Selecting and Customizing a Mereology Ontology for its Reuse in a Pharmaceutical Product Ontology

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Abstract. This paper presents our experience in reusing mereology ontologies in a Pharmaceutical Product ontology, an ontology built by the EU NeOn project. It shows a set of mereology ontologies implemented in different machine interpretable languages and analyzes them according to the different types of mereology identified by Varzi. Then, it describes the specifications of mereology modeling necessities for Pharmaceutical Product. Finally, it presents the ontology which fits best with the specifications. One of the results of this work is a procedure to reuse general (also called common) ontologies.

Keywords. Mereology, implemented ontology, pattern reuse, competency question

Introduction

The part-whole relationship has been analyzed over the ages by philosophers. In the Ancient Greece, by the atomists Plato and Aristotle, in the Middle Ages, by Thomas Aquinas and Raymond Llull, in the Age of Enlightenment by Kant and, at the end of the XIX century and beginning of the XX, by Brentano and Husserl. However, none of them formulated a precise theory on this part-whole relationship. It was Lesniewiski [1] who coined the word mereology (from the Greek word méros, meaning part) in 1927 to refer to a formal theory he devised in his papers published between 1916 and 1931. However, because Lesniewiski wrote all his papers in Polish, his theory was unknown by most of his contemporary scientists. Leonard and Goodman’s work “The Calculus of the Individuals” [2] in 1940 made that this formal theory began to be studied in Logics and Ontology. Later on, authors such as Simons [3], Casati and Varzi [4][5],

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Smith [6][7] and Lambrix [8], among others, made relevant contributions to this field. Lambrix is well known for his contribution to the application of mereology to information systems.

In this paper we have adopted the definition of ontology proposed by Studer et al. ([9], page 185, based on Gruber’s definition [10]), “an ontology is a formal, explicit specification of a shared conceptualization”. When explaining such a definition, the authors interpret the word shared as agreed, and the word formal as machine interpretable. Therefore, if this definition holds, we can say that a mereology ontology is an agreed mereology implemented in a machine-interpretable language.

Recently, researchers like Gangemi et al. [11] and Massolo et al. [12] have proposed the use of mereology in ontology construction. This idea is embodied in the work of Borst [13], who built and used a mereology ontology in an engineering application for modeling, simulating and designing physical systems. In this article we intend to describe our experience in reusing ontologies that implement mereology ontologies in an EU Project. The main difference between the work shown in this section and Borst’s is that we analyze, reuse and customize a mereology ontology already built, and that we do not develop a mereology ontology from scratch.

In Section 1, following Varzi’s study, we present the different formalizations that the notion part-whole has undergone. In Section 2, we provide a list of the different ontologies that implement mereological definitions and then, we analyze them according to the formalization variants presented in section 1. In Section 3, we show a case in which these ontologies have been reused for building a Pharmaceutical Products ontology. Finally, in Section 4 we present the conclusions and future lines of research.

The Pharmaceutical Product ontology (PPO) will be used as a bridge between proprietary systems for managing financial and product knowledge interoperability in pharmaceutical laboratories, companies and distributors in Spain [14]. The composition of drugs, the interaction between them, etc., require the formalization of the part of relation. Consequently, it seems reasonable to consider the reuse of a mereology ontology.

1. Mereologies

A mereology is a formal theory of parts and associated concepts [13][15]. We have said ‘a mereology’ instead of ‘the mereology’ because different assumptions can be taken into account in the formalization of the part-whole relationship. Therefore, different mereologies can be proposed.

Theory M

Part-of, otherwise subclass-of, is a relation between individuals. Most of the authors agree on the following core of axioms (named with an A) and definitions (named with a D) [5]:

A1) Reflexivity. Every object of the universe of discourse is part of itself. For instance, the European Union (EU) is part of the EU.
A2) Antisymmetry. If an object \( x \) is part of \( y \), and \( y \) is part of \( x \), then \( x \) and \( y \) are the same object. For instance, if the territory \( T_1 \) is part of the territory \( T_2 \), then the only way for \( T_2 \) to be part of \( T_1 \) is by being \( T_1 \) and \( T_2 \) the same territory.

