
mendeleev Documentation

Release 0.15.0

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CONTENTS

1	Getting started	3
1.1	Overview	3
1.2	Contributing	3
1.3	Citing	3
1.4	Related projects	4
1.5	Funding	4
2	Installation	5
3	Tutorials	7
3.1	Quick start	7
3.2	Bulk data access	16
3.3	Electronic configuration	23
3.4	Ions	25
3.5	Visualizing custom periodic tables	27
3.6	Advanced visualization tutorial	29
3.7	Jupyter notebooks	32
4	Data	33
4.1	Elements	33
4.2	Isotopes	37
4.3	Isotope Decay Modes	37
5	Accessing data	39
5.1	Individual Elements	39
5.2	Fetching data in bulk	39
5.3	Computed properties	40
5.4	Database session and engine	41
6	Electronegativities	43
6.1	Allen	43
6.2	Allred and Rochow	44
6.3	Cottrell and Sutton	44
6.4	Ghosh	44
6.5	Gordy	45
6.6	Li and Xue	45
6.7	Martynov and Batsanov	45
6.8	Mulliken	46
6.9	Nagle	46
6.10	Pauling	46
6.11	Sanderson	46

6.12	Fetching all electronegativities	47
7	API Reference	49
7.1	mendelev.db	49
7.2	mendelev.cli	50
7.3	mendelev.econf	50
7.4	mendelev.electronegativity	50
7.5	mendelev.fetch	51
7.6	mendelev.mendelev	52
7.7	mendelev.models	52
7.8	mendelev.ion	53
7.9	mendelev.vis.periodictable	53
7.10	mendelev.vis.bokeh	53
7.11	mendelev.vis.plotly	54
7.12	mendelev.vis.seaborn	54
7.13	mendelev.vis.utils	54
7.14	mendelev.utils	54
8	Bibliography	55
9	mendelev Changelog	57
9.1	v0.15.0 (26.12.2023)	57
9.2	v0.14.0 (07.06.2023)	57
9.3	v0.13.1 (24.04.2023)	57
9.4	v0.13.0 (11.04.2023)	57
9.5	v0.12.1 (28.11.2022)	58
9.6	v0.12.0 (9.10.2022)	58
9.7	v0.11.0 (29.09.2022)	58
9.8	v0.10.0 (17.07.2022)	58
9.9	v0.9.0 (24.09.2021)	59
9.10	v0.8.0 (22.08.2021)	59
9.11	v0.7.0 (20.03.2021)	59
9.12	v0.6.1 (03.11.2020)	59
9.13	v0.6.0 (10.04.2020)	60
9.14	v0.5.2 (29.01.2020)	60
9.15	v0.5.1 (26.08.2019)	60
9.16	v0.5.0 (25.08.2019)	60
9.17	v0.4.5 (17.03.2018)	60
9.18	v0.4.4 (10.12.2018)	60
9.19	v0.4.3 (16-07-2018)	61
9.20	v0.4.2 (26-12-2018)	61
9.21	v0.4.1 (03-12-2017)	61
9.22	v0.4.0 (22-11-2017)	61
9.23	v0.3.6 (17-09-2017)	61
9.24	v0.3.5 (07-09-2017)	61
9.25	v0.3.4 (28-06-2017)	62
9.26	v0.3.3 (16-05-2017)	62
9.27	v0.3.2 (01-05-2017)	62
9.28	v0.3.1 (25-01-2017)	62
9.29	v0.3.0 (09-01-2017)	62
9.30	v0.2.17 (08-01-2017)	63
9.31	v0.2.16 (06-01-2017)	63
9.32	v0.2.15 (02-01-2017)	63
9.33	v0.2.14 (02-01-2017)	63

9.34	v0.2.13 (01-01-2017)	63
9.35	v0.2.12 (21-12-2016)	63
9.36	v0.2.11 (10-11-2016)	63
9.37	v0.2.10 (18-10-2016)	64
9.38	v0.2.9 (16-10-2016)	64
9.39	v0.2.8 (29-08-2016)	64
9.40	v0.2.7 (02-04-2016)	64
9.41	v0.2.6 (02-04-2016)	64
9.42	v0.2.5 (02-04-2016)	64
9.43	v0.2.4 (05-02-2016)	65
9.44	v0.2.3 (27-01-2016)	65
9.45	v0.2.2 (29-11-2015)	65
9.46	v0.2.1 (26-10-2015)	66
9.47	v0.2.0 (22-10-2015)	66
9.48	v0.1.0 (11-07-2015)	67
10	License	69
11	Indices and tables	71
	Bibliography	73
	Python Module Index	79
	Index	81

This package provides an API for accessing various properties of elements from the periodic table of elements.

Periodic Table																		
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H Hydrogen 1.008																	2 He Helium 4.00260
2	3 Li Lithium 6.940	4 Be Beryllium 9.01218											5 B Boron 10.810	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.99840	10 Ne Neon 20.1797
3	11 Na Sodium 22.98977	12 Mg Magnesium 24.305											13 Al Aluminum 26.98154	14 Si Silicon 28.085	15 P Phosphorus 30.97376	16 S Sulfur 32.060	17 Cl Chlorine 35.450	18 Ar Argon 39.948
4	19 K Potassium 39.0983	20 Ca Calcium 40.078	21 Sc Scandium 44.95591	22 Ti Titanium 47.887	23 V Vanadium 50.9415	24 Cr Chromium 51.9961	25 Mn Manganese 54.93804	26 Fe Iron 55.845	27 Co Cobalt 58.93319	28 Ni Nickel 58.6934	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.630	33 As Arsenic 74.92159	34 Se Selenium 78.971	35 Br Bromine 79.904	36 Kr Krypton 83.798
5	37 Rb Rubidium 85.4678	38 Sr Strontium 87.62	39 Y Yttrium 88.90584	40 Zr Zirconium 91.224	41 Nb Niobium 92.90637	42 Mo Molybdenum 95.95	43 Tc Technetium [87.80721]	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.90550	46 Pd Palladium 106.42	47 Ag Silver 107.8682	48 Cd Cadmium 112.414	49 In Indium 114.818	50 Sn Tin 118.710	51 Sb Antimony 121.760	52 Te Tellurium 127.60	53 I Iodine 126.90447	54 Xe Xenon 131.293
6	55 Cs Cesium 132.90545	56 Ba Barium 137.327	71 Lu Lutetium 174.9668	72 Hf Hafnium 178.49	73 Ta Tantalum 180.94788	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.217	78 Pt Platinum 195.084	79 Au Gold 196.96657	80 Hg Mercury 200.592	81 Tl Thallium 204.380	82 Pb Lead 207.2	83 Bi Bismuth 208.98040	84 Po Polonium [209]	85 At Astatine [210]	86 Rn Radon [222]
7	87 Fr Francium [223]	88 Ra Radium [226]	103 Lr Lawrencium [262]	104 Rf Rutherfordium [267]	105 Db Dubnium [268]	106 Sg Seaborgium [271]	107 Bh Bohrium [274]	108 Hs Hassium [280]	109 Mt Meitnerium [278]	110 Ds Darmstadtium [281]	111 Rg Roentgenium [281]	112 Cn Copernicium [285]	113 Nh Nihonium [286]	114 Fl Flerovium [289]	115 Mc Moscovium [288]	116 Lv Livermorium [293]	117 Ts Tennessine [294]	118 Og Oganesson [294]
			57 La Lanthanum 138.90547	58 Ce Cerium 140.116	59 Pr Praseodymium 140.90766	60 Nd Neodymium 144.242	61 Pm Promethium [144.91276]	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.92535	66 Dy Dysprosium 162.500	67 Ho Holmium 164.93033	68 Er Erbium 167.259	69 Tm Thulium 168.93422	70 Yb Ytterbium 173.04		
			89 Ac Actinium [227]	90 Th Thorium 232.0377	91 Pa Protactinium 231.03588	92 U Uranium 238.02891	93 Np Neptunium [237]	94 Pu Plutonium [244]	95 Am Americium [243]	96 Cm Curium [247]	97 Bk Berkelium [247]	98 Cf Californium [251]	99 Es Einsteinium [252]	100 Fm Fermium [257]	101 Md Mendelevium [258]	102 No Nobelium [259]		

GETTING STARTED

1.1 Overview

This package provides an API for accessing various properties of elements from the periodic table of elements. The repository is hosted on [github](#).

1.2 Contributing

All contributions are welcome!

If you would like to suggest an improvement or report a bug or data inconsistency please consider creating an [issue on github](#). I would be especially grateful for references to possible data updates and sources and recommendations of new data.

1.3 Citing

If you use *mendelev* in a scientific publication, please consider citing the software as

L. M. Mentel, *mendelev* - A Python resource for properties of chemical elements, ions and isotopes. , 2014– . Available at: <https://github.com/lmmentel/mendelev>.

Here's the reference in the [BibLaTeX](#) format

```
@software{mendelev2014,
  author = {Mentel, Łukasz},
  title = {{mendelev} -- A Python resource for properties of chemical elements, ions,
↪and isotopes},
  url = {https://github.com/lmmentel/mendelev},
  version = {0.15.0},
  date = {2014--},
}
```

or the older [BibTeX](#) format

```
@misc{mendeleev2014,
  auhor = {Mentel, Łukasz},
  title = {mendeleev} -- A Python resource for properties of chemical elements, ions,
↪and isotopes, ver. 0.15.0},
  howpublished = {\url{https://github.com/lmmentel/mendeleev}},
  year = {2014--},
}
```

1.4 Related projects

periodictable

This package provides a periodic table of the elements with support for mass, density and xray/neutron scattering information.

periodic

Periodic is an open source simple python API/command line script for the periodic table.

1.5 Funding

This project is supported by the RCN (The Research Council of Norway) project number 239193.

INSTALLATION

The package can be installed using `pip`

```
pip install mendelev
```

You can also install the most recent version from the repository:

```
pip install git+https://github.com/lmmentel/mendelev.git
```

If you use `conda` you can install the package from [my anaconda channel](#) by

```
conda install -c lmmentel mendelev=0.15.0
```


TUTORIALS

3.1 Quick start

This simple tutorial will illustrate the basic capabilities of the package.

3.1.1 Table of Contents

- *Basic interactive usage*
 - *Getting single elements*
 - *Getting-list-of-elements*
- *Extended attributes*
 - *Oxidation states*
 - *Ionization energies*
 - *Isotopes*
 - *Ionic radii*
 - *Electronic configuration*
- *Useful functions for calculating properties*
- *Electronegativity*
- *CLI utility*

3.1.2 Basic interactive usage

Getting single elements

The simplest way of accessing the elements is importing them directly from `mendeleev` by symbols

```
[1]: from mendeleev import Si, Fe, O
print("Si's name: ", Si.name)
print("Fe's atomic number:", Fe.atomic_number)
print("O's atomic weight: ", O.atomic_weight)
```

```
Si's name: Silicon
Fe's atomic number: 26
O's atomic weight: 15.999
```

An alternative interface to the data is through the `element` function that returns a single `Element` object or a list of `Element` object depending on the arguments.

