PubChem Periodic Table and Element Pages

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Abstract:

PubChem (https://pubchem.ncbi.nlm.nih.gov) is one of the top five most visited chemistry web sites in the world, with 3.5 million unique users per month at peak. About half of them are between ages 18 and 24, suggesting that PubChem is heavily used by undergraduate or graduate students at academic institutions. Therefore, PubChem has a great potential as an online resource for chemical education. This paper describes the PubChem Periodic Table and Element pages, which were recently introduced to celebrate the 150th anniversary of the periodic table. These new services help users navigate the abundant chemical element data available within PubChem, while providing a convenient entry point to explore additional information, such as bioactivities and health and safety data, available in PubChem Compound pages for specific elements and their isotopes.

Introduction

The periodic table of chemical elements is one of the most recognized tools in science. Its simplicity and grace may make it easy to overlook the wealth of information contained therein. The periodic table organizes all known elements in a tabular format in order of increasing atomic number. The tabular organization (left to right and top to bottom) is very important, reflecting key trends and commonalities. There is much students in the classrom can learn about chemistry from the periodic table and they should get familar with it.

The periodic table in its present form is considered to be first introduced in 1869 by a Russian chemist, Dimitry Mendeleev, although there had been earlier attempts to classify elements by their similarities. As we mark the 150th anniversary of the periodic table, the scientific community has declared 2019 to be “The International Year of the Periodic

Table".[1] PubChem (**Figure 1**) (https://pubchem.ncbi.nlm.nih.gov) [2-4] joins this celebration by launching the PubChem Periodic Table and corresponding Element pages.

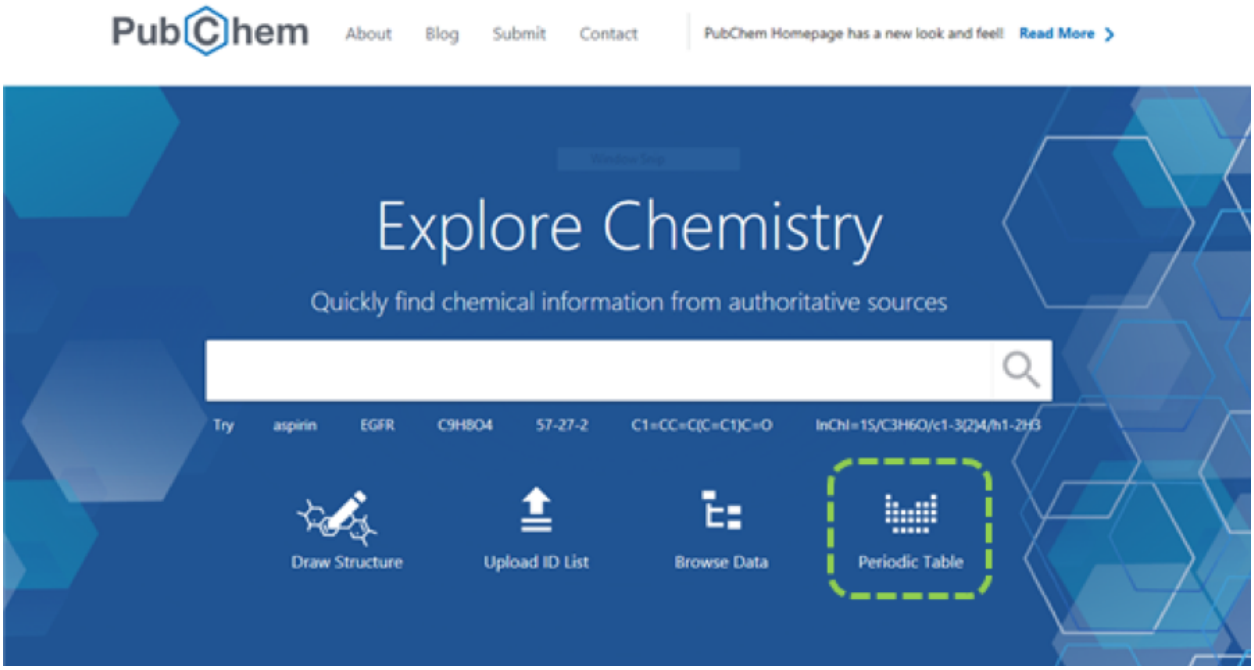

Figure 1. *Snapshot of PubChem Homepage (https://pubchem.ncbi.nlm.nih.gov). The PubChem Periodic Table can be accessed by clicking the Periodic Table icon (indicated with the green box).*

PubChem is a public chemical information resource, developed and maintained by the U.S. National Institutes of Health. With 3.5 million unique users per month at peak, it is considered as one of the top five chemistry web sites in the world in terms of web traffic. About 40% of PubChem users are aged between 18 and 24, many of which are likely to be students enrolled in academic institutions. This suggests PubChem's great potential as a chemical education resource.

