

CBB Ontology User Guide

Version 1.0

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I. Introduction to Ontology

I.A. What is an Ontology?

As a philosophical discipline, ontology is the branch of metaphysics that deals with “the nature and relations of being.” Notably, one of the questions in the study of ontology is whether certain things exist and how to possibly sort them.

For our concerns it suffices to say that **an ontology is a machine-readable vocabulary** that formalizes the concepts in a particular discipline and *the relationships* between said concepts. Specifically, ontologies are vocabularies for the Semantic Web as standardized by the World Wide Web Consortium. The goal of the standard is to allow compatibility between databases.

I.B. Why have an Ontology?

By formalizing the definitions of and relationships between concepts across disciplines, we can **more easily communicate with our peers**. Additionally, ontologies are created such that a computer can utilize the information.

As a simple example, say one wanted to analyze the relation between number of authors on a paper and the number of citations. Some available databases use the term “author” whereas others use “contributor.” By defining the relationship (in this case equivalency) between the terms “author” and “contributor” we can more easily perform analysis using data from both types of database.

So, if an ontology contained all of the relevant terms in a particular field not only can colleagues better understand each other, but it would allow for automated connection between related concepts across similar fields.

But why use an *Ontology*?

The key distinction between an ontology and other organization strategies is the presentation of both information and explicit relationships.

Whereas a Wiki, say, contains information on a range of topics and indeed permits the interconnection of topics by way of hyperlinks, the lack of a formal definition makes the

relationship hard for a computer to parse. The relationships are too vague. A human reader can use context clues to understand the relationship between linked Wiki articles, but such a prospect is significantly harder to codify for computer use.

On the other hand, a taxonomy is too restrictive, organizing concepts under a single classification scheme without including other forms of relationships.

Ontologies include a formal hierarchy and explicit relationships between terms. This makes them both rigid in their framework but extremely flexible in their application.

Why does the CBB need an ontology?

As a center that includes researchers in several different fields, it is important to have a resource available to help facilitate conversation between colleagues. In particular, **being able to relate concepts across disciplines will permit new collaborations.**

I.C. What content should go into the CBB ontology?

Any technical information that **first year graduate student in the field should know.** For example this includes:

- Techniques (e.g. DFT, XPS, STM, KPFM)
- Materials (e.g. different superconductors, different photocathodes)
- Instruments and their constituent parts (e.g. linear accelerator, aberration corrector)
- Parameters (e.g. brightness, emittance, aperture)
- Specific facilities (e.g. NSLS-II, TRIUMF, CBB)

DO NOT INCLUDE individual CBB members

Each of these topics should have the following content:

- Definition of the term
- Any synonyms
- Relationships to other terms
- Comments/questions
- Useful resources to learn more (**papers**/relevant URLs)

II. Getting Started as a User

II.A. Creating user account

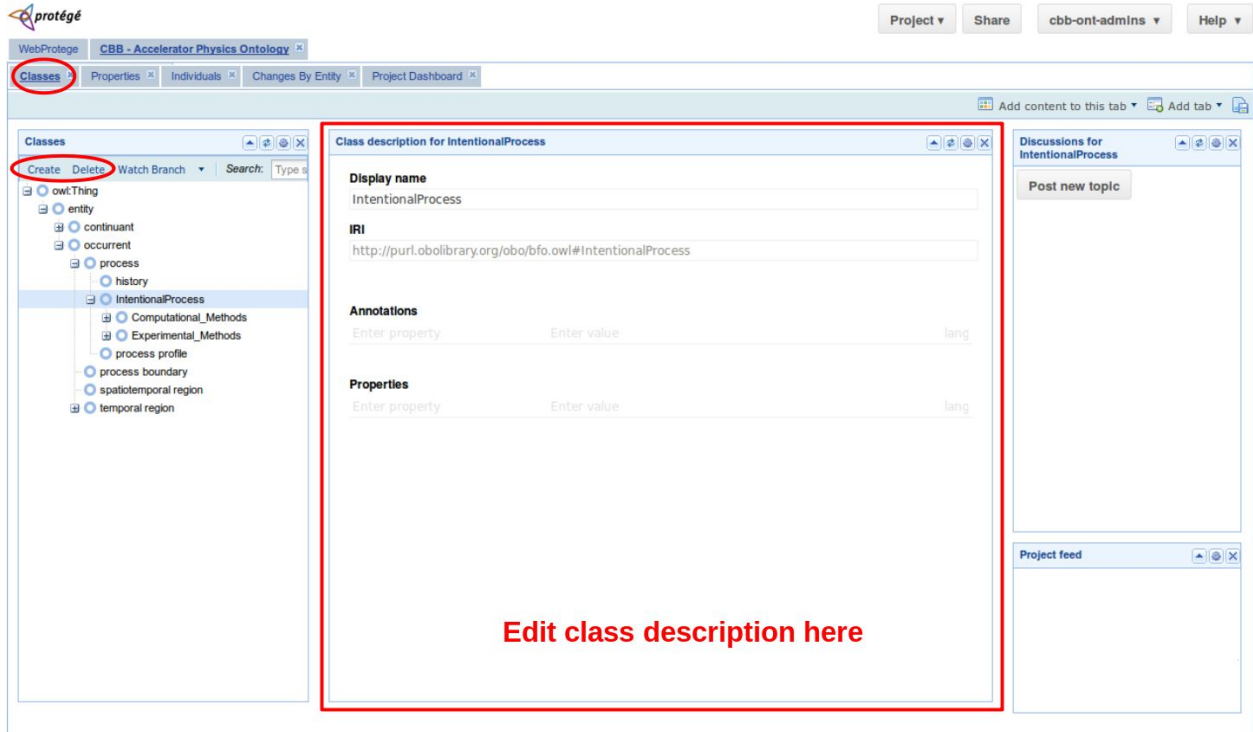
1. Create user account at <https://webprotege.cbb.cornell.edu/> by clicking “Sign up for account” on the top right corner.
2. Enter email, username, password.
3. Send your **username** to cbb-ontology-admin-l@list.cornell.edu to obtain editing rights for the ontology.

