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PubChem Periodic Table and Element pages: improving access to information on chemical elements from authoritative sources

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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 more than five million unique users per month (as of March 2020). Many of these users are educators, undergraduate students, and 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 services help users navigate the abundant chemical element data available within PubChem, while providing a convenient entry point to explore additional chemical content, such as biological activities and health and safety data available in PubChem Compound pages for specific elements and their isotopes. The PubChem Periodic Table and Element pages are also available as widgets, which enable web developers to display PubChem's element data on web pages they design. The elemental data can be downloaded in common file formats and imported into data analysis programs (e.g., spreadsheet software, like Microsoft Excel and Google Sheets, and computer scripts, such as python and R). Overall, the PubChem Periodic Table and Element pages improve access to chemical element data from authoritative sources.

Keywords: chemical database; chemical element; periodic table; PubChem.

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 that students in the classroom can learn about chemistry from the periodic table and they should get familiar with it.

The periodic table in its present form was first introduced in 1869 by a Russian chemist, Dimitry Mendeleev, although there had been earlier attempts to classify elements by their similarities. As we marked the

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150th anniversary of the periodic table in 2019, the scientific community declared 2019 to be “The International Year of the Periodic Table” (International Union of Pure and Applied Chemistry [IUPAC], 2019). PubChem (Figure 1) (<https://pubchem.ncbi.nlm.nih.gov>) (Kim, 2016; Kim et al., 2016, 2019) joined this celebration by launching the PubChem Periodic Table and corresponding Element pages, which are useful resources for chemical education at the high school, undergraduate, and graduate levels.

PubChem is a public chemical information resource, developed and maintained by the U.S. National Institutes of Health. With more than five million unique users per month (as of March 2020), it is one of the top five chemistry web sites in the world in terms of web traffic. Many of PubChem users are undergraduate and graduate students enrolled in academic institutions. In addition, many educators use PubChem within their curriculum to help teach chemical information literacy among other topics. In general, PubChem provides many opportunities as a chemical education resource.

Among many features, PubChem provides a Compound summary, a comprehensive overview of all information available within PubChem for a given chemical. While the Compound Summary page is appropriate to present data for discrete 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.

This article provides an overview of the PubChem Periodic Table and Element pages. It was originally presented at an online conference hosted by the Committee on Computers in Chemical Education (CCCE) of the American Chemical Society (ACS) Division of Chemical Education (CHED) (Kim, Gindulyte, Zhang, Thiessen, & Bolton, 2019). The present paper is modified from its original version to reflect discussions with chemical educators during the conference as well as technical updates since made.

Periodic table

PubChem Periodic Table (Figures 2, 3, 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/periodic-table/>

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

- Table View (<https://pubchem.ncbi.nlm.nih.gov/periodic-table/#view=table>) (Figure 2) 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

Figure 1: Snapshot of the PubChem homepage (<https://pubchem.ncbi.nlm.nih.gov>). The PubChem Periodic Table can be accessed by clicking the Periodic Table icon (as indicated by the dotted green box in the lower right-hand side).

Periodic Table of Elements

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TABLE LIST W/PROPERTIES GAME

1 H Hydrogen Nonmetal

2 He Helium Noble Gas

3 Li Lithium Alkali Metal
4 Be Beryllium Alkaline E...

11 Na Sodium Alkali Metal
12 Mg Magnesium Alkaline E...

19 K Potassium Alkali Metal
20 Ca Calcium Alkaline E...

21 Sc Scandium Transition ...
22 Ti Titanium Transition ...
23 V Vanadium Transition ...
24 Cr Chromium Transition ...
25 Mn Manganese Transition ...
26 Fe Iron Transition ...
27 Co Cobalt Transition ...
28 Ni Nickel Transition ...
29 Cu Copper Transition ...
30 Zn Zinc Transition ...
31 Ga Gallium Post-Trans...
32 Ge Germanium Metalloid
33 As Arsenic Metalloid
34 Se Selenium Nonmetal
35 Br Bromine Halogen
36 Kr Krypton Noble Gas