The function can be imported directly from the `mendeleev` package

```
[2]: from mendeleev import element
```

The `element` method accepts unique identifiers: **atomic number**, **atomic symbol** or **element's name** in English. To retrieve the entries on Silicon by symbol type

```
[3]: si = element('Si')
```

```
[4]: si
```

```
[4]: Element(
    abundance_crust=282000.0,
    abundance_sea=2.2,
    annotation='',
    atomic_number=14,
    atomic_radius=110.0,
    atomic_radius_rahm=231.99999999999997,
    atomic_volume=12.1,
    atomic_weight=28.085,
    atomic_weight_uncertainty=None,
    block='p',
    c6=305.0,
    c6_gb=308.0,
    cas='7440-21-3',
    covalent_radius_bragg=117.0,
    covalent_radius_cordero=111.00000000000001,
    covalent_radius_pyykko=115.99999999999999,
    covalent_radius_pyykko_double=107.0,
    covalent_radius_pyykko_triple=102.0,
    cpk_color='#daa520',
    density=2.3296,
    description="Metalloid element belonging to group 14 of the periodic table. It
    ↳is the second most abundant element in the Earth's crust, making up 25.7% of it by
    ↳weight. Chemically less reactive than carbon. First identified by Lavoisier in 1787
    ↳and first isolated in 1823 by Berzelius.",
    dipole_polarizability=37.3,
    dipole_polarizability_unc=0.7,
    discoverers='Jöns Berzelius',
    discovery_location='Sweden',
    discovery_year=1824,
    ec=<ElectronicConfiguration(conf="1s2 2s2 2p6 3s2 3p2")>,
    econf='[Ne] 3s2 3p2',
    electron_affinity=1.3895211,
    en_allen=11.33,
    en_ghosh=0.178503,
    en_pauling=1.9,
    evaporation_heat=383.0,
    fusion_heat=50.6,
    gas_basicity=814.1,
    geochemical_class='major',
```

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```

    glawe_number=85,
    goldschmidt_class='litophile',
    group=<Group(symbol=IVA, name=Carbon group)>,
    group_id=14,
    heat_of_formation=450.0,
    ionic_radii=[IonicRadius(
    atomic_number=14,
    charge=4,
    coordination='IV',
    crystal_radius=40.0,
    econf='2p6',
    id=379,
    ionic_radius=26.0,
    most_reliable=True,
    origin='',
    spin='',
), IonicRadius(
    atomic_number=14,
    charge=4,
    coordination='VI',
    crystal_radius=54.0,
    econf='2p6',
    id=380,
    ionic_radius=40.0,
    most_reliable=True,
    origin='from r^3 vs V plots, ',
    spin='',
)],
    is_monoisotopic=None,
    is_radioactive=False,
    isotopes=[<Isotope(Z=14, A=22, mass=22.0361(5), abundance=None)>, <Isotope(Z=14,
↪ A=23, mass=23.0257(5), abundance=None)>, <Isotope(Z=14, A=24, mass=24.01154(2),
↪ abundance=None)>, <Isotope(Z=14, A=25, mass=25.00411(1), abundance=None)>,
↪ <Isotope(Z=14, A=26, mass=25.9923338(1), abundance=None)>, <Isotope(Z=14, A=27,
↪ mass=26.9867047(1), abundance=None)>, <Isotope(Z=14, A=28, mass=27.9769265344(6),
↪ abundance=92.254(4))>, <Isotope(Z=14, A=29, mass=28.9764946643(6), abundance=4.67(2))>,
↪ <Isotope(Z=14, A=30, mass=29.97377014(2), abundance=3.074(2))>, <Isotope(Z=14, A=31,
↪ mass=30.97536320(5), abundance=None)>, <Isotope(Z=14, A=32, mass=31.9741515(3),
↪ abundance=None)>, <Isotope(Z=14, A=33, mass=32.9779770(8), abundance=None)>,
↪ <Isotope(Z=14, A=34, mass=33.9785380(9), abundance=None)>, <Isotope(Z=14, A=35,
↪ mass=34.98455(4), abundance=None)>, <Isotope(Z=14, A=36, mass=35.98665(8),
↪ abundance=None)>, <Isotope(Z=14, A=37, mass=36.9929(1), abundance=None)>,
↪ <Isotope(Z=14, A=38, mass=37.9955(1), abundance=None)>, <Isotope(Z=14, A=39, mass=39.
↪ 0025(1), abundance=None)>, <Isotope(Z=14, A=40, mass=40.0061(1), abundance=None)>,
↪ <Isotope(Z=14, A=41, mass=41.0142(3), abundance=None)>, <Isotope(Z=14, A=42, mass=42.
↪ 0181(3), abundance=None)>, <Isotope(Z=14, A=43, mass=43.0261(4), abundance=None)>,
↪ <Isotope(Z=14, A=44, mass=44.0315(5), abundance=None)>, <Isotope(Z=14, A=45, mass=45.
↪ 0398(6), abundance=None)>],
    jmol_color='#f0c8a0',
    lattice_constant=5.43,
    lattice_structure='DIA',
    mendelev_number=88,

```

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```

    metallic_radius=117.0,
    metallic_radius_c12=138.0,
    molar_heat_capacity=19.99,
    molcas_gv_color='#f0c8a0',
    name='Silicon',
    name_origin='Latin: silex, silicus, (flint).',
    period=3,
    pettifor_number=85,
    phase_transitions=[14 Tm=1687.15 Tb=3538.15],
    proton_affinity=837.0,
    screening_constants=[<ScreeningConstant(Z= 14, n= 1, s=s, screening= 0.
↪4255)>, <ScreeningConstant(Z= 14, n= 2, s=p, screening= 4.0550)>,
↪<ScreeningConstant(Z= 14, n= 2, s=s, screening= 4.9800)>, <ScreeningConstant(Z= 14, n= 3, s=p, screening= 9.7148)>, <ScreeningConstant(Z= 14, n= 3, s=s, screening= 9.0968)>],
    sources='Makes up major portion of clay, granite, quartz (SiO2), and sand. Commercial production depends on a reaction between sand (SiO2) and carbon at a temperature of around 2200 °C.',
    specific_heat_capacity=0.712,
    symbol='Si',
    thermal_conductivity=149.0,
    uses='Used in glass as silicon dioxide (SiO2). Silicon carbide (SiC) is one of the hardest substances known and used in polishing. Also the crystalline form is used in semiconductors.',
    vdw_radius=210.0,
    vdw_radius_alvarez=219.0,
    vdw_radius_batsanov=210.0,
    vdw_radius_bondi=210.0,
    vdw_radius_dreiding=426.99999999999994,
    vdw_radius_mm3=229.0,
    vdw_radius_rt=None,
    vdw_radius_truhlar=None,
    vdw_radius_uff=429.5,
)

```

Similarly to access the data by atomic number or element names type

```
[5]: al = element(13)
print(al.name)
```

```
Aluminum
```

```
[6]: o = element('Oxygen')
print(o.atomic_number)
```

```
8
```


Getting list of elements

The `element` method also accepts list or tuple of identifiers and then returns a list of `Element` objects

```
[7]: c, h, o = element(['C', 'Hydrogen', 8])
      print(c.name, h.name, o.name)
```

```
Carbon Hydrogen Oxygen
```

3.1.3 Extended attributes

Next to simple attributes returning `str`, `int` or `float`, there are extended attributes

- `oxistates`, returns a list of oxidation states
- `ionenergies`, returns a dictionary of ionization energies
- `isotopes`, returns a list of `Isotope` objects
- `ionic_radii` returns a list of `IonicRadius` objects
- `ec`, electronic configuration object

Oxidation states

`oxistates` returns a list of most common oxidation states for a given element

```
[8]: fe = element('Fe')
      print(fe.oxistates)
```

```
[2, 3]
```

Ionization energies

The `ionenergies` returns a dictionary with ionization energies in eV as values and degrees of ionization as keys

```
[9]: o = element('O')
      o.ionenergies
```

```
[9]: {1: 13.618054,
      2: 35.12111,
      3: 54.93554,
      4: 77.4135,
      5: 113.8989,
      6: 138.1189,
      7: 739.32679,
      8: 871.40985}
```

Isotopes

The `isotopes` attribute returns a list of `Isotope` objects with the following attributes per isotope

- `abundance`
- `abundance_uncertainty`
- `atomic_number`
- `discovery_year`
- `g_factor`
- `g_factor_uncertainty`
- `half_life`
- `half_life_uncertainty`
- `half_life_unit`
- `is_radioactive`
- `mass`
- `mass_number`
- `mass_uncertainty`
- `parity`
- `quadrupole_moment`
- `quadrupole_moment_uncertainty`
- `spin`

[]:

```
[10]: print("{0:^4s} {1:^4s} {2:^10s} {3:8s} {4:6s} {5:5s}\n{6}".format("AN", "MN", "Mass", "
↳ "Unc.", "Abu.", "Rad.", "-" * 42))
for iso in fe.isotopes:
    print('{0:4d} {1:4d} {2:10.5f} {3:8.2e} {4:} {5:}'.format(
        iso.atomic_number, iso.mass_number, iso.mass, iso.mass_uncertainty, iso.
↳ abundance, iso.is_radioactive))
```

AN	MN	Mass	Unc.	Abu.	Rad.

26	45	45.01547	3.04e-04	None	True
26	46	46.00130	3.22e-04	None	True
26	47	46.99235	5.37e-04	None	True
26	48	47.98067	9.90e-05	None	True
26	49	48.97343	2.60e-05	None	True
26	50	49.96299	9.00e-06	None	True
26	51	50.95686	1.50e-06	None	True
26	52	51.94811	1.92e-07	None	True
26	53	52.94531	1.79e-06	None	True
26	54	53.93961	3.68e-07	5.845	False
26	55	54.93829	3.30e-07	None	True
26	56	55.93494	2.87e-07	91.754	False
26	57	56.93539	2.87e-07	2.119	False

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26	58	57.93327	3.39e-07	0.282	False
26	59	58.93487	3.54e-07	None	True
26	60	59.93407	3.66e-06	None	True
26	61	60.93675	2.80e-06	None	True
26	62	61.93679	3.00e-06	None	True
26	63	62.94027	4.62e-06	None	True
26	64	63.94099	5.39e-06	None	True
26	65	64.94502	5.49e-06	None	True
26	66	65.94625	4.40e-06	None	True
26	67	66.95093	4.10e-06	None	True
26	68	67.95288	2.07e-04	None	True
26	69	68.95792	2.15e-04	None	True
26	70	69.96040	3.22e-04	None	True
26	71	70.96572	4.29e-04	None	True
26	72	71.96860	5.37e-04	None	True
26	73	72.97425	5.37e-04	None	True
26	74	73.97782	5.37e-04	None	True
26	75	74.98422	6.44e-04	None	True
26	76	75.98863	6.44e-04	None	True

Accessing isotopes

Similarly to `element` function that can be used to fetch specific isotopes by:

- `atomic_number` and `mass_number` or
- `symbol` and `mass_number`

```
[11]: from mendeleev import isotope
```

```
[12]: isotope("Fe", mass_number=57)
```

```
[12]: <Isotope(Z=26, A=57, mass=56.9353920(3), abundance=2.12(3))>
```

```
[13]: # tritium
isotope(1, 3)
```

```
[13]: <Isotope(Z=1, A=3, mass=3.01604928132(8), abundance=None)>
```

Radioactive isotopes can have multiple decay modes and that data is available as `decay_modes` attribute for each `Isotope`

```
[14]: isotope("Li", 11).decay_modes
```

```
[14]: [<IsotopeDecayMode(id=40, isotope_id=39, mode='B-', intensity=100.0)>,
<IsotopeDecayMode(id=41, isotope_id=39, mode='B-n', intensity=86.3)>,
<IsotopeDecayMode(id=42, isotope_id=39, mode='2n', intensity=4.1)>,
<IsotopeDecayMode(id=43, isotope_id=39, mode='3n', intensity=1.9)>,
<IsotopeDecayMode(id=44, isotope_id=39, mode='B-A', intensity=1.7)>,
<IsotopeDecayMode(id=45, isotope_id=39, mode='B-d', intensity=0.013)>,
<IsotopeDecayMode(id=46, isotope_id=39, mode='B-t', intensity=0.0093)>]
```

Ionic radii

Another composite attribute is `ionic_radii` which returns a list of `IonicRadius` object with the following attributes

- `atomic_number`, atomic number of the ion
- `charge`, charge of the ion
- `econf`, electronic configuration of the ion
- `coordination`, coordination type of the ion
- `spin`, spin state of the ion (HS or LS)
- `crystal_radius`, crystal radius in pm
- `ionic_radius`, ionic radius in pm
- `origin`, source of the data
- `most_reliable`, recommended value, (see the original paper for more information)

```
[15]: for ir in fe.ionic_radii:
      print(ir)

charge= 2, coordination=IV   , crystal_radius=77.000, ionic_radius=63.000
charge= 2, coordination=IVSQ , crystal_radius=78.000, ionic_radius=64.000
charge= 2, coordination=VI   , crystal_radius=75.000, ionic_radius=61.000
charge= 2, coordination=VI   , crystal_radius=92.000, ionic_radius=78.000
charge= 2, coordination=VIII , crystal_radius=106.000, ionic_radius=92.000
charge= 3, coordination=IV   , crystal_radius=63.000, ionic_radius=49.000
charge= 3, coordination=V    , crystal_radius=72.000, ionic_radius=58.000
charge= 3, coordination=VI   , crystal_radius=69.000, ionic_radius=55.000
charge= 3, coordination=VI   , crystal_radius=78.500, ionic_radius=64.500
charge= 3, coordination=VIII , crystal_radius=92.000, ionic_radius=78.000
charge= 4, coordination=VI   , crystal_radius=72.500, ionic_radius=58.500
charge= 6, coordination=IV   , crystal_radius=39.000, ionic_radius=25.000
```

