



**DL TR 02001**

# **The CLRC Scientific Metadata Model**

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## Foreword

The Central Laboratory of the Research Councils (CLRC) in the UK is one of Europe's largest multidisciplinary research support organisations. From its three sites, CLRC operates several large scale scientific facilities for the UK research and industrial community including accelerators, lasers, telescopes, satellites and supercomputers, which all create copious quantities of data. Currently CLRC is holding data in excess of 50 TB, deployed through a number of data centres incl. 1 World Data Centre, 3 National Data Centres and a range of facilities for particular user communities or instruments. However, it is expected that much more data will be collected in the future with the advent of new instruments, facilities (DIAMOND) and projects (LHC Challenge), which will lead to data volumes in excess of several PB within the next 5-6 years. The data held at CLRC covers most major science areas e.g. Astronomy, Biology, Chemistry, Environmental Science, Physics. These data resources are stored in many file systems and databases physically distributed throughout the organisation with, at present, no common way of accessing or searching them to find what data is available. It is often necessary to open and read the actual data files to find out what information they contain. There is little consistency in the information, which is recorded for each dataset held and sometimes this information may not even be available on-line, only in experimenters' logbooks. This situation could potentially lead to serious under-utilisation of these data resources or to the wasteful re-generation of data. It could also hinder the development of cross-discipline research as this requires good facilities for locating and combining relevant data across traditional disciplinary boundaries.

To address these problems, a web-based data portal is being developed with the aim of offering a single method of browsing and searching the contents of all the CLRC data resources. Central to the DataPortal is the philosophy that each facility/data centre is responsible for its own data and metadata and that ownership and residence are untouched by the Portal. Each facility/data centre is expected to have or develop its own metadata catalogue, which will provide at least a given set of common information held in a chosen local format. Interaction with the metadata catalogues and interchange between them is based on a metadata model for representing scientific data, which has been developed by the project and version 1 is described in this document.

The preferred solution for the interchange metadata schema would have been the reuse or adaptation of an existing tool, however a distinguishing feature of CLRC's requirement is the necessary *Generality* of the Metadata model. Other metadata approaches are either usually closely associated with a particular scientific domain (e.g. CERA – Environmental Science), or else are metadata design frameworks (e.g. RDF, XMI). Some of the initiatives studied were: XSIL from Caltech, work of the OODT group and the activities surrounding the *Dublin Core*. The Extensible Scientific Interchange Language (XSIL) is a flexible, hierarchical, extensible, transport language for scientific data objects. At a lower level than CLRC's metadata model it allows the definition of the data array and the transport of those arrays: it is used on LIGO - Laser Interferometer Gravitational-Wave Observatory

(<http://www.cacr.caltech.edu/SDA/xsil/index.html>). The Object Oriented Data Technology group (OODT) at the Jet Propulsion Lab <http://oodt.jpl.nasa.gov> is also producing a generic framework for connecting XML based metadata profiles, and uses a CORBA based OO-system to provide a distributed resource location service. A good deal of activity also surrounds the *Dublin Core* metadata <http://dublincore.org/>. This provides a basic set of elements (15 in the original definition), but is unfortunately not detailed enough for CLRC's purposes. Elements of CLRC's model could be mapped onto the Dublin Core - an important feature for interoperability, especially with Digital Libraries. Therefore CLRC decided to develop its own metadata schema for scientific data.

**In the context of scientific data and this paper, we consider metadata to be all the information, additional to the raw data itself, which a potential user of the data would need to know to be able to make full and accurate use of the data in a subsequent scientific analysis.**

The raw data may have been collected or generated in many ways, such as by measurements or observation of the environment, by carrying out an analytical experiment or by running a computer simulation.

When developing our metadata model, we aimed to provide a high-level generic model, which can be specialized to specific scientific disciplines.

The resulting model has been implemented as an XML schema and a relational database model and is currently in use in the prototype implementation of the CLRC DataPortal (<http://esc.dl.ac.uk:9000>).

Kerstin Kleese van Dam

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## 1. INTRODUCTION

This document contains the 1. Version of the CLRC Scientific Metadata Schema. It aims to provide a high-level generic model, which can be specialised to specific scientific disciplines.

Based on discussions with various departments at CLRC it was initially tailored to the needs of the data holdings of those facilities. Nevertheless, the model will abstract away from the specific requirements of these facilities in order to capture scientific data from any discipline.

Other influences come from the CIP metadata catalogue for Earth Observation and the DDI metadata description for Social Science data.

## 2. APPROACH

As a framework, we follow the categorisation of metadata from Keith Jeffery, dividing metadata into three main divisions and several subdivisions beneath that.

- **Schematic**

The data model: a (logical) description of the structure of the resource, the relationship between the elements of the resource, and any constraints.

- **Concrete**

Provides a machine view close to physical representation - data formats, fields, strings, code interfaces.

- **Abstract:**

Provides a user view, near the real-world - abstract entities and relationships between them

- **Mappings**

Capturing the relationships between levels and domains; one abstract to many concrete.

- **Navigational**

Provides the information on where resources and their sub-components are located. Often tends to be mixed up in other metadata. Ideally, kept separate from other information.

- **Associative**

All other information about a resource.

- **Descriptive:**  
what the resource is about and where it comes from.
- **Restrictive:**  
how the resource can be used.
- **Supportive:**  
the context in which the resource sits.

The metadata is structured into categories which correspond to this framework.

This provides a set of top-level categories. To specialise to a particular domain of interest, we use an *object inheritance* mechanism, providing an initial class hierarchy of metadata objects in this document.

We shall use UML class diagrams to illustrate the relationships between the components of the metadata model.

We shall also supply XML and RDF bindings of the metadata model.

### 3. THE DOMAIN OF INTEREST

#### 3.1 Modelling Scientific Activity

The data model attempts to capture scientific activities at different levels: generically, all activities are called **Studies**. Each study has an **Investigator** that describes who is undertaking the activity, and the **Study Information** that captures the details of this particular study.

Studies can be of different kinds.

**Programmes:** are studies that have a common theme, and usually a common source of funding, instigated by a principal investigator or institution. Programmes can be single projects (such as EPSRC projects, or application for beam time on ISIS), linked sequences of projects; for example an EPSRC Faraday project would have a set of linked projects. Each programme can thus be associated (linked) with a series of sub-investigations. Programmes are not expected to have direct links to data, but rather through the set of investigations within the programmes.

**Investigations:** are studies that have links directly to data holdings. More specific types of investigations include experiments, measurements or simulations.<sup>1</sup>

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<sup>1</sup> Further types of investigation may be added. For example, extending the model to social science data may well introduce the additional investigation *Survey* representing a study comprising of a questionnaire completed by a sample of the population.

**Experiments:** investigations into the physical behaviour of the environment usually to test an hypothesis, typically involving an instrument operating under some instrumental settings and environmental conditions, and generating data sets in files. E.g. the subjection of a material to bombardment by X-Rays of known frequency generated by the SR source at Daresbury, with the result diffraction pattern recorded.

**Measurements:** investigations that record the state of some aspect of the environment over a sequence of point in time and space, using some passive detector. E.g. measurement of temperature at a point on the earth surface taken hourly using a thermometer of known accuracy.

**Simulations:** investigations that test a model of part of the world, and a computer simulation of the state space of that model. This will typically involve a computer program with some initial parameters, and generate a dataset representing the result of the simulation. E.g. a computer simulation of fluid flow over a body using a specific program, with input parameters the shape of the body, and the velocity and viscosity of the fluid, generating a data set of fluid velocities

### 3.2 The Data Holdings

The metadata format given here is designed for use on general scientific data holdings. These data holdings have three layers: the experiment, the logical data, and the physical files.

Each investigation (experiment, measurement or simulation) has a particular purpose and uses a particular experimental set up of instruments or computer systems. Experiments may be organised within larger studies or projects, which themselves may be organised into programmes of linked studies.

An investigation generates raw data. This raw data can then be processed via set processing tools, forming on the way intermediate stages, which may or may not be held in the data holding. The final processing step generates the final data set.

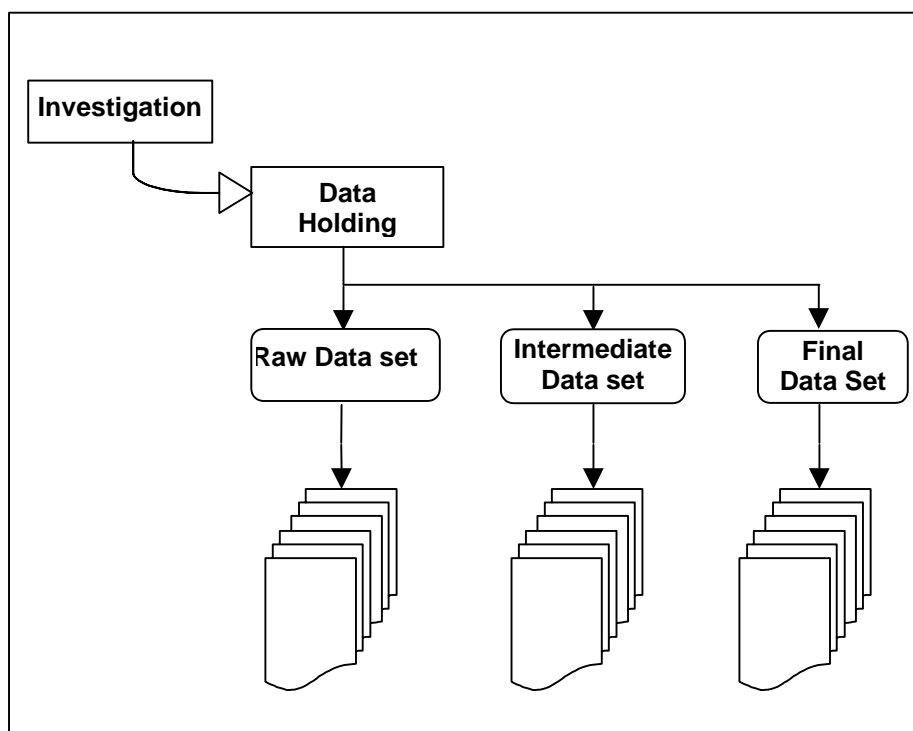
Each stage of the data process stores data in a set of physical files with a physical location.

It is possible that there may be different versions of the data-sets in the holding.

Thus each **data holding** takes the form of a hierarchy: one *investigation* generates a *sequence* of logical data sets, and each data set is instantiated via a *set* of physical files.

The design of the metadata model is tailored to capture such an organisation of data holdings.

A single metadata record in this model can provide sufficient metadata to access *all* the components of the data holding either all together or separately.



**Figure 1: Hierarchy of scientific data holdings**

### 3.3 Example

As an example of this scientific metadata model, consider the SXD information from ISIS.

The *study* in this case would be an application for beam-time, uniquely identified with an ‘RB number’, which covers a programme of investigations, and is described by a description of the purpose in the original study application. This programme is in turn broken down into a series of individual investigations, each of which are experiments on the SXD detector. Each investigation may have a sequence of *runs*, each generating a data set. Each run keeps the major parameters of the experiment the same (e.g. temperature of study), but alter some other parameter (e.g. orientation of the sample in the target). This information will need to be preserved in the metadata model.

For example an investigation with name *Benzene, variable temperature study: 150K*, would have user, purpose and date and time information associated with it. It should have a unique ID – this is not necessarily the RB number as that may relate to a programme of investigations, but it might be generated from it. It will have associated with it a set of RAW files, for example:

SXD10091 : Benzene, variable temperature study: 150K

SXD10092 : Benzene, variable temperature study: 150K

SXD10093 : Benzene, variable temperature study: 150K

SXD10094 : Benzene, variable temperature study: 150K

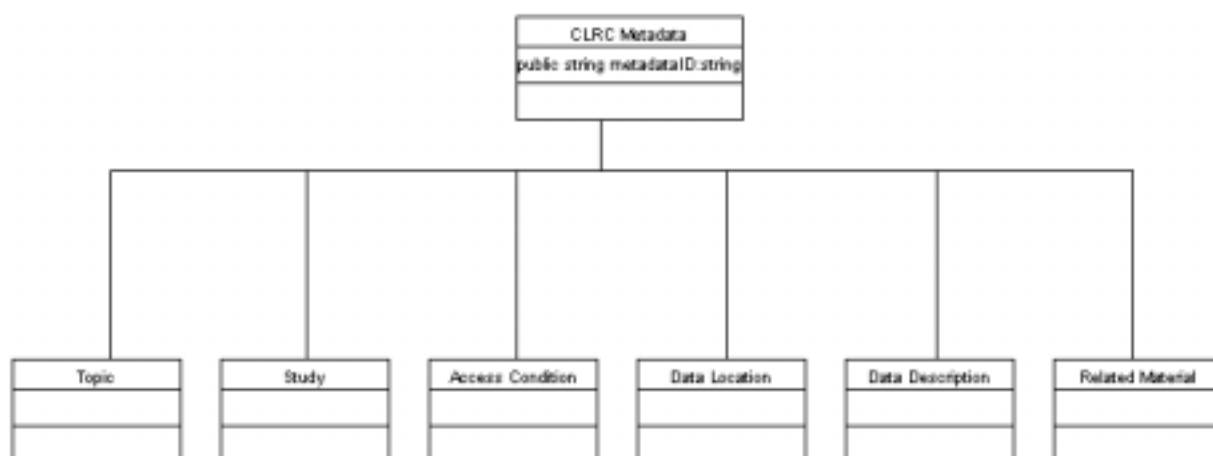
SXD10095 : Benzene, variable temperature study: 150K

It may also have a set of intermediate SXD files, and it also may have set of processed final files in standard data formats for specific programs, such as .HKL, .INS and .RES files. The system should keep track of the relationship between files, and record which have been processed and which not.

#### 4. TOP-LEVEL METADATA

A single metadata record in the CLRC Metadata record will have the following format. This will relate all the information for a single *study*, as defined above. Thus it will either describe a programme, and thus have links to all the related study record within that programme, or an investigation, and thus it will record the data holdings relevant to that investigation.

Each metadata record is provided with its unique identifier within the set of metadata records.



The CLRC Scientific metadata description will contain 6 major data areas, forming the top-level categorisation of the metadata. These are as follows:

Metadata Category	Description
Topic	Keywords from restricted vocabulary giving the hierarchical subject categorisation within each discipline; the discipline and the categorisation within the discipline are taken from controlled vocabularies.
Study	The type of entry which this metadata description is capturing. Description of the study within which the dataset has been generated. Includes investigator, experimental conditions, and purpose.
Access Conditions	Access rights and conditions on the data referred to within this entry.. Includes ownership and access control information.
Data Description	Description of the datasets.
Data Location	Location of data sets together with any copies, mirrors etc.

Related Material	Contextual information: domain definitional information; links to literature, related studies, user communities,
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Additionally, each metadata record will have a unique identifier for reference.

We break down these top-level categories further.

## 5. TOPIC

The topic gives a set of keywords relevant to the particular study, describing the subject domain with which it is concerned. It thus forms the “encyclopaedia” categorisation of the study.

Keywords will usually come from a particular domain specific restricted vocabulary, and correspond with some named thesaurus or glossary of terms. Thus in the Topic, we allow for not only the keyword, but also the discipline and source of the term. Thus for *each* keyword, we have three fields (the first two are optional):

Discipline	The subject domain (e.g. chemistry, astronomy, ecology etc).
Source	A pointer (such as URL) to a reference work providing the definition of the restricted vocabulary.
Keyword	The term itself.

This approach should help overcome inappropriate hits being returned to the user. For example, the term *Field* has quite distinct meanings in Mathematics (an algebraic structure), Physics (the region of influence of some physical phenomenon), and Geography (a region of farmed land). Searches can be qualified by discipline to prevent results in one domain being returned in response to a query in another.

Controlled vocabularies may be arranged in hierarchies or more complicated ontologies. This structure currently does not attempt to capture such structures or reason over them in the search mechanism. This would be the subject of further development of this model.

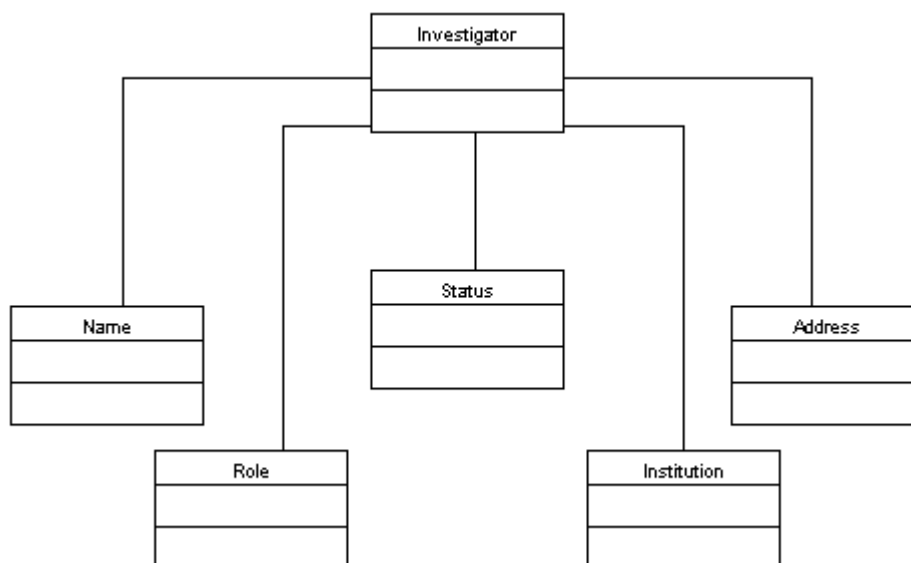
## 6. STUDY DESCRIPTION

The study description describes the current investigation being undertaken.

Category	Description
Name	Full name of the Study
Study Id	One or more identifier of the Study provided as a reference number by the user; e.g. a grant number, or a run number. Could be qualified by the source of the identifier; e.g. EPSRC, ISIS. <i>Issue – should this institutional qualifier be mandatory?</i>
Investigator	One or more people involved in the study.
Study Information	A description of the study being undertaken
Notes	Any additional miscellaneous notes that may be added to the study.

### 6.1 The Investigator

The investigator category defines *one or more* people involved in the study; one person can be distinguished as the principle investigator in the study. Others may include experimenters, students, contact staff at the facility, data processors, technicians etc.



**Figure: the Investigator and its relations**

Each person has the following fields:



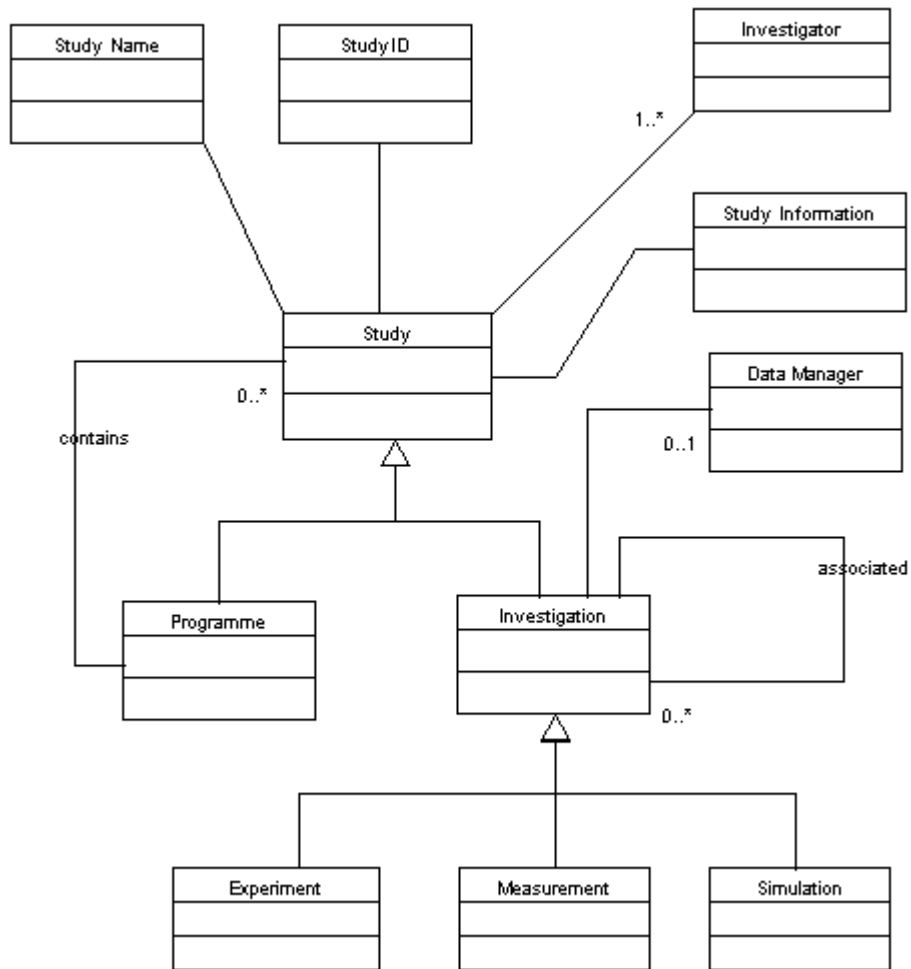
Name	Name of the person
Role	Role of the person in this study, e.g. principal investigator, co-investigator experimenter, data analyst etc.
Status	Position of the person within the institution, e.g. professor, student, team leader etc.
Institution	The institution of the person. May also categorise the type of institution (e.g. academic, government, military, commercial non-profit etc).
Address	Contact details

## 6.2 The Study Information

The information about this study has the following fields:

Funding source	Source of funds of the study, including grant-funding body, and reference number
Time	Date, time and duration of study. Can be either a point time and date, or a begin time and end time. We expect it to be in a standard format: dd/mm/yyyy for dates; hh:mm:ss for times.  <i>Issue: we should probably put time information on specific files/data sets.</i>
Purpose	Description of purpose of study, including <ul style="list-style-type: none"> <li>• Free text abstract of investigation</li> <li>• Keywords categorising subject of investigation – preferably selected from a controlled vocabulary. This is a repeat of the top-level topic and will normally be left out (or just pointed to).</li> <li>• Study type: a field which can be used to indicate the type of study being undertaken – such as a calibration run.</li> </ul>
Status of Study	Status of study, ( <i>not-started, in progress, complete...</i> ).
Resources	Statement of the resources being used, e.g. which facility.