PubChem provides for a given chemical a Compound Summary page, a comprehensive overview of all information available within PubChem for that chemical. While the Compound Summary page is appropriate to present data for most chemicals, it is not designed for displaying information specific to elements (such as electronegativity and electron configuration). The PubChem Periodic Table and Element pages help you navigate the abundant chemical element data available within PubChem, while providing a convenient entry point to explore additional information, such as bioactivities, health and safety data, available in PubChem Compound pages for specific elements and their isotopes. The present paper provides an overview of the PubChem Periodic Table and Element pages.

Periodic Table

PubChem Periodic Table (**Figures 2-4**) can be accessed by clicking the Periodic Table icon on the PubChem homepage (https://pubchem.ncbi.nlm.nih.gov) (**Figure 1**). Alternatively, it can also be directly accessed via the following URL: https://pubchem.ncbi.nlm.nih.gov/ptable/

The PubChem Periodic Table provides three distinct views: Table View, List View, and Game View.

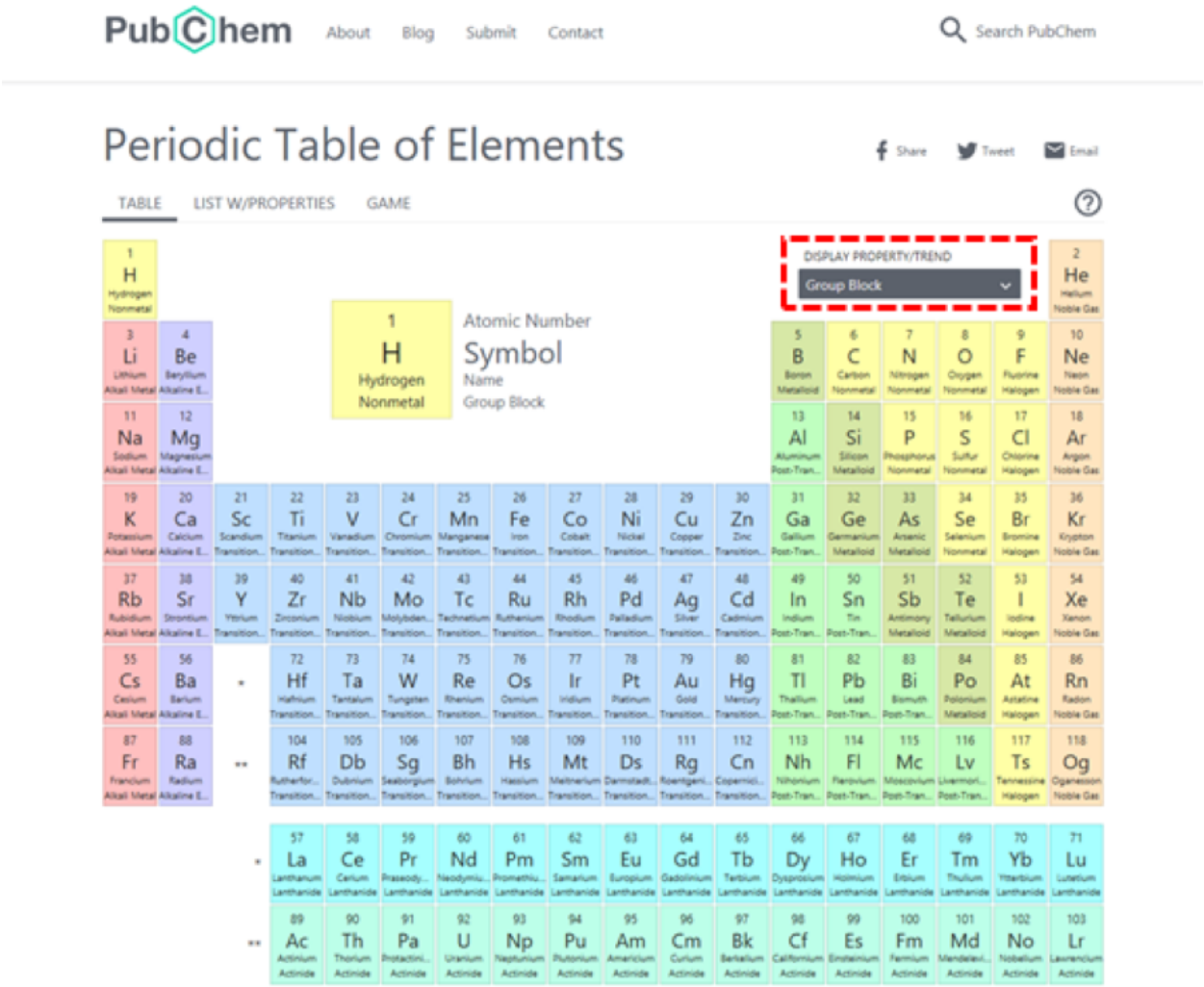

Figure 2. *Snapshot of the Table View of PubChem Periodic Table (https://pubchem.ncbi.nlm.nih.gov/ptable/). The elements can be colored according to their properties, by using the drop-down menu available at the upper-right corner of the table.*

• The Table View (https://pubchem.ncbi.nlm.nih.gov/ptable/#view=table) is the traditional periodic table any scientist would instantly recognize. The elements can be colored according to various elemental properties (atomic mass, standard state, group block, electron configuration, etc.) with the selected property value displayed for each element, by using the drop-down menu available at the top-right corner.