3.1.4 Useful functions for calculating properties

Next to stored attributes there is a number of useful functions

```
[16]: si = element('Si')
```

```
[17]: # get the number of valence electrons
      si.nvalence()
```

```
[17]: 4
```

```
[18]: # calculate softness for an ion
      si.softness(charge=2)
```

```
[18]: 0.058318712346158874
```

```
[19]: # calcualte hardness for an ion
      si.hardness(charge=4)
```

```
[19]: 60.812605
```

```
[20]: # calculate the effective nuclear charge for a subshell using Slater's rules
      si.zeff(n=3, o='s')
```

```
[20]: 4.149999999999999
```

```
[21]: # calculate the effective nuclear charge for a subshell using Clementi's and Raimondi's
      ↪ exponents
      si.zeff(n=3, o='s', method='clementi')
```

```
[21]: 4.9032
```

Electronegativity

Currently there are 9 electronegativity scales implemented that can be accessed through the common electronegativity method, the scales are:

- allen
- allred-rochow
- cottrell-sutton
- ghosh
- gordy
- li-xue
- martynov-batsanov
- mulliken
- nagle
- pauling
- sanderson

More information can be found in the [documentation](#).

```
[22]: si.electronegativity(scale='pauling')
```

```
[22]: 1.9
```

```
[23]: si.electronegativity(scale='allen')
```

```
[23]: 11.33
```

```
[24]: # calculate mulliken electronegativity for a neutral atom or ion
      si.electronegativity(scale="mulliken", charge=1)
```

```
[24]: 12.248764000000001
```

3.1.5 CLI utility

For those who work in the terminal there is a simple command line interface (CLI) for printing the information about a given element. The script name is `element.py` and it accepts either the symbol or name of the element as an argument and prints the data about it. For example, to print the properties of silicon type

```
[25]: !element.py Si
/usr/bin/sh: 1: element.py: not found
```

3.2 Bulk data access

This tutorial explains how to retrieve full tables from the database into `pandas DataFrames`.

3.2.1 The following tables are available from mendelev

- elements
- ionicradii
- ionizationenergies
- oxidationstates
- groups
- series
- isotopes

All data is stored in a sqlite database that is shipped together with the package. You can interact directly with the database if you need more flexibility but for convenience `mendelev` provides a few functions in the `fetch` module to retrieve data.

To fetch whole tables you can use `fetch_table`. The function can be imported from `mendelev.fetch`

```
[1]: from mendelev.fetch import fetch_table
```

To retrieve a table call the `fetch_table` with the table name as argument. Here we'll get probably the most important table `elements` with basis data on each element

```
[3]: ptable = fetch_table('elements')
```

Now we can use `pandas`' capabilities to work with the data.

```
[4]: ptable.info()
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 118 entries, 0 to 117
Data columns (total 70 columns):
#   Column                Non-Null Count  Dtype
---  -
0   annotation            118 non-null   object
1   atomic_number         118 non-null   int64
2   atomic_radius         90 non-null    float64
3   atomic_volume         91 non-null    float64
```

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4	block	118 non-null	object
5	boiling_point	96 non-null	float64
6	density	95 non-null	float64
7	description	109 non-null	object
8	dipole_polarizability	117 non-null	float64
9	electron_affinity	77 non-null	float64
10	electronic_configuration	118 non-null	object
11	evaporation_heat	88 non-null	float64
12	fusion_heat	75 non-null	float64
13	group_id	90 non-null	float64
14	lattice_constant	87 non-null	float64
15	lattice_structure	91 non-null	object
16	melting_point	100 non-null	float64
17	name	118 non-null	object
18	period	118 non-null	int64
19	series_id	118 non-null	int64
20	specific_heat	81 non-null	float64
21	symbol	118 non-null	object
22	thermal_conductivity	66 non-null	float64
23	vdw_radius	103 non-null	float64
24	covalent_radius_cordero	96 non-null	float64
25	covalent_radius_pyykko	118 non-null	float64
26	en_pauling	85 non-null	float64
27	en_allen	71 non-null	float64
28	jmol_color	109 non-null	object
29	cpk_color	103 non-null	object
30	proton_affinity	32 non-null	float64
31	gas_basicity	32 non-null	float64
32	heat_of_formation	89 non-null	float64
33	c6	43 non-null	float64
34	covalent_radius_bragg	37 non-null	float64
35	vdw_radius_bondi	28 non-null	float64
36	vdw_radius_truhlar	16 non-null	float64
37	vdw_radius_rt	9 non-null	float64
38	vdw_radius_batsanov	65 non-null	float64
39	vdw_radius_dreiding	21 non-null	float64
40	vdw_radius_uff	103 non-null	float64
41	vdw_radius_mm3	94 non-null	float64
42	abundance_crust	88 non-null	float64
43	abundance_sea	81 non-null	float64
44	molcas_gv_color	103 non-null	object
45	en_ghosh	103 non-null	float64
46	vdw_radius_alvarez	94 non-null	float64
47	c6_gb	86 non-null	float64
48	atomic_weight	118 non-null	float64
49	atomic_weight_uncertainty	74 non-null	float64
50	is_monoisotopic	21 non-null	object
51	is_radioactive	118 non-null	bool
52	cas	118 non-null	object
53	atomic_radius_rahm	96 non-null	float64
54	geochemical_class	76 non-null	object
55	goldschmidt_class	118 non-null	object

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```

56 metallic_radius          56 non-null    float64
57 metallic_radius_c12      63 non-null    float64
58 covalent_radius_pyykko_double 108 non-null    float64
59 covalent_radius_pyykko_triple 80 non-null     float64
60 discoverers              118 non-null    object
61 discovery_year            105 non-null    float64
62 discovery_location        106 non-null    object
63 name_origin               118 non-null    object
64 sources                   118 non-null    object
65 uses                      112 non-null    object
66 mendelev_number           118 non-null    int64
67 dipole_polarizability_unc  117 non-null    float64
68 pettifor_number           103 non-null    float64
69 glawe_number              103 non-null    float64
dtypes: bool(1), float64(46), int64(4), object(19)
memory usage: 63.8+ KB

```

For clarity let's take only a subset of columns

```
[5]: cols = ['atomic_number', 'symbol', 'atomic_radius', 'en_pauling', 'block',
            ↪ 'vdw_radius_mm3']
```

```
[6]: ptable[cols].head()
```

```

[6]:   atomic_number  symbol  atomic_radius  en_pauling  block  vdw_radius_mm3
0         1         H         25.0         2.20      s         162.0
1         2        He        120.0         NaN      s         153.0
2         3        Li        145.0         0.98      s         255.0
3         4        Be        105.0         1.57      s         223.0
4         5         B         85.0         2.04      p         215.0

```

It is quite easy now to get descriptive statistics on the data.

```
[7]: ptable[cols].describe()
```

```

[7]:   atomic_number  atomic_radius  en_pauling  vdw_radius_mm3
count    118.000000     90.000000    85.000000     94.000000
mean      59.500000    149.844444     1.748588    248.468085
std       34.207699     40.079110     0.634442     36.017828
min        1.000000     25.000000     0.700000    153.000000
25%       30.250000    135.000000     1.240000    229.000000
50%       59.500000    145.000000     1.700000    244.000000
75%       88.750000    178.750000     2.160000    269.250000
max      118.000000    260.000000     3.980000    364.000000

```


3.2.2 Isotopes table

Let try and retrieve another table, namely isotopes

```
[8]: isotopes = fetch_table('isotopes', index_col='id')
```

```
[9]: isotopes.info()
```

```
<class 'pandas.core.frame.DataFrame'>
Int64Index: 406 entries, 1 to 406
Data columns (total 11 columns):
#   Column                Non-Null Count  Dtype
---  -
0   atomic_number         406 non-null   int64
1   mass                  377 non-null   float64
2   abundance             288 non-null   float64
3   mass_number           406 non-null   int64
4   mass_uncertainty      377 non-null   float64
5   is_radioactive        406 non-null   bool
6   half_life             121 non-null   float64
7   half_life_unit        85 non-null    object
8   spin                  323 non-null   float64
9   g_factor              323 non-null   float64
10  quadrupole_moment     320 non-null   float64
dtypes: bool(1), float64(7), int64(2), object(1)
memory usage: 35.3+ KB
```

Merge the elements table with the isotopes

We can now perform SQL-like merge operation on two DataFrames and produce an [outer](#) join

```
[10]: import pandas as pd
```

```
[11]: merged = pd.merge(ptable[cols], isotopes, how='outer', on='atomic_number')
```

now we have the following columns in the merged DataFrame

```
[12]: merged.info()
```

```
<class 'pandas.core.frame.DataFrame'>
Int64Index: 406 entries, 0 to 405
Data columns (total 16 columns):
#   Column                Non-Null Count  Dtype
---  -
0   atomic_number         406 non-null   int64
1   symbol                406 non-null   object
2   atomic_radius         328 non-null   float64
3   en_pauling            313 non-null   float64
4   block                 406 non-null   object
5   vdw_radius_mm3        350 non-null   float64
6   mass                  377 non-null   float64
7   abundance             288 non-null   float64
8   mass_number           406 non-null   int64
```

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```

9  mass_uncertainty  377 non-null  float64
10 is_radioactive    406 non-null  bool
11 half_life         121 non-null  float64
12 half_life_unit    85 non-null   object
13 spin              323 non-null  float64
14 g_factor          323 non-null  float64
15 quadrupole_moment 320 non-null  float64
dtypes: bool(1), float64(10), int64(2), object(3)
memory usage: 51.1+ KB

```

```
[13]: merged.head()
```

```

[13]:   atomic_number  symbol  atomic_radius  en_pauling  block  vdw_radius_mm3  \
0           1      H         25.0         2.2      s         162.0
1           1      H         25.0         2.2      s         162.0
2           1      H         25.0         2.2      s         162.0
3           2      He        120.0         NaN      s         153.0
4           2      He        120.0         NaN      s         153.0

      mass  abundance  mass_number  mass_uncertainty  is_radioactive  \
0  1.007825  0.999720           1      6.000000e-10          False
1  2.014102  0.000280           2      8.000000e-10          False
2      NaN      NaN           3      NaN              True
3  3.016029  0.000002           3      2.000000e-08          False
4  4.002603  0.999998           4      4.000000e-10          False

      half_life  half_life_unit  spin  g_factor  quadrupole_moment
0      NaN      None          0.5  5.585695          0.000000
1      NaN      None          1.0  0.857438          0.00286
2      NaN      None          0.5  5.957994          0.000000
3      NaN      None          0.5 -4.254995          0.000000
4      NaN      None          0.0  0.000000          0.000000

```

To display all the isotopes of Silicon

```
[14]: merged[merged['symbol'] == 'Si']
```

```

[14]:   atomic_number  symbol  atomic_radius  en_pauling  block  vdw_radius_mm3  \
28           14      Si         110.0         1.9      p         229.0
29           14      Si         110.0         1.9      p         229.0
30           14      Si         110.0         1.9      p         229.0

      mass  abundance  mass_number  mass_uncertainty  is_radioactive  \
28  27.976927  0.92191           28      3.000000e-09          False
29  28.976495  0.04699           29      3.000000e-09          False
30  29.973770  0.03110           30      2.000000e-08          False

      half_life  half_life_unit  spin  g_factor  quadrupole_moment
28      NaN      None          0.0  0.000000          0.0
29      NaN      None          0.5 -1.11058          0.0
30      NaN      None          0.0  0.000000          0.0