A3) Transitivity. If \( x \) is part of \( y \), and \( y \) is part of \( z \), then \( x \) is part of \( z \). For instance, Madrid is part of Spain, and Spain is part of EU, therefore, Madrid is part of EU.

A number of additional mereological predicates can be then introduced by definition. For example:

D1) Proper part. A proper part is a part that is other than the individual itself. For example, Spain is a proper part of EU, since Spain is part of EU and they are different entities.

D2) Direct part. \( X \) is a direct part of \( y \) if and only if \( x \) is a proper part of \( y \) and there is no part between \( x \) and \( y \). For example, Italy is a direct part of EU, but Madrid is not, since Madrid is part of EU through Spain.

D3) Overlap. The relation overlap is defined as a sharing part. That is, \( x \) and \( y \) overlap if and only if there is a \( z \) such that \( z \) is part of \( x \) and part of \( y \). For instance, Spain and Africa overlap, since Spain has territories in Africa (Canaries, Ceuta, Melilla, etc.).

D4) Underlap. The relation underlap is defined as a sharing whole. That is, \( x \) and \( y \) underlap if and only if there is a \( z \) such that \( x \) and \( y \) are parts of \( z \). For example, Portugal, Spain, France and Italy underlap because they share a common whole: EU.

D5) Disjoint. The disjoint relation is the logical negation of overlaps. For example, EU and USA territories are disjoint.

Theory \( M \) may be viewed as the embodiment of the common core of any mereological theory. A.1-A.3 should be extended to build a mereology.

**Minimal Mereology (MM)**

A way to extend \( M \) is to assume the following decomposition principle [5]:

A4) Weak supplementation principle. Every object \( x \) with a proper part \( y \) has another part \( z \) that is disjoint of \( y \). The domain of territories fulfils this principle. For example, given that Spain is a proper part of the European Union (EU), then EU has other parts that are disjoint of Spain: Portugal, France, Italy, etc.

Most of the authors maintain that A.4 should be incorporated to \( M \) as a further fundamental principle of the meaning of part-of. Other authors provide scenarios that could be counterexamples of this principle (see [4]). However, it has not been

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demonstrated yet that such supposed counterexamples have implications in computer applications.

**Extensional Mereology (EM)**

Another stronger way to express decomposition is the following:

A5) *Strong supplementation*. If \( y \) is not part of \( x \), then there is a part of \( y \) that does not overlap with \( x \). For example, given that Spain is not part of Africa, there is a part of Spain (e.g. Madrid) that is not part of Africa.

A.5 implies A.4.

This theory is called ‘extensional’ because a theorem that can be demonstrated is

T1) for all \( x \)’s and \( y \)’s, such that \( x \) has proper parts or \( y \) has proper parts, \( x \) and \( y \) are identical if and only if \( x \) and \( y \) have the same proper parts, that is, for all \( z \)’s, \( z \) is proper part of \( x \) if and only if \( z \) is part of \( y \). For example, the territory of the Community of Madrid is the same as that of the province of Madrid because both territories are composed of the same proper parts, that is, by the same municipalities.

**Closure Mereology (CM)**

Another way of extending \( M \) is by composition [4]

A6) *Sum principle*. If \( x \) and \( y \) underlap, then there is a \( z \) such that, for all \( w \)’s, \( w \) overlaps \( z \) if and only if \( w \) overlaps \( x \) or \( w \) overlaps \( y \). That is, if two objects underlap, then it may be assumed that there is a smallest object of which they are part (an object that exactly and completely exhausts both).

According to (A6), there is an object made up exactly of Madrid and Barcelona.

