently used in publications are selected in the list of functions and arguments, and their corresponding synonyms in the original plot are defined by an additional attribute. It is much more difficult to switch from one unit of measurement to another when comparing function values. The problem is that the transition coefficients may depend on parameters (e.g., thermodynamic) which values are not explicitly defined in the text of the publication. Finally, when analyzing the quality of citations, there is a problem caused by the lack of citation culture and stemming from the implicit definition of the cited plot.

Some of the tasks of systematization and classifying plots have been partially solved [12, 13]. The results of the analysis of the quality of citation have pointed to the need to introduce an additional type of "expert citing plot", i.e., a citing plot for which the decision of an expert is required, for example, for the solution of the problem indicated in the last sentence of the preceding paragraph.

3. Functionality of the GrafOnto system

The functionality of the IS is determined by what domain tasks in it are solved within the framework of information technology. Along with the traditional information tasks (classification of resources, resource search, statistical data on resources, etc.), solved in the

GrafOnto IS and defined by the knowledge cycle [14], the fundamental task is the task of assessing the quality of information resources available in the information system.

Information tasks in GrafOnto IS are divided into two groups. At the administrative level of GrafOnto IS management graphical resources are collected, composite plots and figures are decomposed into primitive plots, which are then digitized, virtual pairs "citing - cited plots" are constructed, database of primitive and composite plots and figures and their metadata is formed and individual ontologies of graphic information resources are automatically created.

At this level, a comprehensive search for a cited plot for a given citing plot is supported, in which the cited publication is found first, and then the difference score used to select the citing plot is calculated. Then a virtual pair of cited and citing plots is created associated with the metadata characterizing the pair. One feature of this search is that it automatically translates the measurement units.

The functionality of GrafOnto IS available to users includes different kinds of searches (attributive, contextual, semantic) of graphical resources, statistics of plots by substances and functions, results of plot citation quality analysis, evaluation of citation quality by substances, etc.

Table 1 shows the statistics by type of plot. It demonstrates that the greatest number of primitive plots are original, the number of citing plots is one-fifth of the collection, and the number of plots requiring peer review is less than 10%. The abbreviations contained in the third column are used in the names of ontology classes and individuals. The fourth and fifth columns list restrictions on the number and quantity of primitive plots of different types.

Table 1. Statistics of plots and figures from the GrafOnto collection

Figure type	Plot type	Abbreviation of plots and figures	Restrictions	Quantity
Primitive Figure	*Primitive Plots*			6542
	Original primitive plot	OPP		4694
	Citing primitive plot	CPP		1255
	Expert citing primitive plot	ECPP		260
	Expert primitive plot	EPP		333
	Composite Plots			1433
	Original composite plot	nOPP	n>1	889
	Citing composite plot	nOPP+mCPP	m≥1, n+m>1	205
	Specific composite plot	OPP + CCP		691
	Multipaper composite plot	nOPP+mCPP+kOCiP	k≥1,k+n+m≥2	339
Composite Figure		nOPP+mCPP+kOCiP+pCCP	k+n+m+p≥2	258

Figure 1 shows histograms characterizing the number of citing plots in the GrafOnto IS for molecules and mixtures. The abscissa shows the difference percentage between plots, and the ordinate shows the number of "citing - cited plots" pairs. Note that a difference of 50% indicates a difference of two times the values of the compared plots. This difference is explained by the absence of values of thermodynamic quantities in the publications or incorrect transition coefficients between different measurement units.

