Ontological Derivation of Mendeleev's Periodic Table of Chemical Elements

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Abstract

Given 63 chemical elements identified 150 years ago, Mendeleev developed his first version of the Periodic Table of Chemical Elements. To celebrate the 150th anniversary, we asked whether ontology could be used to derive the major features of Periodic Table. Using two criteria (e.g., oxidation and atomic weights), we were able to regenerate the major structure of Mendeleev's Periodic Table in ontology. The characteristics of new elements could also be predicted using ontology.

Keywords:

Chemical Element; Periodic Table; Ontology.

Introduction

In 1869, Mendeleev generated the first version of his Periodic Table of Chemical Elements by carefully arranging the 63 known chemical elements (among which Didymium is indeed a mixture of two elements) (1). Based on the Table, we were also able to predict the characteristics of three unknown elements, germanium, gallium, and scandium. In this study, we hypothesized that ontological generation and inference would be able to predict the framework of the chemical elements with the same information that Mendeleev had.

Methods

The basic atom information of the 62 known elements was extracted using Ontofox (http://ontofox.hegroup.org) from the Chemical Entities of Biological Interest Ontology (ChEBI; http://www.obofoundry.org/ontology/chebi.html), and the information formed the basis of the resulting Ontology of Chemical Elements (OCE). Protege-OWL editor was used for OCE editing and reasoning. Key attributes of chemical elements were identified and added to the OCE, and used to generate ontology axioms and support inference and prediction.

Results

One major criterion Mendeleev used is the oxidation condition for each element, in the format of R_2O, R_2O_2, R_2O_3, R_2O_4, R_2O_5, R_2O_6, R_2O_7, R_2O_8 or RO_4 (1). For example, using the oxidation condition, we could generate an axiom as equivalent class definition for Group 2 atom (Figure 1):

'has function' some 'able to form RO'

With this axiom, Calcium atom is infered as a Group 2 atom. In the modern era, such feature can also be expressed using valence electron number, which is the number of electons on the outer electron shell of the atom. The valence electron number determines the level of oxidation of the atom and is also responsible for chemical properties such as electrical conductivity. Metallic elements typically have high electronical conductivity when in the solid state.

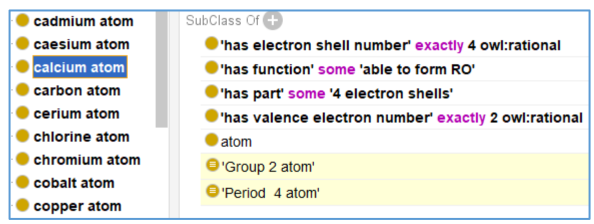

Figure 1. Definition and classification of Calcium atom.

The combination of the Group classification and the atomic weights was able to derive Mendeleev's basic Periodic Table structure. Instead of using atomic weights, the current ordering of the elements in the Periodic table uses an atomic number or proton number. The electron configuration and the atomic number together define the framework of the current Periodic Table structure.

Using the same methods defined above, Mendeleev correctly predicted the positions of three then unknown elements Germanium, Gallium and Scandium. The characteristics of these elements could also be predicted by comparing the features of their neighboring chemical elements.

Conclusions

With proper attributes and axiom definitions, ontology could be used to regenerate Mendeleev's Periodic Table of Chemical Elements and predict unknown elements' characteristics. Therefore, given proper logical definitions, ontology supports entity classification and feature prediction.

References

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