```

3.2.3 Ionic radii

The function to fetch ionic radii is called `fetch_ionic_radii` and can either fetch ionic or crystal radii depending on the `radius` argument.

```
[2]: from mendelev.fetch import fetch_ionic_radii
```

```
[3]: irs = fetch_ionic_radii(radius="ionic_radii")
      irs.head(10)
```

```
[3]: coordination      I      II      III  IIIPY      IV  IVPY  IVSQ  IX   V   \
      atomic_number charge
1          1      -38.0  -18.0      NaN      NaN      NaN      NaN      NaN      NaN
3          1          NaN      NaN      NaN      NaN      59.0      NaN      NaN      NaN
4          2          NaN      NaN      16.0      NaN      27.0      NaN      NaN      NaN
5          3          NaN      NaN      1.0      NaN      11.0      NaN      NaN      NaN
6          4          NaN      NaN      -8.0      NaN      15.0      NaN      NaN      NaN
7          -3          NaN      NaN      NaN      NaN      146.0      NaN      NaN      NaN
              3          NaN      NaN      NaN      NaN      NaN      NaN      NaN      NaN
              5          NaN      NaN      -10.4      NaN      NaN      NaN      NaN      NaN
8          -2          NaN      135.0      136.0      NaN      138.0      NaN      NaN      NaN
9          -1          NaN      128.5      130.0      NaN      131.0      NaN      NaN      NaN

      coordination      VI  VII   VIII   X  XI  XII  XIV
      atomic_number charge
1          1          NaN      NaN      NaN      NaN      NaN      NaN      NaN
3          1          76.0      NaN      92.0      NaN      NaN      NaN      NaN
4          2          45.0      NaN      NaN      NaN      NaN      NaN      NaN
5          3          27.0      NaN      NaN      NaN      NaN      NaN      NaN
6          4          16.0      NaN      NaN      NaN      NaN      NaN      NaN
7          -3          NaN      NaN      NaN      NaN      NaN      NaN      NaN
              3          16.0      NaN      NaN      NaN      NaN      NaN      NaN
              5          13.0      NaN      NaN      NaN      NaN      NaN      NaN
8          -2          140.0      NaN      142.0      NaN      NaN      NaN      NaN
9          -1          133.0      NaN      NaN      NaN      NaN      NaN      NaN
```

3.2.4 Ionization energies

To fetch ionization energies use `fetch_ionization_energies` that takes a `degree` (default is `degree=1`) argument that can either be a single integer or a list of integers to fetch multiple ionization energies.

```
[17]: from mendelev.fetch import fetch_ionization_energies
```

```
[25]: ies = fetch_ionization_energies(degree=2)
      ies.head(10)
```

```
[25]:      IE2
      atomic_number
1          NaN
2          54.417763
3          75.640094
4          18.211153
5          25.154830
```

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```

6          24.384500
7          29.601250
8          35.121110
9          34.970810
10         40.962960

```

```
[24]: ies_multiple = fetch_ionization_energies(degree=[1, 3, 5])
      ies_multiple.head(10)
```

```
[24]:
```

	IE1	IE3	IE5
atomic_number			
1	13.598434	NaN	NaN
2	24.587388	NaN	NaN
3	5.391715	122.454354	NaN
4	9.322699	153.896198	NaN
5	8.298019	37.930580	340.226008
6	11.260296	47.887780	392.090500
7	14.534130	47.445300	97.890130
8	13.618054	54.935540	113.898900
9	17.422820	62.708000	114.249000
10	21.564540	63.423310	126.247000

3.2.5 Electronegativities

To fetch all data from electronegativity scales use `fetch_electronegativities`. This can take a few seconds since most of the values need to be computed.

```
[26]: from mendeleeev.fetch import fetch_electronegativities
```

```
[27]: ens = fetch_electronegativities()
      ens.head(10)
```

```
[27]:
```

	Allen	Allred-Rochow	Cottrell-Sutton	Ghosh	Gordy	\
atomic_number						
1	13.610	0.000977	0.176777	0.263800	0.031250	
2	24.590	0.000803	0.192241	0.442712	0.036957	
3	5.392	0.000073	0.098866	0.105093	0.009774	
4	9.323	0.000187	0.138267	0.144986	0.019118	
5	12.130	0.000360	0.174895	0.184886	0.030588	
6	15.050	0.000578	0.208167	0.224776	0.043333	
7	18.130	0.000774	0.234371	0.264930	0.054930	
8	21.360	0.001146	0.268742	0.304575	0.072222	
9	24.800	0.001270	0.285044	0.344443	0.081250	
10	28.310	0.001303	0.295488	0.384390	0.087313	
						Li-Xue \
atomic_number						
1	{('I', 'I'): -3.540721753312244, ('II', 'I'): -2...					
2	{}					
3	{('IV', 'I'): 1.7160634314550876, ('VI', 'I'): 1...					
4	{}					

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5					{}
6					{}
7					{}
8					{}
9					{}
10					{}
	Martynov-Batsanov	Mulliken	Nagle	Pauling	Sanderson
atomic_number					
1	3.687605	6.799217	0.605388	2.20	2.187771
2	6.285107	12.293694	1.130639	NaN	1.000000
3	2.322007	2.695857	0.182650	0.98	0.048868
4	3.710381	4.661350	0.375615	1.57	0.126847
5	4.877958	4.149010	0.526974	2.04	0.254627
6	6.083300	5.630148	0.707393	2.55	0.427525
7	7.306768	7.267065	0.877498	3.04	0.577482
8	8.496136	6.809027	1.042218	3.44	0.941649
9	9.701808	8.711410	1.232373	3.98	1.017681
10	10.918389	NaN	1.443255	NaN	1.000000

3.3 Electronic configuration

ec attribute is an object from the `ElectronicConfiguration` class that has additional method for manipulating the configuration. Internally the configuration is represented as a `OrderedDict` from the `collections` module where tuples (n, s) (n is the principal quantum number and s is the subshell label) are used as keys and shell occupations are the values

```
[1]: from mendeleeev import Si
```

```
[2]: Si.ec.conf
```

```
[2]: OrderedDict([(1, 's'), 2],
                  [(2, 's'), 2],
                  [(2, 'p'), 6],
                  [(3, 's'), 2],
                  [(3, 'p'), 2]])
```

the occupation of different subshells can be access supplying a proper key

```
[3]: Si.ec.conf[(1, 's')]
```

```
[3]: 2
```

to calculate the number of electrons per shell type

```
[4]: Si.ec.electrons_per_shell()
```

```
[4]: {'K': 2, 'L': 8, 'M': 4}
```

get the largest value of the pricipal quantum number

```
[5]: Si.ec.max_n()
```

```
[5]: 3
```

Get the largest value of azimuthal quantum number for a given value of principal quantum number

```
[6]: Si.ec.max_l(n=3)
```

```
[6]: 'p'
```

Find the large noble gas-like core configuration

```
[7]: Si.ec.get_largest_core()
```

```
[7]: ('Ne', <ElectronicConfiguration(conf="1s2 2s2 2p6")>)
```

Get the total number of electrons

```
[8]: Si.ec.ne()
```

```
[8]: 14
```

Last subshell

```
[9]: Si.ec.last_subshell()
```

```
[9]: ((3, 'p'), 2)
```

Get unpaired electrons

```
[10]: Si.ec.unpaired_electrons()
```

```
[10]: 2
```

Remove electrons by ionizing returns a new configuration with an electron removed

```
[11]: ionized = Si.ec.ionize()
```

```
print(ionized)
```

```
1s2 2s2 2p6 3s2 3p1
```

We can check that it actually has less electrons:

```
[12]: ionized.ne()
```

```
[12]: 13
```

Spin occupations by subshell

```
[13]: Si.ec.spin_occupations()
```

```
[13]: OrderedDict([(1, 's'), {'pairs': 1, 'alpha': 1, 'beta': 1, 'unpaired': 0}],
                  ((2, 's'), {'pairs': 1, 'alpha': 1, 'beta': 1, 'unpaired': 0}),
                  ((2, 'p'), {'pairs': 3, 'alpha': 3, 'beta': 3, 'unpaired': 0}),
                  ((3, 's'), {'pairs': 1, 'alpha': 1, 'beta': 1, 'unpaired': 0}),
                  ((3, 'p'), {'pairs': 0, 'alpha': 2, 'beta': 0, 'unpaired': 2})])
```

Calculate the spin only magnetic moment

```
[14]: Si.ec.spin_only_magnetic_moment()
```

```
[14]: 2.8284271247461903
```

Calculate the screening constant using Slater's rules for 2s orbital

```
[15]: Si.ec.slater_screening(n=2, o='s')
```

```
[15]: 4.1499999999999995
```

3.3.1 Standalone use

You can use the `ElectronicConfiguration` as a standalone class and use all of the methods shown above.

```
[16]: from mendeleev.econf import ElectronicConfiguration
```

```
[17]: ec = ElectronicConfiguration("1s2 2s2 2p6 3s1")
```

Get the valence only configuration

```
[18]: ec.get_valence()
```

```
[18]: <ElectronicConfiguration(conf="3s1")>
```

3.4 Ions

You can use the `Ion` class to work with ions instead of elements. Ions can be created from elements and charge information.

```
[1]: from mendeleev.ion import Ion
```

```
[2]: fe_2 = Ion("Fe", 2)
```

You can access variety of properties of the ion

```
[3]: fe_2.charge
```

```
[3]: 2
```

```
[4]: fe_2.electrons
```

```
[4]: 24
```

```
[5]: fe_2.Z
```

```
[5]: 26
```

```
[6]: fe_2.name
```

```
[6]: 'Iron 2+ ion'
```

you can also print the unicode ion symbol

```
[7]: fe_2.unicode_ion_symbol()
```

```
[7]: 'Fe2+'
```

Ionic radii for this ion are available under `radius` attribute

```
[8]: fe_2.radius
```

```
[8]: [IonicRadius(
      atomic_number=26,
      charge=2,
      coordination='IV',
      crystal_radius=77.0,
      econf='3d6',
      id=149,
      ionic_radius=63.0,
      most_reliable=False,
      origin='',
      spin='HS',
    ),
    IonicRadius(
      atomic_number=26,
      charge=2,
      coordination='IVSQ',
      crystal_radius=78.0,
      econf='3d6',
      id=150,
      ionic_radius=64.0,
      most_reliable=False,
      origin='',
      spin='HS',
    ),
    IonicRadius(
      atomic_number=26,
      charge=2,
      coordination='VI',
      crystal_radius=75.0,
      econf='3d6',
      id=151,
      ionic_radius=61.0,
      most_reliable=False,
      origin='estimated, ',
      spin='LS',
    ),
    IonicRadius(
      atomic_number=26,
      charge=2,
      coordination='VI',
      crystal_radius=92.0,
      econf='3d6',
      id=152,
      ionic_radius=78.0,
      most_reliable=True,
      origin='from r^3 vs V plots, ',
```

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```

        spin='HS',
    ),
    IonicRadius(
        atomic_number=26,
        charge=2,
        coordination='VIII',
        crystal_radius=106.0,
        econf='3d6',
        id=153,
        ionic_radius=92.0,
        most_reliable=False,
        origin='calculated, ',
        spin='HS',
    )
]
```

Appropriate value of ionization energy and electron affinity are available under `ie` and `ea` attributes

```
[9]: fe_2.ie
```

```
[9]: 30.651
```

```
[10]: fe_2.ea
```

```
[10]: 16.1992
```

compute ionic potential

```
[11]: fe_2.ionic_potential()
```

```
[11]: 0.02564102564102564
```

3.5 Visualizing custom periodic tables

In this tutorial you'll learn how to use `mendeleev` to create customized visualizations of the periodic table.

The most convenient method to use for this is `periodic_table` function from `mendeleev.vis` module.

```
[1]: from mendeleev.vis import periodic_table
```

Make sure you have optional `vis` dependencies installed when installing `mendeleev`. If you are using `pip` install with

```
pip install mendeleev[vis]
```

To see the default visualization of the periodic table simply call the imported function

```
[2]: periodic_table()
```

Data type cannot be displayed: application/vnd.plotly.v1+json, text/html

mendelev stores also two color schemes for atoms that are frequently used for visualizing molecular structures. One set is stored in the `cpk_color` column and refers to **CPK** coloring, another is stored in `jmol_color` column and is used by the **Jmol** program, finally there is also coloring scheme from **MOLCAS GV** program store in the `molcas_gv_color` attribute. They can be displayed either by hovering of the element to display a tooltip or used directly to color the element cells.

```
[3]: periodic_table(colorby='jmol_color', title="JMol Colors")
```

Data type cannot be displayed: application/vnd.plotly.v1+json, text/html

```
[4]: periodic_table(colorby='cpk_color', title='CPK Colors')
```

Data type cannot be displayed: application/vnd.plotly.v1+json, text/html

```
[5]: periodic_table(colorby='molcas_gv_color', title='MOLCAS GV Colors')
```

Data type cannot be displayed: application/vnd.plotly.v1+json, text/html

3.5.1 Visualizing properties

Any of the properties in mendelev can now be visualized and color coded. This means that the value of selected attribute will be visible on each element and also it is possible to use the attribute to color code the background of each element.