A7) *Product principle*. If \( x \) overlaps \( y \), then there is a \( z \) such that for all \( w \)’s, \( w \) is part of \( z \) if and only if \( w \) is part of \( x \) and \( w \) is part of \( y \). That is, if two objects overlap, then it may be assumed that there is the largest object that is part of both (the common part at their junction). For example, Spain and Africa overlap, and it may be assumed that there is the largest object overlapped by both: Canaries, Ceuta, Melilla, etc.

The assumption of (A6) and (A7) is controversial. In fact, it is not obvious that the overlap of Spain and Africa makes an entity.

**Closure Extensional Mereology (CEM)**

The result of adding these axioms to \( MM \) or \( EM \) yields corresponding Minimal or Extensional Closure Mereologies, that is, \( CMM \) and \( CEM \), respectively. In the presence of (A4), (A7) implies (A5). Consequently, \( CMM \) and \( CEM \) are the same theory [4].
The entities whose conditional existence is asserted by (A6) and (A7) must be unique in the presence of extensionality. Thus, \( \text{CEM} \) supports the following definitions:

D6) \textit{Binary sum}. \( X + y \) is the \( z \) that fulfils that for all \( w \)'s, \( w \) overlaps \( z \) if and only if \( w \) overlaps \( x \) or \( w \) overlaps \( y \). That is, \( x + y \) is the smallest object of which \( x \) and \( y \) are part.

D7) \textit{Binary product}. \( X . y \) is the \( z \) that fulfils that for all \( w \)'s, \( w \) is part of \( z \) if and only if \( w \) is part of \( x \) and \( w \) is part of \( y \). That is, \( X . y \) is the largest object that is part of \( x \) and \( y \).

\textbf{General (classical) Mereology (GM)}

Another way of extending \( M \) is through the following axiom schema:

A8) \textit{Unrestricted fusion principle}. For every satisfied property or condition \( \phi \), there is a \( z \) such that for all \( y \)'s, \( y \) overlaps \( z \) if and only if there is an \( x \) such that it satisfies \( \phi \) and overlaps \( y \). That is, there is an entity consisting of all those things that satisfy \( \phi \). For example, suppose that \( \phi \) means “country with more than 10 million inhabitants”, then there is an object that consists of all the countries with more than 10 million inhabitants.

If (A5) is satisfied, then at most one entity can satisfy the consequent of (A8). Therefore, the operation of general sum (\( \sigma \)) can be defined as follows:

D8) \textit{General sum}. The general sum of all \( x \)'s satisfying \( \phi \) is that \( z \) that for every \( y \), it overlaps \( z \) if and only if there is an \( x \) such that it satisfies \( \phi \) and overlaps \( y \). That is, the sum of \( \phi \)'s is the entity that consists of all entities that satisfy \( \phi \).

\textbf{General Extensional Mereology (GEM)}

The extensions of \( MM \) and \( EM \), which yield the same extensional strengthening of \( GM \) [4], is the theory of General Extensional Mereology, or \( GEM \), since (A8) implies (A7) and (A7)+(A4) imply (A5) ([3], page 31). It is also clear that \( GM \) is an extension of \( CM \) and \( GEM \) is an extension of \( CEM \), since (A6) can be deduced from (A8).

\textbf{Atomistic Mereology}

In an atomistic mereological theory, every element is made up of elements that are building blocks or atoms. To describe such a theory, the following definition can be provided:

D9) \textit{Atom}. It is an element that does not have proper parts.

The atomistic axiom can be formulated in the following way:
A9) Atomicity. Every object has at least a part that is an atom. For example, the administrative division of territories follows this axiom, since there are simple divisions that are not divided.

Figure 1 shows a diagram with all the theories presented in this section.

A mereology $X$ (e.g. GEM) extended with the atomicity axiom is known as $AX$ (e.g. AGEM).