37 Rb Rubidium Alkali Metal
38 Sr Strontium Alkaline E...
39 Y Yttrium Transition ...
40 Zr Zirconium Transition ...
41 Nb Niobium Transition ...
42 Mo Molybdenum Transition ...
43 Tc Technetium Transition ...
44 Ru Ruthenium Transition ...
45 Rh Rhodium Transition ...
46 Pd Palladium Transition ...
47 Ag Silver Transition ...
48 Cd Cadmium Transition ...
49 In Indium Post-Trans...
50 Sn Tin Post-Trans...
51 Sb Bismuth Post-Trans...
52 Te Tellurium Metalloid
53 I Iodine Halogen
54 Xe Xenon Noble Gas

55 Cs Cesium Alkali Metal
56 Ba Barium Alkaline E...
57 La Lanthanum Lanthanide
58 Ce Cerium Lanthanide
59 Pr Praseodymium Lanthanide
60 Nd Neodymium Lanthanide
61 Pm Promethium Lanthanide
62 Sm Samarium Lanthanide
63 Eu Europium Lanthanide
64 Gd Gadolinium Lanthanide
65 Tb Terbium Lanthanide
66 Dy Dysprosium Lanthanide
67 Ho Holmium Lanthanide
68 Er Erbium Lanthanide
69 Tm Thulium Lanthanide
70 Yb Ytterbium Lanthanide
71 Lu Lutetium Lanthanide

87 Fr Francium Alkali Metal
88 Ra Radium Alkaline E...
89 Ac Actinium Actinide
90 Th Thorium Actinide
91 Pa Protactinium Actinide
92 U Uranium Actinide
93 Np Neptunium Actinide
94 Pu Plutonium Actinide
95 Am Americium Actinide
96 Cm Curium Actinide
97 Bk Berkelium Actinide
98 Cf Californium Actinide
99 Es Einsteinium Actinide
100 Fm Fermium Actinide
101 Md Mendelevium Actinide
102 No Nobelium Actinide
103 Lr Lawrencium Actinide

104 Rf Rutherfordium Transition ...
105 Db Dubnium Transition ...
106 Sg Seaborgium Transition ...
107 Bh Bohrium Transition ...
108 Hs Hassium Transition ...
109 Mt Meitnerium Transition ...
110 Ds Darmstadtium Transition ...
111 Rg Roentgenium Transition ...
112 Cn Copernicium Post-Trans...
113 Nh Nihonium Post-Trans...
114 Fl Flerovium Post-Trans...
115 Mc Moscovium Post-Trans...
116 Lv Livermorium Post-Trans...
117 Ts Tennessine Post-Trans...
118 Og Oganesson Noble Gas

Figure 2: Snapshot of the table view of PubChem Periodic Table (<https://pubchem.ncbi.nlm.nih.gov/periodic-table/>). The elements can be colored according to their properties, by using the drop-down menu available at the upper-right corner of the table (as indicated by the dotted red box).

selected property value displayed for each element, by using the drop-down menu available at the top-right corner. Clicking on an element in the Table View opens a popup, called the element information card, presenting select properties of that element. The properties in the element information card are hyper-linked to appropriate sections of the corresponding Element page so that users can easily find more information/references for the properties of interest (see below for more details about the Element page).

- List View (<https://pubchem.ncbi.nlm.nih.gov/periodic-table/#view=list>) (Figure 3) 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

Periodic Table of Elements

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TABLE LIST W/PROPERTIES GAME

Element Name, Symbol or Atomic Number

<p>1</p> <p>H</p> <p>Hydrogen</p> <p>Nonmetal</p> <p>Hydrogen Element Page</p>	<p>Standard State: Gas</p> <p>Atomic Mass: 1.0080 u</p> <p>Electron Configuration: 1s¹</p> <p>Oxidation States: +1, -1</p> <p>Electronegativity (Pauling Scale): 2.2</p> <p>Atomic Radius (van der Waals): 120 pm</p> <p>Ionization Energy: 13.598 eV</p> <p>Electron Affinity: 0.754 eV</p> <p>Melting Point: 13.81 K</p> <p>Boiling Point: 20.28 K</p> <p>Density: 0.00008988 g/cm³</p> <p>Year Discovered: 1766</p>
<p>2</p> <p>He</p> <p>Helium</p> <p>Noble Gas</p> <p>Helium Element Page</p>	<p>Standard State: Gas</p> <p>Atomic Mass: 4.00260 u</p> <p>Electron Configuration: 1s²</p> <p>Oxidation States: 0</p> <p>Atomic Radius (van der Waals): 140 pm</p> <p>Ionization Energy: 24.587 eV</p> <p>Melting Point: 0.95 K</p> <p>Boiling Point: 4.22 K</p> <p>Density: 0.0001785 g/cm³</p> <p>Year Discovered: 1868</p>

Figure 3: Snapshot of the list view of PubChem periodic table (<https://pubchem.ncbi.nlm.nih.gov/periodic-table/#view=list>).