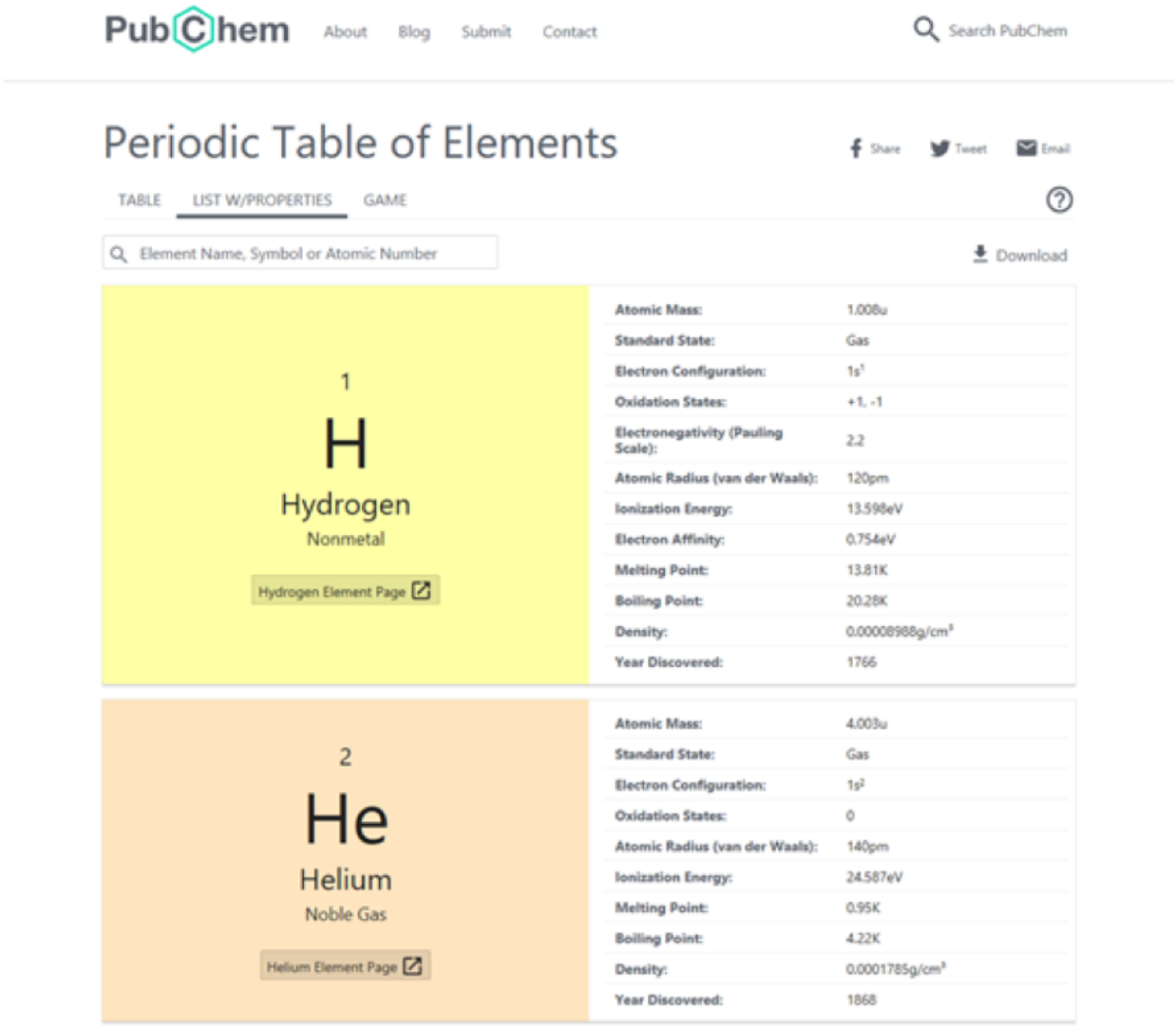

Figure 3. *Snapshot of the List View of PubChem Periodic Table (https://pubchem.ncbi.nlm.nih.gov/ptable/).*

• The List View (https://pubchem.ncbi.nlm.nih.gov/ptable/#view=list) allows one to see a set of properties available for each element all at once. Using the search box at the top-left

corner, one can quickly find an element of interest. The "Download" button at the top-right corner allows one to download all data presented on the Periodic Table.