![Hasse's diagram of mereological theories](http://suo.ieee.org/SUO/ontologies/Guarino.txt)

**Figure 1.** Hasse’s diagram of mereological theories (from weaker to stronger, going uphill) [4].

### 2. Mereology Ontologies

Using a general purpose search engine (Google) and a specific one (Swoogle), we have found a series of mereology ontologies. Some of them have been rejected because they lack documentation; therefore, the final list of ontologies that we have studied is this

- **KACTUS** [16] ontology library, implemented in CML, it is maintained by the University of Amsterdam. Such a library contains the Mereological Ontology (MO), which is an adapted version of Borst’s proposals [13](see foot note 3).
- **DOLCE** is one of the ontologies developed within the WonderWeb European project [12]. It is available in KIF and OWL.
- The **Standard Upper Ontology** [4]: (SUO) is the result of a joint effort to create a large, general-purpose, formal ontology [17]. It is promoted by the IEEE Standard Upper Ontology working group, and its development began in May 2000. This ontology is implemented in KIF and Protégé format; on the other hand, SUO formally describes mereology and topology terms. The general predicates in this section of the ontology are adapted from Barry Smith, Borgo et al.’s work, and from Casati and Varzi’s mereologies.
- **The ontology based on Barry Smith and other authors’ work** [6][7] in KIF, which is referred in the SUO web page. It represents various mereological definitions and axioms concerning boundaries and objects [8].

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The mereology based on the work of Borgo et al., which is another ontology referred in SUO web page. These authors describe a set of definitions and axioms concerning mereology in [18]. Such ontology is currently implemented in KIF\(^7\). The ontology formalizes a CEM mereology (except the product principle).

Casati and Varzi’s [19] mereology can be also found implemented in KIF and is also referred in the SUO web page.

The features of these ontologies with regard to the theories previously presented are shown in table 1.

3. Use Case: a Pharmaceutical Product Ontology Built within the NeOn Project

NeOn\(^8\) is a project co-funded by the European Commission’s Sixth Framework Programme. Its aim is to advance the state of the art of the use of ontologies for large-scale semantic applications in the distributed organizations. Particularly, it aims to improve the capability of handling multiple networked ontologies that exist in a particular context, that are created collaboratively, and that might be highly dynamic and constantly evolving.

The Pharmaceutical Product ontology (PPO) will be part of the supportive collaboration of the pharmaceutical industry, concerned with the infrastructure and its APIs to bridge the currently used proprietary systems for managing financial and product knowledge interoperability in the networks/clusters of pharmaceutical laboratories, companies and distributors in Spain [14]. In this section, we will focus just in four (out of 61) competency questions (CQs) that allow us to explain our idea as best as possible (see table 2).

The activities that we have carried out to identify the mereology terms, axioms and definitions required in the PPO are the following:

I) **Ontology search.** The activity implies finding candidate ontologies or ontology modules to be reused. To perform this activity, we have started from the analysis of the PPO competency questions (CQs):

I.a) **Analysis of the PPO CQs.** The steps carried out are the following:

I.a.1) *To obtain the concepts and their relations that allow us to represent the terms appearing in the CQs.* For our case, the concepts are chemical substance and drug, and the relations are has component and has interaction with (both relations are found between chemical substances), and has main substance and has active ingredient (both relations are found between drugs and chemical substances). Besides, drug is subclass of chemical substance. Drug-drug interaction does not necessarily require the physical interaction between their ingredients. While some drugs might inactivate other drugs by bonding with them, others simply compete for the same receptors without interacting physically.

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\(^7\) http://suo.ieee.org/SUO/ontologies/Guarino.txt

\(^8\) http://www.neon-project.org
Table 1. Features of ontologies that implement mereotopology theories. The characteristics that appear shaded are those required for the Pharmaceutical Product Ontology.