Figure 4: Snapshot of the game view of PubChem periodic table (<https://pubchem.ncbi.nlm.nih.gov/periodic-table/#view=game>).

- quickly find an element of interest. Clicking on an element in the List View directs the user to the corresponding Element page (see section “Element pages” below).
- Game View (<https://pubchem.ncbi.nlm.nih.gov/periodic-table/#view=game>) (Figure 4), 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-left corner of the Periodic Table. By default, the Table View is presented. A printable image of the Periodic Table can be downloaded in PNG or PDF by clicking the “Download” button available at the top-right corner of each view of the Periodic Table. This button also allows one to download the data presented in the Periodic Table (see section “Machine-readable elemental data” below). The Periodic Table uses a responsive design approach and is optimized for both touch- and mouse-based interfaces. In addition, the new page automatically adjusts to the available screen size, making it friendly for desktops, tablets, and phones.

Element pages

The Element page for a given element (Figure 5) presents a wide variety of information on that element, 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 (Allen, 1989; Allred, 1961; Mann, Meek, & Allen, 2000; Mann, Meek, Knight, Capitani, & Allen, 2000; Meija et al., 2016a, 2016b; Myers, 1990; Slater, 1964) and various authoritative data sources, including:

- International Union of Pure and Applied Chemistry (IUPAC) Commission on Isotopic Abundances and Atomic Weights (CIAAW) (<http://ciaaw.org/>).
- National Institute of Standard and Technology (NIST) Physical Measurement Laboratory (<https://www.nist.gov/pml>).
- International Atomic Energy Agency (IAEA) Nuclear Data Section, Atomic Mass Data Center (<https://www.nds.iaea.org/amdc/>).

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PERIODIC TABLE > ELEMENT SUMMARY

Carbon

Carbon is a chemical element with symbol C and atomic number 6. Classified as a nonmetal, carbon is a solid at room temperature.

Atomic Mass: 12.011u
Electron Configuration: [He]2s²2p²
Oxidation States: +4, +2, -4
Year Discovered: Ancient

View All Properties

1 Identifiers

1.1 Element Name

Carbon

PubChem: Commission on Isotopic Abundances and Atomic Weights (CIAAW), International Union of Pure and...

1.2 Element Symbol

C

PubChem: Commission on Isotopic Abundances and Atomic Weights (CIAAW), International Union of Pure and...

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

- Thomas Jefferson National Accelerator Facility (Jefferson Lab) Office of Science Education (<https://education.jlab.org/itselemental/>).
- Los Alamos National Laboratory (LANL) Chemistry Division (<https://periodic.lanl.gov/index.shtml>).

At the top of each Element page there 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 be reached by clicking an element in the Table View (via the element information card) or the List View of the Periodic Table. It 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 Periodic Table and 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 (Kim, Thiessen, Bolton, & Bryant, 2015; Kim, Thiessen, Cheng, Yu, & Bolton, 2018) and PUG-View (Kim, Thiessen, et al., 2019), which are Representational State Transfer (REST)-like interfaces 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

Widgets

Both the PubChem Periodic Table and Element pages are also available as widgets. Web developers can embed them within web pages they design to display PubChem's elemental data on their own web site. Because all data presented through these widgets come directly from PubChem, there is no need to mirror the data content to keep them up to date. Several web sites are already using the widgetized PubChem Periodic Table and a notable example is LibreTexts (<https://libretexts.org/>), which is an open education repository. It uses the PubChem Periodic Table within a reference table page (https://chem.libretexts.org/Bookshelves/Ancillary_Materials/Reference/Periodic_Table_of_the_Elements), which is provided as a supplement to free online chemistry course materials.

Displaying PubChem's element data on a web page can be done simply by including an HTML iframe tag with a proper URL as the 'src' attribute. For instance, to embed the PubChem Periodic Table, the following code needs to be added:

```
<iframe class="pubchem-widget" src="https://pubchem.ncbi.nlm.nih.gov/periodic-table/#view=table&embed=true" style="border: 0; width: 100%;"></iframe>
```

More examples can be found in the PubChem Widgets help document (<https://pubchemdocs.ncbi.nlm.nih.gov/widgets>).