An study itself can either be a project, representing a programme of work (perhaps containing a series of sub-programmes or projects), or an activity which collects data – such as an experiment or (computer) simulation. Each programme can be related to a series of studies; these relations are captured in the following class UML diagram.



**Figure: the Study hierarchy**

Investigations relate to data holdings. They have the distinguished attribute of a possible *Data Manager*.

Data manager	<p>A description of the primary organisation(s) responsible for generating, curating and/or holding the data. Not to be confused with a pure data archive, though they may be the same. E.g. the data manager for meteorological data held at BADC may be the Met Office; BADC is represented in the <i>Data Location</i> segment later.</p> <p>May also include details of a named contact.</p>
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Investigations can be directly related to other investigations, which may be used to feed previously taken measurements into an experiment for example, through the *associated* association.

Particular types of investigations include experiments, measurements and simulations.

### **6.2.1 Experiment**

This class describes the properties of investigations which are experiments undertaken using particular experimental equipment, under particular experimental conditions, usually to test a hypothesis.

Thus the Experiment class has the following additional fields.

Instrument	Name of instruments used. Could have a hierarchical structure.
Experimental Conditions	Environmental conditions within which the experiment was undertaken.
Parameters	Which physical characteristics are being measured and their units (and accuracy?).

We would expect further subclasses of experiment to be defined for particular facilities that are tailored to the special conditions applying in those cases; e.g. Isis experiment, SR experiment, or possibly experiments using particular instruments within those facilities.

Similarly, we would expect subclasses of conditions for different classes of experiments. Thus for ISIS we would have a field for the temperature of the sample. For LHC we might have a field for the beam-energy of the accelerator.

### **6.2.2 Measurements and Observations**

This class describes the properties of investigations which are measurements undertaken using a particular instrument to measure a physical quantity over time or space. It has much the same characteristics as experiments.

Thus the Measurement class has the following additional fields.

Instrument	Name of instruments used
Experimental Conditions	Environmental conditions within which the experiment was undertaken.
Parameters	Which physical characteristics are being measured and their units (and accuracy?).

We would expect further subclasses of experiment to be defined for particular facilities that are tailored to the special conditions applying in those cases; e.g. Isis experiment, SR experiment, or possibly experiments using particular instruments within those facilities.

Similarly, we would expect subclasses of conditions for different classes of experiments. Thus for ISIS we would have a field for the temperature of the sample. For LHC we might have a field for the beam-energy of the accelerator.

### 6.2.3 Simulation

For simulation we would expect the additional fields:

Machine	Description of the machine used to carry out the simulation.
Program	Program used to produce the simulation
Parameters	Input parameters to the simulation program.
Data	Input data to the simulation.

### 6.2.4 Parameters and Conditions

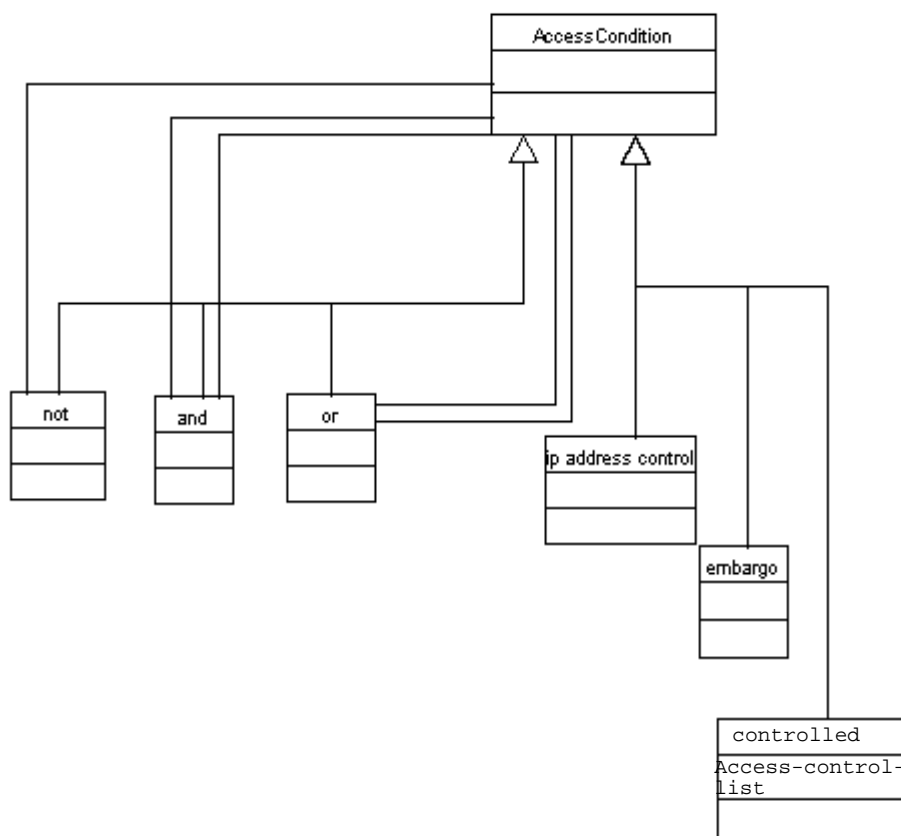
Parameters and conditions have a similar structure in the outset. Each is formed by a triple of *Name*, *Units* and *Value*. E.g. e.g. (Temperature, K, 150), (Atmospheric Pressure, milliBar, 1014). Units and Value are optional - this allows the name to be set and the other entries to be given later.

Name	The name of the parameters set or measured
Units	The unit of measurement in which the value is recorded.  <i>Issue: should the data portal querying system accommodate unit conversion? Should a default set of units (e.g. SI units) be built in?</i>
Value	The value recorded for this parameter/experimental condition.
Range	An optional indication of the range of values this parameter would be expected to take within the tolerances of the study. Typically would have top and bottom values.

## 7. ACCESS CONDITIONS

A description of the conditions that must be satisfied before a data set can be accessed.

Currently, this is left as a place-holder, but would potentially include access control lists, statements on access polices, conditions of use, and information on pricing and payment.



**Figure: Access Control Hierarchy**

Here we suggest one way in which this may be represented, as in the Figure.

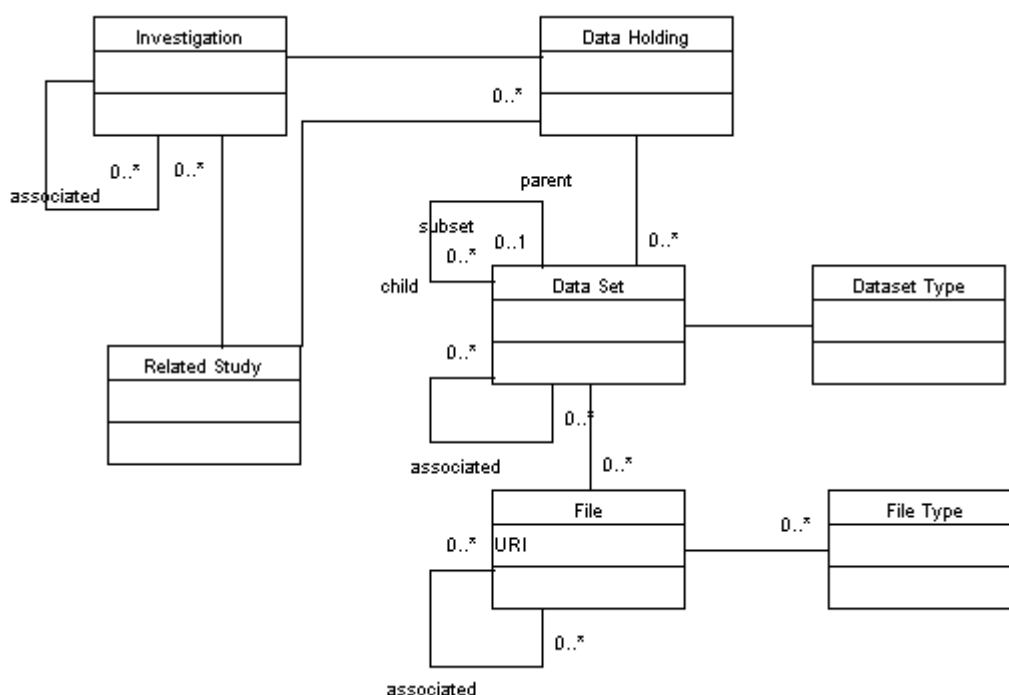
The model provides generic classes for providing access control features within the metadata model. The *Access Condition* class, defines the access control policy being used for this particular study. Some common access control policies, such as embargo until a fixed date, or testing the IP number of the user, or a lookup on an access-control list. Also some constructors (*and*, *or*, *not*) are provided for combining access conditions. Further access conditions can be provided in specific user packages, such as conditions for ISIS, or SRS. These access control policies can include restricting access to view the metadata itself as well as the data holding.

## 8. DATA DESCRIPTION

The data description maintains the description of the data itself.

### 8.1 Data Hierarchy

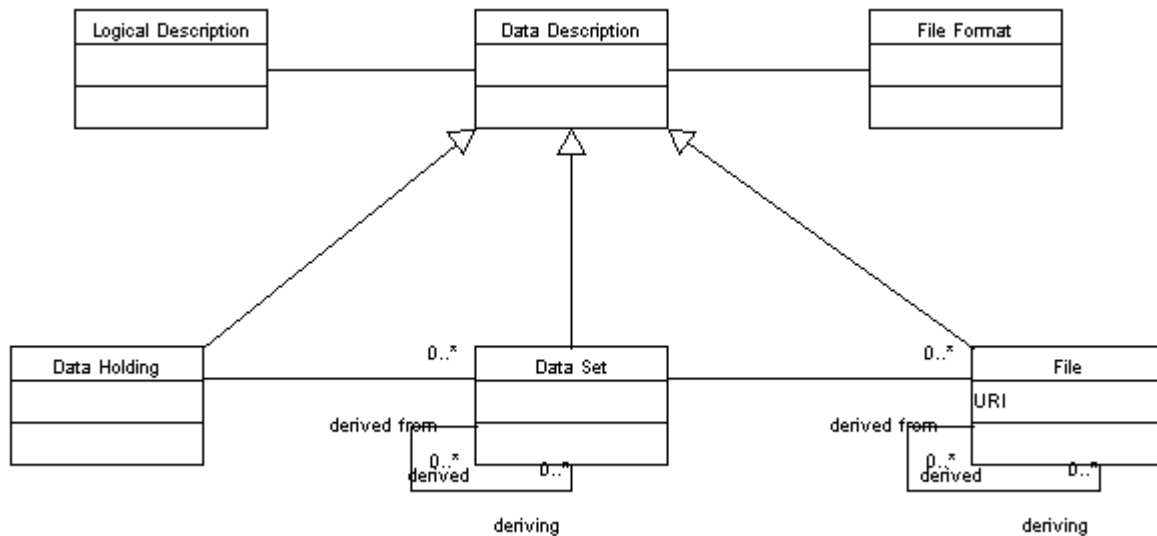
The data description, which relates to a single data holding, can be broken down into a hierarchy. The data description can have references to several related *data sets*, which have their type (e.g. “raw”, “intermediate” and “final”) recorded and general fields which cover all the particular files within each data set (both a logical and file description). Data sets can be further subdivided into a hierarchy of datasets, through a subset (“parent-child”) relation. Within data sets, there are *files*. Each file may have specific metadata, recording its URI, and any specific parameter settings for this file. E.g. in the Birkbeck protein crystallography archive, each image (to all intents and purposes a single file) could have different settings for the Crystal-to-detector distance. This hierarchy is shown in the following figure.



**Figure: Relationship between Investigations and Data Descriptions**

Each Data Holding is in a one to one relationship with a particular investigation. Further, there can be other relationships between data holdings and other investigations; mediated through a *Related Study*. These could include calibration studies, or previous results that are input to the analysis of this study.

Data holdings, datasets and files all share core metadata fields; this is reflected in their being represented as subclasses of the Data Description class in the following diagram.



**Figure: The Data Description class hierarchy.**

Thus a data description may have some general metadata associated with it covering all its data sets, and also one or more datasets. Each data set has a name, some both a logical and file description metadata, and a set of files. Each file has a name, some both a logical and file description metadata. Thus we are constructing a recursive hierarchy of descriptions. If the metadata for an item (say a file) cannot be found, then the parent data set’s metadata should be searched.

## 8.2 Fields for Data Descriptions

All data descriptions provide the following fields.

Name	Name of this particular data set
Type	Type of this data set – raw, intermediate, user, etc.
Status	Status of this data set – e.g. partial, complete, under review, error.
Logical description	Reference to a set of logical description fields.
File format	Reference to a set of file format fields



### 8.3 Logical Description

The logical description is the description of the data in terms of physical entities measured. This would include the following fields, although this is very experiment dependent.

Parameters	Names of parameters being measured, with units, range and value. Usually quantitative measures, with numerical values.
Conditions	Any extra conditions on this particular data set – restriction on <i>which part</i> of this study this covers. Usually qualitative measures – which material this run applies to, what catalyst is used etc.
Sampling rate	Rate of data capture
Coverage	Depending on discipline e.g. geographic location or radiation spectrum used.
Time	Time (range) of data capture.

### 8.4 File Formats

Description of the physical file formats used to store the data.

Typically there would be more than one file format for each data set – representing raw, intermediate and fully analysed data.

Fields could include such information as:

Array size	Size of the array stored in the format.
Record size	Size of the record in each field.
Encoding	Encoding of data for each type (floating point number)
Standard	Reference to some standard file format used.
Software	Reference to Software appropriate for analysing the data in this format.
Processor	Program used to produce this file format.

## 8.5 Additional Fields for Data Holdings.

Fields for the data description:

Data sets	References to the data sets within the data
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## 8.6 Additional Fields for Data Sets

Related Data sets	Data sets in other studies that this data set is dependent upon. Should correspond to an investigation associated with the current investigation.
Parent Data sets	The parent data set (if any) of the hierarchy of data sets.
Child data sets	The child data set in the hierarchy of data sets.
Derived From data sets	References to any data sets this data set has been generated from.

## 8.7 Additional Fields for Files

Related Files	Reference to a set of files which this file has some (non-parent) dependency – configuration, input data etc. Should respect the related data set condition of the bounding data set.
Parent files	References to any files this files has been generated from. Should respect the Parent relation of the bounding dataset.
URI	URI of this file.

**ISSUE:** At the moment, we are considering a file as the smallest “retrieval unit” – that is the smallest item of data which can be identified by the system. However, there may be a requirement to add additional metadata for identifiable sub-parts of files so that they can be retrieved independently. Extraction would frequently be on the basis of a sub-range of values of parameters in the file. There is no reason in principle why this data hierarchy should not be recursively extensible to cover this (W3C recommendations on XPointer and XML Fragments may well be useful in expressing this problem).

## 9. DATA LOCATION

Gives details on the location of the data sets associated with this investigation.

We propose to use a system of Uniform Resource Identifiers (URIs) and Uniform Resource Locators (URLs). *URIs uniquely identify a particular logical resource* - a data-set or subpart of a data set, and any associated programs, machines and other computing resources. *URLs uniquely identify locations on the Web*, typically but not necessarily files. The data location category of maintains a mapping between URIs representing the resources described in this metadata entry and the physical locations of those resources.

This distinction is made because:

- Physical locations of resources can move, while their identity remains the same. By using a URI and maintaining its mapping in one place, we can simply maintain the consistency of the metadata.
- A resource identified with one URI can have more than one physical manifestation in the form of copies, caches and mirrors, located using URLs. The map can maintain the correspondence to all of these and thus offer the user a choice of data source.

We propose to have a URI for each logical data set, and a mapping to URLs maintained in the data location component of the metadata.

This would include maintaining identifiers and locations for raw, intermediate and analysed data sets – the exact configuration of the location information would depend on the data used.

Maintaining a naive map between URIs and sets of URLs would soon get cumbersome and hard to manage (e.g. when a complete data set is moved without changing file names, this would require every URL to be changed individually). Thus we propose an alternative method of data location which reflects the structure of data descriptions given in section 8. This proposes a break down of data holdings into datasets and datasets into files, which have URIs.

Thus for each data holding, we give a set of fields:

Data holding name	The name of the data holding as given in the data holding's name field.
Data holding location	<p>Set of (partial) locators to physical locations; typically this will be to a URL to a directory within the data holders filestore. Each locator can be tagged with:</p> <ul style="list-style-type: none"> <li>• A comment on the nature of the data source (e.g. is primary or a mirror).</li> <li>• A comment on the medium of the storage (e.g. is it CDROM, tape archive, filestore etc).</li> <li>• Possibly a comment on how to access the data.</li> </ul>

For each data set we give a similar set of fields:

Data set name	The name of the data set as given in the data set's name field.
Data set location	<p>Set of (partial) locators to physical locations; typically this will be a directory structure within the data holders filestore. Each locator can be tagged with:</p> <ul style="list-style-type: none"> <li>• A flag indicating whether the locator is absolute or relative. <ul style="list-style-type: none"> <li>– If absolute, this locator can be used directly to locate the dataset – with reference to the data holding's locator.</li> <li>– If relative, combine with (any) of the locators within the parent data holding's data location entry to construct a location where the dataset can be accessed.</li> </ul> </li> <li>• A comment on the nature of the data source (e.g. is primary or a mirror).</li> <li>• A comment on the medium of the storage (e.g. is it CDROM, tape archive, filestore etc).</li> <li>• Possibly a comment on how to access the data.</li> </ul>

For each data file we give a similar set of fields:

Data file URI	The URI of the data set as given in the file's URI field.
Data set location	<p>Set of (partial) locators to physical locations; typically this will be a file within the data holders filestore. Each locator can be tagged with:</p> <ul style="list-style-type: none"> <li>• A flag indicating whether the locator is absolute or relative. <ul style="list-style-type: none"> <li>– If absolute, this locator can be used directly to locate the file – with reference to the data holding's locator.</li> <li>– If relative, combine with (any) of the locators within the parent dataset's data location entry to construct a location where the file can be accessed.</li> </ul> </li> <li>• A comment on the nature of the data source (e.g. is primary or a mirror).</li> <li>• A comment on the medium of the storage (e.g. is it CDROM, tape archive, filestore etc).</li> <li>• Possibly a comment on how to access the data.</li> </ul>

## 10. RELATED MATERIALS

This category would include contextual information associated with the resource being described.

This could include the following types of information:

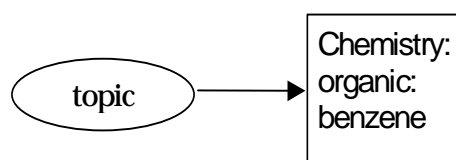
Publications	Publications reporting results derived from this dataset.
References	References to literature relevant to this dataset, but not derived from it.
Thesauri	References to controlled vocabulary describing the subject domain of the resource.
Related work	References to related investigations.
Community	References to the wider community that is working in this area.

## 11. EXAMPLE 1: THE ISIS SXD ARCHIVE

We give an example of a metadata record for an experiment on the ISIS facility, CLRC Neutron Spallation Instrument. The experiment is *Benzene, variable temperature study: 150K*, with the associated data files.

### 11.1 The Metadata Record

This set of data files for one study can be represented in one metadata record. Here we give a diagrammatic representation of this record (following the class-property diagrams of RDF).