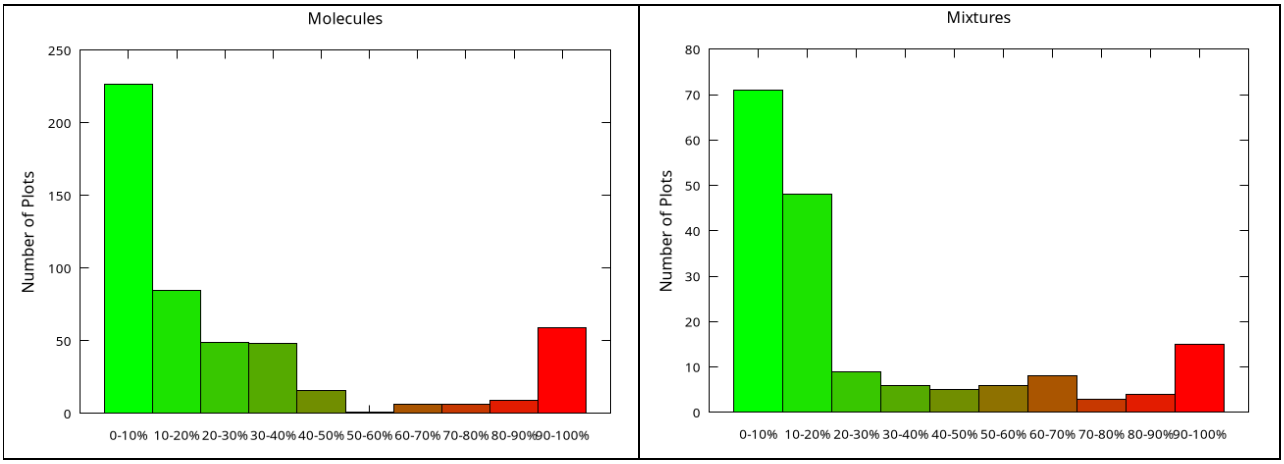
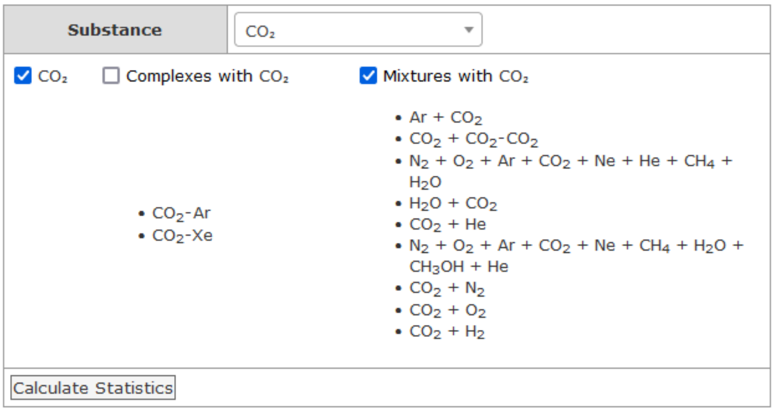


Figure 1. Statistics on the quality of citing plots of the GrafOnto collection by substance groups.

Figure 2 shows the plot citation quality statistics in more detail using the example of a carbon dioxide molecule. The upper part of the figure lists mixtures containing carbon dioxide as well as carbon dioxide itself. At the bottom, the numbers of citing plots in each interval are shown for different intervals of the percentage difference. More than thirty-five percent of these plots don't contain their corresponding citing plots in the plot collection, but the publications in which they are published are available in the GrafOnto IP publication collection.



Citing Plot Type		CO_2	Mixtures with CO_2	Total	Total (%)
Pairs of Linked Plots	0% ≤ R < 10%	40	36	76	39.6
	10% ≤ R < 25%	37	40	77	40.1
	25% ≤ R < 50%	28	5	33	17.2
	50% ≤ R < 100%	2	4	6	3.12
	Total	107	85	192	100
Reference with a Cited Plot					57.7
Reference without a Cited Plot		91	27	118	35.4

Figure 2. Statistics of citing plots by molecule CO_2, stages of processing citing plots and citation quality.