Let's first use the `covalent_radius_pyykko` and display the values with the default color coding by series

```
[6]: periodic_table(attribute='covalent_radius_pyykko', title="Covalent Radii of Pyykko")
```

Data type cannot be displayed: application/vnd.plotly.v1+json, text/html

Now let's use the same attribute but in addition color code by the actual values, by adding `colorby='attribute'` argument

```
[7]: periodic_table(attribute='covalent_radius_pyykko', colorby='attribute',
    ↪ title="Covalent Radii of Pyykko")
```

Data type cannot be displayed: application/vnd.plotly.v1+json, text/html

The color map can also be customized using the `cmap` argument to any of the **standard colormaps** available in matplotlib

```
[8]: periodic_table(attribute='covalent_radius_pyykko', colorby='attribute',
    cmap='spring', title="Covalent Radii of Pyykko")
```

Data type cannot be displayed: application/vnd.plotly.v1+json, text/html

Let also see one of the more modern colormaps: `viridis`, `plasma`, `inferno` and `magma`.

```
[9]: periodic_table(attribute='covalent_radius_pyykko', colorby='attribute',
    cmap='inferno', title="Covalent Radii of Pyykko")
```

Data type cannot be displayed: application/vnd.plotly.v1+json, text/html

Lets try a different property: `atomic_volume`

```
[10]: periodic_table(attribute='atomic_volume', colorby='attribute', title='Atomic Volume')
```

Data type cannot be displayed: application/vnd.plotly.v1+json, text/html

```
[11]: periodic_table(attribute='en_pauling', colorby='attribute',
    title="Pauling's Electronegativity", cmap='viridis')
```

Data type cannot be displayed: application/vnd.plotly.v1+json, text/html

3.5.2 Wide 32-column version

The `periodic_table` function can also present the periodic table in the so-called wide format with the *f*-block between the *s*- and *d*-blocks resulting in 32 columns.

```
[12]: periodic_table(height=600, width=1500, wide_layout=True)
```

Data type cannot be displayed: application/vnd.plotly.v1+json, text/html

3.6 Advanced visualization tutorial

Next to the high level plotting function `mendeleev.vis.periodic_table`, `mendeleev` offers two lower level functions that give you more control over the result. There are two plotting backends supported:

1. `Plotly` (default)
2. `Bokeh`

3.6.1 Note

Depending on your environment being the classic jupyter notebook or jupyterlab you might have to do additional configuration steps, so if you're not getting expected results see plotly of bokeh documentation.

3.6.2 Accessing lower level plotting functions

There are two plotting functions, one for each of the backends:

- `periodic_table_plotly` in `mendelev.vis.plotly`
- `periodic_table_bokeh` in `mendelev.vis.bokeh`

that you can use to customize the visualizations even further.

Both functions take the same keyword arguments as the `periodic_table` function but they also require a `DataFrame` with periodic table data. That dataframe needs to have `x` and `y` columns for each element that play the role of coordinates. You can get the default data using the `create_vis_dataframe` function. Let's start with an example using the `plotly` backend.

```
[1]: from mendelev.vis import create_vis_dataframe, periodic_table_plotly
```

The function has only one required argument which is the data itself.

```
[2]: elements = create_vis_dataframe()
periodic_table_plotly(elements)
```

Data type cannot be displayed: application/vnd.plotly.v1+json, text/html

3.6.3 Custom coloring scheme

To apply a custom color scheme you can assign color to all the elements in the `DataFrame`. This can be done by creating a custom column in the `DataFrame` and then using `colorby` argument to specify which column contains colors. Let's try to color the elements according to the block they belong to.

```
[3]: import seaborn as sns
from matplotlib import colors
blockcmap = {b : colors.rgb2hex(c) for b, c in zip(['s', 'p', 'd', 'f'], sns.color_
    ↳ palette('deep'))}

elements['block_color'] = elements['block'].map(blockcmap)
periodic_table_plotly(elements, colorby='block_color')
```

Data type cannot be displayed: application/vnd.plotly.v1+json, text/html

3.6.4 Custom properties

You can also visualize custom properties using `pandas`' awesome methods for manipulating data. For example let's consider the difference of electronegativity between every element and the Oxygen atom. To calculate the values we will use Allen scale this time and call our new value ENX-ENO.

```
[4]: elements.loc[:, 'ENX-ENO'] = elements.loc[elements['symbol'] == 'O', 'en_allen'].values_
↳- elements.loc[:, 'en_allen']

periodic_table_plotly(elements, attribute='ENX-ENO', colorby='attribute',
                      cmap='viridis', title='Allen Electronegativity wrt. Oxygen')
```

Data type cannot be displayed: application/vnd.plotly.v1+json, text/html

As a second example let's consider a difference between the `covalent_radius_slater` and `covalent_radius_pyykko` values

```
[5]: elements['cov_rad_diff'] = elements['atomic_radius'] - elements['covalent_radius_pyykko']

periodic_table_plotly(elements, attribute='cov_rad_diff', colorby='attribute',
                      title='Covalent Radii Difference', cmap='viridis')
```

Data type cannot be displayed: application/vnd.plotly.v1+json, text/html

3.6.5 Bokeh backend

We can also use the Bokeh backed in the same way but we need to take a few extra steps to render the result in a notebook

```
[6]: from bokeh.plotting import show, output_notebook
from mendeleeev.vis import periodic_table_bokeh
```

First we need to enable notebook output

```
[7]: output_notebook()
```

Data type cannot be displayed: application/javascript, application/vnd.bokehjs_load.v0+json

```
[8]: fig = periodic_table_bokeh(elements)
show(fig)
```

Data type cannot be displayed: application/javascript, application/vnd.bokehjs_exec.v0+json

```
[9]: fig = periodic_table_bokeh(elements, attribute="atomic_radius", colorby="attribute")
show(fig)
```

Data type cannot be displayed: application/javascript, application/vnd.bokehjs_exec.v0+json

3.7 Jupyter notebooks

All tutorials are available as [Jupyter](#) notebooks on [binder](#) where you can explore the examples interactively:

- [Quick start](#)
- [Bulk data access](#)
- [Electronic Configuration](#)
- [Ions](#)
- [Visualizations](#)
- [Advanced visualizations](#)

To find out how to fetch data in bulk, check out the documentation about [data access](#).

4.1 Elements

The following data are currently available:

Name	Type	Comment	Unit	Data Source
abundance_crust	float	Abundance in the Earth's crust	mg/kg	[23]
abundance_sea	float	Abundance in the seas	mg/L	[23]
annotation	str	Annotations regarding the data		
atomic_number	int	Atomic number		
atomic_radius	float	Atomic radius	pm	[53]
atomic_radius_rahm	float	Atomic radius by Rahm et al.	pm	[45, 46]
atomic_volume	float	Atomic volume	cm ³ /mol	
atomic_weight	float	Atomic weight ⁽¹⁾		[35, 63]
atomic_weight_uncertainty	float	Atomic weight uncertainty ^(Page 36, 1)		[35, 63]
block	str	Block in periodic table		
boiling_point	float	Boiling temperature	K	[22]
c6	float	C ₆ dispersion coefficient in a.u.	a.u.	[13, 56]
c6_gb	float	C ₆ dispersion coefficient in a.u. (Gould & Bučko)	a.u.	[21]
cas	str	Chemical Abstracts Service identifier		
covalent_radius_bragg	float	Covalent radius by Bragg	pm	[10]
covalent_radius_cordero	float	Covalent radius by Cordero et al. ⁽²⁾	pm	[16]
covalent_radius_pyykko	float	Single bond covalent radius by Pyykko et al.	pm	[43]

continues on next page

Table 1 – continued from previous page

Name	Type	Comment	Unit	Data Source
cova-lent_radius_pyykko_d	float	Double bond covalent radius by Pyykko et al.	pm	[42]
cova-lent_radius_pyykko_t	float	Triple bond covalent radius by Pyykko et al.	pm	[44]
cpk_color	str	Element color in CPK convention	HEX	[61]
critical_pressure	float	Critical pressure	MPa	[22]
critical_temperature	float	Critical temperature	K	[22]
density	float	Density at 295K ⁽⁹⁾	g/cm ³	[23, 66]
description	str	Short description of the element		
dipole_polarizability	float	Dipole polarizability	a.u.	[51]
dipole_polarizability_	float	Dipole polarizability uncertainty	a.u.	[51]
discoverers	str	The discoverers of the element		
discovery_location	str	The location where the element was discovered		
discovery_year	int	The year the element was discovered		
electron_affinity	float	Electron affinity ⁽³⁾	eV	[6, 23]
electrons	int	Number of electrons		
electrophilicity	float	Electrophilicity index	eV	[39]
en_allen	float	Allen's scale of electronegativity ⁽⁴⁾	eV	[31, 32]
en_ghosh	float	Ghosh's scale of electronegativity		[18]
en_mulliken	float	Mulliken's scale of electronegativity	eV	[36]
en_pauling	float	Pauling's scale of electronegativity		[23]
econf	str	Ground state electron configuration		
evaporation_heat	float	Evaporation heat	kJ/mol	
fusion_heat	float	Fusion heat	kJ/mol	
gas_basicity	float	Gas basicity	kJ/mol	[23]
geochemical_class	str	Geochemical classification		[59]
glawe_number	int	Glawe's number (scale)		[19]
goldschmidt_class	str	Goldschmidt classification		[59, 60]
group	int	Group in periodic table		
heat_of_formation	float	Heat of formation	kJ/mol	[23]

continues on next page

Table 1 – continued from previous page

Name	Type	Comment	Unit	Data Source
inchi	str	International Chemical Identifier		[24]
ionenergy	tuple	Ionization energies	eV	[26]
ionic_radii	list	Ionic and crystal radii in pm ⁽⁸⁾	pm	[29, 52]
is_monoisotopic	bool	Is the element monoisotopic		
is_radioactive	bool	Is the element radioactive		
isotopes	list	Isotopes		
jmol_color	str	Element color in Jmol convention	HEX	[64]
lattice_constant	float	Lattice constant	Angstrom	
lattice_structure	str	Lattice structure code		
mass_number	int	Mass number (most abundant isotope)		
melting_point	float	Melting temperature	K	[22]
mendelev_number	int	Mendelev's number ⁽⁵⁾		[41, 57]
metallic_radius	float	Single-bond metallic radius	pm	[1]
metallic_radius_c12	float	Metallic radius with 12 nearest neighbors	pm	[1]
molar_heat_capacity	float	Molar heat capacity @ 25 C, 1 bar	J/(mol K)	[23]
molcas_gv_color	str	Element color in MOCAS GV convention	HEX	[65]
name	str	Name in English		
name_origin	str	Origin of the name		
neutrons	int	Number of neutrons (most abundant isotope)		
oxistates	list	Commonly occurring oxidation states		[67]
nist_webbook_url	str	URL for the NIST Chemistry Web-Book		[38]
oxistates	list	Oxidation states		
period	int	Period in periodic table		
pettifor_number	float	Pettifor scale		[41]
proton_affinity	float	Proton affinity	kJ/mol	[23]
protons	int	Number of protons		
sconst	float	Nuclear charge screening constants ⁽⁶⁾		[14, 15]

continues on next page

Table 1 – continued from previous page

Name	Type	Comment	Unit	Data Source
series	int	Index to chemical series		
sources	str	Sources of the element		
specific_heat_capacity	float	Specific heat capacity @ 25 C, 1 bar	J/(g K)	[23]
symbol	str	Chemical symbol		
thermal_conductivity	float	Thermal conductivity @25 C	W/(m K)	
triple_point_pressure	float	Triple point pressure	kPa	[22]
triple_point_temperature	float	Triple point temperature	K	[22]
uses	str	Applications of the element		
vdw_radius	float	Van der Waals radius	pm	[23]
vdw_radius_alvarez	float	Van der Waals radius according to Alvarez ⁽⁷⁾	pm	[5, 58]
vdw_radius_batsanov	float	Van der Waals radius according to Batsanov	pm	[8]
vdw_radius_bondi	float	Van der Waals radius according to Bondi	pm	[9]
vdw_radius_dreiding	float	Van der Waals radius from the DREIDING FF	pm	[34]
vdw_radius_mm3	float	Van der Waals radius from the MM3 FF	pm	[3]
vdw_radius_rt	float	Van der Waals radius according to Rowland and Taylor	pm	[48]
vdw_radius_truhlar	float	Van der Waals radius according to Truhlar	pm	[33]
vdw_radius_uff	float	Van der Waals radius from the UFF	pm	[47]

¹ Atomic Weights

Atomic weights and their uncertainties were retrieved mainly from ref. [63]. For elements whose values were given as ranges the *conventional atomic weights* from Table 3 in ref. [35] were taken. For radioactive elements the standard approach was adopted where the weight is taken as the mass number of the most stable isotope. The data was obtained from [CIAAW page on radioactive elements](#). In cases where two isotopes were specified the one with the smaller standard deviation was chosen. In case of Tc and Pm relative weights of their isotopes were used, for Tc isotope 98, and for Pm isotope 145 were taken from [CIAAW](#).