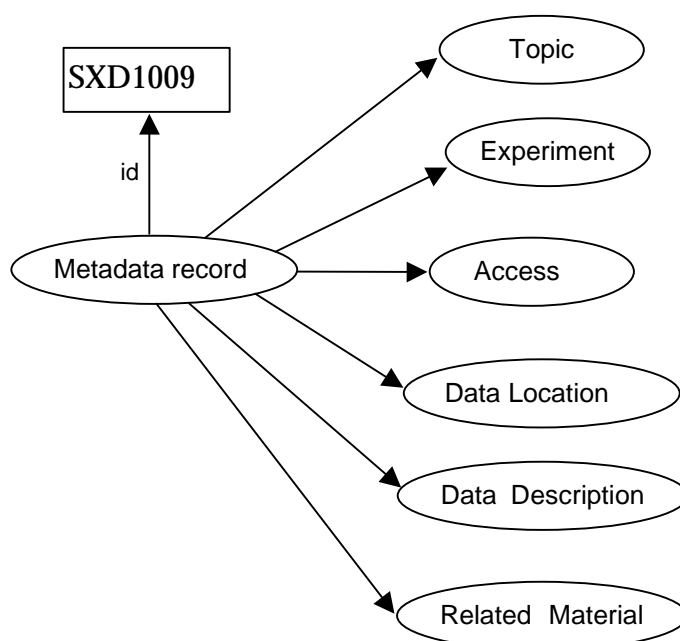


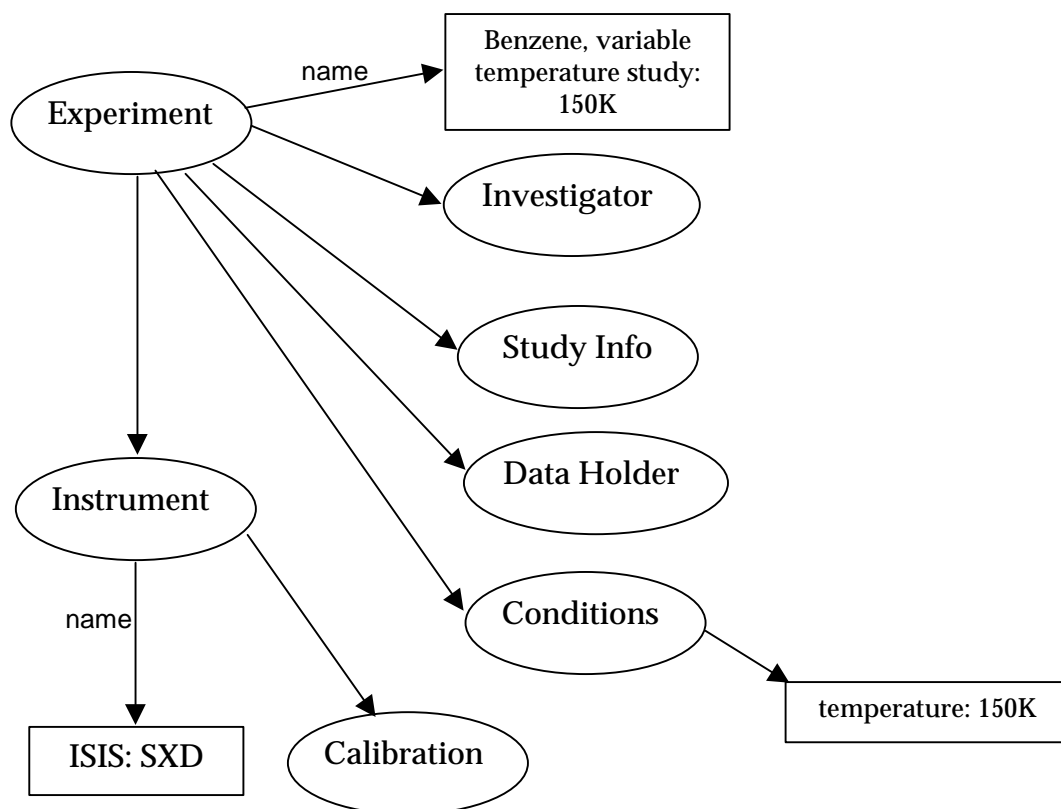
In this case, the Topic will be a structured value in a ontology, such as:

The study description will be an investigation, using the inheritance mechanism.

### 11.2 Tabular Description

We can also express these fields as a set of tables. Some values are pointers to other tables; this is denoted as *#fieldname*. The first table gives the top-level fields.





CLRC Metadata Record	
metadataID	PX0001
Topic	Chemistry: organic: benzene
Study	<i>#experiment</i>
Access	<i>#access</i>
Data location	<i>#location</i>
Data definition	<i>#data-definition</i>
Related material	<i>#related-material</i>



### 11.2.1 The Study Description

The experiment table gives details of this particular study; it is an experiment, as a subtype of study, so it has the additional experimental conditions and instrument fields..

<b>Experiment</b>	
StudyID	SXD10091
Study Name	Benzene, variable temperature study: 150K
Investigator	<i>#investigator</i>
Study Information	<i>#study-information</i>
Data holder	<i>#data-holder</i>
Instrument	<i>#instrument</i>
Environmental Conditions	<i>#conditions</i>
Parameters	??

The Investigator gives details of the people involved in the study.

<b>Investigator</b>	
Name	Anne X. Perimenter
Institution	University of Somewhere
Status	Lecturer
Role	Principal Investigator
Address	Dept of Organic Chemistry, Univ of Somewhere, Somewhere, UK.

Study information gives the information on this study.

<b>Study Information</b>	
Funding Source	EPSRC
Time	1/11/00, 11.45
Purpose	<i>#purpose</i>
Status	Complete
Resources	Beam time on ISIS using the SXD, for 1hr on 1/11/00

The Purpose itself may have several fields.

<b>Purpose</b>	
Abstract	To study the structure of Benzene at a temperature of 150K.
Keywords	Chemistry: organic: benzene: denatured benzene, C6H6, C6D6

The data holder refers to the institution principally responsible for holding the data – this is not a locator in the sense of a URL.

<b>Data Holder</b>	
Institution	ISIS, CLRC Rutherford Appleton Laboratory
Contact	Chick Wilson

The instrument will in this case be the SXD.

<b>Instrument</b>	
Name	ISIS SXD
Calibration	<i>Calibration information.</i>

The conditions in this case just record the temperature under which the sample has been studied.

<b>Conditions</b>	
Temperature	150K

### **11.2.2 Access**

Access is controlled by the access entry in the metadata record; how this is actually done is dependent on the topic area.. For example, there might be an access type, with settings such as “open”, “on application”, “restricted”, “commercial in confidence”. This may be given in conjunction with explicit instructions on how to access the data.

<b>Access</b>	
Access Type	On application
Conditions	The user must be a registered user of the ISIS facility. To register, apply to ISIS, CLRC RAL, UK.

### **11.2.3 Data Location**

The data location provides a mapping between the URI's used in the data definition component of the metadata model, and the actual URL's used in practice. This can provide facilities for describing mirror location for the whole structure, and also for individual files.

This will also have to accommodate different organisations of files – not just the raw/intermediate/final as given in the ISIS model. Giving filetype/directory pairs could do this:

Data holding locations	ftp://ftp.isis.rl.ac.uk/SXD/ SXD1009/  http://www.dooc.uos.ac.uk/~perimenter/bezene/
Data set Directories	(RAW, “raw/”), (Intermediate, “SXD/”), (HKL, “HKL/”), (INS, “INS/”), (RES, “RES/”).

Filenames can then be constructed from URIs.

### 11.2.4 Data Description

The data description would break down into a hierarchy of entries. Firstly the top-level entry, which contains references to the data sets of the study.

Data description	
Data Sets	<i>#raw, #intermediate, #processed</i>

Then the raw data set would have references to the *metadata* for each file (not the file itself):

Raw	
Dataset type	RAW
Files	<i>#SXD10091.RAW, #SXD10092.RAW, #SXD10093.RAW, #SXD10094.RAW, #SXD10095.RAW</i>

Then each file would have a metadata entry, giving its URI:

SXD10091.RAW	
URI	SXD10091.RAW

There will also be a dataset entry for intermediate files.

Intermediate	
Dataset type	Intermediate SXD
Parent Data set	RAW
Processor ( <i>this field would actually be in the file format record for this entry</i> ).	SF
Files	<i>#SXD10091.SF, #SXD10092.SF, #SXD10093.SF,</i>

With corresponding file description:

<b>SXD10091.SF</b>	
Parent files	SXD10091.RAW
URI	SXD10091.SF

Thus the system could track which files have been processed in particular ways.

**ISSUE:** I have not added any information on the parameters set in general, or for each dataset/file, or for any information on the logical and physical formats. This has fields in place in the metadata model, but I have not built them in (partly due to not enough information).

## **12. EXAMPLE: PROTEIN CRYSTALLOGRAPHY FROM BIRKBECK**

Birkbeck College has provided an example of a protein crystallography study.

<b>CLRC Metadata Record</b>	
metadataID	SXD10091
Topic	Chemistry: organic: protein: xxx
Study	<i>#experiment</i>
Access	<i>#access</i>
Data location	<i>#location</i>
Data definition	<i>#data-definition</i>
Related material	<i>#related-material</i>

### **12.1.1 The Study Description**

The experiment table gives details of this particular study; it is an experiment, as a subtype of study, so it has the additional experimental conditions and instrument fields.

<b>Experiment</b>	
StudyID	SXD10091
Study Name	Protein Crystallography on Protein xxx
Investigator	<i>#investigator</i>
Study Information	<i>#study-information</i>
Data holder	<i>#data-holder</i>
Instrument	<i>#instrument</i>
Environmental Conditions	<i>#conditions</i>
Parameters	??

The Investigator gives details of the people involved in the study.

<b>Investigator</b>	
Name	Claire Naylor
Institution	Birkbeck College ,University of London
Status	Lecturer
Role	Principal Investigator
Address	Dept of Crystallography Birkbeck College Malet St LONDON WC1E 7HX tel: 020-7631-6835 fax: 020-7631-6803 c.naylor@mail.cryst.bbk.ac.uk

Study information gives the information on this study.

<b>Study Information</b>	
Funding Source	EPSRC
Time	1/11/00, 11.45
Purpose	<i>#purpose</i>
Status	Complete
Resources	Beam time on SRS for 1hr on 1/11/00

The Purpose itself may have several fields.

<b>Purpose</b>	
Abstract	To study the structure of the protein xxx
Keywords	Chemistry: organic: protein:

The data holder refers to the institution principally responsible for holding the data – this is not a locator in the sense of a URL.

<b>Data Holder</b>	
Institution	SRS, CLRC Daresbury Laboratory
Contact	??

The instrument will in this case be the SRS Beamline – with a detector type (here we are going into the specific local metadata stored with the data at DL or BBK which gives details of the instrument we would not expect to store at the central repository.

<b>Instrument</b>	
Name	SRS, beamline 1,
Calibration	<i>Calibration information.</i>

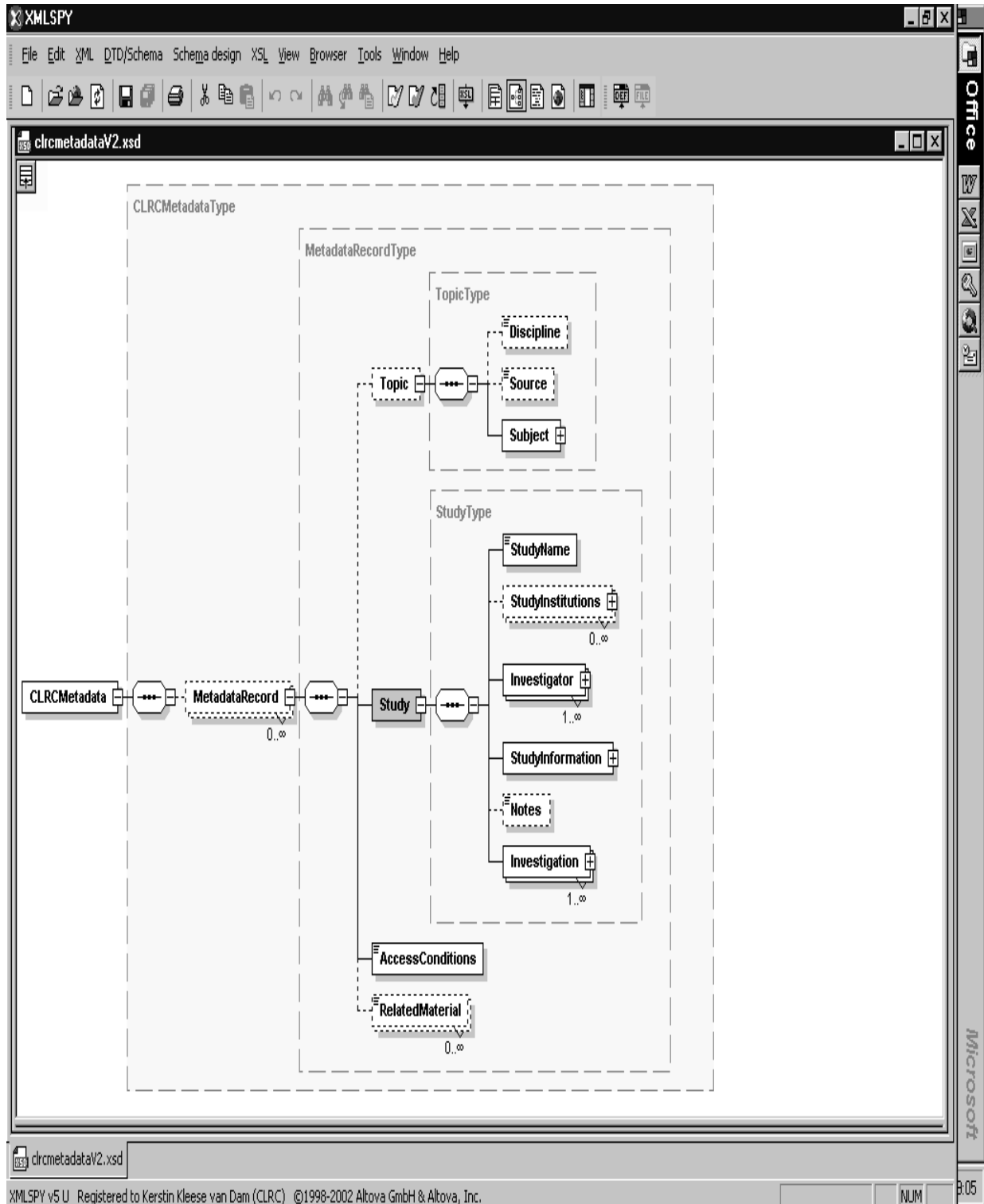
The conditions in this case just record the temperature under which the sample has been studied. Again, these fields are specific to this metadata for this experiment and would be stored at DL/BBK rather than the central repository.

<b>XP Conditions</b>	
Wavelength	
Crystal-to-detector distance	
Beam Centre	
Crystallisation conditions	