4 Citation procedures, citing plot properties and evaluation of plot similarity

When investigating the citation of published plots, the citation procedures used are important as well as finding the qualitative and quantitative characteristics of the difference between the discrete functions corresponding to the cited and the citing plots. The published citing plot, characterized by a discrete function, is compared to a previously published original plot from another publication, also characterized by a discrete function. Function values are stored in the GrafOnto database. A published citing plot presented graphically in a publication assumes that for the corresponding cited plot there exist values of the function in graphical or tabular representation in another previously published publication.

A plot is called citing if the publication containing it includes a bibliographic reference to a previously published article in which a similar set of coordinate pairs is presented in analytical, graphical or tabular form.

In order to compare the citing and cited plots, it is necessary to bring the physical quantities referring to the corresponding coordinate system axes to the same units and to check the availability of the values of thermodynamic parameters included in the formulas for calculating the transition coefficients between these units. Sometimes working with the reference to the cited plot involves calculating the values of an analytical function or using tabular data. Bringing plots to the same units of measurement requires additional calculations.

Let us distinguish three variants of the citation procedure when working with plots. The first option includes comparisons of discrete functions of plots and does not require additional calculations. The second variant includes comparisons in which it is necessary to recalculate the units of functions representing physical quantities. The third variant of the procedure requires calculations of values of the discrete function of the cited plot presented in analytical or tabular representation. The first two variants of the citation procedure are implemented in the GrafOnto IS and further considered as passive citation. The procedure of the third variant will be called an active citation. At present, this citation option is not supported in the information system.

The results of the citing and cited plots comparison are stored in the metadata of the citing plot and are described by three attributes. The first attribute describes the difference in the number of discrete function values corresponding to these plots. It can be equal, partial or redundant, which characterizes citation completeness. The second attribute describes the interval of values along the abscissa axis, at which the functions being compared intersect in the measurement units of the citing plot. The third attribute characterizes the percentage difference of the compared discrete functions [15].

Estimation of similarity of a pair of plots is used to solve two tasks: search for a cited plot in the GrafOnto collection and automatic selection of plots from the collection close to an arbitrary original plot of the collection for purposes of citation. The second task is somewhat broader in comparison to the first one. For example, on the one hand, the user can select a set of cited plots based on proximity criterion, and on the other hand, they can find published plots that potentially miss a citation.