II.B. Navigating the CBB Accelerator Physics Ontology

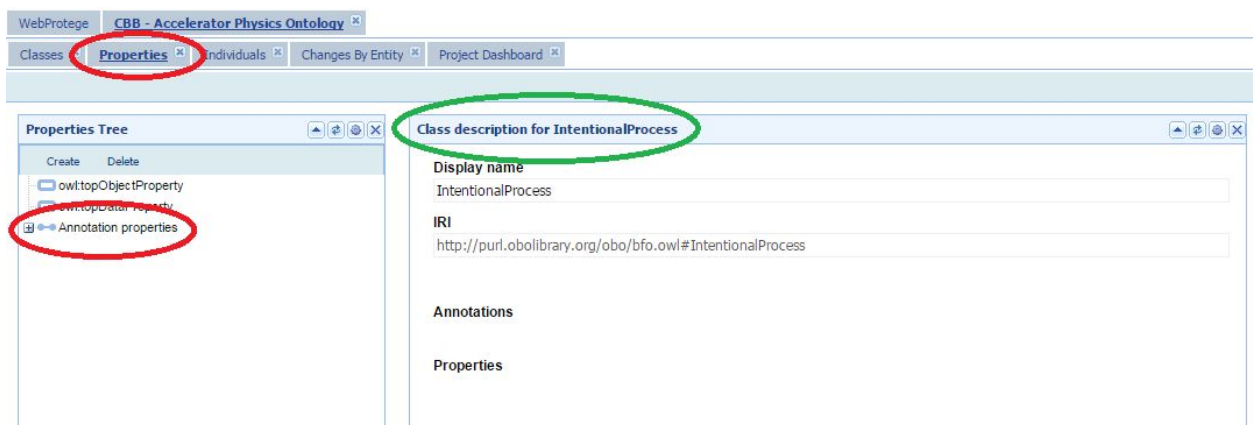
1. Sign in to your account at <https://webprotege.cbb.cornell.edu/>.
2. Under “Home” tab in <https://webprotege.cbb.cornell.edu/>, click at “CBB - Accelerator Physics Ontology”.

The screenshot displays the WebProtégé web interface. At the top left is the Protégé logo and the text "WebProtégé". At the top right, there are two buttons: "cbb-ont-admins" with a dropdown arrow and "Help" with a dropdown arrow. Below the header, there are two buttons: "* Create Project ..." and "† Upload Project ...". A navigation sidebar on the left contains "Home" (highlighted in blue), "Owned By Me", and "Trash". The main content area features a table with the following columns: "Project Name", "Description", "Owner", and "Download". The table contains one entry: "CBB - Accelerator Physics Ontology" (circled in red), "An ontology describing the field of accelerator physics that is being developed at the Center for Bright Beams, a NSF-funded Science and Technology Center. Visit us at http://cbb.cornell.edu.", "cbb-ont-admins", and a download icon. At the bottom of the table, there are navigation icons and the text "1-1 of 1". A footer at the very bottom contains the text: "WebProtégé is developed by the Protégé team in the Biomedical Informatics Research Group (BMIR) at Stanford University, California, USA. The work is supported by Grant GM103316 from the National Institute of General Medical Sciences at the United States National Institute of Health. [Privacy Policy](#) [Terms of Use](#)."