### 13. APPENDIX A – SCHEMA

Fig. 1: Top level metadata structure



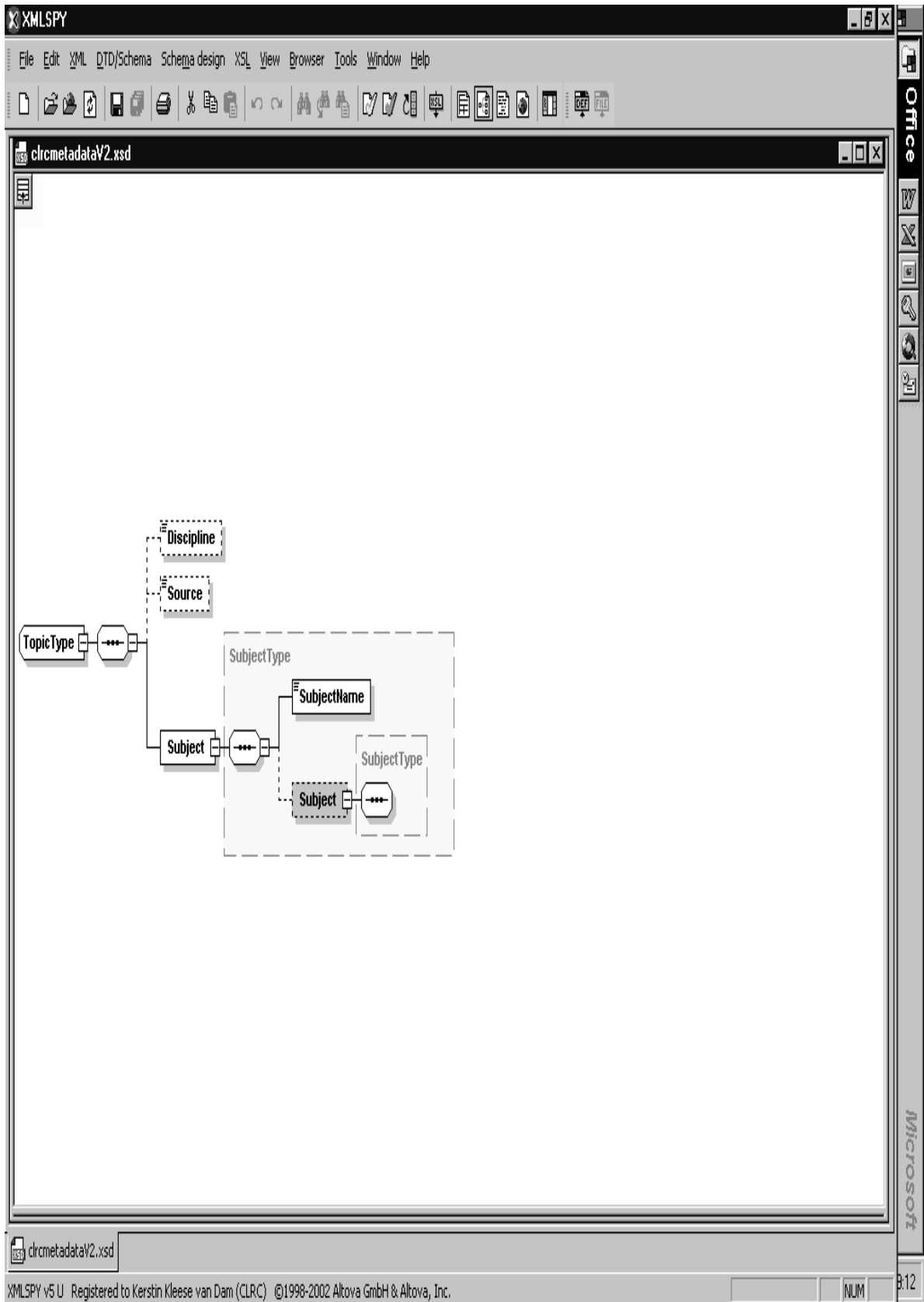


Fig. 2: Topic Metadata

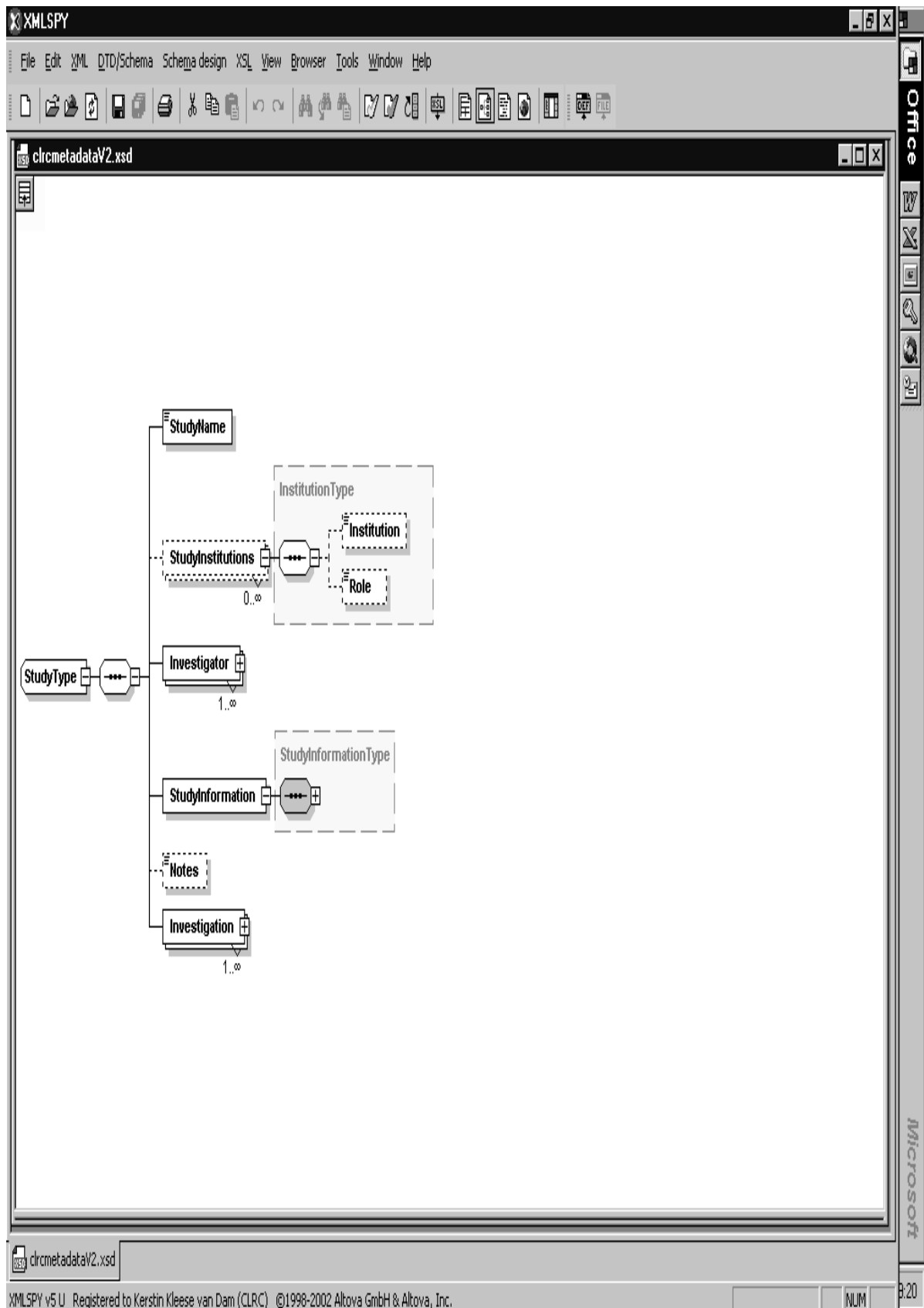


Fig. 3: Top Level Study Information

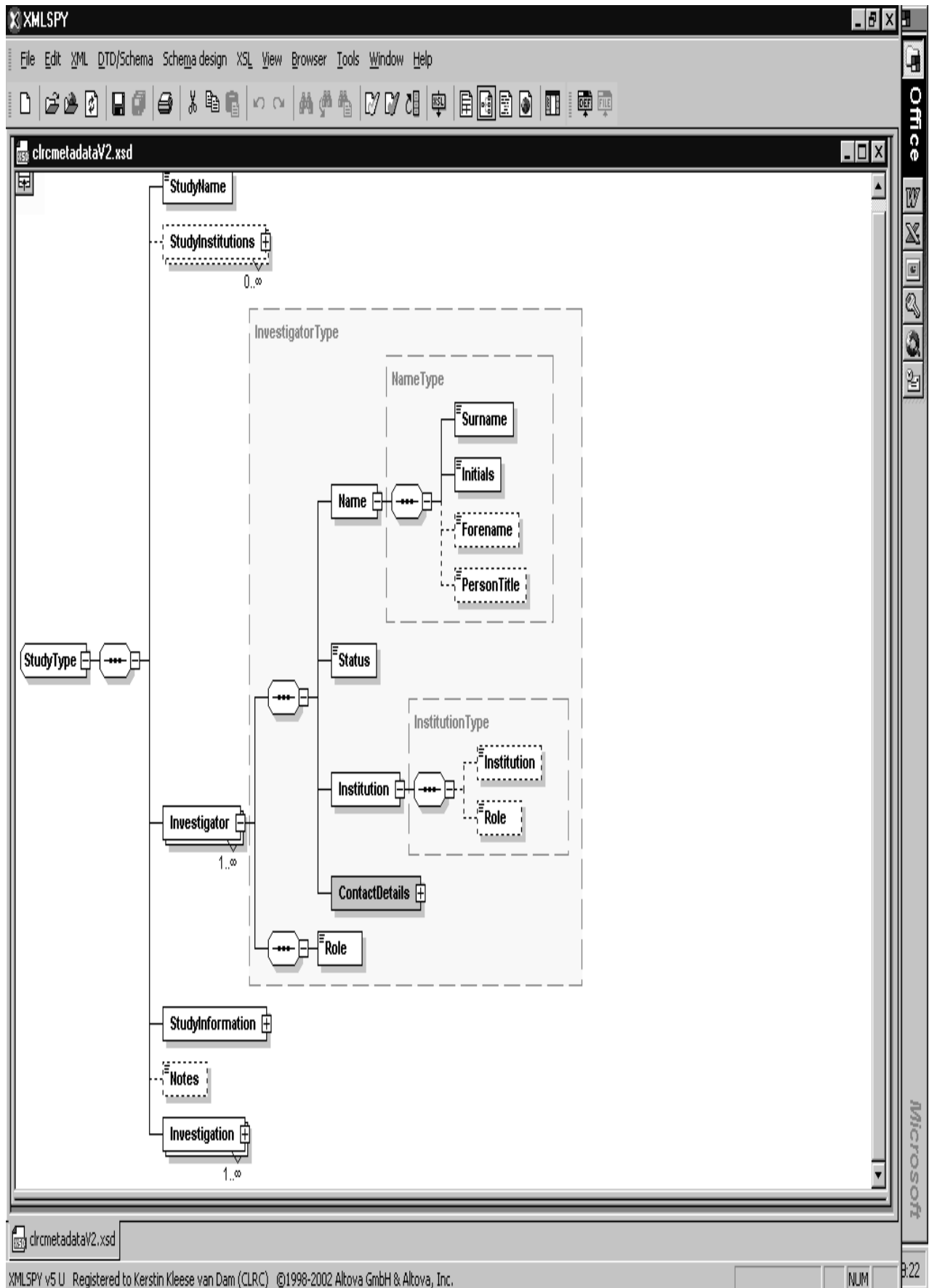


Fig. 4: Top Level Investigator Information

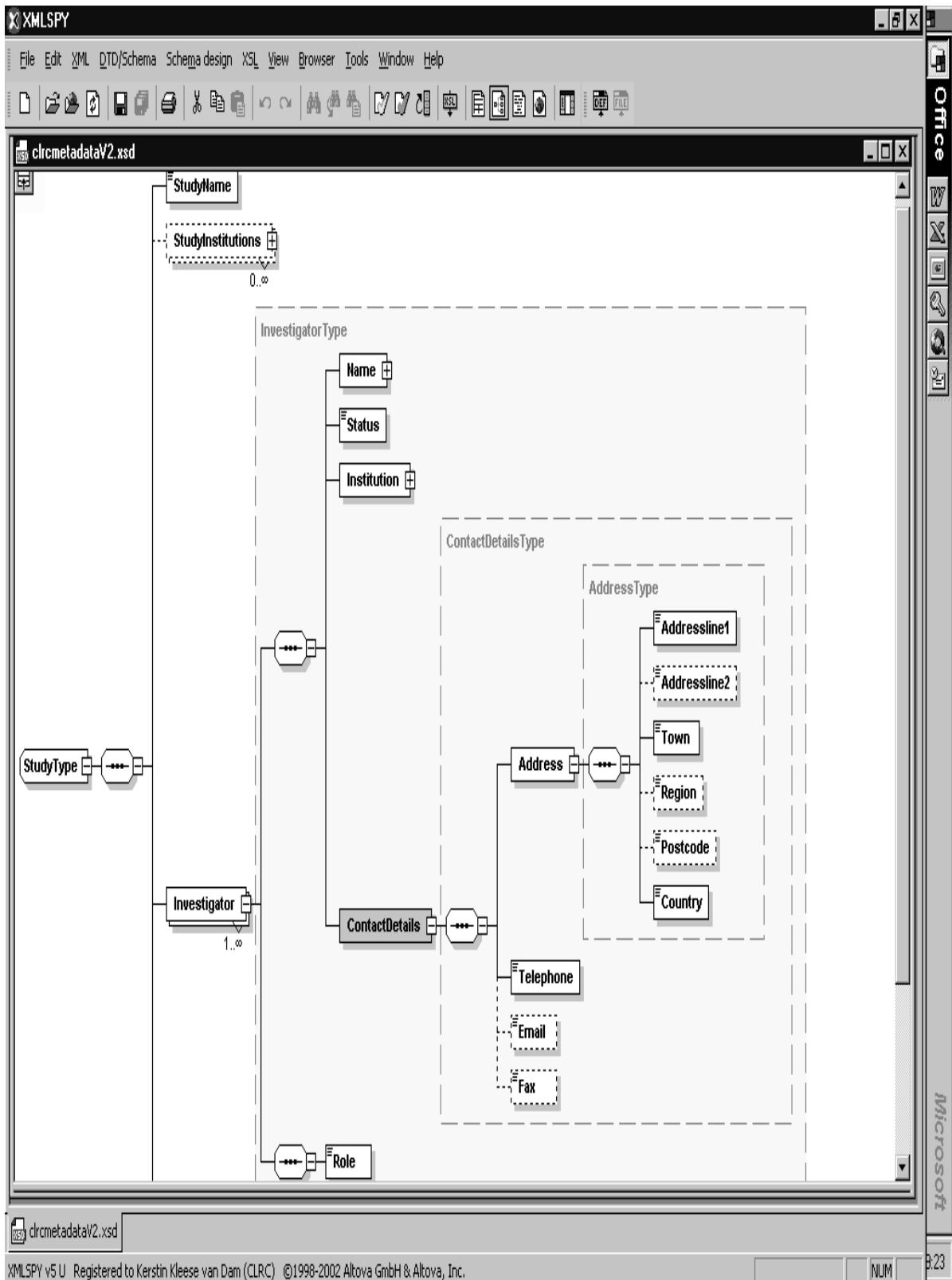


Fig. 5: Contact Detail Description for Investigators

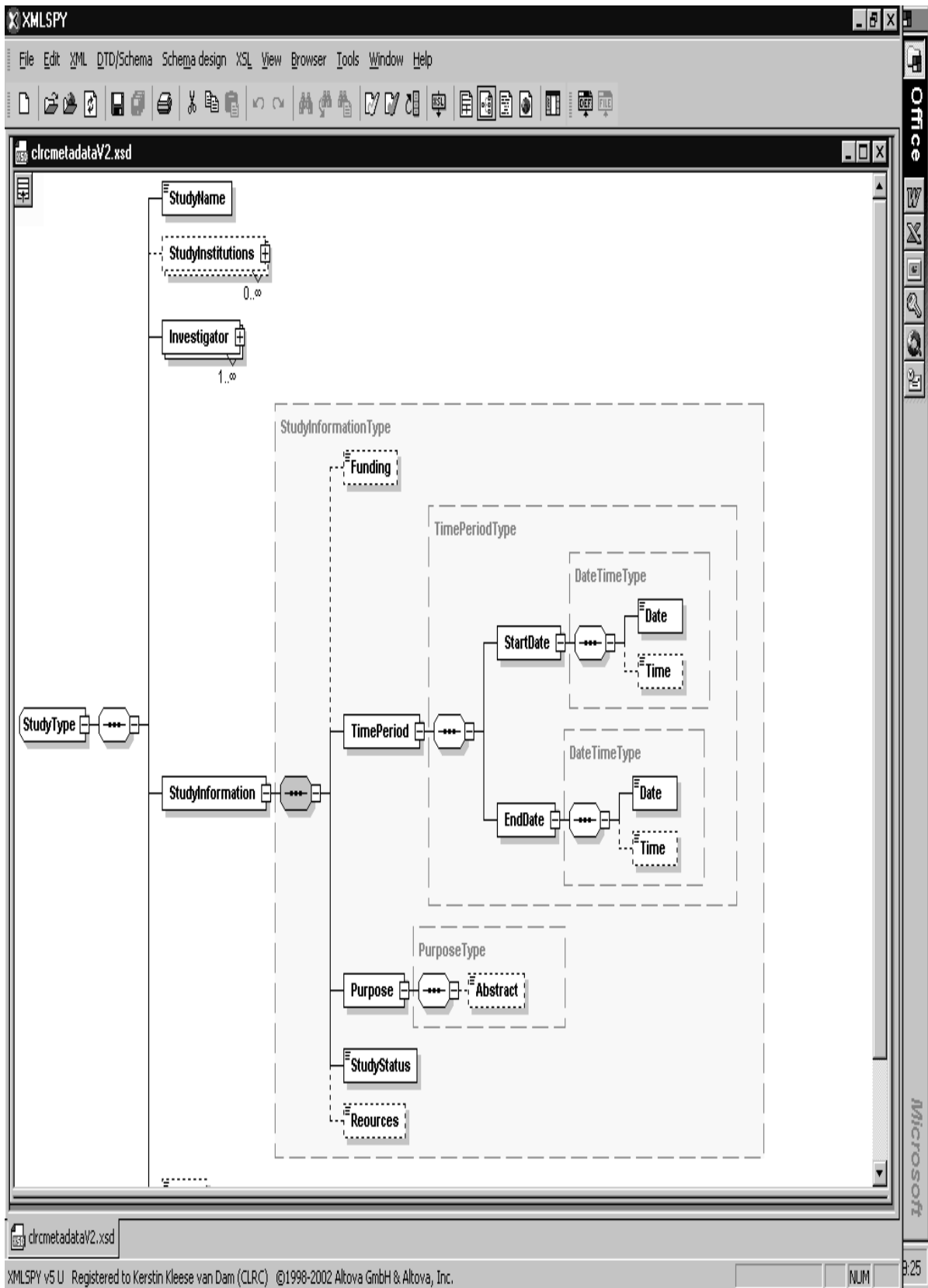


Fig. 6: General Study Information



Fig. 7: Top Level Metadata for Study - Investigation

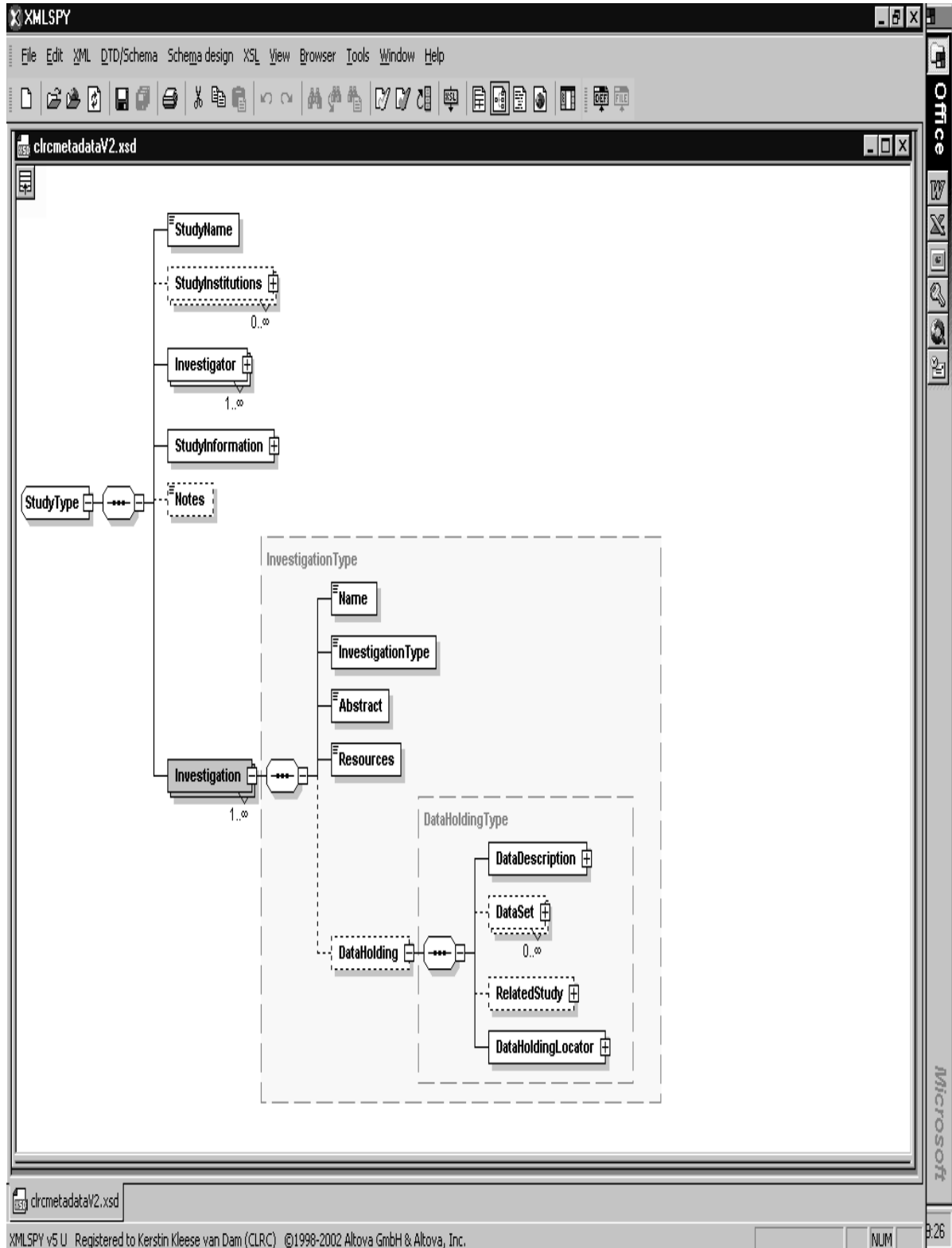
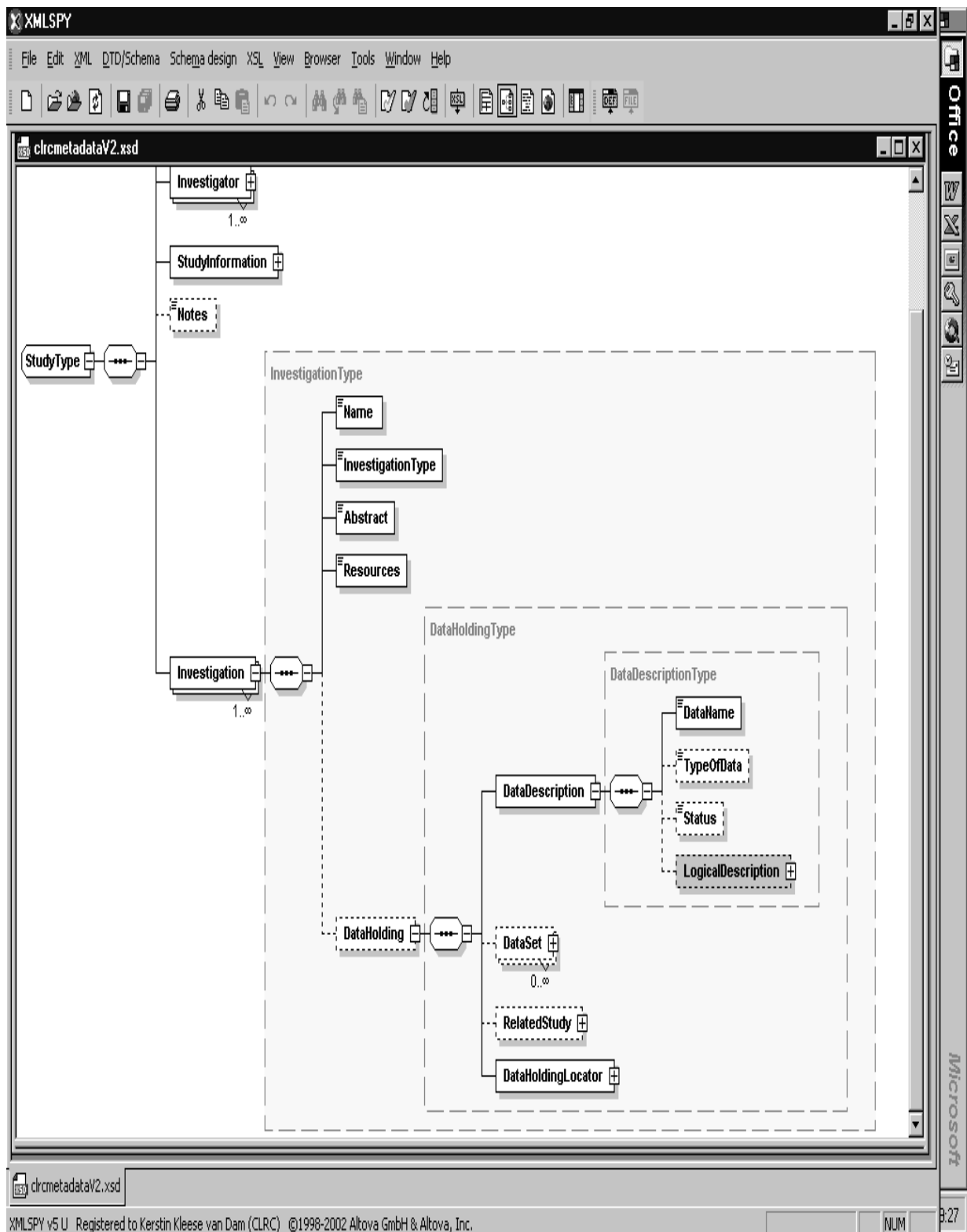




Fig. 8: Study – Investigation – Top Level Data Holding Metadata



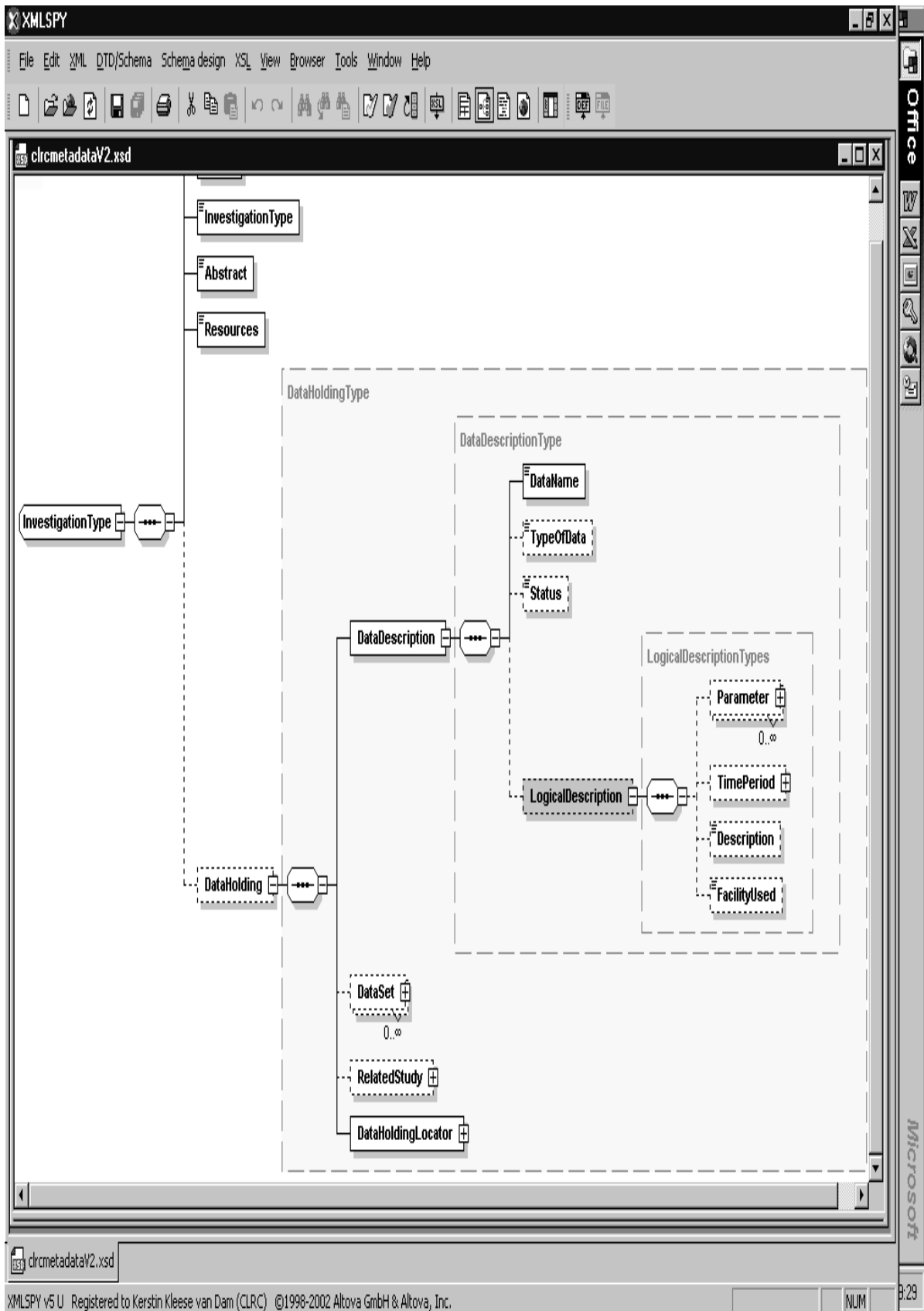


Fig. 9: Study – Investigation – Data Holding – Data Description – Top Level Logical Description Metadata