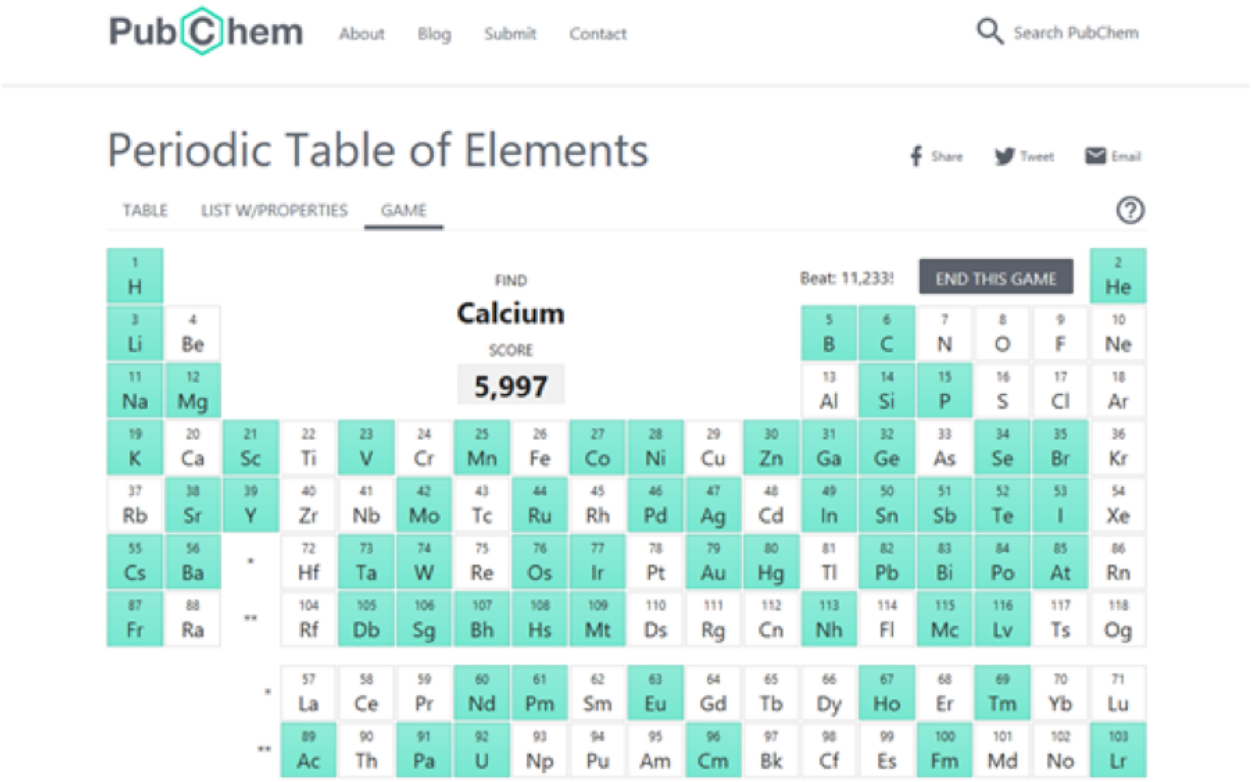

Figure 4. *Snapshot of the Game View of PubChem Periodic Table (https://pubchem.ncbi.nlm.nih.gov/ptable/).*

• The Game View (https://pubchem.ncbi.nlm.nih.gov/ptable/#view=game), added as an educational feature, helps test one's knowledge of element names and symbols. The game has three levels of difficulty (easy, medium, and hard).

One can select one of the three views by clicking the "TABLE", "LIST W/ PROPERTIES" and "GAME" tabs, available above the upper-right corner of the Periodic Table. By default, the Table View is presented. The Periodic Table is optimized for printing and/or saving as the Portable Document Format (PDF), hiding unnecessary user interface (UI) components (e.g., the icons and dropdown menu).

Element Pages

Clicking an element in the Table or List Views of PubChem Periodic Table directs you to the corresponding Element page (**Figure 5**). This page presents a wide variety of element information, including atomic properties (electron affinity, electronegativity, ionization potential, oxidation states, electron configuration, etc.) as well as isotopes, history, uses, and, most importantly, information source. PubChem Element page content comes from scientific articles[5-12] and various authoritative data sources, such as the International Union of Pure and Applied Chemistry (IUPAC) Commission on Isotopic Abundances and Atomic Weights (CIAAW)[13], National Institute of Standard and Technology (NIST)[14], International Atomic Energy Agency (IAEA)[15], Thomas Jefferson National Accelerator Facility (Jefferson Lab)[16], and Los Alamos National Laboratory[17].