- To add/edit/delete classes, navigate through the classes in the “Classes” window under the “Classes” tab by expanding the class tree. Then, create a new class under an existing class, or select an existing class you want to edit or delete.



To check for existing Annotation properties to go under the “Annotations” description, click the “Properties” tab.

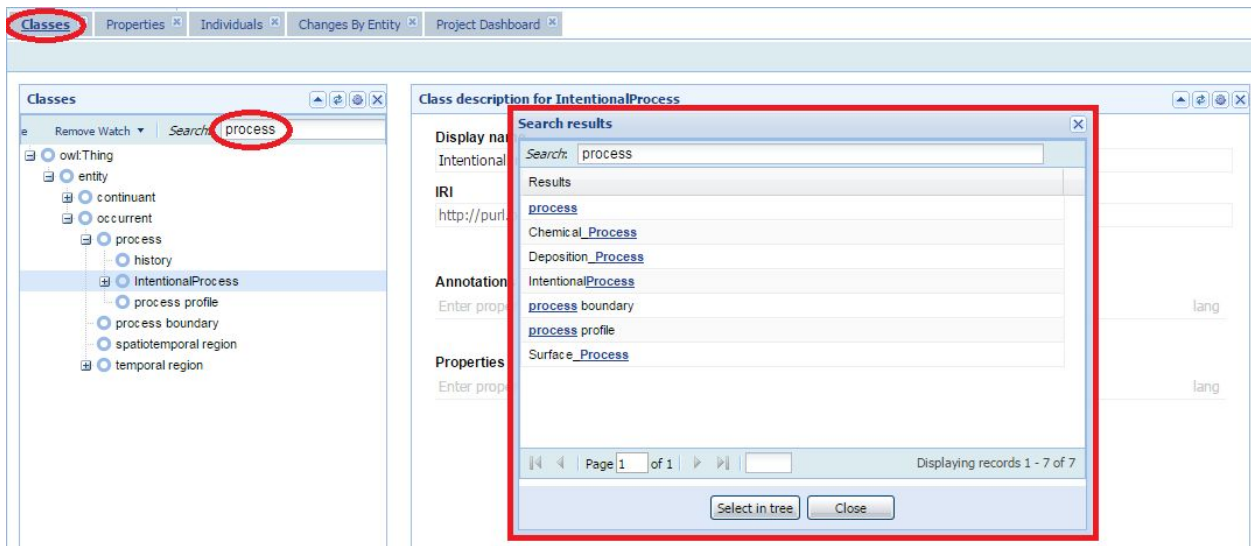


Typically relevant annotation properties for a class entry:

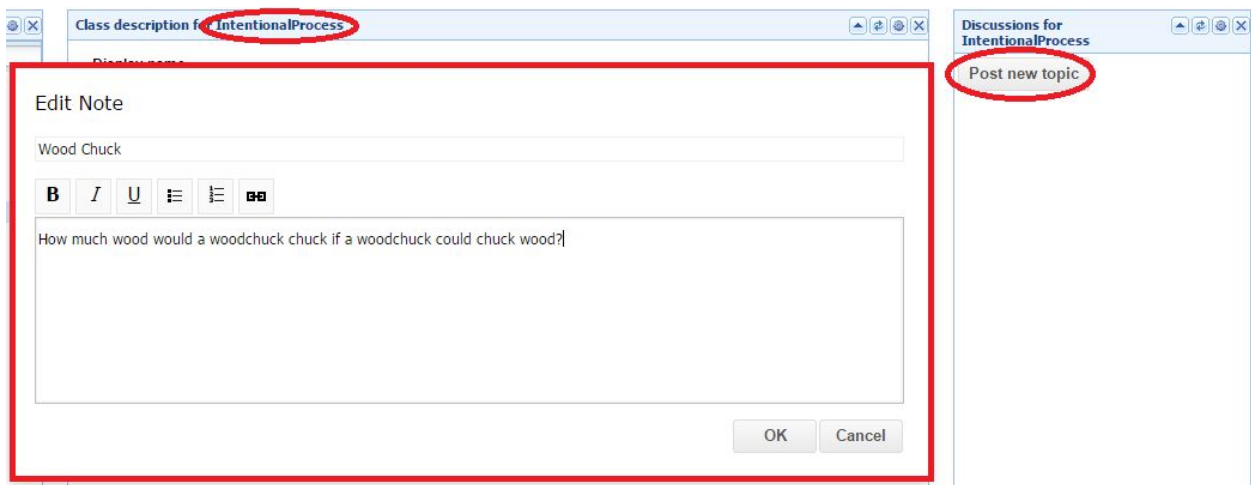
- **rdfs:label** = class name = “Display name”
- **alternative term**: synonyms, acronyms, and alternative terms for the entry