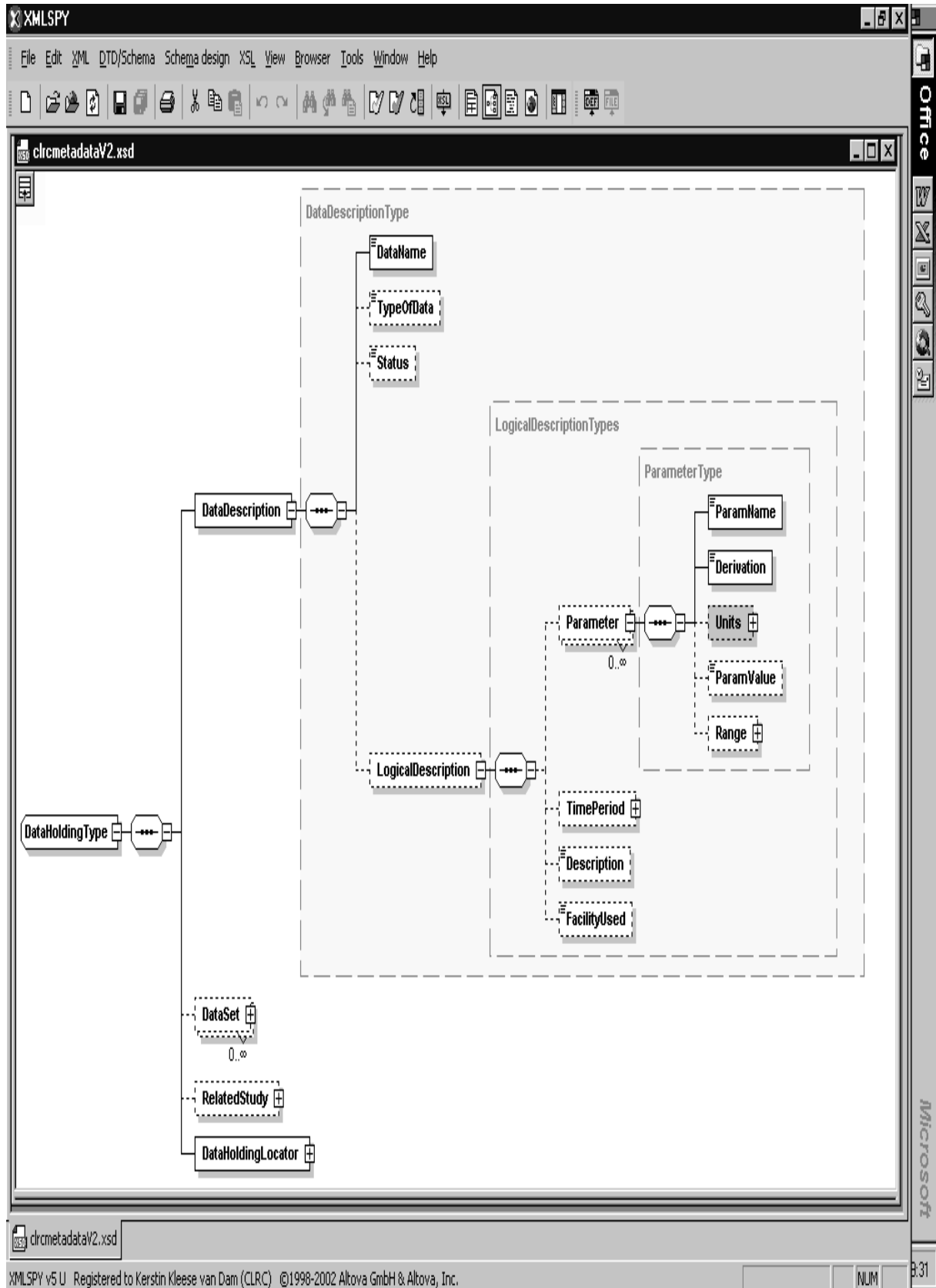


Fig. 10: Study – Investigation – Data Holding – Data Description – Logical Description – Top Level Parameter Metadata

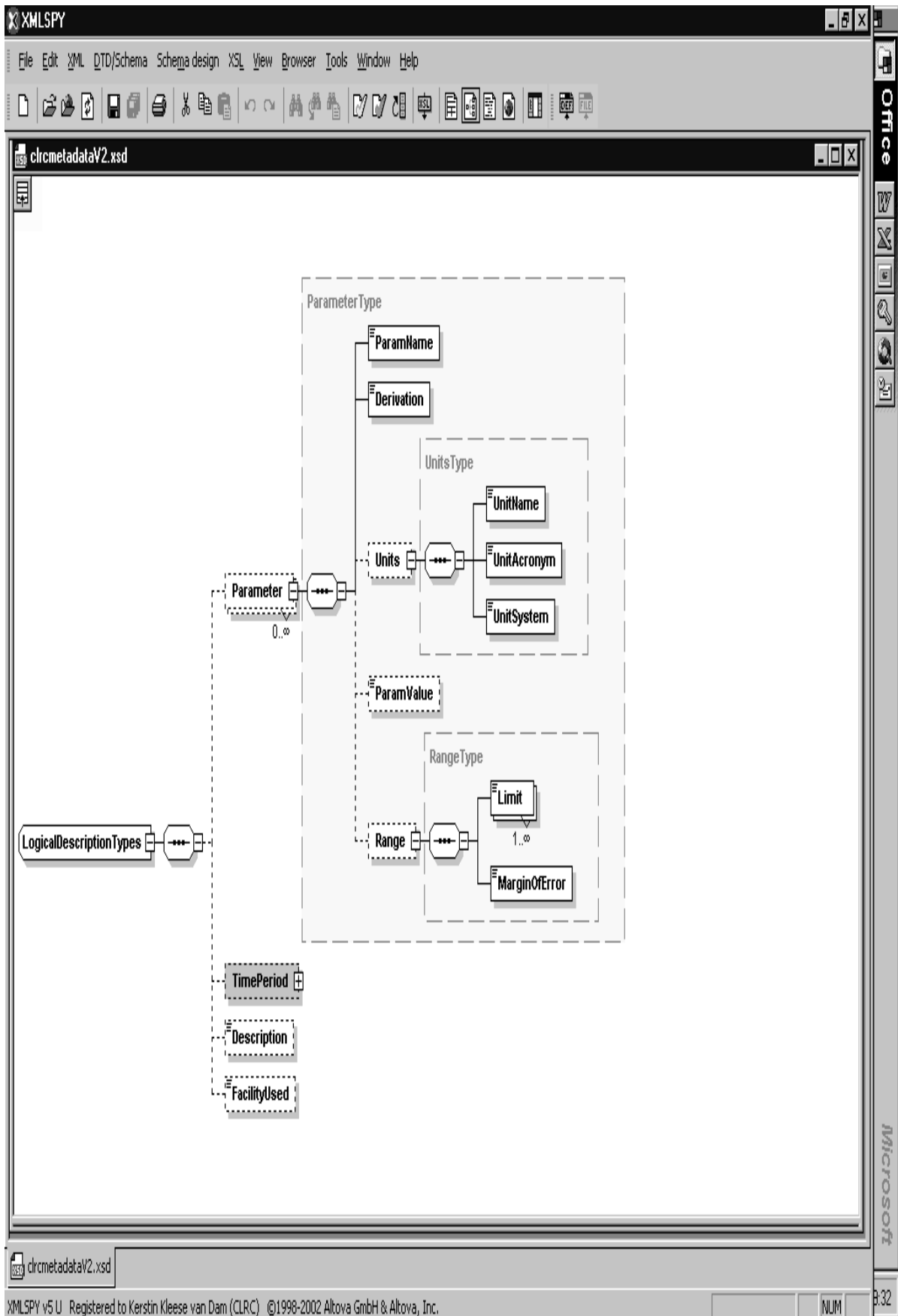


Fig. 11: Study – Investigation – Data Holding – Data Description – Logical Description – Parameter Metadata

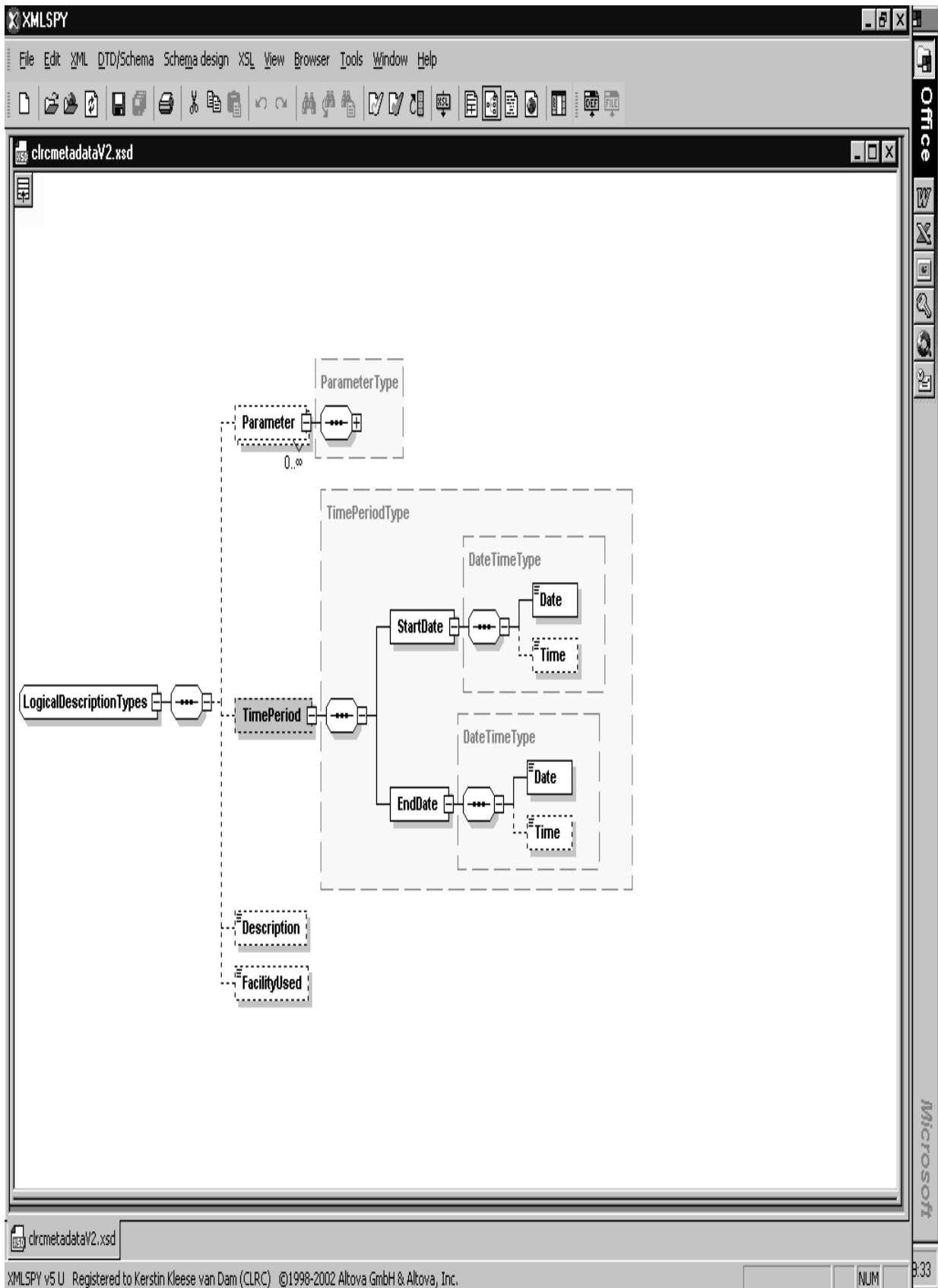


Fig. 12: Study – Investigation – Data Holding – Data Description – Logical Description – Time Period Metadata