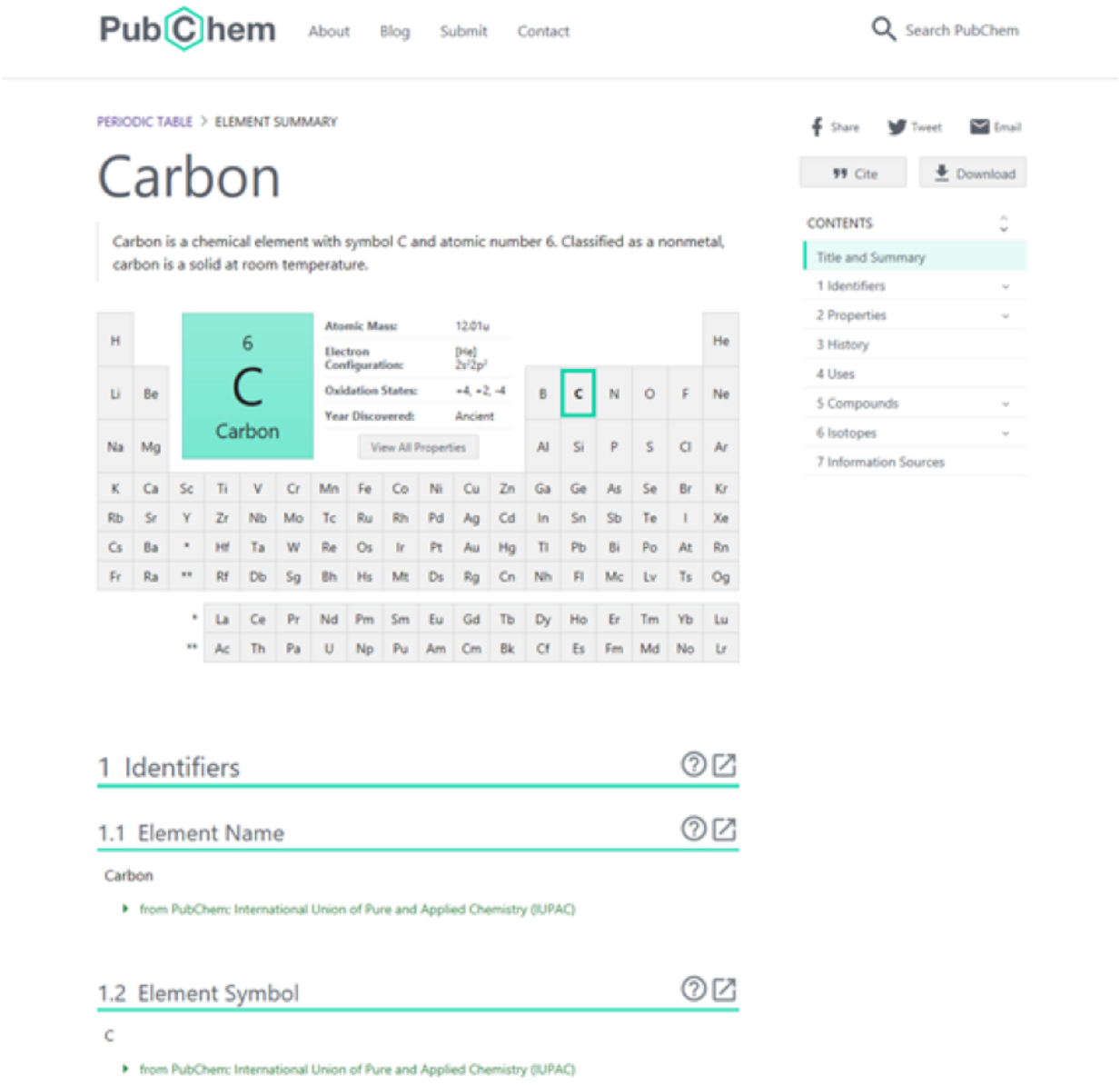

Figure 5. *Snapshot of the Element page for carbon, accessible via the URL: https://pubchem.ncbi.nlm.nih.gov/element/Carbon.*

At the top of each Element page is a periodic table, which allows one to quickly move to other elements' pages. The Table of Contents on the right column helps the user to readily locate desired information. The data presented on the Element page can be downloaded using the "Download" button at the top-right corner.

The element page can also be reached directly via URLs that includes atomic number, symbol, or name (all case-insensitive). For example, the following URLs are for the Element page for carbon:

https://pubchem.ncbi.nlm.nih.gov/element/Carbon

https://pubchem.ncbi.nlm.nih.gov/element/C

https://pubchem.ncbi.nlm.nih.gov/element/6

Machine-Readable Elemental Data

The data presented in the Periodic Table and Element pages can be downloaded by clicking the "Download" button available at the top-right corner of the List View of the Periodic Table and the respective element pages. The data are available in various formats, including XML, JSON, ASNT, and CSV (for the Periodic Table data only). Programmatic access to these data are supported through PUG-REST and PUG-View, which are Representational State Transfer (REST)-like interface to PubChem information. For example, the following PUG-REST request URL allows one to retrieve key elemental data presented in the Periodic Table in CSV format:

https://pubchem.ncbi.nlm.nih.gov/rest/pug/periodictable/CSV

It is also possible to download the annotations presented on the Element page using the following PUG-View request (with hydrogen as an example):

https://pubchem.ncbi.nlm.nih.gov/rest/pug_view/data/element/1/JSON

Conclusions

The PubChem Periodic Table and Element pages help users navigate the abundant chemical element data available within PubChem, while providing a convenient entry point to explore additional information, such as bioactivities and health and safety data, available in PubChem Compound pages for specific elements and their isotopes. The data presented on the Periodic

Table and Element pages are integrated from scientific articles and authoritative data sources. These data can be downloaded in machine-readable formats through the web browser or programmatically, giving the user access to the data in his or her own program.

Acknowledgments

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Contributions

AG generated the user interface. JZ compiled and integrated element information. PT created the PUG REST interface. EB contributed to the design. SK wrote the initial draft and SK, AG, JZ, PT, and EB revised it. All authors read and approved the final manuscript.

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