<table>
<thead>
<tr>
<th>Theory</th>
<th>Principles and definitions</th>
<th>KACTUS</th>
<th>DOLCE</th>
<th>SUO</th>
<th>Smith et al.</th>
<th>Borgo et al.</th>
<th>Casati and Varzi</th>
</tr>
</thead>
<tbody>
<tr>
<td>M</td>
<td>A.1) Reflexivity</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td></td>
<td>A.2) Antisymmetry</td>
<td>Yes</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td></td>
<td>A.3) Transitivity</td>
<td>Yes</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td></td>
<td>D.1) Proper part</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td></td>
<td>D.2) Direct part</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td></td>
<td>D.3) Overlap</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td></td>
<td>D.4) Underlap</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td></td>
<td>D.5) Disjoint</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>MM = M + (P4)</td>
<td>A.4) Weak supplementation</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
<td>Inferred</td>
<td>No</td>
</tr>
<tr>
<td>EM = M + (A5)</td>
<td>A.5) Strong supplementation</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td>CM = M + (A6) + (A7)</td>
<td>A.6) Sum principle</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td></td>
<td>A.7) Product principle</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>CEM = CM + (A5)</td>
<td>D.6) Binary sum</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td></td>
<td>D.7) Binary product</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>GM = M + (A8)</td>
<td>A.8) Unrestricted fusion principle</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>GEM = GM + (A5)</td>
<td>D.8) General sum</td>
<td>No</td>
<td>Yes</td>
<td>No</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>AX = (A9) + a mereology X</td>
<td>D.9) Atom</td>
<td>No</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td></td>
<td>A.9) Atomicity</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
</tr>
</tbody>
</table>
Table 2. Competency question analysis for mereology ontology reuse

<table>
<thead>
<tr>
<th>Identifier</th>
<th>Competency question</th>
<th>Competency question using the vocabulary of mereology</th>
<th>Extracted terms</th>
</tr>
</thead>
<tbody>
<tr>
<td>CQ1</td>
<td>What is the composition of the drug?</td>
<td>Which are the parts of the drug?</td>
<td>- part of</td>
</tr>
<tr>
<td>CQ2</td>
<td>Which is the main active ingredient (molecule) of the drug?</td>
<td>(It does not directly require mereotopology)</td>
<td>- active ingredient</td>
</tr>
<tr>
<td></td>
<td></td>
<td>This term requires the definition of: part of</td>
<td></td>
</tr>
<tr>
<td>CQ3</td>
<td>Which is the main substance of the composition?</td>
<td>(It does not directly require mereotopology)</td>
<td>- main substance</td>
</tr>
<tr>
<td></td>
<td></td>
<td>This term requires the definition of: part of</td>
<td></td>
</tr>
<tr>
<td>CQ4</td>
<td>Does the drug have interaction with another drug?</td>
<td>Are there parts of the drug that interact with parts of another drug?</td>
<td>- part of</td>
</tr>
</tbody>
</table>

I.a.ii) To apply a pattern of reuse of mereologies (inspired by [20][21]), which answers the question ¿what relations are candidate to be renamed so that mereology definitions and axioms can be reused? The pattern involves the use of the following rules:

- **Rule 1.** If the relation establishes a (partial) order, then this relation (or its inverse) is candidate to be a kind of part-of. An example that adheres to this rule is component of, since a substance \( x \) can be a component of \( y \), \( y \) can be a component of \( z \), etc, in such a way that an order \( x < y < z \) is established. Note that the engineer could have decided to model the relation has component instead of component of.

- **Rule 2.** If we can find a super-relation that establishes an order, then this relation is candidate to be modeled in terms of a mereology, even though it is not itself a type of part-of. For example, that \( x \) has as a main substance \( y \) implies that \( y \) is part of \( x \).