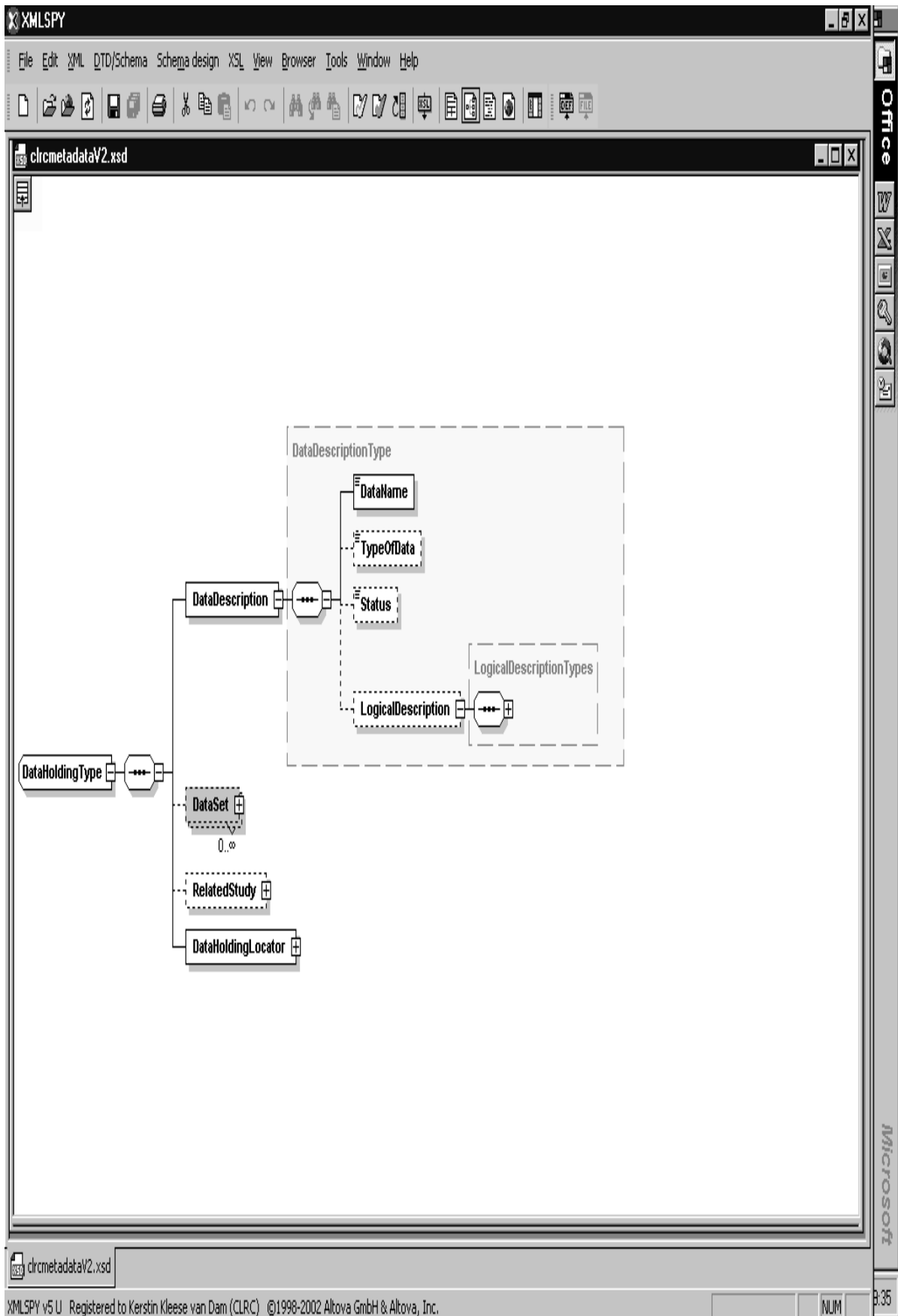


Fig. 13: Study – Investigation – Top Level Data Holding Metadata

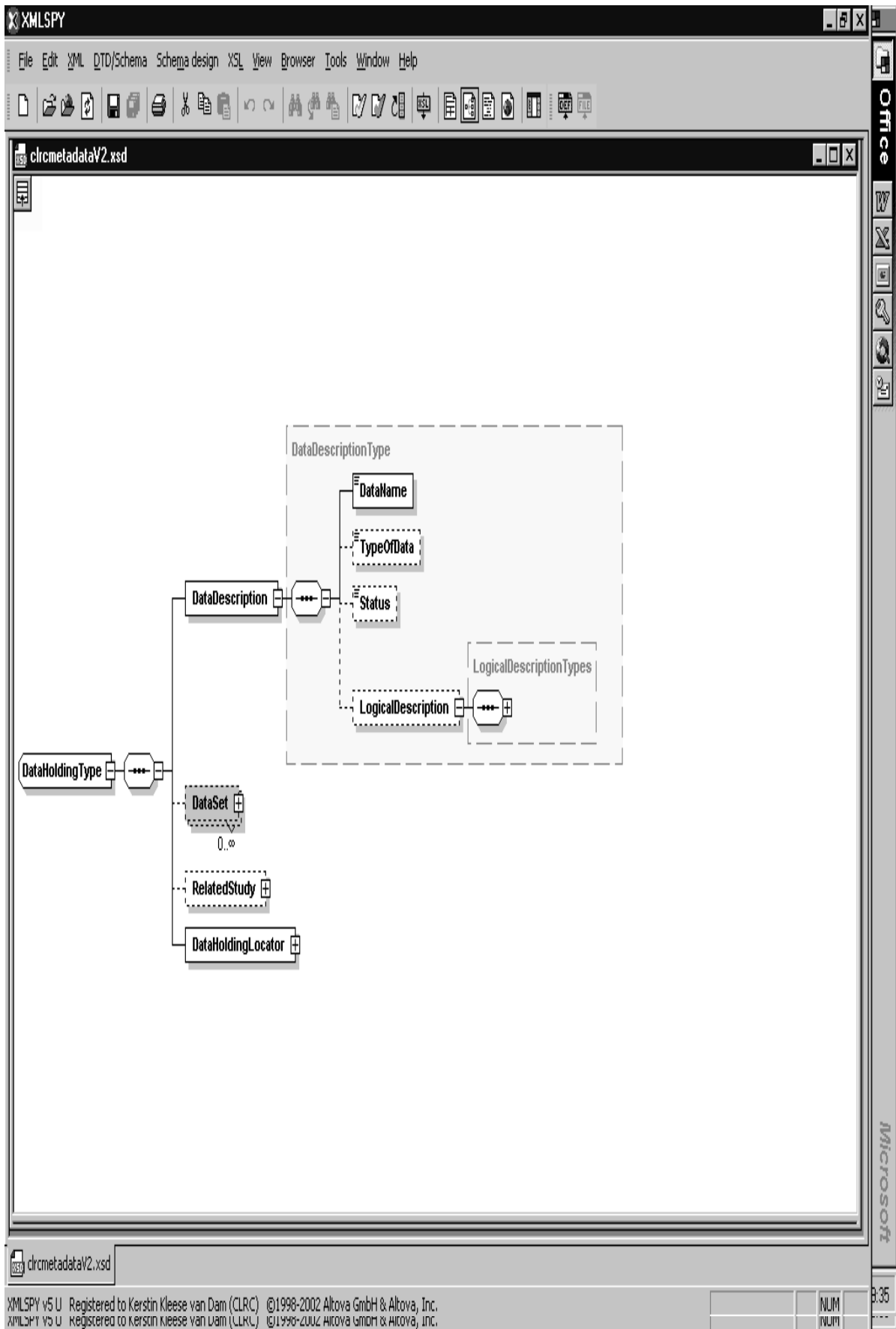


Fig. 14: Study – Investigation – Data Holding Metadata

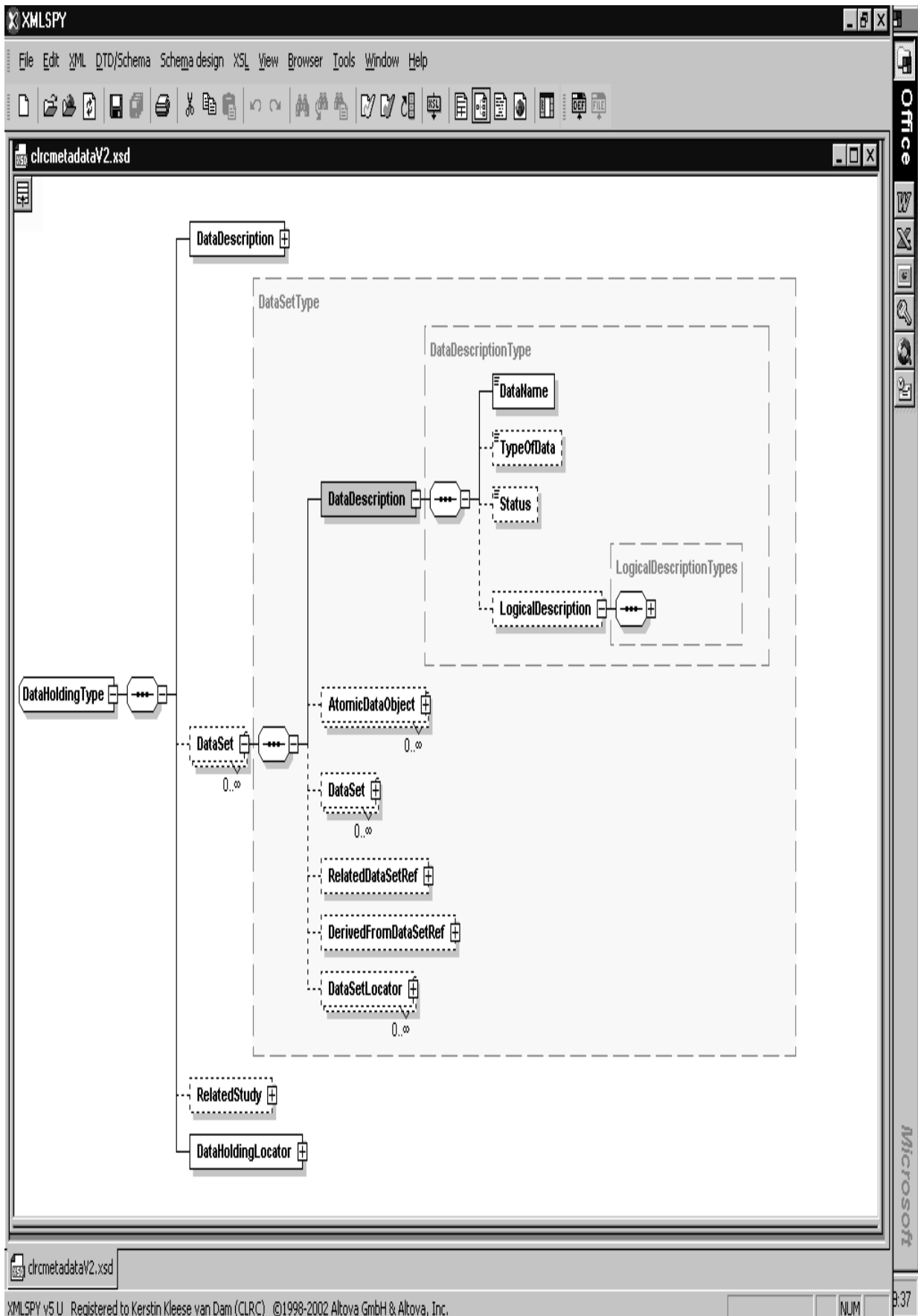


Fig. 15: Study – Investigation – Data Holding – Top Level Data Set Metadata



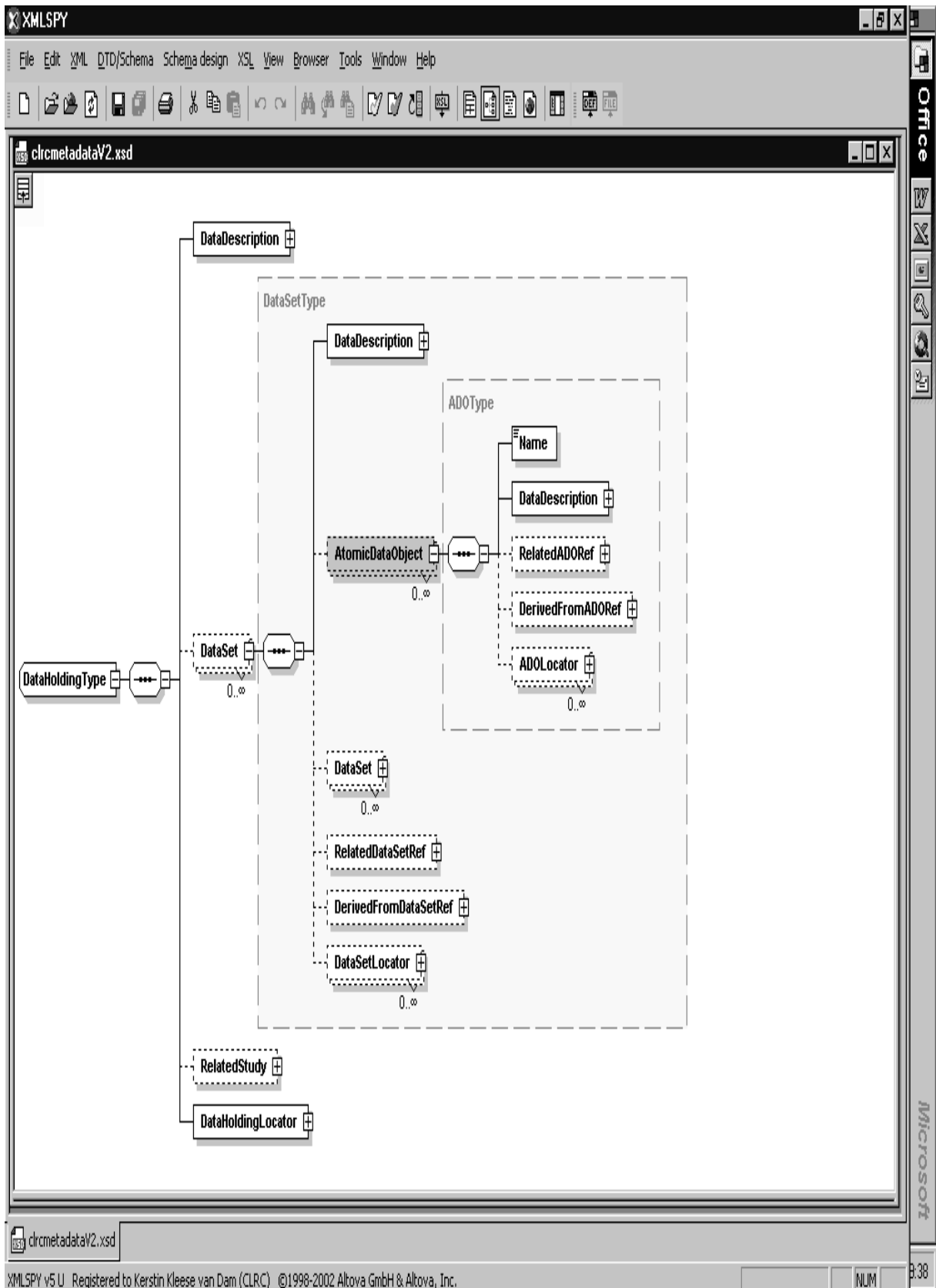


Fig. 16: Study – Investigation – Data Holding – Data Set – Top Level Atomistic Data Object Metadata

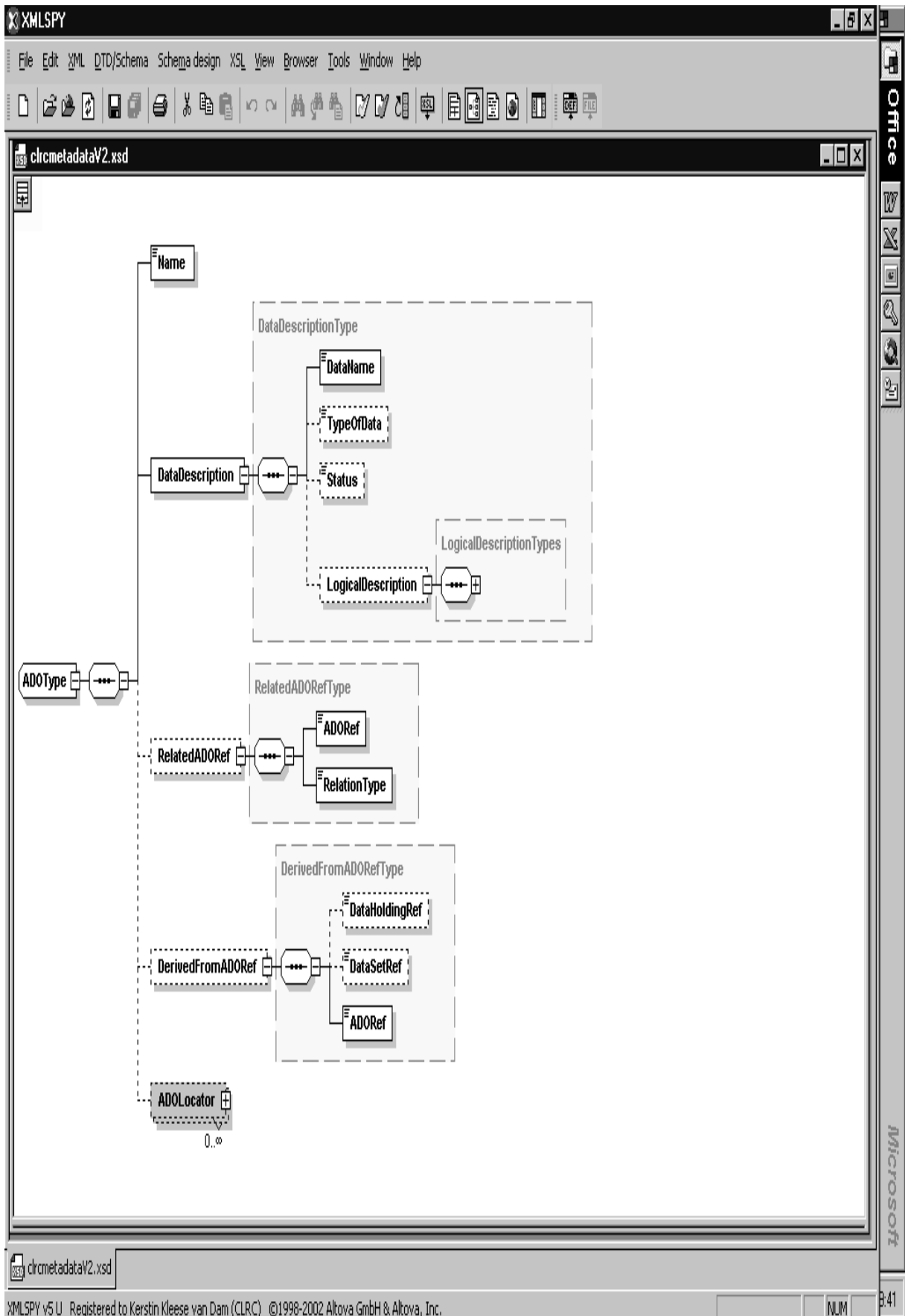


Fig. 17: Study – Investigation – Data Holding – Data Set – Atomistic Data Object Metadata (1)

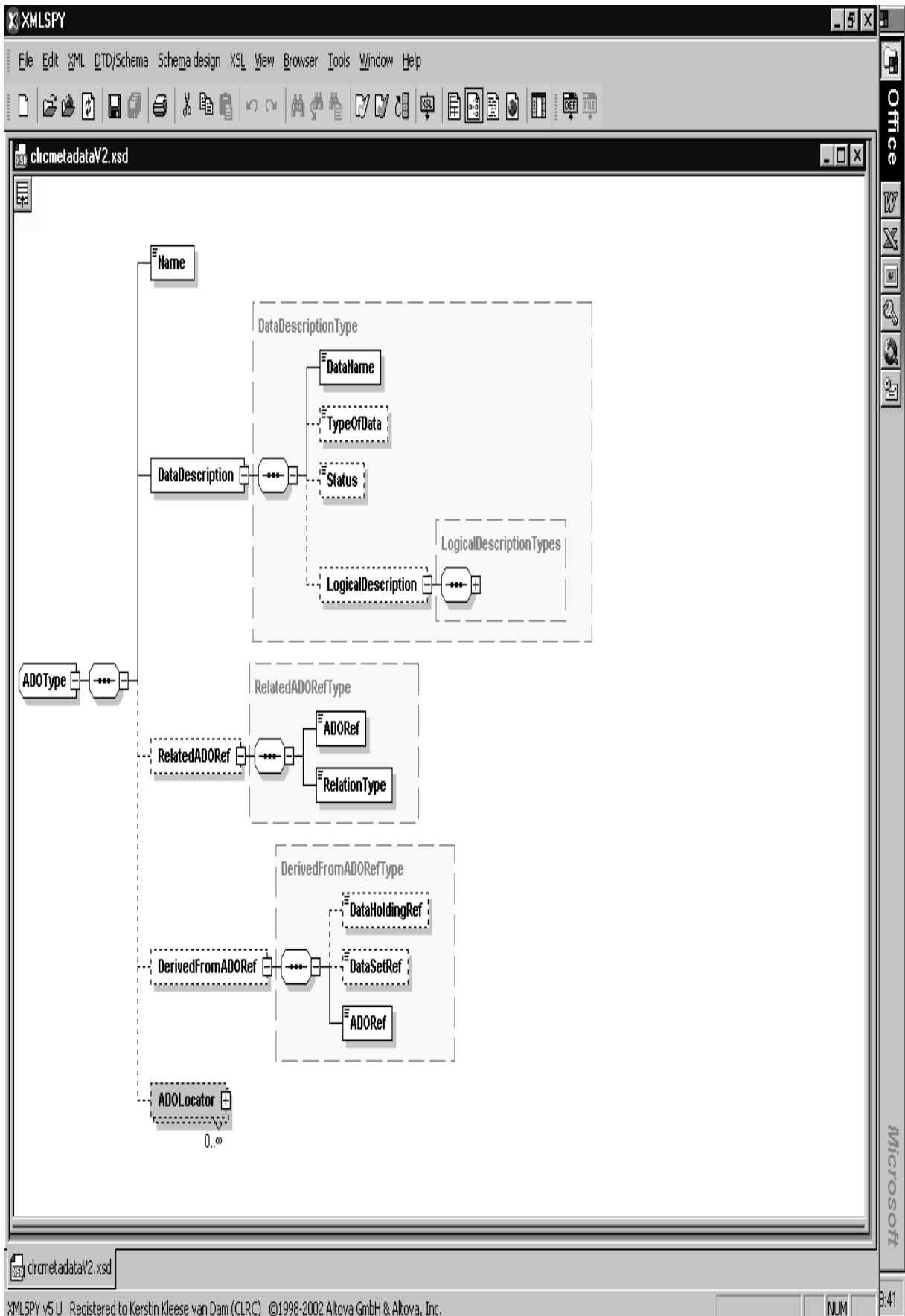


Fig. 18: Study – Investigation – Data Holding – Data Set – Atomistic Data Object Metadata (2)

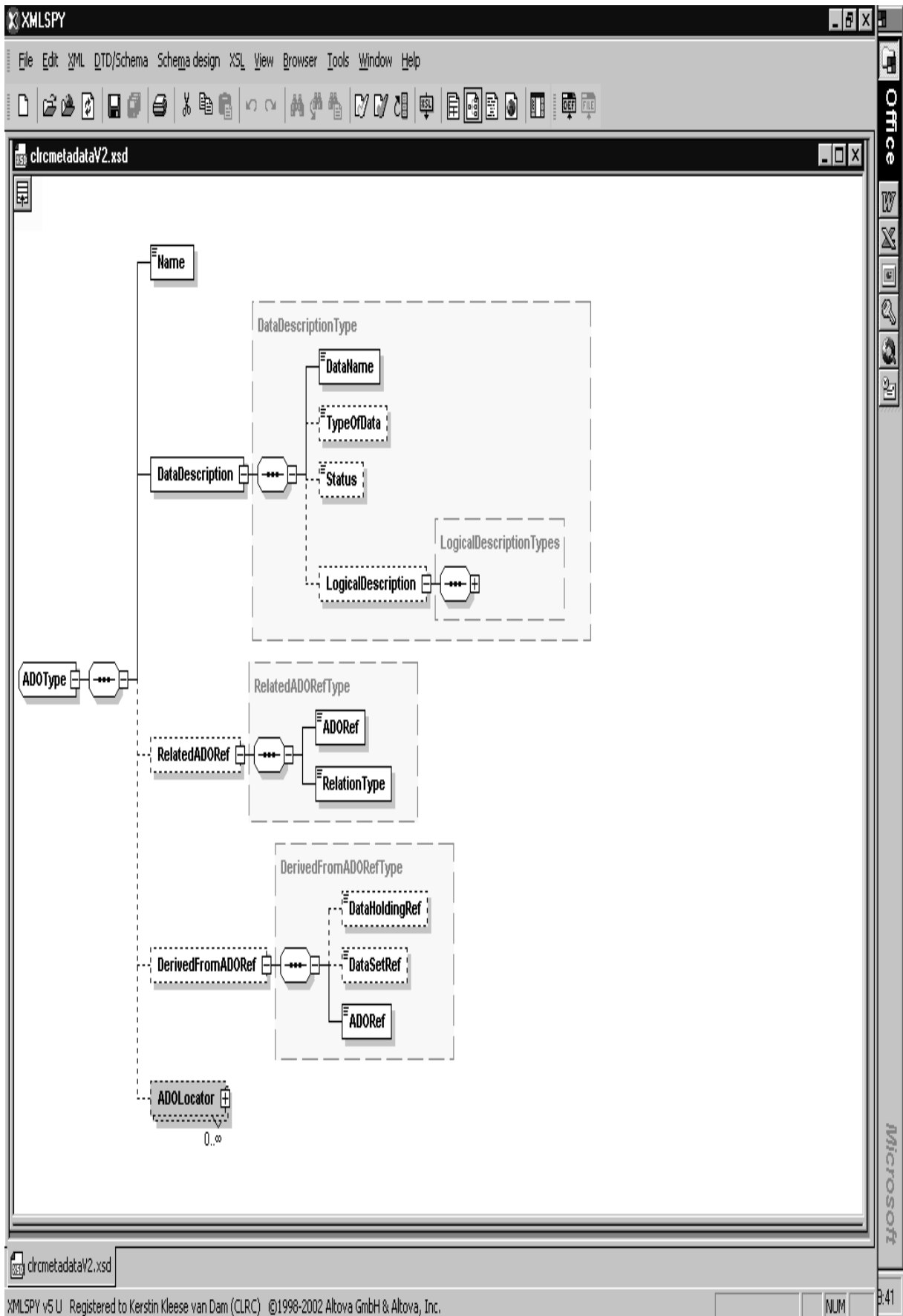


Fig. 19: Study – Investigation – Data Holding – Top Level Data Set Metadata (2)

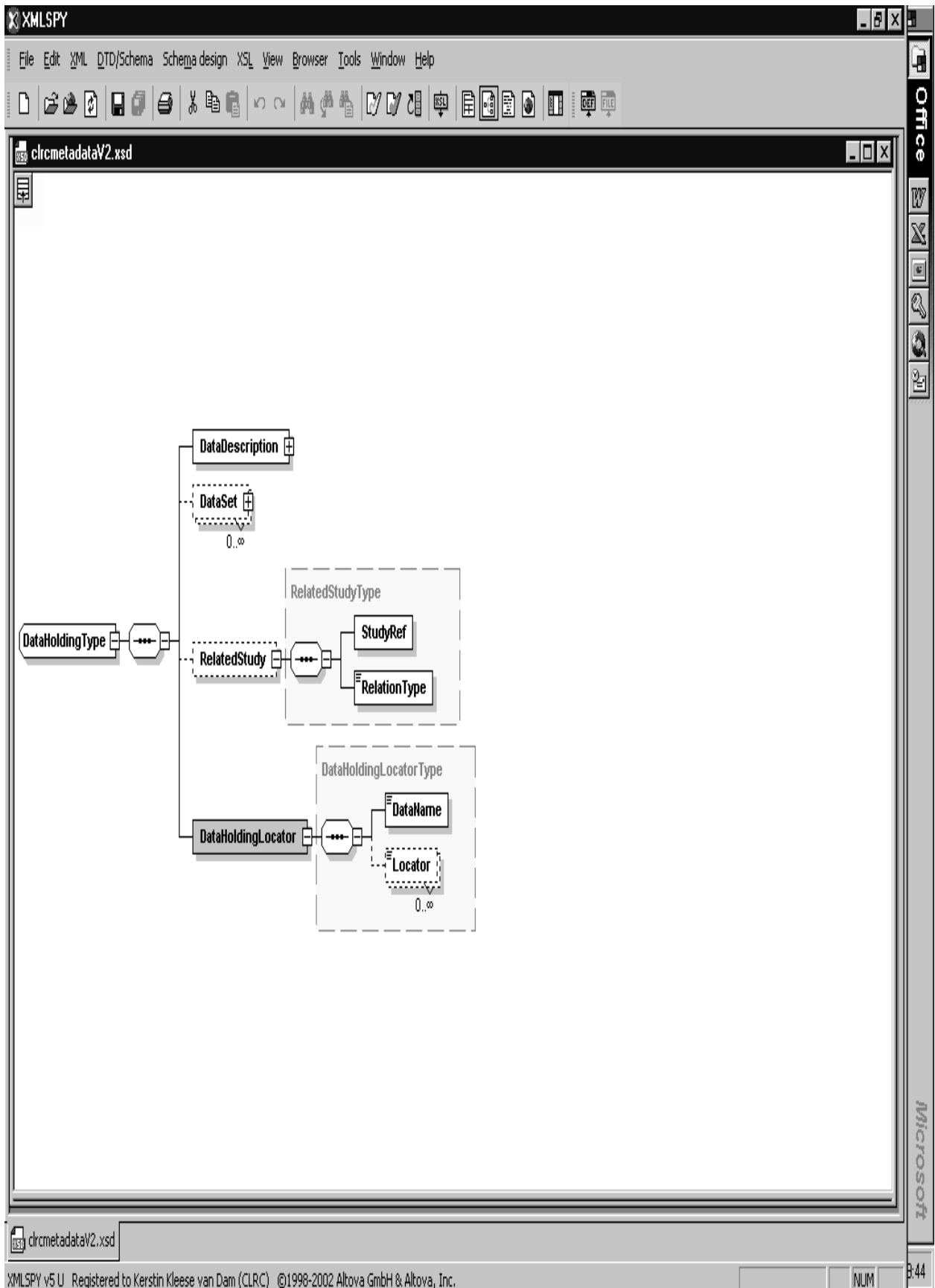


Fig. 20: Study – Investigation – Top Level Data Holding Metadata (2)