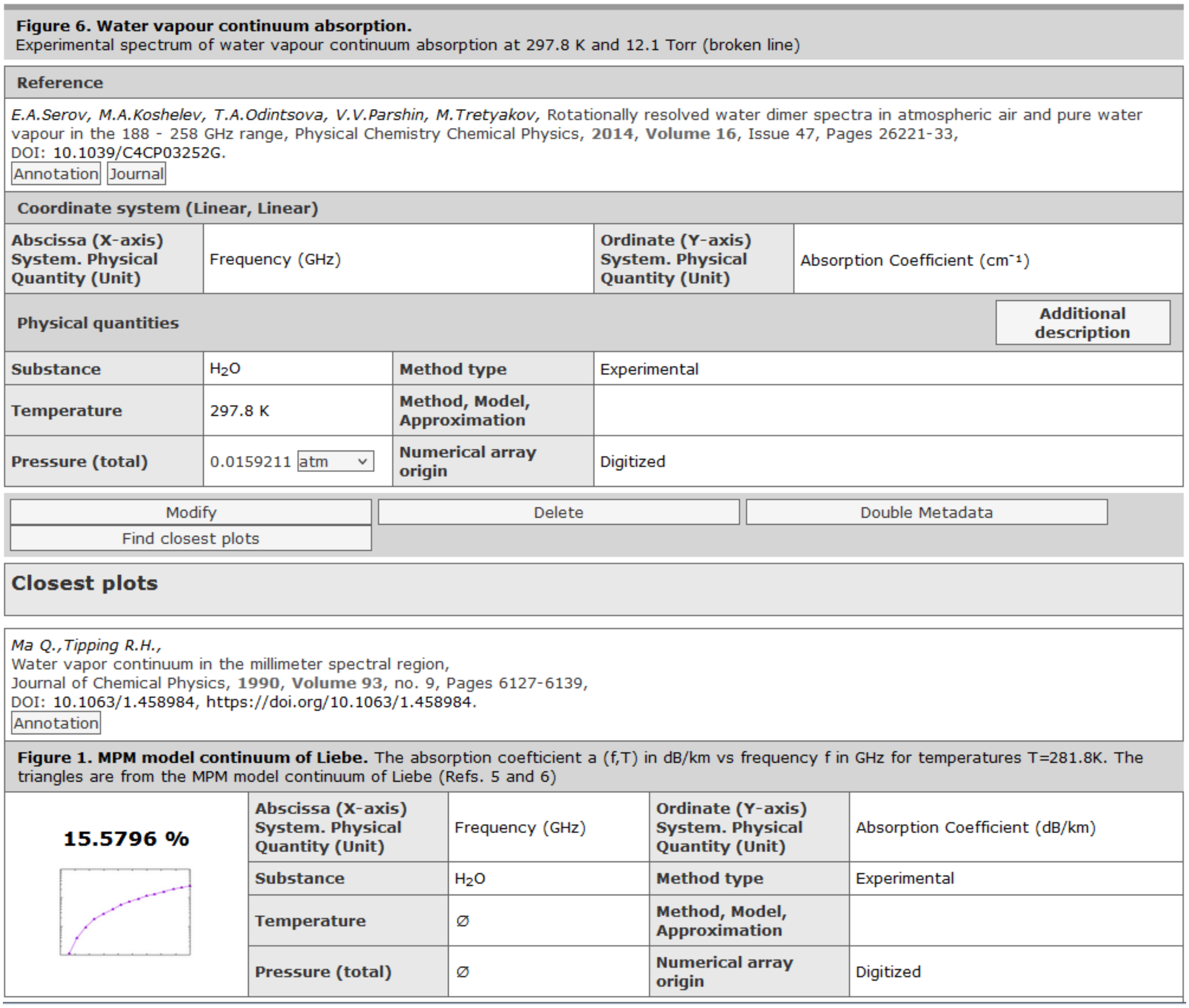


Figure 3. User interface for viewing closest plots.

The interface for viewing the results of plot selection in GrafOnto is shown in Figure 3. The ontological description of the closest plots is given below.

5 Extension of the graphical resources ontology

The results of analyzing the quality of plot citation and determining the similarity of plots in the collection led to the introduction of several new properties and a significant number of individuals in the ontology, therefore the running time of the reasoners started to exceed twenty-four hours. For this reason, the ontologies were divided into modules, one for each substance.
A description of individual structures and an example of constraints for class definition are given below.

5.1 Properties for ontological description of primitive plots

Analyzing the quality of citing plots and clustering information resources required the introduction of additional properties and the development of the structure of ontology individuals. Additional properties to the ontology describing the quality of citing plots and the similar plots are shown in Table 2.

Table 2. Properties of the three types of primitive plots (original, citing and similar)