² Covalent Radius by Cordero et al.

In order to have a more homogeneous data for covalent radii taken from ref. [16] the values for 3 different valences for C, also the low and high spin values for Mn, Fe Co, were respectively averaged.

⁹ Densities

Density values for solids and liquids are always in units of grams per cubic centimeter and can be assumed to refer to temperatures near room temperature unless otherwise stated. Values for gases are the calculated ideal gas densities at 25°C and 101.325 kPa.

Original values for gasses are converted from g/L to g/cm³.

For elements where several allotropes exist, the density corresponding to the most abundant are reported (for full list refer to [23]), namely:

4.2 Isotopes

Name	Type	Comment	Unit	Data Source
abundance	float	Relative Abundance		[25]
abundance_uncertainty	float	Uncertainty of relative abundance		[25]
atomic_number	int	Atomic number		
decay_modes	obj	Decay modes with intensities		[25]
discovery_year	int	Year the isotope was discovered		[25]
g_factor	float	Nuclear g-factor		[55]
g_factor_uncertainty	float	Uncertainty of the nuclear g-factor		[55]
half_life	float	Half life of the isotope		[25]
half_life_uncertainty	float	Uncertainty of the half life		[25]
half_life_unit	str	Unit in which the half life is given		[25]
is_radioactive	bool	Is the isotope radioactive		[62]
mass	float	Atomic mass	Da	[62]
mass_number	int	Mass number of the isotope		[62]
mass_uncertainty	float	Uncertainty of the atomic mass	Da	[62]
parity	str	Parity, if present, it can be either + or -		[25]
quadrupole_moment	float	Nuclear electric quadrupole moment	b [100 fm ²]	[54]
quadrupole_moment_uncertainty	float	Nuclear electric quadrupole moment	b [100 fm ²]	[54]
spin	str	Nuclear spin quantum number		[25]

4.3 Isotope Decay Modes

Name	Type	Comment	Unit	Data Source
isotope_id	int	ID of the isotope		
mode	str	ASCII symbol of the decay mode		[25]
relation	str	Uncertainty of relative abundance		[25]
intensity	float	Intensity of the decay mode	%	[25]
is_allowed_not_observed	bool	If <i>True</i> decay mode is energetically allowed, but not experimentally observed		[25]
is_observed_intensity_unknown	bool	If <i>True</i> decay mode is observed, but its intensity is not experimentally known		[25]

The different modes in the table are stores as ASCII representations for compatibility. The table below provides expla-

- Antimony (gray)
- Berkelium (form)
- Carbon (graphite)
- Phosphorus (white)
- Selenium (gray)
- Sulfur (rhombic)
- Tin (white)

For elements where experimental data is not available, theoretical estimates taken from [66] are used, namely for:

- Astatine
- Francium
- Einsteinium
- Fermium
- Mendelevium
- Nobelium

4.2. Isotopes

- Lawrencium
- Rutherfordium
- Dubnium
- Seaborgium
- Bohrium

nations of the symbols.

ASCII	Unicode	Description
A	α	α emission
p	p	proton emission
2p	2p	2-proton emission
n	n	neutron emission
2n	2n	2-neutron emission
EC	ϵ	electron capture
e+	e^+	positron emission
B+	β^+	β^+ decay ($\beta^+ = \epsilon + e^+$)
B-	β^-	β^- decay
2B-	$2\beta^-$	double β^- decay
2B+	$2\beta^+$	double β^+ decay
B-n	$\beta^- n$	β^- -delayed neutron emission
B-2n	$\beta^- 2n$	β^- -delayed 2-neutron emission
B-3n	$\beta^- 3n$	β^- -delayed 3-neutron emission
B+p	$\beta^+ p$	β^+ -delayed proton emission
B+2p	$\beta^+ 2p$	β^+ -delayed 2-proton emission
B+3p	$\beta^+ 3p$	β^+ -delayed 3-proton emission
B-A	$\beta^- \alpha$	β^- -delayed α emission
B+A	$\beta^+ \alpha$	β^+ -delayed α emission
B-d	$\beta^- d$	β^- -delayed deuteron emission
B-t	$\beta^- t$	β^- -delayed triton emission
IT	IT	internal transition
SF	SF	spontaneous fission
B+SF	$\beta^+ \text{SF}$	β^+ -delayed fission
B-SF	$\beta^- \text{SF}$	β^- -delayed fission
24Ne	24Ne	heavy cluster emission

Data Footnotes

The screening constants were calculated according to the following formula

$$\sigma_{n,l,m} = Z - n \cdot \zeta_{n,l,m}$$

where n is the principal quantum number, Z is the atomic number, $\sigma_{n,l,m}$ is the screening constant, $\zeta_{n,l,m}$ is the optimized exponent from [14, 15].

For elements Nb, Mo, Ru, Rh, Pd and Ag the exponent values corresponding to the ground state electronic configuration were taken (entries with superscript a in Table II in [15]).

For elements La, Pr, Nd and Pm two exponent were reported for 4f shell denoted 4f and 4f' in [15]. The value corresponding to 4f were used since according to the authors these are the dominant ones.

⁷ **van der Waals radii according to Alvarez**

The bulk of the radii data was taken from Ref. [5], but the radii for noble gasses were update according to the values in Ref. [58].

ACCESSING DATA

5.1 Individual Elements

The easiest way to access individual elements is simply by importing them from the *mendeleev* directly using their symbols:

```
>>> from mendeleev import H, C, O, Og
>>> [x.name for x in [H, C, O, Og]]
['Hydrogen', 'Carbon', 'Oxygen', 'Oganesson']
```

An alternative method of access is through the `element()` function that returns either a single `Element` instance or a tuple of those instances depending on the input. It provides a more flexible interface since it accepts element names, atomic numbers and symbols as well as their combinations.

5.2 Fetching data in bulk

If you want a whole set of data you can retrieve one of the tables from the database as `pandas.DataFrame` through the `fetch_table()`. The following tables are available:

- elements
- groups
- ionicradii
- ionizationenergies
- isotopes
- oxidationstates
- screeningconstants
- series

fetch_table(*table*: str, ***kwargs*) → `pandas.DataFrame`

Return a table from the database as `pandas.DataFrame`

Parameters

- **table** – Name of the table from the database
- **kwargs** – A dictionary of keyword arguments to pass to the `pandas.read_sql()`

Returns

Pandas DataFrame with the contents of the table

Return type`df (pandas.DataFrame)`**Example**

```
>>> from mendelev.fetch import fetch_table
>>> df = fetch_table('elements')
>>> type(df)
pandas.core.frame.DataFrame
```

fetch_ionization_energies(*degree: List[int] | int = 1*) → `pandas.DataFrame`Fetch a `pandas.DataFrame` with ionization energies for all elements indexed by atomic number.**Parameters****degree** – Degree of ionization, either as int or a list of ints. If a list is passed then the output will contain ionization energies corresponding to particular degrees in columns.**Returns**

ionization energies, indexed by atomic number

Return type`df (pandas.DataFrame)`**fetch_ionic_radii**(*radius: str = 'ionic_radius'*) → `pandas.DataFrame`

Fetch a pandas DataFrame with ionic radii for all the elements.

Parameters**radius** – The radius to be returned either *ionic_radius* or *crystal_radius***Returns****a table with atomic numbers, symbols and ionic radii for all coordination numbers****Return type**`df (pandas.DataFrame)`

5.3 Computed properties

Some properties need to be computed rather than directly retrieved from the database. *Electronegativities***fetch_electronegativities**(*scales: List[str] = None*) → `pandas.DataFrame`Fetch electronegativity scales for all elements as `pandas.DataFrame`**Parameters****scales** – list of scale names, defaults to all available scales**Returns**

Pandas DataFrame with the contents of the table

Return type`df (pandas.DataFrame)`

5.4 Database session and engine

For those how want to interact with the database through a layer of [SQLAlchemy](#) there are methods for getting the session or the engine:

get_session(*dbpath*: *str* = *None*) → Session

Return the database session connection.

get_engine(*dbpath*: *str* = *None*) → Engine

Return the db engine

ELECTRONEGATIVITIES

Since electronegativity is useful concept rather than a physical observable, several scales of electronegativity exist and some of them are available in *mendeleev*. Depending on the definition of a particular scale the values are either stored directly or recomputed on demand with appropriate formulas. The following scales are stored:

- *Allen*
- *Ghosh*
- *Pauling*

Moreover there are electronegativity scales that can be computed from their respective definition and the atomic properties available in *mendeleev*:

- *Allred-Rochow*
- *Cottrell-Sutton*
- *Gordy*
- *Li and Xue*
- *Martynov and Batsanov*
- *Mulliken*
- *Nagle*
- *Sanderson*

For a short overview on electronegativity see this [presentation](#).

All the examples shown below are for Silicon:

```
>>> from mendeleev import element
>>> Si = element('Si')
```

6.1 Allen

The electronegativity scale proposed by Allen in ref [2] is defined as:

$$\chi_A = \frac{\sum_x n_x \varepsilon_x}{\sum_x n_x}$$

where: ε_x is the multiplet-averaged one-electron energy of the subshell x and n_x is the number of electrons in subshell x and the summation runs over the valence shell.

The values that are tabulated were obtained from refs. [31] and [32].

Example:

```
>>> Si.en_allen
11.33
>>> Si.electronegativity('allen')
11.33
```

6.2 Allred and Rochow

The scale of Allred and Rochow [4] introduces the electronegativity as the electrostatic force exerted on the electron by the nuclear charge:

$$\chi_{AR} = \frac{e^2 Z_{\text{eff}}}{r^2}$$

where: Z_{eff} is the effective nuclear charge and r is the covalent radius.

Example:

```
>>> Si.electronegativity('allred-rochow')
0.00028240190249702736
```

6.3 Cottrell and Sutton

The scale proposed by Cottrell and Sutton [17] is derived from the equation:

$$\chi_{CS} = \sqrt{\frac{Z_{\text{eff}}}{r}}$$

where: Z_{eff} is the effective nuclear charge and r is the covalent radius.

Example:

```
>>> Si.electronegativity('cottrell-sutton')
0.18099342720014772
```

6.4 Ghosh

Ghosh [18] presented a scale of electronegativity based on the absolute radii of atoms computed as

$$\chi_{GH} = a \cdot (1/R) + b$$

where: R is the absolute atomic radius and a and b are empirical parameters.

Example:

```
>>> Si.en_ghosh
0.178503
```

6.5 Gordy

Gordy's scale [20] is based on the potential that measures the work necessary to achieve the charge separation, according to:

$$\chi_G = \frac{eZ_{\text{eff}}}{r}$$

where: Z_{eff} is the effective nuclear charge and r is the covalent radius.

Example:

```
>>> Si.electronegativity('gordy')
0.03275862068965517
```

6.6 Li and Xue

Li and Xue [27, 28] proposed a scale that takes into account different valence states and coordination environment of atoms and is calculated according to the following formula:

$$\chi_{LX} = \frac{n^* \sqrt{I_j / Ry}}{r}$$

where: n^* is the effective principal quantum number, I_j is the j 'th ionization energy in eV , Ry is the Rydberg constant in eV and r is either the crystal radius or ionic radius.