Suggested use cases and applications

The PubChem Periodic Table can be used to find select properties of elements and their trend or periodicity across rows and columns. In addition to this traditional use case, it serves as an entry point to the respective Element pages, which provide more detailed information on chemical elements. The Game View of the Periodic Table helps students memorize the position of each element in the Periodic Table. As mentioned in section "Widgets", the Periodic Table can be embedded within a web page outside PubChem for free. This feature is useful for those who develop online educational resources.

Importantly, PubChem provides the data underlying the PubChem Periodic Table in a machine readable format, as described in section "Machine-readable elemental data". Therefore, it is possible to develop various learning activities exploiting the machine readable element data. For instance, as illustrated in Figure 6, students can download element data from PubChem, import them in spreadsheet software or a computer script, make a plot of an elemental property (e.g., the ionization potential) against the atomic number, and analyze the trend or periodicity observed in the plot.

Discussion

The PubChem Periodic Table and Element pages provides three important features:

- Interactive: the web interface is designed to help the user to more readily explore chemical element data in PubChem. Each element on the Periodic Table provides links to the relevant sections of the corresponding Element page that presents all information for that element available within PubChem.
- Machine readable: the elemental data can be downloaded in common file formats and imported into data analysis programs (spreadsheet software like Microsoft Excel and Google Sheets or computer scripts in python or R).

Figure 6: An example of learning activities of the machine-readable chemical element data from the PubChem Periodic Table. Students can download the chemical element data, import them in Excel, create a plot of the ionization potential against the atomic number, and analyze the observed trend or periodicity.

- **Widgetized:** these services are also available as widgets, which enable one to display PubChem's element data on his or her own web page. Because the widget gets the data directly from PubChem, they always show the most current information in PubChem.

One of the goals of the PubChem Periodic Table and Element pages is to provide users with elemental data from authoritative sources. However, even among these sources, variations and discrepancies in data exist. For example, as shown in Figure 7, while the atomic weights of carbon from Jefferson Lab and LANL are given as values (12.0107 and 12.01, respectively), those from both CIAAW and NIST are given as a range of values (12.0096, 12.0116). In general, PubChem does not determine which one is the best among these variations in the same kind of annotations collected from different sources. Instead, PubChem presents all variations together, along with data provenance information (i.e., where does this data come from?), as shown in Figure 7. An exception to this general rule is a case in which it is not feasible to present multiple values. For example, it is not straightforward to list multiple variations of the atomic mass of an element in a small cell within the Periodic Table or a spreadsheet. Therefore, the atomic mass data used in the Periodic Table are all hard-coded based on the values provided by CIAAW and IAEA. These mass data are included in the machine-readable element data (available through the Download button on the Periodic Table or through programmatic access using PUG-REST) (see section “Machine-readable elemental data”).

Essentially, the Periodic Table and Element pages play a role as a one-stop shop for chemical element data, because it enables users to readily get desired element data scattered across multiple authoritative sources, without directly visiting each source. In addition, these data are not only available through the web interfaces but also programmatically through PUG-REST and PUG-View. As a result, the Periodic Table and Element pages improve the accessibility of element data from those authoritative sources. However, as with any online resource,

The screenshot shows the PubChem interface for the element Carbon. At the top, there is a header with the element name 'Carbon (Element)' and a 'CONTENTS' button. Below this, the section '2.1 Atomic Weight' is highlighted. Under this section, several atomic weight values are listed with their corresponding authoritative sources:

- [12.0096, 12.0116] Commission on Isotopic Abundances and Atomic Weights (CIAAW), I...
- 12.0107 Jefferson Lab, U.S. Department of Energy
- 12.01 Los Alamos National Laboratory, U.S. Department of Energy
- [12.0096, 12.0116] NIST Physical Measurement Laboratory

Figure 7: Snapshot of the Atomic Weight section of the Element page for carbon, accessible via the URL: <https://pubchem.ncbi.nlm.nih.gov/element/Carbon#section=Atomic-Weight>.

including PubChem, the user should always critically assess the source, accuracy, reliability, and context of the data. Allowing users to see the difference in values from authoritative sources, it helps to demonstrate that science is constantly evolving, and this includes even the most basic information, including the atomic weights and masses in the periodic table. This makes for an excellent lesson for any budding scientist.

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 direct access to the data as needed.

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Author contributions: AG designed and implemented 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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