Domain	Object property	Range	Abbr.
PrimitivePlotDescription	hasSubstance	Substance	Op1
PrimitivePlotDescription	hasCurveType	CurveType	Op2
Description	hasReference	Reference	Op3
PrimitivePlotDescription	hasOriginType	OriginType	Op4
PrimitivePlotDescription	hasCS	CoordinateSystem	Op5
PrimitivePlotDescription	hasPlotType	PlotType	Op6
PrimitivePlotDescription	hasCSType	CSType	Op7
CoordinateSystem	hasX-axis	X-axis	Op8
CoordinateSystem	hasY-axis	Y-axis	Op9
X-axis	hasSX-axis	SystemPhysicalQuantityDepended	Op10
Y-axis	hasSY-axis	SystemPhysicalQuantityIndepended	Op11
X-axis	hasPX-axis	SystemPhysicalQuantityDepended	Op12
Y-axis	hasPY-axis	SystemPhysicalQuantityIndepended	Op13
X-axis or Y-axis	hasAxisScale	AxisScale	Op14
Y-axis	hasMethodType	MethodType	Op15
Y-axis	hasMethod	Method	Op16
Description	hasCitingReference	Reference	Op17
CitedPrimitivePlotDescription	hasOriginalPlot	OriginalPrimitivePlotDescription	Op18
CitingPrimitivePlotDescription	hasTypeOfCitingProcedure	Citing_Procedure	Op19
CitingPrimitivePlotDescription	hasQualitativeDifference	Qualitative_Difference	Op20
OriginalPrimitivePlotDescription	hasSimilarOPPD	SimilarOPPD	Op21
SimilarOPPD	hasSPOPPD	OriginalPrimitivePlotDescription	Op22
Domain	Datatype property	Range	
ResearchPlotDescription	isPrimitiveFigure	xs:boolean	Dp1
ResearchPlotDescription	hasNumberOfPoints	xs:int	Dp2
ResearchPlotDescription	hasFigureCaption	xs:string	Dp3
PrimitivePlotDescription	hasOriginalPlotInformation	xs:anyURI	Dp4
ResearchPlotDescription	hasSystemFigureNumber	xs:int	Dp5
ResearchPlotDescription	hasOriginalImageOfPlot	xs:anyURI	Dp6
ResearchPlotDescription	hasSystemImageOfPlot	xs:anyURI	Dp7
Reference	hasBibliographicReference	xs:string	Dp8
CitingPrimitivePlotDescription	hasMaximumXOverlapInterval	xs:float	Dp9
CitingPrimitivePlotDescription	hasMinimumXOverlapInterval	xs:float	Dp10
CitingPrimitivePlotDescription	hasEstimationOfDeviation	xs:float	Dp11
SimilarOPPD	hasPercentageDifference	xs:float	Dp12

Properties Op1-Op16 and Dp1-Dp8 characterize the classification of plots, properties Op17-Op20 and Dp9-Dp11 describe the results of citation quality assessment and properties Op21, Op22 and Dp12 represent the results of the problem of finding the closest plots to a given plot.

5.2 The main types of individuals that characterize primitive plots

Being the equivalents of figures and plots from the published graphical resources, the images generated in the GrafOnto system are associated with the description of their metadata, which constitute the most significant part of the ontology individuals included in its A-box. The types of figures and plots given in [8,9] are determined by the values of the hasPlotType property (primary or original plot, citing plot, expert citing plot (the plot which expert should determine whether it will be a citation in accordance with the contents of the GrafOnto database), expert primitive plot (which type is determined by expert) and cited plot (the plot to which the publication should contain a corresponding bibliographic reference).
The names of such individuals use the abbreviation of the corresponding values (for example, OCP - Original Composite Plot). Fig. 4 shows the structures of three types of primitive plots. Ovals denote ontology individuals, rectangles denote literals, and directed arcs denote object (OP) and data (DP) properties.