Example:

```
>>> Si.en_li_xue(charge=4)
{'u'IV': 13.16033405547733, 'u'VI': 9.748395596649873}
>>> Si.electronegativity('li-xue', charge=4)
{'u'IV': 13.16033405547733, 'u'VI': 9.748395596649873}
```

6.7 Martynov and Batsanov

Martynov and Batsanov [7] used the square root of the averaged valence ionization energy as a measure of electronegativity:

$$\chi_{MB} = \sqrt{\frac{1}{n_v} \sum_{k=1}^{n_v} I_k}$$

where: n_v is the number of valence electrons and I_k is the k th ionization potential.

Example:

```
>>> Si.en_martynov_batsanov()
5.0777041564076963
>>> Si.electronegativity(scale='martynov-batsanov')
5.0777041564076963
```

6.8 Mulliken

Mulliken scale [36] is defined as the arithmetic average of the ionization potential (IP) and the electron affinity (EA):

$$\chi_M = \frac{IP + EA}{2}$$

Example:

```
>>> Si.en_mulliken()
4.0758415
>>> Si.electronegativity('mulliken')
4.0758415
```

6.9 Nagle

Nagle [37] derived his scale from the atomic dipole polarizability:

$$\chi_N = \sqrt[3]{\frac{n}{\alpha}}$$

Example:

```
>>> Si.electronegativity('nagle')
0.47505611644667534
```

6.10 Pauling

Pauling's thermochemical scale was introduced in [40] as a relative scale based on electronegativity differences:

$$\chi_A - \chi_B = \sqrt{E_d(AB) - \frac{1}{2}[E_d(AA) + E_d(BB)]}$$

where: $E_d(XY)$ is the bond dissociation energy of a diatomic XY . The values available in *mendelev* are taken from ref. [23].

Example:

```
>>> Si.en_pauling
1.9
>>> Si.electronegativity('pauling')
1.9
```

6.11 Sanderson

Sanderson [49, 50] established his scale of electronegativity based on the stability ratio:

$$\chi_S = \frac{\rho}{\rho_{ng}}$$

where: ρ is the average electron density $\rho = \frac{Z}{4\pi r^3/3}$, and ρ_{ng} is the average electron density of a hypothetical noble gas atom with charge Z .

Example:

```
>>> Si.en_sanderson()
0.3468157872145231
>>> Si.electronegativity()
0.3468157872145231
```

6.12 Fetching all electronegativities

If you want to fetch all the available scales for all elements you can use the `fetch_electronegativities` function, that collect all the values into a `DataFrame`.

API REFERENCE

Here you'll find API documentation of the mendelev's modules.

<code>mendelev.db</code>	
<code>mendelev.cli</code>	
<code>mendelev.econf</code>	Implementation of the abstraction for the electronic configuration object.
<code>mendelev.electronegativity</code>	Electronegativity scale formulas.
<code>mendelev.fetch</code>	
<code>mendelev.mendelev</code>	
<code>mendelev.models</code>	module specifying the database models
<code>mendelev.ion</code>	
<code>mendelev.vis.periodictable</code>	
<code>mendelev.vis.bokeh</code>	
<code>mendelev.vis.plotly</code>	
<code>mendelev.vis.seaborn</code>	
<code>mendelev.vis.utils</code>	
<code>mendelev.utils</code>	

7.1 mendelev.db

Functions

<code>get_engine([dbpath])</code>	Return the db engine
<code>get_package_dbpath()</code>	Return the default database path
<code>get_session([dbpath])</code>	Return the database session connection.

7.2 mendelev.cli

Functions

<code>clielement()</code>	CLI for convenient printing of properties for a given element
---------------------------	---

7.3 mendelev.econf

Implementation of the abstraction for the electronic configuration object.

Functions

<code>get_l(subshell)</code>	Return the orbital angular momentum quantum number for a given subshell
<code>get_spin_strings(sodict[, average])</code>	spin strings as numpy arrays
<code>print_spin_occupations(sodict[, average])</code>	Pretty format for the spin occupations
<code>shell_capacity(shell)</code>	Return the shell capacity (max number of electrons)
<code>subshell_capacity(subshell)</code>	Return the subshell capacity (max number of electrons)
<code>subshell_degeneracy(subshell)</code>	Return the degeneracy of a given subshell

Classes

<code>ElectronicConfiguration([conf, atomre, shellre])</code>	Electronic configuration handler
---	----------------------------------

7.4 mendelev.electronegativity

Electronegativity scale formulas.

Functions

<code>allred_rochow(zeff, radius)</code>	Calculate the electronegativity of an atom according to the definition of Allred and Rochow
<code>cottrell_sutton(zeff, radius)</code>	Calculate the electronegativity of an atom according to the definition of Allred and Rochow
<code>generic(zeff, radius[, rpow, apow])</code>	Calculate the electronegativity from a general formula
<code>gordy(zeff, radius)</code>	Calculate the electronegativity of an atom according to the definition of Allred and Rochow
<code>li_xue(ionization_energy, radius, valence_pqn)</code>	Calculate the electronegativity of an atom according to the definition of Li and Xue
<code>martynov_batsanov(ionization_energies)</code>	Calculates the electronegativity value according to Martynov and Batsanov as the average of the ionization energies of the valence electrons
<code>mulliken(ionization_energy, electron_affinity)</code>	Return the absolute electronegativity (Mulliken scale).
<code>nagle(nvalence, polarizability)</code>	Calculate the electronegativity of an atom according to the definition of Nagle
<code>sanderson(radius, noble_gas_radius)</code>	Calculate Sanderson's electronegativity

7.5 mendelev.fetch

Functions

<code>add_plot_columns(elements)</code>	Add columns needed for the creating the plots
<code>fetch_electronegativities([scales])</code>	Fetch electronegativity scales for all elements as <code>pandas.DataFrame</code>
<code>fetch_ionic_radii([radius])</code>	Fetch a pandas DataFrame with ionic radii for all the elements.
<code>fetch_ionization_energies([degree])</code>	Fetch a <code>pandas.DataFrame</code> with ionization energies for all elements indexed by atomic number.
<code>fetch_neutral_data()</code>	Get extensive set of data from multiple database tables as <code>pandas.DataFrame</code>
<code>fetch_table(table, **kwargs)</code>	Return a table from the database as <code>pandas.DataFrame</code>
<code>get_app_data()</code>	write a file with the neutral data
<code>get_zeff(an[, method])</code>	A helper function to calculate the effective nuclear charge.

7.6 mendeleev.mendeleev

Functions

<code>deltaN(id1, id2[, charge1, charge2, ...])</code>	Calculate the approximate fraction of transferred electrons between elements or ions <i>id1</i> and <i>id2</i> with charges <i>charge1</i> and <i>charge2</i> respectively according to the expression
<code>element(ids)</code>	Based on the type of the <i>ids</i> identifier return either an Element object from the database, or a list of Element objects if the <i>ids</i> is a list or a tuple of identifiers.
<code>get_all_elements()</code>	Get all elements as a list
<code>ids_to_attr(ids[, attr])</code>	Convert the element ids: atomic numbers, symbols, element names or a combination of the above to a list of corresponding attributes.
<code>isotope(symbol_or_atn, mass_number)</code>	Get an Isotope based on the element symbol and mass number or atomic number and mass number.

7.7 mendeleev.models

module specifying the database models

Functions

<code>estimate_from_group(atomic_number, attr_name)</code>	Evaluate a value <i>attribute</i> for element by interpolation or extrapolation of the data points from elements from <i>group</i> .
<code>fetch_attrs_for_group(attrs[, group])</code>	A convenience function for getting a specified attribute for all the members of a given group.
<code>with_uncertainty(value, uncertainty[, digits])</code>	Format a value with uncertainty using scientific notation.

Classes

<code>Element(**kwargs)</code>	Chemical element.
<code>Group(**kwargs)</code>	Name of the group in the periodic table.
<code>IonicRadius(**kwargs)</code>	Effective ionic radii and crystal radii in pm retrieved from [1] .
<code>IonizationEnergy(**kwargs)</code>	Ionization energy of an element
<code>Isotope(**kwargs)</code>	<p>param abundance Abundance of the isotope</p>
<code>IsotopeDecayMode(**kwargs)</code>	<p>param mode ASCII symbol for the decay mode</p>
<code>OxidationState(**kwargs)</code>	Oxidation states of an element
<code>PhaseTransition(**kwargs)</code>	Phase Transition Conditions
<code>ScreeningConstant(**kwargs)</code>	Nuclear screening constants from Clementi, E., & Raimondi, D.
<code>Series(**kwargs)</code>	Name of the series in the periodic table.

7.8 mendeleev.ion

Classes

<code>Ion(label[, q])</code>	Class representating atomic ions
------------------------------	----------------------------------

7.9 mendeleev.vis.periodictable

Functions

<code>periodic_table([attribute, height, width, ...])</code>	High level api for visualizing periodic tables.
--	---

7.10 mendeleev.vis.bokeh

Functions

<code>periodic_table_bokeh(elements[, attribute, ...])</code>	Use Bokeh backend to plot the periodic table.
---	---

7.11 mendeleeev.vis.plotly

Functions

<code>create_annotation(row, attr[, size, ...])</code>	Create an annotation from pandas series
<code>create_tile(element, color[, x_offset, y_offset])</code>	Create tile shape
<code>periodic_table_plotly(elements[, attribute, ...])</code>	Create a periodic table visualization with plotly.Figure

7.12 mendeleeev.vis.seaborn

Functions

<code>heatmap(elements, prop[, style, figsize, ...])</code>	Plot a heatmap of the given property
---	--------------------------------------

7.13 mendeleeev.vis.utils

Functions

<code>add_tile_coordinates(df[, x_coord, y_coord, ...])</code>	Calculate coordinates for the tile centers
<code>colormap_column(elements, column[, cmap, ...])</code>	Return a new DataFrame with the same size (and index) as <i>elements</i> with a column <i>cmap</i> containing HEX color mapping from <i>cmap</i> colormap.
<code>create_vis_dataframe([x_coord, y_coord, ...])</code>	Base DataFrame for visualizations

7.14 mendeleeev.utils

Functions

<code>coeffs(a[, b])</code>	Return stoichiometric coefficients from oxidation states
<code>n_effective(n[, source])</code>	Effective principal quantum number

BIBLIOGRAPHY

MENDELEEV CHANGELOG

9.1 v0.15.0 (26.12.2023)

- [FIX] Fix a few issues with README.md by @paulromano in #119
- [MNT] Remove six dependency by @paulromano in #120
- [FIX] Update abundance for ¹²⁶Te isotope by @Immentel in #123
- [MNT] add python 3.12 support and bump various package versions @Immentel in #134

9.2 v0.14.0 (07.06.2023)

- Fix Mulliken electronegativity by @Immentel in #116
- [FIX] Enable fetch of phase transition data by @Immentel in #112

9.3 v0.13.1 (24.04.2023)

- Fix URL in references.bib by @paulromano in #108
- Fix import warning for declarative_base by @Immentel in #109
- Add vis extra by @Immentel in #110

9.4 v0.13.0 (11.04.2023)

- [MNT] Relax dependencies for sqlalchemy and pandas and drop python 3.7 by @Immentel in #103
- Bump ipython from 7.34.0 to 8.10.0 by @dependabot in #104
- [MNT] Add API docs for vis module by @Immentel in #105

9.5 v0.12.1 (28.11.2022)

- Add CodeQL workflow for GitHub code scanning by @lgtn-com in #89
- Fix number of valence electrons (#91) for Pd by @Immentel in #92
- Add missing type hints by @Immentel in #93

9.6 v0.12.0 (9.10.2022)

- Configure concurrency in github actions by @Immentel in #82
- Fix abundancies for isotopes with one naturally occurring isotope by @Immentel in #80
- Add IsotopeDecayMode model and data by @Immentel in #84
- Update boiling and melting point data and add triple point and critical temperature and pressure, by @Immentel in #88
- Include compatibility with python 3.11.