- **definition:** definition of the entry
- **dc:contributor:** name of people who contribute to the entry
- **useful resource:** useful papers/references for the entry

4. To search for a particular class entry, type the desired keyword into the *Search* bar under the “Classes” window.

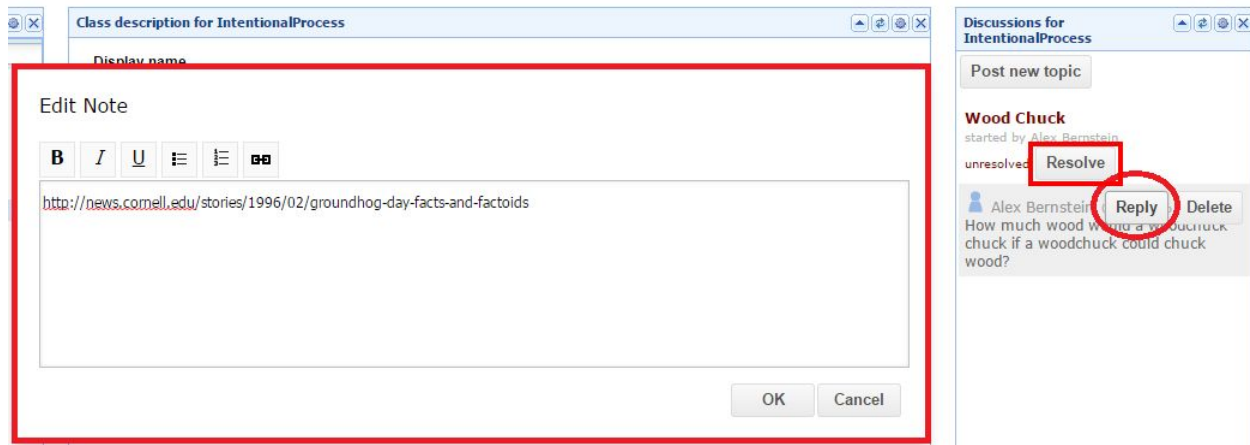


5. To ask questions or give comments on a particular class/entry, select the class, and then click “Post new topic” under the “Discussions for <class name>” window



- To respond to a question/comment, hover over the question/comment and click “Reply”.

- **For original asker/commenter only:** To mark a question/comment as resolved, click the “Resolve” button on your question/comment.



II.C. Ontology structure & language

The CBB ontology is structured according to the **Basic Formal Ontology (BFO) structure** guideline and uses the **Web Ontology Language (OWL)** as the underlying language. This section only covers the basics; please refer to Section IV for links for further information regarding BFO and OWL.

II.C.1. BFO structure

Under the Basic Formal Ontology (BFO), all entries, called *entities*, in the ontology fall under one of two categories: Continuants and Occurrents. Continuants are objects that continue existing over time, i.e. they are timeless and have no definite beginning or end. Occurrents are processes that occur in a given moment, and thus cease to exist after the duration of that moment.

Furthermore, Continuants are divided into Independent Continuants and Dependent Continuants. Independent Continuants are entities that exist on their own, and Dependent Continuants are entities that need another Continuant in order to exist.

These three branches can be thought about in the following way:

- Independent Continuants are **nouns**.

- Dependent Continuants are **adjectives**.
- Occurrents are **verbs**.

Examples:

- Your **body** and your **legs** are independent continuants.
- Your body's **shape** and **size** are dependent continuants.
- The processes of **eating** and **sleeping** are occurrents.

The most fundamental relationship in an ontology is that **each entity is a subclass of another**, which forms the basis of the ontology hierarchy; this means that *every single entity is a class*. At the top of the hierarchy is the class Entity, and all Continuants and Occurrents are a type of Entity.

A common problem is to use other kinds of relationships instead of the subclass when building the hierarchy of the ontology. For example, Leg would not be a type of Body, but rather is a part of the Body, and thus Leg should not be a subclass of Body in the ontology.