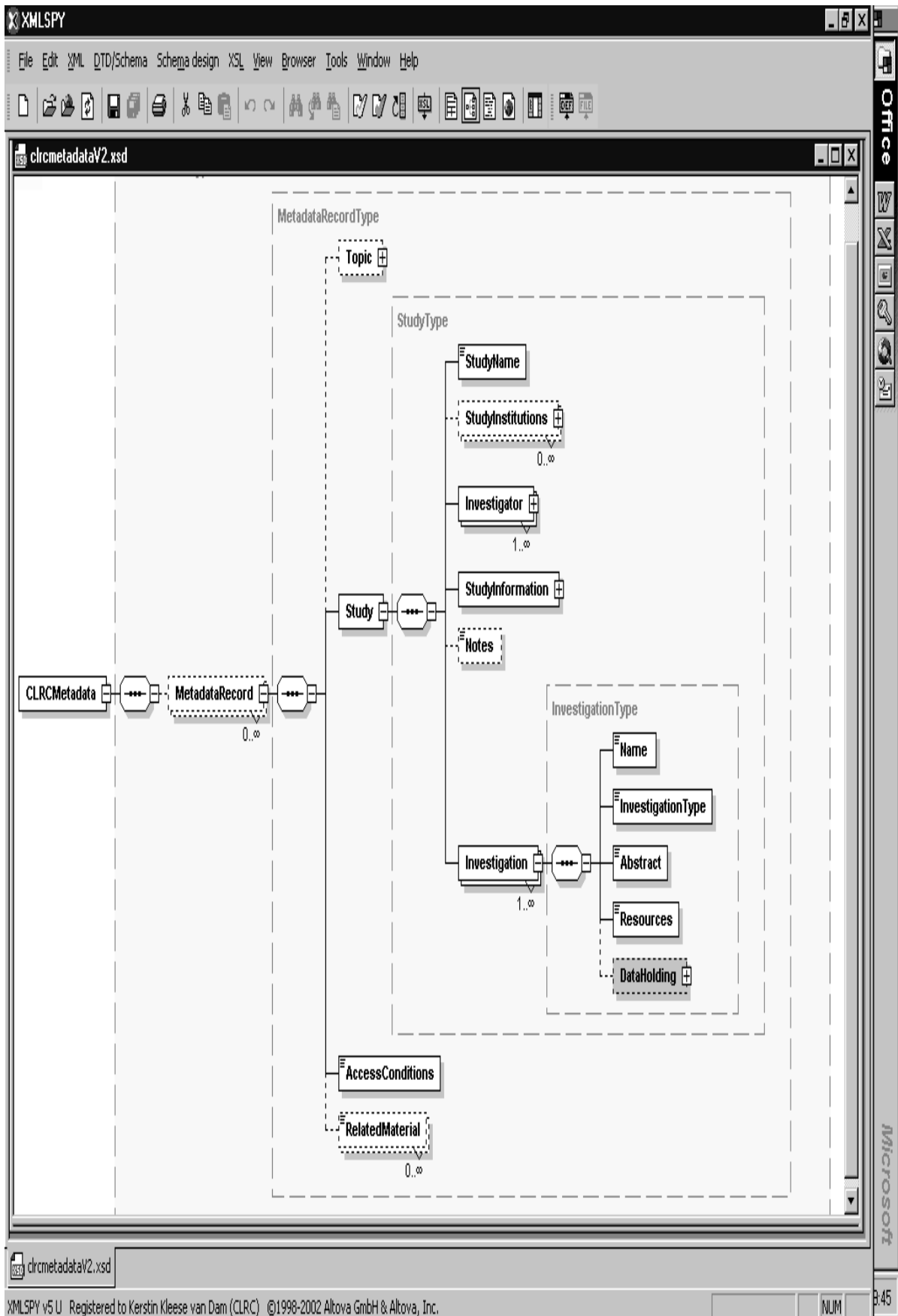


Fig. 21: Top Level Study Metadata (2)

## 14. APPENDIX B – CLRC SCIENTIFIC METADATA DTD

```
<!-- ***** -->
<!-- clrcmetadata.dtd -->
<!-- v.1.3.2 -->
<!-- 15/05/02 -->
<!-- -->
<!-- A DTD to represent the CLRC Scientific -->
<!-- Metadata format. -->
<!-- -->
<!-- (changes made by Shoaib Sufi, E-Science) -->
<!-- Brian Matthews -->
<!-- Data Portal Project -->
<!-- ITD-CLRC -->
<!-- -->
<!-- Based on the first draft CLRC Metadata -->
<!-- November 2000. -->
<!-- -->
<!-- This represents a first pass to provide a common -->
<!-- understanding and initial implementation. -->
<!-- This is not likely to prove the best approach and -->
<!-- a move to XML Schema and/or RDF is more suitable -->
<!-- for the design of the metadata model. -->
<!-- -->
<!-- CHANGE HISTORY -->
<!-- Created: 29/11/00 -->
<!-- 27/01/01 - StudyID missing in Study - added. -->
<!-- 31/01/01 -->
<!-- - DataHolder changed to DataManager.
- DataManager Moved to Investigation
- studyref attribute type changed to IDREF
```

- StudyID changed from #PCDATA to studyid attribute
- optional Institution added to StudyID
- StudyID source attribute changed to institutionref
  
- CLRCMetadata changed to MetadataEntry
- new top level CLRCMetadata element - groups a list of MetadataEntry elements.
  
- element Calibration removed.
  
- elements Parameter and Condition given a structure of triples  
(ParamName, Units, Value).
- Units taken out of LogicalDescription - subsumed into Parameter
  
- Role moved from PersonClass to Investigator
  
- added Time, Date, TimeRange and more structure to TimePeriod.
- added TimePeriod to LogicalDescription.

-->

<!-- 06/02/01 -->

- <!-- - MetadataRecord changed from optional %DataDescriptionClass;  
to optional DataHolding
- dataid attribute added to DataDescription elements,  
dataidref attribute added to DataLocation elements.

-->

<!-- 13/02/01 - v.1.3.0 -->

- <!-- - Topic under Purpose removed - just have top-level topic  
to remove confusion
- Range moved to be an optional value on a Parameter.
- Limit elements, with possible top and bottom attributes  
added explicitly to range.
- ChildDataSetRef added.



```

- DerivedFromDataSetRef added.

- ParentFileRef changed to DerivedFromFileRef

- Optional DataSetRef and DataHolding (should it be Study - yes?) added to
  DerivedFromFileRef

- Optional DataHolding (should it be Study - yes?) added to Derived from
  data set. ParentDataSet does not need this as has to be in same data holding.

- added Condition to LogicalDescription.

-->

<!-- 21/02/01 - v.1.3.1 -->

<!-- - Timeperiod changed to give start and optional end date - no
- infinite regress.

-->

<!-- 15/05/02 -v.1.3.2 some changes made for easier integration of -->

<!-- XMLWrappers -->

<!-- -->

<!-- ***** -->

<!-- Entity definitions to "represent" the OO model -->

<ENTITY % InvestigationClass 'Experiment | Measurement | Simulation'>

<ENTITY % StudyClass '(Programme | %InvestigationClass;)'>

<ENTITY % Study 'StudyName, StudyID*, Investigator+, StudyInformation, Notes?*>

<ENTITY % Studyatts ">

<ENTITY % Investigation '%Study;, DataManager'>

<!-- associated refer to other CLRCMetadata element IDs. -->

<ENTITY % Investigationatts "%Studyatts; associated IDREFS #IMPLIED">

<!-- Top Level -->

<ELEMENT CLRCMetadata (MetadataRecord*)>

<ELEMENT MetadataRecord (Topic, %StudyClass;, AccessConditions, DataHolding?, DataHoldingLocator?,
RelatedMaterial?)*>

<ATTLIST MetadataRecord
  metadataID ID #REQUIRED
>

<!-- Topic categorisation -->

<ELEMENT Topic (Discipline?, Source?, Subject+)*>

```

```

<!ELEMENT Discipline (#PCDATA)>
<!ELEMENT Subject (#PCDATA)>
<!ELEMENT Source (#PCDATA)>
<!-- Then these entities are used like this to build the class hierarchy. -->
<!-- subStudies refer to other CLRCMetadata element IDs. -->
<!ELEMENT Programme (%Study;)>
<!ATTLIST Programme
    %Studyatts;
    subStudies IDREFS #IMPLIED
>
<!-- There will be further subtypes of both Experiment and Simulation -->
<!-- but for the central repository, where these are fixed, we can ignore them, and stick to this DTD -->
<!ELEMENT Experiment (%Investigation;, Instrument, Condition*, Parameter*)>
<!ATTLIST Experiment
    %Investigationatts;
>
<!-- Measurement currently the same as Experiment - probably shouldn't be -->
<!ELEMENT Measurement (%Investigation;, Instrument, Condition*, Parameter*)>
<!ATTLIST Measurement
    %Investigationatts;
>
<!ELEMENT Simulation (%Investigation;, Machine, Program, Parameter*, Data*)>
<!ATTLIST Simulation
    %Investigationatts;
>
<!-- Breakdown of the study information -->
<!ELEMENT StudyName (#PCDATA)>
<!ELEMENT StudyID (Institution?)>
<!-- studyid - the identifier given by the institution -->
<!-- institutionref - a reference to an institution - should be a reference to a key -->
<!-- XML Schema should be able to do better here -->
<!ATTLIST StudyID

```

```

    studyid CDATA #REQUIRED

    institutionref CDATA #IMPLIED
>
<!-- Investigator - it may be going into too much detail -->
<!-- we have fixed a person to have one institution - this may cause problems in future -->
<ENTITY % PersonClass "Name, Status, Institution, ContactDetails">
<!-- an Investigator has a Role in this study. -->
<ELEMENT Investigator (%PersonClass;, Role)>
<ELEMENT Name (Surname, Initials, Forename*, PersonTitle?)>
<ELEMENT Surname (#PCDATA)>
<ELEMENT Initials (#PCDATA)>
<ELEMENT Forename (#PCDATA)>
<ELEMENT PersonTitle (#PCDATA)>
<ELEMENT Role (#PCDATA)>
<ELEMENT Status (#PCDATA)>
<ELEMENT Institution (#PCDATA)>
<!ATTLIST Institution
    institutionID CDATA #IMPLIED
    institutiontype (academic | government | military | commercial | nonprofit | other) #IMPLIED
>
<!-- institutiontype is a bit of an "extra", might miss out -->
<ELEMENT ContactDetails (Address, Telephone, Email?, Fax?)>
<!-- breaking this contact detail down like this is likely to be too much -->
<!-- detail for the purpose of metadata searching -->
<ELEMENT Address (Addressline1, Addressline2?, Town, Region?, Postcode?, Country)>
<ELEMENT Addressline1 (#PCDATA)>
<ELEMENT Addressline2 (#PCDATA)>
<ELEMENT Town (#PCDATA)>
<ELEMENT Region (#PCDATA)>
<ELEMENT Country (#PCDATA)>
<!-- from ISO Standard country codes -->
<!ATTLIST Country

```

```

countryabbrev CDATA ""
>
<!ELEMENT Postcode (#PCDATA)>
<!ELEMENT Telephone (#PCDATA)>
<!ELEMENT Email (#PCDATA)>
<!ELEMENT Fax (#PCDATA)>
<!-- Study Information -->
<!ELEMENT StudyInformation (Funding, TimePeriod, Purpose, StudyStatus, Resources?)>
<!ELEMENT Funding (#PCDATA)>
<!-- Time point or range over which the study was undertaken. -->
<!-- Do we want to put time information onto individual data items?-->
<!ELEMENT TimePeriod (StartDate, EndDate?)>
<!ELEMENT StartDate (Date, Time?)>
<!ELEMENT EndDate (Date, Time?)>
<!ELEMENT Date (#PCDATA)>
<!-- expect this to be in dd/mm/yyyy format-->
<!ELEMENT Time (#PCDATA)>
<!-- expect this to be in hh:mm:ss format -->
<!-- Purpose
    An abstract, study type and any other information.
    Topic keywords also form part of this, but are kept in the top-level topic to
    avoid confusion.
-->
<!ELEMENT Purpose (Abstract?, StudyType?)>
<!ELEMENT Abstract (#PCDATA)>
<!-- should we accept HTML? At the moment, treat as free text -->
<!ELEMENT StudyType (#PCDATA)>
<!-- should some be enumerated? -->
<!ELEMENT StudyStatus (#PCDATA)>
<!-- should some be enumerated?
    e.g.
<! ELEMENT StudyStatus (#PCDATA | COMPLETE | INPROGRESS | PENDING) >

```

```

<! ELEMENT COMPLETE EMPTY >

<! ELEMENT INPROGRESS EMPTY >

<! ELEMENT PENDING EMPTY>

-->

<!ELEMENT Resources (#PCDATA)>

<!-- Data Holder -->

<!ELEMENT DataManager (Institution, Contact*)>

<!ELEMENT Contact (%PersonClass;)>

<!-- Note the reuse of the person class entity -->

<!-- Notes -->

<!ELEMENT Notes (#PCDATA)>

<!-- Fields of Experiment -->

<!-- Parameters and Conditions - essentially similar. -->

<!-- these are proposed to be triples formed of:

      (Name, Units, Value)

      e.g. (Temperature, K, 150)

      (Pressure, Bar, 300)

      units and value are optional - this allows the name to be set and the
      other entries to be given later.

-->

<!ENTITY % ParameterType "ParamName, Units?, ParamValue?, Range?">

<!ELEMENT Instrument (#PCDATA)>

<!-- should this have a hierarchical structure? -->

<!ELEMENT Condition (%ParameterType;)>

<!ELEMENT Parameter (%ParameterType;)>

<!ELEMENT ParamValue (#PCDATA)>

<!ELEMENT Units (#PCDATA)>

<!ELEMENT ParamName (#PCDATA)>

<!-- Fields of Simulation -->

<!-- Currently, I have no more information about these than that they are free text -->

<!-- This will probably have to do for the prototype, but will not be satisfactory in the future. -->

```

```

<!ELEMENT Program (#PCDATA)>
<!ELEMENT Machine (#PCDATA)>
<!ELEMENT Data (#PCDATA)>
<!-- Access Conditions -->
<!-- At the moment, not much more than free text - but will require more. -->
<!ELEMENT AccessConditions (#PCDATA)>
<!-- Data Location -->
<ENTITY % locationatts 'dataidref CDATA #REQUIRED'>
<!-- should be an IDREF -->
<!--<!ELEMENT DataHoldingLocator (DataHoldingLocator, DataSetLocator*, FileLocator*)>-->
<ELEMENT DataHoldingLocator (DataName, Locator*, DataSetLocator*, FileLocator*)>
<!ATTLIST DataHoldingLocator
    %locationatts;
>
<ELEMENT DataSetLocator (DataName, Locator*)>
<!ATTLIST DataSetLocator
    %locationatts;
>
<ELEMENT FileLocator (URI, Locator*)>
<!ATTLIST FileLocator
    %locationatts;
>
<ELEMENT Locator (URL, DataSourceType?, DataSourceAccess?)>
<!ATTLIST Locator
    type (absolute | relative) "absolute"
>
<!ELEMENT URL (#PCDATA)>
<!ELEMENT DataSourceType (#PCDATA)>
<!ELEMENT DataSourceAccess (#PCDATA)>
<!-- Data Description entities -->
<ENTITY % DataDescriptionClass 'DataHolding | DataSet | File'>
<ENTITY % DataDescription 'DataName, TypeOfData?, Status?, LogicalDescription?, FileFormat?'>

```

```

<ENTITY % datadescatts 'dataid CDATA #REQUIRED'>

<!-- should be an ID -->

<!-- Data Description elements -->

<ELEMENT DataHolding (%DataDescription;, DataSet*, RelatedStudy*)>

<!ATTLIST DataHolding
    %datadescatts;
>

<ELEMENT RelatedStudy (StudyRef, RelationType)>

<ELEMENT StudyRef EMPTY>

<!-- StudyRef refers to a metadataID -->

<!ATTLIST StudyRef
    studyref IDREF #REQUIRED
>

<!-- should refer to the id of a study -->

<ELEMENT RelationType (#PCDATA)>

<!-- Data sets -->

<ELEMENT DataSet (%DataDescription;, File*, RelatedDataSetRef*, ParentDataSetRef?, ChildDataSetRef*,
DerivedFromDataSetRef*)>

<!ATTLIST DataSet
    %datadescatts;
>

<ELEMENT RelatedDataSetRef (DataSetRef, RelationType)>

<ELEMENT ParentDataSetRef (#PCDATA)>

<ELEMENT ChildDataSetRef (#PCDATA)>

<ELEMENT DerivedFromDataSetRef (DataHoldingRef?, DataSetRef)>

<ELEMENT DataSetRef (#PCDATA)>

<ELEMENT DataHoldingRef (#PCDATA)>

<!-- Should point to a named data set in a named study -->

<ELEMENT File (%DataDescription;, URI, RelatedFileRef*, DerivedFromFileRef*)>

<!ATTLIST File
    %datadescatts;
>

<ELEMENT URI (#PCDATA)>

```

```

<!ELEMENT RelatedFileRef (FileRef, RelationType)>

<!ELEMENT DerivedFromFileRef (DataHoldingRef?, DataSetRef?, FileRef)>

<!ELEMENT FileRef (#PCDATA)>

<!-- Should point to a named data set in a named study -->

<!ELEMENT DataName (#PCDATA)>

<!ELEMENT TypeOfData (#PCDATA)>

<!ELEMENT LogicalDescription (#PCDATA | Parameter | Condition | Coverage | TimePeriod)*>

<!-- expect just one time period -->

<!-- this is an arbitrary list - will change -->

<!ELEMENT Range (Limit)+>

<!ELEMENT Limit (#PCDATA)>

<!ATTLIST Limit
    bound (top | bottom | other) #IMPLIED
>

<!ELEMENT Coverage (#PCDATA)>

<!ELEMENT FileFormat (#PCDATA)>

<!-- keep as a single lump at the moment - may make more detailed -->

<!-- Related Materials -->

<!ELEMENT RelatedMaterial (#PCDATA | Publications | References | RelatedInvestigations | CommunityInformation)*>

<!ELEMENT Publications (#PCDATA)>

<!ELEMENT References (#PCDATA)>

<!ELEMENT RelatedInvestigations (#PCDATA)>

<!ELEMENT CommunityInformation (#PCDATA)>

```



## 14. APPENDIX C – XML SCHEMA

```
<?xml version="1.0" encoding="UTF-8"?>

<xsd:schema xmlns:xsd="http://www.w3.org/2001/XMLSchema">

  <xsd:annotation>

    <xsd:documentation xml:lang="en">

      General Scientific Meta-Data Format Schema

      for eScience Data Portal.

    </xsd:documentation>

  </xsd:annotation>

  <!-- maybe the class type definitions should go here -->

  <!-- defining the actual elements in the document -->

  <xsd:element name="CLRCMetadata" type="CLRCMetadataType"/>

  <xsd:complexType name="CLRCMetadataType">

    <xsd:sequence>

      <xsd:element name="MetadataRecord" type="MetadataRecordType" minOccurs="0"
maxOccurs="unbounded"/>

    </xsd:sequence>

  </xsd:complexType>

  <xsd:complexType name="MetadataRecordType">

    <xsd:sequence>

      <xsd:element name="Topic" type="TopicType" minOccurs="0"/>

      <xsd:element name="Study" type="StudyType"/>

      <xsd:element name="AccessConditions" type="xsd:string"/>

      <xsd:element name="RelatedMaterial" type="RelatedMaterialTypes" minOccurs="0"
maxOccurs="unbounded"/>

    </xsd:sequence>

    <xsd:attribute name="metadataID" type="metadataIDKeyType" use="required"/>

    <xsd:attribute name="facility" type="xsd:string" use="required"/>

  </xsd:complexType>

  <!-- metadataID uniquely identified one record - logically it consists of the -->

  <!-- name of the data archive (which has to be unique in the dataportal ) -->
```

```

<!-- and something which identifies unique records in the data archive -->
<xsd:simpleType name="metadataIDKeyType">
  <xsd:restriction base="xsd:ID">
    <xsd:pattern value="[0-9A-Za-z]*-[0-9A-Za-z]*"/>
  </xsd:restriction>
</xsd:simpleType>
<xsd:complexType name="TopicType">
  <xsd:sequence>
    <xsd:element name="Discipline" type="xsd:string" minOccurs="0"/>
    <xsd:element name="Source" type="xsd:string" minOccurs="0"/>
    <xsd:element name="Subject" type="SubjectType"/>
  </xsd:sequence>
</xsd:complexType>
<xsd:complexType name="SubjectType">
  <xsd:sequence>
    <xsd:element name="SubjectName" type="xsd:string"/>
    <xsd:element name="Subject" type="SubjectType" minOccurs="0"/>
  </xsd:sequence>
</xsd:complexType>
<xsd:complexType name="StudyType">
  <xsd:sequence>
    <xsd:element name="StudyName" type="xsd:string"/>
    <xsd:element name="StudyInstitutions" type="InstitutionType" minOccurs="0" maxOccurs="unbounded"/>
    <xsd:element name="Investigator" type="InvestigatorType" maxOccurs="unbounded"/>
    <xsd:element name="StudyInformation" type="StudyInformationType"/>
    <xsd:element name="Notes" type="xsd:string" minOccurs="0"/>
    <xsd:element name="Investigation" type="InvestigationType" maxOccurs="unbounded"/>
  <!-- sc -->
  </xsd:sequence>
</xsd:complexType>
<xsd:complexType name="InvestigationType">
  <xsd:sequence>