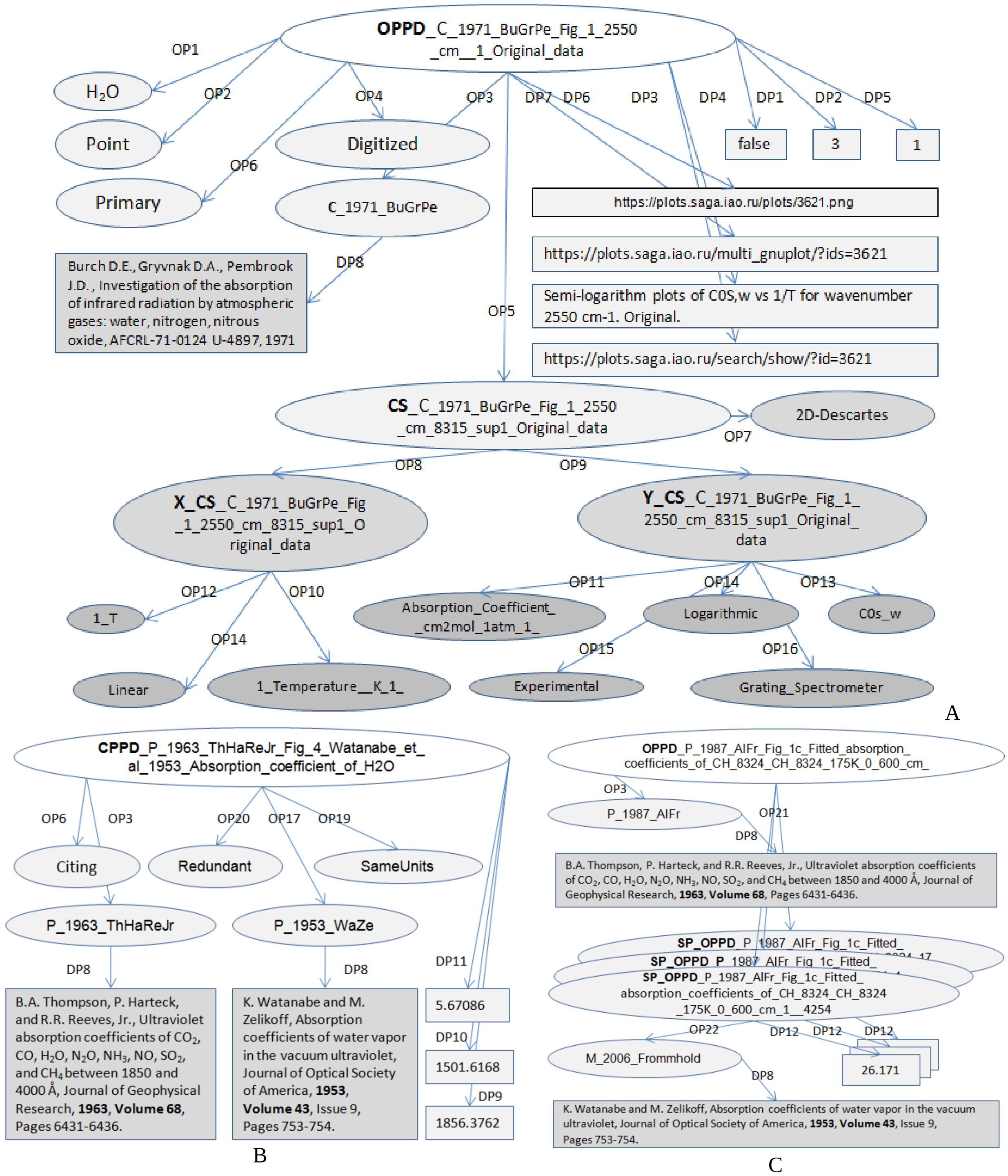


Figure 4. Characteristic structures of the three types of ontological individuals of graphical resources in spectroscopy. A. The structure of the original primitive plot individual [16], B. A fragment of the structure of the citing plot individual [17,18], C. A fragment of the structure of the original primitive plot individual with related similar plots [19].

Figure 4A contains the structure of the original primitive plot, for which in the GrafOnto plot collection there are no plots similar to it within the proximity criterion δ [14] (e.g., δ < 20%). Figure 4B contains a fragment of the structure of the citing plot and a number of Op20, Op19, Dp10, Dp11 and Dp9 property values characterizing the citing procedure, maximum and minimum values of the argument of the compared (citing and cited) plots and the value of their similarity. Figure 4C contains a fragment of the structure of a primitive plot, for which in the GrafOnto collection there are plots similar to it within the proximity criterion δ. Evaluating the proximity of such graphs allows users to construct a set of plot to compare for citation purposes.