9.7 v0.11.0 (29.09.2022)

- Update data.rst by @Eben60 in #66
- Set discovery_location for Zinc to null by @Immentel in #68
- Change “Oxidation states” to “Commonly occurring oxidation states” by @Eben60 in #69
- Add International Chemical Identifier property by @Immentel in #76
- Update data for isotopes by @Immentel in #74
- Update oxidation states and add method to fetch values by @Immentel in #77
- Documentation fixes by @Immentel in #78

9.8 v0.10.0 (17.07.2022)

- Corrected specific heat capacity values with *CRC Handbook of Chemistry and Physics* as the data source [Issue #60](#)
- Renamed *specific_heat* attribute to *specific_heat_capacity* [PR #61](#) (for backwards compatibility *specific_heat* will still work)
- Added *molar_heat_capacity* property from *CRC Handbook of Chemistry and Physics* [PR #61](#)
- Corrected wrong units in the docs for *specific_heat* [Issue #59](#)
- Fixed usage of *pytest.approx* after api change [PR #62](#)
- Refactored *format* call to f-strings [PR #62](#)
- Updated locked dependencies to eliminate known vulnerabilities [PR #63](#)
- Added python 3.10 to CI workflows to increase test coverage [PR #62](#)

9.9 v0.9.0 (24.09.2021)

- Correct density data with *CRC Handbook of Chemistry and Physics* as the data source [PR #39](#) that fixes [issue #38](#).
- Fixed plotly based visualizations not rendering at <https://mendeleev.readthedocs.io>.
- Added DOI number.

9.10 v0.8.0 (22.08.2021)

- Enable visualizations of periodic tables with `plotly` as well as `bokeh` backends through `mendeleev.vis.plotly.periodic_table_plotly` and `mendeleev.vis.bokeh.periodic_table_bokeh` functions.
- Add `mendeleev.vis.periodic_table` function for convenient periodic table plotting wrapping both plotting backends.
- Refactored the `mendeleev.vis` module so it can be easily extended with plotting backends.
- Add `CITATION.cff` file.

9.11 v0.7.0 (20.03.2021)

- Update ionic and crystal radii for III+ actinoids.
- Refactor electronegativity calculations for easier calculation and retrieval of the different scales.
- Add `fetch.py` module with methods for accessing bulk data.
- Add `oxides` methods to `Element` that returns possible oxides ([Issue #17](#)).
- Add tutorials on fetching data and electronic configuration.
- `tables.py` is renamed to `models.py`.
- Switch from `pipenv` to `poetry` for development.
- Switch from Travis CI to Github Actions and extend testing matrix to Win and MacOS.
- Documentation update.

9.12 v0.6.1 (03.11.2020)

- Add *electrophilicity* index.
- Pin *sqlalchemy* version to prevent further issues with old versions, see [Issue #22](#)

9.13 v0.6.0 (10.04.2020)

- Add *Ion* class to handle atomic ions.
- Add Github templates for bug reports, feature requests and pull requests.
- Update the values of *atomic_radius_rahm* according to corrigendum, (PR #13).
- Switch the default documentation theme to material with [sphinx-material](#).

9.14 v0.5.2 (29.01.2020)

- Fix a UnicodeDecodeError from README.md while installing on windows.
- Code quality improvements based on [lgtm.com](#)

9.15 v0.5.1 (26.08.2019)

- Fix [issue #3](#), `get_table('elements')` throwing an error

9.16 v0.5.0 (25.08.2019)

- Migrate the package from bitbucket to github
- Add Pettifor scale: `pettifor_number` attribute
- Add Glawe scale: `glawe_number` attribute
- Restore default printing of isotopic abundancies, fix issue #9
- Correct the oxidation states for Xe, fix issue #10

9.17 v0.4.5 (17.03.2018)

- Update dipole polarizability value to the latest recommended (2018)
- Fix [issues/8/typeerror-on-some-of-the-element](#)

9.18 v0.4.4 (10.12.2018)

- Fix [issues/6/type-of-block-is-wrong](#)

9.19 v0.4.3 (16-07-2018)

- Added `mendelev_number` attribute to elements.
- Added footnotes to the data documentation.

9.20 v0.4.2 (26-12-2018)

- Fixed issue #3: encoding issue in `econf.py`.

9.21 v0.4.1 (03-12-2017)

- Corrected passing integers to the CLI script.
- Various documentation readability and structure improvements.

9.22 v0.4.0 (22-11-2017)

- The elements can now be directly imported from *mendelev* by symbols.
- Added `sphinxcontrib.bibtex` extension to the docs to handle BibTeX style references to improve handling of the bibliographic entries.
- Added `nbsphinx` to include Jupyter Notebook tutorials in the docs.

9.23 v0.3.6 (17-09-2017)

- Added API documentation
- Corrected the sphinx configuration
- Updated the documentation

9.24 v0.3.5 (07-09-2017)

- Added a module with functions to scrape data from ciaaw.org
- Added new `Element` attributes, `name_origin`, `uses` and `sources`
- Added new `Element` attributes related to the discovery: `discoverers`, `discovery_location`, `discovery_year`

9.25 v0.3.4 (28-06-2017)

- Fixed python2.7 compatibility issue
- Added double and triple bond covalent radii from Pyykko
- Corrected minor error in the documentation
- Replaced lazy loading with eager in db queries

9.26 v0.3.3 (16-05-2017)

- Corrected the coordination of Br5+ ion in the ionic radii table

9.27 v0.3.2 (01-05-2017)

- Added `metallic_radius`
- Added Goldschmidt and geochemical classifications
- Corrected the docs configuration
- Added cas number attribute
- Added atomic radii by Rahm et al.
- Created a conda recipe
- Added a citation information to the readme
- Electronic configuration code was split into a separate module

9.28 v0.3.1 (25-01-2017)

- Added new properties of isotopes: `spin`, `g_factor`, `quadrupole_moment`

9.29 v0.3.0 (09-01-2017)

- Updates of the documentation and tutorials
- Added radioactive isotope half-lives

9.30 v0.2.17 (08-01-2017)

- Extended the schema for isotopes with additional attributes and updated the values of abundancies, half lifes and mass uncertainties.
- Updates to the tutorials and docs.

9.31 v0.2.16 (06-01-2017)

- Corrected the radioactive attribute of Th, Pa and U elements.

9.32 v0.2.15 (02-01-2017)

- Patched the sphinx configuration.

9.33 v0.2.14 (02-01-2017)

- Patched typos in README.

9.34 v0.2.13 (01-01-2017)

- Updated atomic weight with the newest IUPAC and CIAAW recommendations.
- Added `is_radioactive` and `is_monoisotopic` attributes.
- Updated the docs.

9.35 v0.2.12 (21-12-2016)

- Got rid of the scipy dependency.

9.36 v0.2.11 (10-11-2016)

- Updated the names and symbols of elements 113, 115, 117, 118.
- Updated the docs.

9.37 v0.2.10 (18-10-2016)

- Added the C6 coefficients from Gould and Bucko.
- Added van der Waals radii from Alvarez.

9.38 v0.2.9 (16-10-2016)

- Added a scale of electronegativities by Ghosh.

9.39 v0.2.8 (29-08-2016)

- Updated the electron affinity of Pb and Co.
- Updates of the docs.

9.40 v0.2.7 (02-04-2016)

- Maintenance.

9.41 v0.2.6 (02-04-2016)

- Mainly maintenance updates to docs, `sphinx conf.py`, `setup.py`, requirements.

9.42 v0.2.5 (02-04-2016)

9.42.1 Features added

- Added calculation of Martynov and Batsanov scale of electronegativity in `en_martynov_batsanov` method in the `Element` class
- Added `abundance_crust` and `abundance_sea` with element abundancies in the crust and seas
- Added `molcas_gv_color` attribute with **MOLCAS GV** colors

9.42.2 Bugs fixed

- Restored Python 3.x compatibility

9.43 v0.2.4 (05-02-2016)

9.43.1 Features added

- Extended and corrected the documentation and Jupyter notebook tutorials on basic usage electronegativities, plotting and tables

9.43.2 Bugs fixed

- Corrected `raise` to `return` when calling `en_sanderson` from `electronegativity`
- Fixed and tested the formula for calculating the Li and Xue scale of electronegativity in `en_lie-xue`

9.44 v0.2.3 (27-01-2016)

9.44.1 Features added

- Added new vdW radii: `vdw_radius_batsanov`, `vdw_radius_bondi`, `vdw_radius_dreiding`, `vdw_radius_mm3`, `vdw_radius_rt`, `vdw_radius_truhlar`, `vdw_radius_uff`
- Added an option to plot the long (wide) version of the periodic table in `periodic_plot`

9.44.2 Bugs fixed

- Typos in the docstrings

9.45 v0.2.2 (29-11-2015)

9.45.1 Features added

- Added new covalent radii: `covalent_radius_bragg`, `covalent_radius_slater`
- Added the c6 dispersion coefficients
- Added `gas_basicity`, `proton_affinity` and `heat_of_formation`
- Added `periodic_plot` function for producing *bokeh* <<https://bokeh.org/>> based plots of the periodic table
- Added `jmol_color` and `cpk_color` with different coloring schemes for atoms

9.45.2 Bug fixes

- Changed the series of elements 113, 114, 115, 116 to poor metals

9.46 v0.2.1 (26-10-2015)

9.46.1 Features added

- Extended the list of options for calculating Mulliken electronegativities in `en_mulliken`
- Added `electrons_per_shell` method
- Added a function to calculate linear interpolation of radii required for calculation of Sandersons electronegativity
- Added hybrid attributes `electrons`, `protons`, `neutrons` and `mass_number`

9.46.2 Bug fixes

- Changed the type of the `melting_point` from `str` to `float`

9.47 v0.2.0 (22-10-2015)

9.47.1 Features added

- Instead of `covalent_radius` added `covalent_radius_2008` and `covalent_radius_2009`
- Instead of `electronegativity` added `en_pauling` and `en_mulliken`
- Added a method for getting ionic radii
- Improved the method for calculating the nuclear screening constants
- Added `ElectronicConfiguration` class initialized as `Element` attribute
- Added nuclear screening constants from Clementi and Raimondi
- Added a method to calculate the absolute softness, absolute hardness and absolute electronegativity
- Added `get_table` method to retrieve the tables as `pandas DataFrames`

9.47.2 Bug fixes

- Added missing electronic configurations
- Converted ionic radii from Angstrom to pico meters

9.48 v0.1.0 (11-07-2015)

First tagged version with the initial structure of the package and first version of the database and the python interface

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INDICES AND TABLES

- `genindex`
- `modindex`
- `search`

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PYTHON MODULE INDEX

m

- `mendelev.cli`, 50
- `mendelev.db`, 49
- `mendelev.econf`, 50
- `mendelev.electronegativity`, 50
- `mendelev.fetch`, 51
- `mendelev.ion`, 53
- `mendelev.mendelev`, 52
- `mendelev.models`, 52

F

`fetch_electronegativities()` (in module `mendeleev.fetch`), 40
`fetch_ionic_radii()` (in module `mendeleev.fetch`), 40
`fetch_ionization_energies()` (in module `mendeleev.fetch`), 40
`fetch_table()` (in module `mendeleev.fetch`), 39

G

`get_engine()` (in module `mendeleev.db`), 41
`get_session()` (in module `mendeleev.db`), 41

M

`mendeleev.cli`
 module, 50
`mendeleev.db`
 module, 49
`mendeleev.econf`
 module, 50
`mendeleev.electronegativity`
 module, 50
`mendeleev.fetch`
 module, 51
`mendeleev.ion`
 module, 53
`mendeleev.mendeleev`
 module, 52
`mendeleev.models`
 module, 52
`mendeleev.utils`
 module, 54
`mendeleev.vis.bokeh`
 module, 53
`mendeleev.vis.periodictable`
 module, 53
`mendeleev.vis.plotly`
 module, 54
`mendeleev.vis.seaborn`
 module, 54
`mendeleev.vis.utils`
 module, 54
 module

`mendeleev.cli`, 50
`mendeleev.db`, 49
`mendeleev.econf`, 50
`mendeleev.electronegativity`, 50
`mendeleev.fetch`, 51
`mendeleev.ion`, 53
`mendeleev.mendeleev`, 52
`mendeleev.models`, 52
`mendeleev.utils`, 54
`mendeleev.vis.bokeh`, 53
`mendeleev.vis.periodictable`, 53
`mendeleev.vis.plotly`, 54
`mendeleev.vis.seaborn`, 54
`mendeleev.vis.utils`, 54