Examples of CBB Accelerator Physics Ontology entities/entries:

- **Density Functional Theory (computational method for electronic structures):**
 occurrent > process > IntentionalProcess > Computational_Methods > Electronic_Structure_Methods > Density_Functional_Theory_(DFT)
- **Nb₃Sn (superconducting material):**
 continuant > independent continuant > material entity > object > Material > Material_for_Superconducting_Cavities > Nb3Sn

II.C.2. OWL language

The Web Ontology Language (OWL) is an ontology for the web written in XML. Every element in OWL is an online resource represented by a URI. These resources are then explained using Annotation Properties and related to each other using Data Properties. These properties are themselves represented by URIs.

There are several default Annotation Properties given by OWL present in our ontology:

- **owl:backwardCompatibleWith** -- Indicates that a given ontology is backward compatible with another ontology.
- **owl:incompatibleWith** -- Indicates that a given ontology is incompatible with another ontology.
- **owl:deprecated** -- Indicates that a given entity is deprecated.
- **owl:priorVersion** -- Indicates predecessor to current ontology.
- **owl:versionInfo** -- Provides version information on an ontology or OWL construct.

In addition to OWL there is the Resource Description Framework Schema (RDFS) which is also written in XML. RDFS also has several default Annotation Properties:

- **rdfs:label** -- A human readable name for the subject resource.
- **rdfs:isDefinedBy** -- The definition of the subject resource (given by URI).
- **rdfs:comment** -- A description of the subject resource.
- **rdfs:seeAlso** -- Further information about the subject resource.

All of these default Annotation Properties are defined by URIs in a W3 standard online.

You are technically free to make your own custom Annotation Properties and Data Properties, and these will automatically generate URIs in WebProtege itself. However, ***please check the “Properties” tab in WebProtege*** (see section II.B #3) to see what properties have already been ***defined before you create a new one to reduce redundancy.***

III. Step-by-step Examples

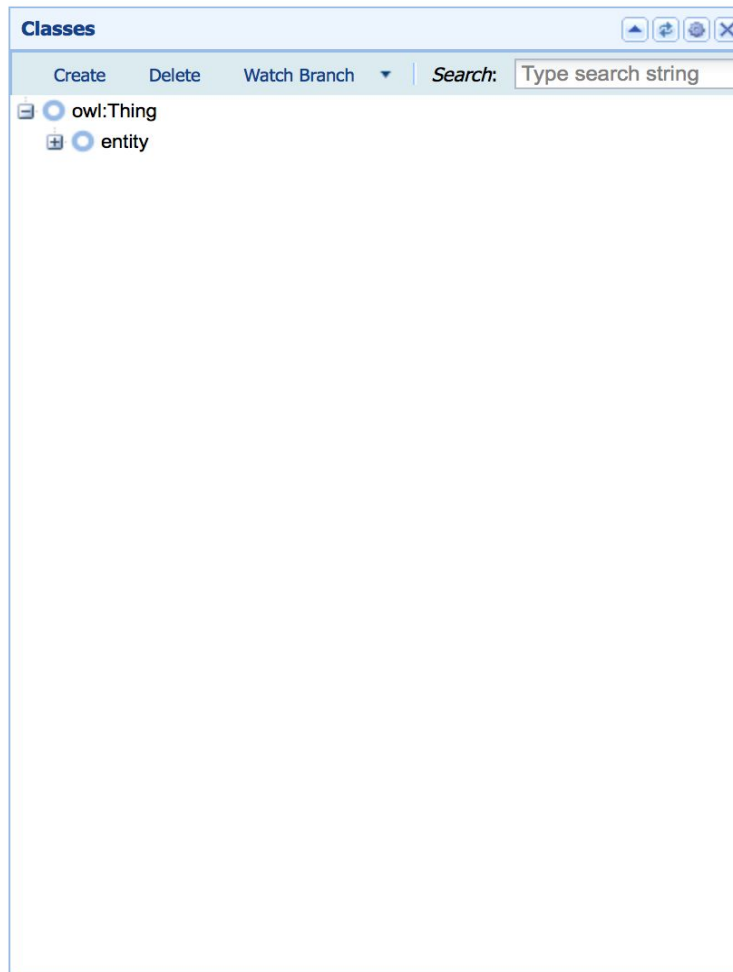
First, sign in at <https://webprotege.cbb.cornell.edu/> and click the “CBB - Accelerator Physics Ontology” as described in Section II.