5.3 Definition of ontology classes

Queries for searching information resources in the collection are performed through the corresponding interface of the GrafOnto IS. OWL ontologies were created for agent-based technologies, in particular for the task of finding the closest plots for all plots in the collection. This task facilitates finding a family of plots close, for example, to a particular user plot loaded into GrafOnto system. In the plot ontology, the proximity δ of plots is specified by a property hasPercentageDifference, which is inherent to individuals of the SimilarOPPD class extension. If, however, a specific quantification is required, e.g., δ <10%, the ontology has a template of class SimilarOPPPDLessThan10 defined by the expression (see Table 2)

(hasPercentageDifference some not xsd:float[> 10.0f]) and (hasPercentageDifference min 1 rdfs:Literal)
.

It contains individuals of all pairs of close plots within the collection with δ < 20%.
The template class OPPD_P_1986_CoDoNe_Fig_3 defined by the expression

((hasPercentageDifference some not (xsd:float[> 10. 0f])) and (hasPercentageDifference min 1 rdfs:Literal)) and (hasSPOPPD value OPPD_P_1986_CoDoNe_Fig_3_Experimentally_determined _absorption_band_ 243K_50_700_cm_1_)

allows to define all the plots closest to the individual P_1986_CoDoNe_Fig_3_ Experimentally_determined_absorption_band_243K_50_700_cm_1_.
Similar class templates exist for citation quality assessment in GrafOnto plot collection.

5.4 Metrics for some applied ontologies

In a subject domain, ontology metrics are used to compare ontologies of different parts of the subject domain (continuum absorption (in spectroscopy)), properties of a group of specific substances (weakly bound complexes), or different subject domains, e.g., absorption cross sections (in spectroscopy and atmospheric chemistry), characterizing quantitative and qualitative features of the ontological description. In different collections of plots, comparison of collections is necessary to understand the quantitative composition of collections, the granularity of their ontological description, and so on. In OWL ontologies, the number of object properties characterizes the number of pairwise relations between individuals. Some of these individuals can be quantified. Evaluated relations are described by datatype properties.

Table 3. Ontology metrics, characterizing the graphical resources collection. DL expressivity of the ontologies is ALCO(D).

	Continuum	Complexes	Cross Sections	CO_2	CH_4
Metrics					
Axiom	148723	32512	11059	38638	3907
Logical axiom count	121153	25963	8829	30512	3020
Declaration axiom count	21615	5107	1749	6585	650
Class count	585	312	69	193	67
Object properties count	30	30	30	30	30
Datatype properties count	14	14	14	14	14
Individual count	21254	4946	1645	6322	552
Individual axioms					
Class assertion	1062	397	230	317	59
Object properties assertion	77489	16597	5546	18929	1665
Datatype properties assertion	41425	8294	28136	10805	1066
Annotation axioms					
Annotation assertions	5955	1442	481	1541	237

Table 3 shows the metrics of three applied ontologies of scientific plots characterizing the process of continuous absorption of molecules (Continuum), absorption in weakly bonded molecular complexes (Complexes) and molecules in the ultraviolet range (Cross Sections), as well as metrics of ontologies of methane and carbon dioxide molecules. The DL expressivity of these ontologies is ALCO(D). The difference in the number of classes indicates the use of more spectral functions in the Continuum problem compared to the Complex and Cross Section problems.
The GrafOnto collection ontologies can be found at https://plots.saga.iao.ru/search/onto/.

Conclusion

The article describes the stages of systematization of scientific plots in the GrafOnto information system and the current functionality of this system, which provides quality control of citing primitive plots and ontology of graphical resources of the system taking into account quantitative assessments of the quality of citing plots.
Further development of the GrafOnto IS is connected with clustering each collection for different domains and calculating quality estimates of plots in different clusters of the collection and assessing the confidence in the results of studies in different spectral and temperature ranges. Depending on the results of the cluster analysis, we could develop proposals for studies in clusters with low confidence estimates.
The technical direction of improving the GrafOnto system is to provide the tools to upload personal primitive plots and build composite plots and figures to researchers with a full set of metadata, including the list of system's recommended plots for comparison

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