I.a.iii) To try to reformulate the competency questions in terms of mereology by following the results of the pattern rules. Table 2 shows how these CQs require mereology terms in PPO. The competency question, *What is the drug main active ingredient (molecule)*? has led to the formalization of the term *active ingredient* by means of the following SWRL rule:

\[
R1) \text{hasActiveIngredient(?x, ?y)} \rightarrow \text{partOf(?y, ?x)}
\]

The competency question, *Which is the main substance of the composition*? has led to the formalization of the term *main substance* by means of the following SWRL rule:
The competency question, *Does the drug have interaction with another drug?* has led to the following SWRL rule concerning the term *interaction with*:

\[
\text{R3)}\ \text{chemicalSubstance(?chs1)} \land \text{chemicalSubstance(?chs2)} \land \\
\text{partOf(?chs11, ?chs1)} \land \\
\text{partOf(?chs21, ?chs2)} \land \\
\text{hasInteractionWith(?chs11, ?chs21)} \rightarrow \\
\text{hasInteractionWith(?chs1, ?chs2)}
\]

that is, if a part of a chemical substance $chs1$ interacts with another part of a chemical substance $chs2$, then $chs1$ interacts with $chs2$. In other words, the interaction is inherited from the parts to the whole [22].

The analysis of other competency questions produces rules that link chemical substance terms to mereology terms.

I.b) *Identification of the features of the mereology ontology to be reused.*

Section 1 and, particularly, table 1 permits us to identify which features the reused mereology ontology should have.

Some properties (e.g. transitivity) were not clearly determined by competence questions. This fact indicates that the meaning of the CQs was not completely clear. That is, the study of the axioms and definitions shown in table 1 has helped us to identify ambiguities and, as will be seen in the further paragraphs, to precise the meaning of the CQs.

For the PPO case, the following formalization has been necessary:

A.1) *Reflexivity.* To ensure the right meaning of the ontology terms.

   Thus, for example, if *part of* is not reflexive, then rule (R3) may not work for a query where $chs1$ is identical to $chs11$ or $chs2$ is identical to $chs21$.

A.2) *Antisymmetry.* To help the user to check constraints.

A.3) *Transitivity.* To be modeled if the different levels of the structure of components are provided. For example, Frenadol® is composed of paracetamol, dextrometorphan, and clorfenamine. Paracetamol, in its turn, is composed of an alcohol, an amino group and a carbonyl group. The alcohol is composed of oxygen and hydrogen, etc. Given that the inclusion of the transitivity axiom is low cost, we have opted to include all the components in the answer of CQs.
D.1) Proper part. The formalization of this term eases the interpretation of the competency questions. Thus, the very substance should not be a result of CQ1, but a result of CQ4 instead, since the very substance can interact with a part of another substance.

D.2) Direct part. This term allows answering CQ1 just in a level. Therefore, CQ1 has been split into two competency questions: (CQ1’) What is the drug composition? (considering only a level) and (CQ1”) idem (considering all the components).

A.4) Weak supplementation principle. This axiom helps the user to check constraints.

D.3) Overlap. It is necessary to formalize (A4).

D.4) Underlap. It is not necessary for the PPO at the moment.

D.5) Disjoint. It is necessary to formalize (A4).

A.5) Strong supplementation principle is not true if the bounds between atoms are not taken into account. We should remember that (A5) implies that two not atomic entities are identical if and only if they have the same parts. However, isomers are not ruled out in the Pharmaceutical Product ontology. An isomer is a chemical compound with the same number and kind of atoms as another but different structural arrangement. If the structure of drugs is required, then a topology ontology is needed.

D.6 and more) Sums and product. We do not find necessary to define sums and products.

D.10) Atom. As will be seen, the term atom will be used to represent the weak supplementation principle.

A.9) Atomicity. We do not think that atomicity is needed in the PPO.

The aforementioned features are shadowed in table 1.

II) Selection of a mereology ontology. This activity involves choosing the most suitable ontologies or ontology modules among those available in an ontology repository or library, for a concrete domain of interest and associated tasks. No mereology ontology completely fulfills all criteria, but KACTUS MO is the ontology that best fits the required features. This ontology has the added advantage of having been built to be easily reused in knowledge based systems.