```

```

<xsd:element name="Name" type="xsd:string"/>

<xsd:element name="InvestigationType" type="InvestigationTypes"/>

<xsd:element name="Abstract" type="xsd:string"/>

<xsd:element name="Resources" type="xsd:string"/>

<xsd:element name="DataHolding" type="DataHoldingType" minOccurs="0"/>

<!-- perhaps this should be at dataset and dataobject level also -->

</xsd:sequence>

<xsd:attribute name="InvestigationID" type="xsd:ID" use="required"/>

</xsd:complexType>

<xsd:simpleType name="InvestigationTypes">
  <xsd:restriction base="xsd:string">
    <xsd:enumeration value="experiment"/>
    <xsd:enumeration value="measurement"/>
    <xsd:enumeration value="simulation"/>
    <xsd:enumeration value="other"/>
  </xsd:restriction>
</xsd:simpleType>

<!-- detail all the things in StudyType before we start inheriting from it -->

<!-- wonder if it matters -->

<xsd:complexType name="InstitutionType">
  <xsd:sequence>
    <xsd:element name="Institution" minOccurs="0">
      <xsd:complexType>
        <xsd:simpleContent>
          <xsd:extension base="xsd:string">
            <xsd:attribute name="institutionID" type="xsd:string" use="optional"/>
            <xsd:attribute name="institutiontype" type="institutionTypes" use="required"/>
          </xsd:extension>
        </xsd:simpleContent>
      </xsd:complexType>
    <!-- adding attributes to an element -->
  </xsd:element>

```

```

    <xsd:element name="Role" type="xsd:string" minOccurs="0"/>

    <!-- <xsd:element name="Institution" type="xsd:string" minOccurs="0" maxOccurs="1"> -->

    <!-- above line is incorrect file would not validate - we have to extend the type -->

    <!-- to add some attributes -->

</xsd:sequence>

</xsd:complexType>

<!-- turn the attribute choices into a type -->

<xsd:simpleType name="institutionTypes">
    <xsd:restriction base="xsd:string">
        <xsd:enumeration value="academic"/>
        <xsd:enumeration value="government"/>
        <xsd:enumeration value="military"/>
        <xsd:enumeration value="commercial"/>
        <xsd:enumeration value="nonprofit"/>
        <xsd:enumeration value="other"/>
    </xsd:restriction>
</xsd:simpleType>

<!-- example of a list type - not used yet -->

<xsd:simpleType name="institutionsType">
    <xsd:list itemType="institutionTypes"/>
</xsd:simpleType>

<!-- started to get into some 'inheritance' now - i.e PersonType and InvestigatorType -->

<xsd:complexType name="PersonType">
    <xsd:sequence>
        <xsd:element name="Name" type="NameType"/>
        <xsd:element name="Status" type="StatusTypes"/>
        <xsd:element name="Institution" type="InstitutionType"/>
        <xsd:element name="ContactDetails" type="ContactDetailsType"/>
    </xsd:sequence>
</xsd:complexType>

<xsd:simpleType name="StatusTypes">
    <xsd:restriction base="xsd:string">

```

```

<xsd:enumeration value="professor"/>
<xsd:enumeration value="Professor"/>
<xsd:enumeration value="Prof."/>
<xsd:enumeration value="doctor"/>
<xsd:enumeration value="Doctor"/>
<xsd:enumeration value="Dr."/>
<xsd:enumeration value="student"/>
<xsd:enumeration value="Student"/>
<xsd:enumeration value="Post Doctoral Research Assistant"/>
<xsd:enumeration value="pdra"/>
<xsd:enumeration value="PDRA"/>
<xsd:enumeration value="other"/>
</xsd:restriction>
</xsd:simpleType>
<!-- some of the contact details in the DTD hinted at being overkill -->
<xsd:complexType name="InvestigatorType">
  <xsd:complexContent>
    <xsd:extension base="PersonType">
      <xsd:sequence>
        <xsd:element name="Role" type="xsd:string"/>
      </xsd:sequence>
    </xsd:extension>
  </xsd:complexContent>
</xsd:complexType>
<xsd:complexType name="NameType">
  <xsd:sequence>
    <xsd:element name="Surname" type="xsd:string"/>
    <xsd:element name="Initials" type="xsd:string"/>
    <xsd:element name="Forename" type="xsd:string" minOccurs="0"/>
    <xsd:element name="PersonTitle" type="xsd:string" minOccurs="0"/>
  </xsd:sequence>
</xsd:complexType>

```

```

<xsd:complexType name="ContactDetailsType">
  <xsd:sequence>
    <xsd:element name="Address" type="AddressType"/>
    <xsd:element name="Telephone" type="xsd:string"/>
    <xsd:element name="Email" type="xsd:string" minOccurs="0"/>
    <xsd:element name="Fax" type="xsd:string" minOccurs="0"/>
  </xsd:sequence>
</xsd:complexType>

<xsd:complexType name="AddressType">
  <xsd:sequence>
    <xsd:element name="Addressline1" type="xsd:string"/>
    <xsd:element name="Addressline2" type="xsd:string" minOccurs="0"/>
    <xsd:element name="Town" type="xsd:string"/>
    <xsd:element name="Region" type="xsd:string" minOccurs="0"/>
    <xsd:element name="Postcode" type="xsd:string" minOccurs="0"/>
    <xsd:element name="Country">
      <xsd:complexType>
        <xsd:simpleContent>
          <xsd:extension base="xsd:string">
            <xsd:attribute name="countryabbrev" type="xsd:string"/>
          </xsd:extension>
        </xsd:simpleContent>
      </xsd:complexType>
      <!-- again we don't mention the type above as we have to extend it -->
    </xsd:element>
  </xsd:sequence>
</xsd:complexType>

<!-- expanding on the study information type -->
<xsd:complexType name="StudyInformationType">
  <xsd:sequence>
    <xsd:element name="Funding" type="xsd:string" minOccurs="0"/>
    <xsd:element name="TimePeriod" type="TimePeriodType"/>
  </xsd:sequence>
</xsd:complexType>

```

```

<xsd:element name="Purpose" type="PurposeType"/>

<xsd:element name="StudyStatus" type="xsd:string"/>

<xsd:element name="Reources" type="xsd:string" minOccurs="0"/>

<!-- perhaps the following should be an enumerated list - even held in a different file -->

<!-- and included here - note taken from the DTD -->

</xsd:sequence>

</xsd:complexType>

<xsd:complexType name="TimePeriodType">

  <xsd:sequence>

    <xsd:element name="StartDate" type="DateTimeType"/>

    <xsd:element name="EndDate" type="DateTimeType"/>

  </xsd:sequence>

</xsd:complexType>

<!-- no equivalent to this following type in DTD - as you can't constrain the contents -->

<!-- of the element in this way in a DTD -->

<xsd:complexType name="DateTimeType">

  <xsd:sequence>

    <xsd:element name="Date" type="xsd:date"/>

    <xsd:element name="Time" type="xsd:time" minOccurs="0"/>

    <!-- note however rather than the dd/mm/ccyy representation mentioned in the DTD -->

    <!-- this format will be CCYY-MM-DD as this is the lexical format for the 'date' -->

    <!-- datatype in XMLSchema - not sure if this is going to be a problem otherwise -->

    <!-- we could just use a string and validate it ourselves - perhaps ? -->

    <!-- the 'date' type also supports an optional timezone component - not sure -->

    <!-- how useful this would be - apparently the 'date' type adheres to the ISO8601 -->

    <!-- standard on representing dates- however the right-truncated format of the date -->

    <!-- appears to be only a subset of what is allowable in ISO8601 -->

    <!-- the format of the time attribute is hh:mm:ss.sss with an optional timezone information -->

    <!-- section - the DTD states a preference for hh:mm:ss -->

    <!-- might be worth just using our own standard and holding them in string - depends if -->

    <!-- the XML Schema forms get in the way - then again date validation if more thoroughly -->

    <!-- enforced using the schema -->

```

```

    </xsd:sequence>
</xsd:complexType>
<xsd:complexType name="PurposeType">
    <xsd:sequence>
        <xsd:element name="Abstract" type="xsd:string" minOccurs="0"/>
        <!-- note in the DTD that maybe we should accept HTML -->
        <!-- again perhaps the following should be an enumerated type -->
    </xsd:sequence>
</xsd:complexType>
<!-- e.g. of the enumeration - perhaps the DTD has more flexibility - as you can have -->
<!-- a PCDATA as well as any of the choices ? -->
<!--

<xsd:simpleType name="StudyTypes">
    <xsd:restriction base="xsd:string">
        <xsd:enumeration value="COMPLETE"/>
        <xsd:enumeration value="INPROGRESS"/>
        <xsd:enumeration value="PENDING"/>
    </xsd:restriction>
</xsd:simpleType>

-->

<xsd:complexType name="DataHoldingType">
    <xsd:sequence>
        <xsd:element name="DataDescription" type="DataDescriptionType"/>
        <xsd:element name="DataSet" type="DataSetType" minOccurs="0" maxOccurs="unbounded"/>
        <xsd:element name="RelatedStudy" type="RelatedStudyType" minOccurs="0"/>
        <xsd:element name="DataHoldingLocator" type="DataHoldingLocatorType"/>
    </xsd:sequence>
    <xsd:attribute name="InvestigationID" type="xsd:ID" use="required"/>
    <!-- again following attribute type should really be a CDATA equivalent -->
    <!-- but can't seem to find it -->

```



```

</xsd:complexType>
<xsd:complexType name="ParameterType">
  <xsd:sequence>
    <xsd:element name="ParamName" type="xsd:string"/>
    <xsd:element name="Derivation" type="DerivationTypes"/>
    <xsd:element name="Units" type="UnitsType" minOccurs="0"/>
    <xsd:element name="ParamValue" type="xsd:string" minOccurs="0"/>
    <xsd:element name="Range" type="RangeType" minOccurs="0"/>
  </xsd:sequence>
</xsd:complexType>
<xsd:complexType name="UnitsType">
  <xsd:sequence>
    <xsd:element name="UnitName" type="xsd:string"/>
    <xsd:element name="UnitAcronym" type="xsd:string"/>
    <xsd:element name="UnitSystem" type="xsd:string"/>
  </xsd:sequence>
</xsd:complexType>
<xsd:simpleType name="DerivationTypes">
  <xsd:restriction base="xsd:string">
    <xsd:enumeration value="fixed"/>
    <xsd:enumeration value="measured"/>
    <xsd:enumeration value="calculated"/>
    <xsd:enumeration value="environment"/>
    <xsd:enumeration value="other"/>
  </xsd:restriction>
</xsd:simpleType>
<xsd:complexType name="RangeType">
  <xsd:sequence>
    <xsd:element name="Limit" maxOccurs="unbounded">
      <xsd:complexType>
        <xsd:simpleContent>
          <xsd:extension base="xsd:string">

```

```

        <xsd:attribute name="bound" type="boundTypes" use="optional"/>
    </xsd:extension>
</xsd:simpleContent>
</xsd:complexType>
</xsd:element>
<xsd:element name="MarginOfError" type="xsd:string"/>
</xsd:sequence>
</xsd:complexType>
<xsd:simpleType name="boundTypes">
    <xsd:restriction base="xsd:string">
        <xsd:enumeration value="upper"/>
        <xsd:enumeration value="lower"/>
        <xsd:enumeration value="other"/>
    </xsd:restriction>
</xsd:simpleType>
<xsd:complexType name="LogicalDescriptionTypes">
    <xsd:sequence>
        <xsd:element name="Parameter" type="ParameterType" minOccurs="0" maxOccurs="unbounded"/>
        <xsd:element name="TimePeriod" type="TimePeriodType" minOccurs="0"/>
        <xsd:element name="Description" type="xsd:string" minOccurs="0"/>
        <xsd:element name="FacilityUsed" type="xsd:string" minOccurs="0"/>
        <!-- even coverage information stored in Parameters now -->
    </xsd:sequence>
</xsd:complexType>
<xsd:complexType name="DataDescriptionType">
    <xsd:sequence>
        <xsd:element name="DataName" type="xsd:string"/>
        <xsd:element name="TypeOfData" type="TypesOfData" minOccurs="0"/>
        <xsd:element name="Status" type="xsd:string" minOccurs="0"/>
        <xsd:element name="LogicalDescription" type="LogicalDescriptionTypes" minOccurs="0"/>
        <!-- need to use a union type as LogicalDescription can be of one or more type -->
    </xsd:sequence>

```

```

</xsd:complexType>

<xsd:simpleType name="TypesOfData">
  <xsd:restriction base="xsd:string">
    <xsd:enumeration value="File"/>
    <xsd:enumeration value="BLOB"/>
    <xsd:enumeration value="other"/>
  </xsd:restriction>
</xsd:simpleType>

<xsd:complexType name="DataSetType">
  <xsd:sequence>
    <xsd:element name="DataDescription" type="DataDescriptionType"/>
    <xsd:element name="AtomicDataObject" type="ADOType" minOccurs="0" maxOccurs="unbounded"/>
    <xsd:element name="DataSet" type="DataSetType" minOccurs="0" maxOccurs="unbounded"/>
    <xsd:element name="RelatedDataSetRef" type="RelatedDataSetRefType" minOccurs="0"/>
    <xsd:element name="DerivedFromDataSetRef" type="DerivedFromDataSetRefType" minOccurs="0"/>
    <xsd:element name="DataSetLocator" type="DataSetLocatorType" minOccurs="0"
maxOccurs="unbounded"/>
    <!-- <xsd:element name="ParentDataSetRef" type="xsd:string" minOccurs="0" maxOccurs="1"/> -->
    <!-- <xsd:element name="ChildDataSetRef" type="xsd:string" minOccurs="0"/> -->
  </xsd:sequence>
  <xsd:attribute name="dataid" type="xsd:ID" use="required"/>
  <!-- again the following is stated as a CDATA type in the original DTD -->
</xsd:complexType>

<xsd:complexType name="DerivedFromDataSetRefType">
  <xsd:sequence>
    <xsd:element name="DataHoldingRef" type="xsd:string" minOccurs="0"/>
    <xsd:element name="DataSetRef" type="xsd:string"/>
  </xsd:sequence>
</xsd:complexType>

<xsd:complexType name="RelatedDataSetRefType">
  <xsd:sequence>
    <xsd:element name="DataSetRef" type="xsd:string"/>
    <xsd:element name="RelationType" type="xsd:string"/>
  </xsd:sequence>
</xsd:complexType>

```

```

    </xsd:sequence>
</xsd:complexType>
<xsd:complexType name="ADOType">
  <xsd:sequence>
    <xsd:element name="Name" type="xsd:string"/>
    <xsd:element name="DataDescription" type="DataDescriptionType"/>
    <xsd:element name="RelatedADORef" type="RelatedADORefType" minOccurs="0"/>
    <xsd:element name="DerivedFromADORef" type="DerivedFromADORefType" minOccurs="0"/>
    <xsd:element name="ADOLocator" type="ADOLocatorType" minOccurs="0" maxOccurs="unbounded"/>
  </xsd:sequence>
  <xsd:attribute name="dataid" type="xsd:ID" use="required"/>
</xsd:complexType>
<!-- how to use the specialisation parent/child class/subclass 'feature' : -->
<!--
<root_element
  xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
  ...
  >
  ...
  ...<ADOLocator xsi:type="FileLocator">
  ...
  -->
<xsd:complexType name="FileLocator">
  <xsd:complexContent>
    <xsd:extension base="ADOLocatorType">
      <xsd:sequence>
        <xsd:element name="Media" type="xsd:string"/>
        <xsd:element name="Filetype" type="xsd:string"/>

```

```

        </xsd:sequence>
    </xsd:extension>
</xsd:complexContent>
</xsd:complexType>
<xsd:complexType name="BLOBLocator">
    <xsd:complexContent>
        <xsd:extension base="ADOLocatorType">
            <xsd:sequence>
                <xsd:element name="DatabaseType" type="xsd:string"/>
                <xsd:element name="DatabaseVersion" type="xsd:string"/>
                <xsd:element name="Host" type="xsd:string"/>
                <xsd:element name="Instance" type="xsd:string" minOccurs="0"/>
                <xsd:element name="Database" type="xsd:string"/>
                <xsd:element name="Port" type="xsd:string" minOccurs="0"/>
                <xsd:element name="Table" type="xsd:string"/>
                <xsd:element name="Column" type="xsd:string"/>
                <xsd:element name="DataFormat" type="xsd:string"/>
            </xsd:sequence>
        </xsd:extension>
    </xsd:complexContent>
</xsd:complexType>
<xsd:complexType name="RelatedADORefType">
    <xsd:sequence>
        <xsd:element name="ADORef" type="xsd:string"/>
        <xsd:element name="RelationType" type="xsd:string"/>
    </xsd:sequence>
</xsd:complexType>
<xsd:complexType name="DerivedFromADORefType">
    <xsd:sequence>
        <xsd:element name="DataHoldingRef" type="xsd:string" minOccurs="0"/>
        <xsd:element name="DataSetRef" type="xsd:string" minOccurs="0"/>
        <xsd:element name="ADORef" type="xsd:string"/>
    </xsd:sequence>

```

```

    </xsd:sequence>
</xsd:complexType>
<!-- in the following the compact syntax works because a complex type defined without -->
<!-- any simpleContent or complexContent is interpreted as shorthand for complex -->
<!-- content that restricts anyType -->
<xsd:complexType name="RelatedStudyType">
    <xsd:sequence>
        <xsd:element name="StudyRef">
            <xsd:complexType>
                <xsd:attribute name="studyref" type="xsd:IDREF" use="required"/>
            </xsd:complexType>
        </xsd:element>
        <xsd:element name="RelationType" type="xsd:string"/>
    </xsd:sequence>
</xsd:complexType>
<!-- The DataLocationTypes -->
<xsd:complexType name="DataHoldingLocatorType">
    <xsd:sequence>
        <xsd:element name="DataName" type="xsd:string"/>
        <xsd:element name="Locator" type="LocatorTypes" minOccurs="0" maxOccurs="unbounded"/>
    </xsd:sequence>
    <xsd:attribute name="dataidref" type="xsd:string" use="required"/>
    <!-- type of this attribute should really be a CDATA - no equivalent in XMLSchema -->
</xsd:complexType>
<xsd:simpleType name="LocatorTypes">
    <xsd:restriction base="xsd:string">
        <xsd:enumeration value="absolute"/>
        <xsd:enumeration value="relative"/>
    </xsd:restriction>
</xsd:simpleType>
<xsd:complexType name="DataSetLocatorType">
    <xsd:sequence>

```

```

    <xsd:element name="DataName" type="xsd:string"/>

    <xsd:element name="Locator" type="LocatorTypes" minOccurs="0" maxOccurs="unbounded"/>
</xsd:sequence>

<xsd:attribute name="dataidref" type="xsd:string" use="required"/>

<!-- type of this attribute should really be a CDATA - no equivalent in XMLSchema -->
</xsd:complexType>

<xsd:complexType name="ADOLocatorType">
  <xsd:sequence>

    <xsd:element name="URI" type="xsd:string"/>

    <xsd:element name="AccessMethod" type="xsd:string" minOccurs="0"/>

    <xsd:element name="Size" type="xsd:string" minOccurs="0"/>

    <xsd:element name="offset" type="xsd:string" minOccurs="0"/>

    <xsd:element name="length" type="xsd:string" minOccurs="0"/>

  </xsd:sequence>

  <xsd:attribute name="dataidref" type="xsd:string" use="required"/>

  <xsd:attribute name="type" type="LocatorTypes" use="optional" default="absolute"/>

  <!-- type of this attribute should really be a CDATA - no equivalent in XMLSchema -->
</xsd:complexType>

<!-- Related Materials as a type -->

<xsd:simpleType name="Publications">
  <xsd:restriction base="xsd:string"/>
</xsd:simpleType>

<xsd:simpleType name="References">
  <xsd:restriction base="xsd:string"/>
</xsd:simpleType>

<xsd:simpleType name="RelatedInvestigations">
  <xsd:restriction base="xsd:string"/>
</xsd:simpleType>

<xsd:simpleType name="CommunityInformation">
  <xsd:restriction base="xsd:string"/>
</xsd:simpleType>

<xsd:simpleType name="RelatedMaterialTypes">

```

```
<xsd:union memberTypes="xsd:string Publications References RelatedInvestigations CommunityInformation"/>  
</xsd:simpleType>  
</xsd:schema>
```



## 15. APPENDIX D – EXAMPLE METADATA RECORD

```
<?xml version="1.0" encoding="UTF-8" ?>
<!DOCTYPE CLRCMetadata (View Source for full doctype...)>
- <CLRCMetadata>
- <MetadataRecord metadataID="WOCE_Bottle_OnetimeData">
- <Topic>
  <Discipline>ocean chemistry</Discipline>
  <Subject>observational data</Subject>
</Topic>
- <Experiment>
  <StudyName>WOCE Hydrographic Onetime Survey Bottle Data</StudyName>
  <StudyID studyid="WOCE_Bottle_OnetimeData" institutionref="I2000061" />
- <Investigator>
- <Name>
  <Surname>Koltermann</Surname>
  <Initials>Klaus-Peter -</Initials>
  </Name>
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