III.A. Making a first entry

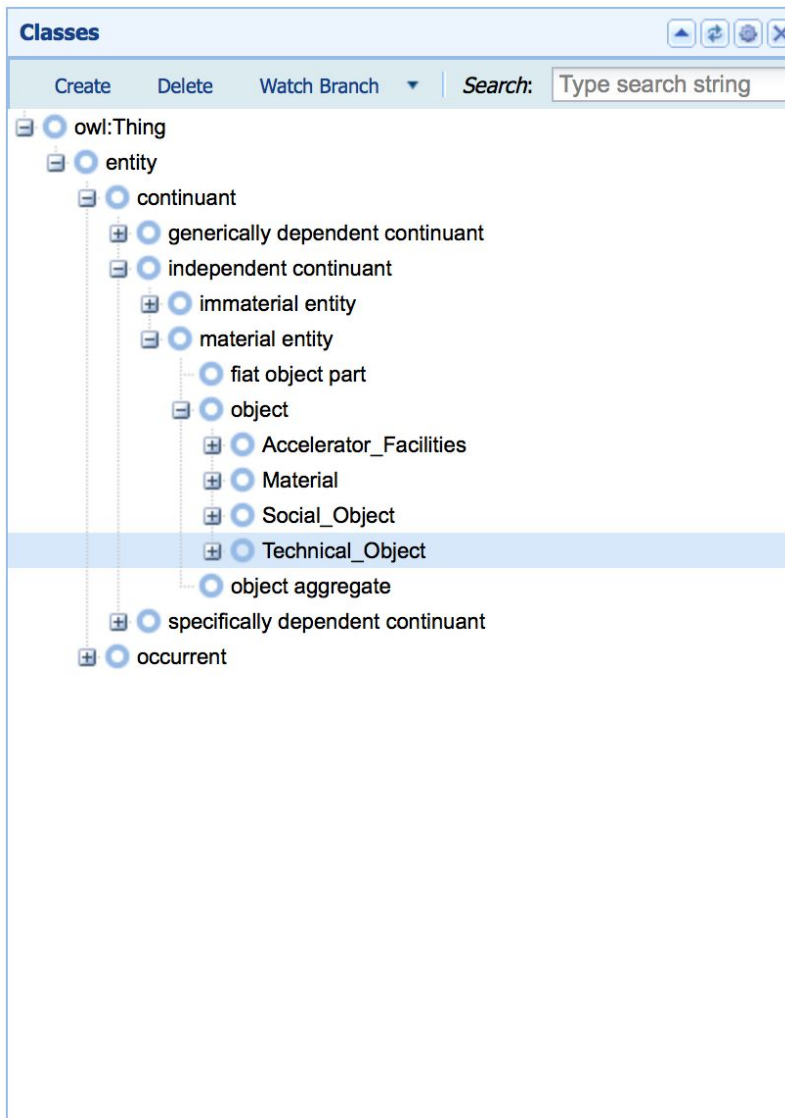
There are two steps to generating an entry, (1) generating a class and (2) annotating a class with information.

Step 1: Generate a Class

All classes in WebProtege begin with the class called “owl:Thing” followed by the class called “entity”. To explore the hierarchy further, simply click the “+” button to the left of the “entity” and all items created under it will show.



Let's create a new class. Suppose we wish to share information about infrared spectrometer, a tool that uses infrared radiation to interrogate chemical bonds to identify their functional group. In the OWL class hierarchy, we need to find an object where `infrared_spectrometer` fits.



In the class window, you can see that under objects, there is a class titled "Technical_Object" there are subclasses that have been generated by other Ontology users which include technical instrumentation such as `Scanning_Probe_Microscope` and `Superconducting_Cavity`.

Click the Create button in the Classes window to create a new class, "Infrared_Spectrometer". You should now see a new class and a mostly blank window that will contain annotations pertaining to `Infrared_Spectrometer`. This is what we need to annotate.

Step 2: Annotate a Class

To annotate a class, click on the annotations, you must specify the type of annotation you will add. Let's add a broad definition, alternative terms, useful resources, and who populated the entry. In OWL these are considered *properties of the class* and you must specify them before adding an annotation. (See the existing Annotation properties in the "Properties" tab as instructed in sections II.B and II.C.2.)

The screenshot shows the Protege software interface for editing a class. The window title is "Class description for Infrared_Spectrometer".