Note however that the rest of the ontologies cover more characteristics that are not considered in the current CQs than KACTUS MO does. In this step, therefore,
we have decided to reuse more the mereology ontology within the current version of the ontology, and to reuse it less in further versions.

III) **Customization of the chosen mereology ontology.** This activity involves adapting an ontology to a specific user’s needs. We have carried out the following subactivities: (1) pruning the reused ontology according to the features really necessary; (2) enriching the ontology (e.g. with the part of reflexivity axiom); (3) translating from CML into OWL + SWRL; and (4) evaluating the ontology obtained. The result of this activity is the tree shown in Figure 2 (the concepts in italic have been added during activity (IV), and a series of OWL definitions and SWRL rules. Some of them are the following:

D.1') MereologicalIndividual ⊆ owl:thing

D.2') mereologicalIndividualNotFWSPrinciple\(^9\) ≡ mereologicalIndividual ∩ not mereologicalIndividualFWSPrinciple

D.3’) atom ≡ mereologicalIndividualFWSPrinciple ∩ (= 0 properPart mereologicalIndividual)

Asymmetry of *proper part of*:

R.4) properPartOf(?x, ?y) ∧ properPartOf(?z, ?x) → differentFrom(?y, ?z)

Transitivity of *proper part of*:

R.5) properPartOf(?x, ?y) ∧ properPartOf(?y, ?z) → properPart(?x, ?z)

*Weak supplementation* principle:

R.6) properPartOf(?x, ?y) ∧ properPartOf(?z, ?y) ∧ differentFrom(?z, ?x) → mereologicalIndividualFWSPrinciple(?y)

This principle is completed with the *atom* definition (D.3’).

IV) **Integration of the chosen mereology ontology in the PPO.** The product of the activity (III) has been included in the PPO. Besides the bridge rules (R1), (R2) and (R3), the following definitions have been incorporated to obtain the ontology to be newly evaluated:

D.4) chemicalSubstance ⊆ mereologicalIndividualFWSPrinciple

D.5) drug ≡ chemicalSubstance ∩ (≥ 1 hasActiveIngredient chemicalSubstance) ∩ (≥ 1 hasMainSubstance chemicalSubstance)

\(^9\) FWS means ‘fulfilling weak supplementation principle’.
4. Conclusions and Future Directions

In this paper, we have presented the study of different mereologies following Varzi’s work [5], and have analyzed a set of mereology ontologies according to the principles and definitions previously identified. Then, we have specified the mereology modeling necessities in the Pharmaceutical Product ontology in the NeOn European project. We have observed that the formalization of the reflexivity, antisymmetry and transitivity axioms, together with the weak supplementation principle and the proper part of and direct part of definitions are useful for the development of the ontology. Moreover, in the future, it is possible to incorporate axioms that imply extensionality, if a detailed structure of drugs is modeled in the ontology. Future investigation lines should include the analysis of other types of part-of different to the functional one and the reuse of patterns for other types of common ontologies (e.g. topologies).

After analyzing the candidate mereology ontologies, we select KACTUS MO to model the part-whole relationship in the NeOn Pharmaceutical Product.

One of the results of this work is the procedure to reuse mereology ontologies, which refines the one presented in [23] for time ontologies. Such a procedure consists in: (I) searching the candidate mereology ontologies; (II) selecting the mereology ontology that best matches the modeling necessities; (III) adapting the chosen mereology ontology; and (IV) integrating the mereology ontology in the host ontology. Activity (I) requires analyzing the CQs of the ontology where the mereology ontology will be reused, and identifying the features required by the mereology ontology. We provide a table explaining the features of the most well-known mereology ontologies. The table also indicates which of these features have been useful in the real case presented in the paper. It must be added that the analysis of CQs may imply their redefinition. Another result of our work is the OWL+SWRL mereology ontology.
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