- Display name:** Infrared_Spectrometer
- IRI:** http://webprotege.stanford.edu/RC29iuYMBie76BunfM5uEoT
- Annotations:**
 - rdfs:label:** Infrared_Spectrometer (lang)
 - definition:** A spectroscopic tool that uses infrared radiation to interrogate the vibrational frequencies of chemical bonds in gases, liquids, and solids. (lang)
 - alternative term:** IR spectrometer (lang)
 - dc:contributor:** Will DeBenedetti, Kevin Nangoi (lang)
 - useful resource:** Selection rules for molecules on surfaces
https://doi.org/10.1016/0167-5729(88)90011-8 (lang)
- Properties:** (Empty table with "Enter property" and "Enter value" headers)

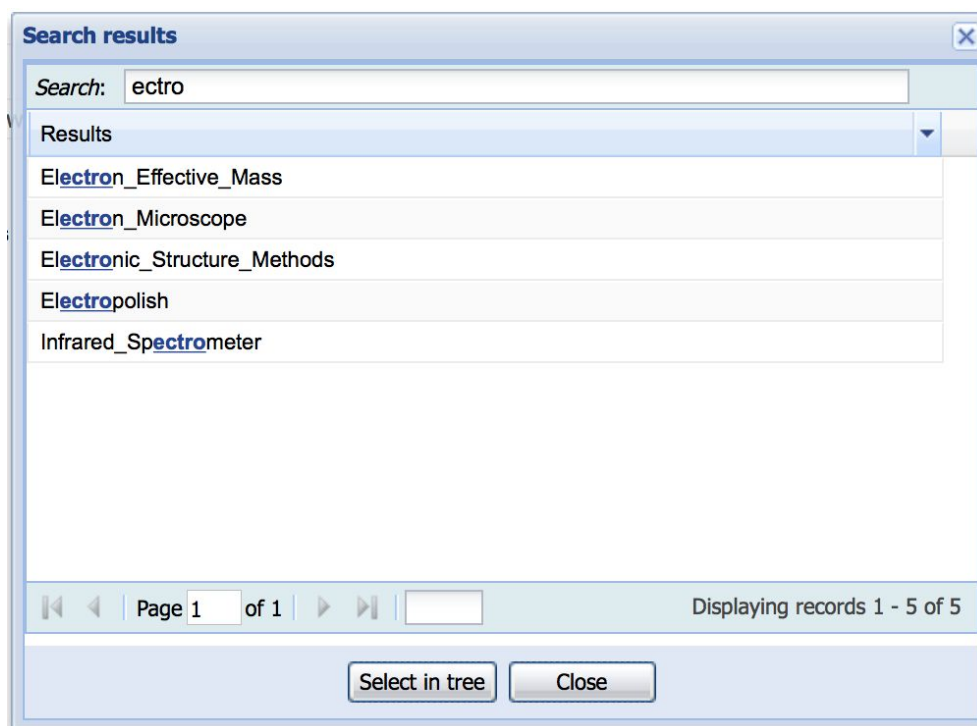
We have now added some class descriptions that broadly define infrared spectrometer, a resource from the literature, and who generated the entry.

Notes:

- If you want to **edit the class name**, simply **edit the "rdfs:label"** property.
- To add **synonyms, acronyms, or alternative terms** for the entry, use the **"alternative term"** property.
- The annotation property for **useful papers/references** is **"useful resource"**. Enter separate references in separate "useful resource" properties (i.e. one "useful resource" property for each reference).
- If you **contribute** to a particular class (e.g. generating it or editing the properties), be sure to **put your name** in using **"dc:contributor"** property.

III.B. Searching for an existing entry

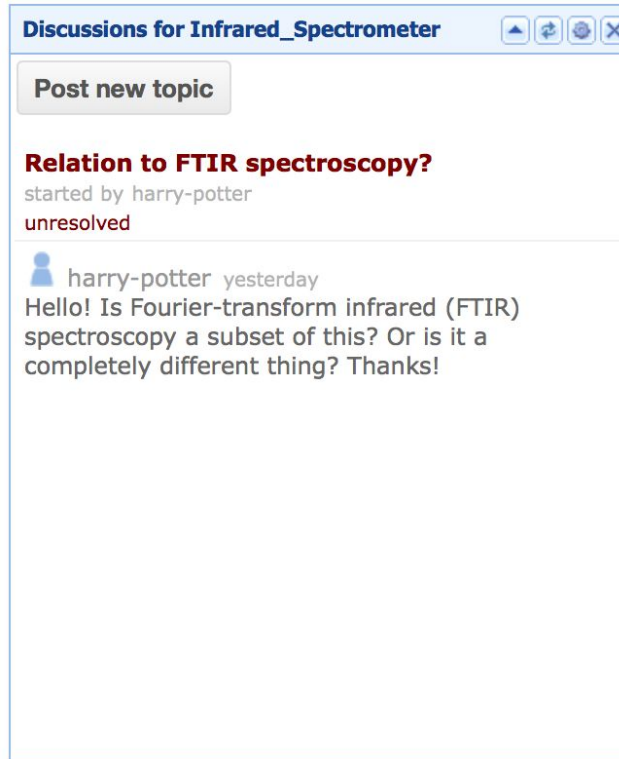
Suppose we want to search for existing classes whose names contain the letters “ectro”. Just simply type “ectro” in the search bar under “Classes” window and hit Enter on the keyboard. A Window will pop up containing the list of all such classes:



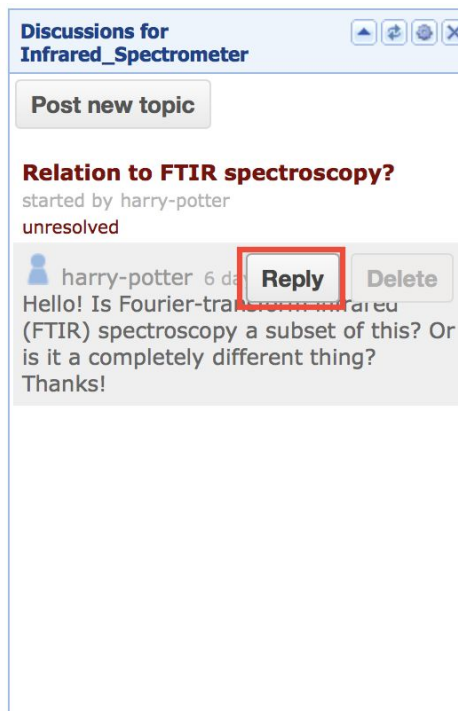
Double click on the class you want to go to from the list.

III.C. Asking questions/adding comments and responding to them

Now suppose we want to ask a question on the Infrared_Spectrometer entry. Click on the “Post new topic” under the “Discussions for Infrared_Spectrometer” window, and the “Edit Note” window will pop up. Type the question title in the “Topic” field and the question in the main field. After clicking “Ok”, the question will show up under the “Discussions for Infrared_Spectrometer” window. It will be marked as “unresolved” by default.



To answer this question, hover the mouse over the question, and click “Reply”.



Type the response in the window that pops up. The reply will show up after clicking “Ok”.

Discussions for Infrared_Spectrometer

Post new topic

Relation to FTIR spectroscopy?
started by harry-potter
unresolved

harry-potter 8 days ago
Hello! Is Fourier-transform infrared (FTIR) spectroscopy a subset of this? Or is it a completely different thing? Thanks!

cbb-ont-admins Less than one minute ago
Yes, FTIR spectroscopy is a type of infrared spectroscopy. Note that "spectroscopy" technically refers to the method, whereas "spectrometer" (as in infrared spectrometer) refers to the tool used for the method.

It's always a good idea to mark a resolved question/comment as "resolved". *Note that this can only be done by the original asker/commenter.* In this example, harry-potter, the original asker, marks the question as being resolved by clicking the "Resolve" button.

Discussions for Infrared_Spectrometer

Post new topic

Relation to FTIR spectroscopy?
started by harry-potter
resolved Re-open

harry-potter 8 days ago
Hello! Is Fourier-transform infrared (FTIR) spectroscopy a subset of this? Or is it a completely different thing? Thanks!

cbb-ont-admins one minute ago
Yes, FTIR spectroscopy is a type of infrared spectroscopy. Note that "spectroscopy" technically refers to the method, whereas "spectrometer" (as in infrared spectrometer) refers to the tool used for the method.

IV. Further Resources

- [Ontology Development 101](#) by WebProtege developers
- WebProtege user guide:
<http://protegewiki.stanford.edu/wiki/WebProtegeUsersGuide>
- Introduction to OWL: http://w3schools.sinsixx.com/rdf/rdf_owl.asp.htm
- OWL guide: <https://www.w3.org/TR/owl-guide/>
- OWL FAQ: <https://www.w3.org/2003/08/owlfaq>
- BFO main website: <http://ifomis.uni-saarland.de/bfo/>
- BFO video tutorial: <https://www.youtube.com/watch?v=bGPVCkuKTo4>

Questions/comments/suggestions? Email CBB ontology admins at cbb-ontology-admin-l@list.cornell.edu.