
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	28
3.6	Advanced visualization tutorial	30
3.7	Jupyter notebooks	33
4	Data	35
4.1	Elements	35
4.2	Isotopes	39
4.3	Isotope Decay Modes	39
5	Accessing data	41
5.1	Individual Elements	41
5.2	Fetching data in bulk	41
5.3	Computed properties	42
5.4	Database session and engine	43
6	Electronegativities	45
6.1	Allen	45
6.2	Allred and Rochow	46
6.3	Cottrell and Sutton	46
6.4	Ghosh	46
6.5	Gordy	47
6.6	Li and Xue	47
6.7	Martynov and Batsanov	47
6.8	Mulliken	48
6.9	Nagle	48
6.10	Pauling	48
6.11	Sanderson	48

6.12	Fetching all electronegativities	49
7	API Reference	51
7.1	mendelev.db	51
7.2	mendelev.cli	52
7.3	mendelev.econf	52
7.4	mendelev.electronegativity	52
7.5	mendelev.fetch	53
7.6	mendelev.mendelev	54
7.7	mendelev.models	54
7.8	mendelev.ion	55
7.9	mendelev.vis.periodictable	55
7.10	mendelev.vis.bokeh	55
7.11	mendelev.vis.plotly	56
7.12	mendelev.vis.seaborn	56
7.13	mendelev.vis.utils	56
7.14	mendelev.utils	56
8	Bibliography	57
9	mendelev Changelog	59
9.1	v0.15.0 (26.12.2023)	59
9.2	v0.14.0 (07.06.2023)	59
9.3	v0.13.1 (24.04.2023)	59
9.4	v0.13.0 (11.04.2023)	59
9.5	v0.12.1 (28.11.2022)	60
9.6	v0.12.0 (9.10.2022)	60
9.7	v0.11.0 (29.09.2022)	60
9.8	v0.10.0 (17.07.2022)	60
9.9	v0.9.0 (24.09.2021)	61
9.10	v0.8.0 (22.08.2021)	61
9.11	v0.7.0 (20.03.2021)	61
9.12	v0.6.1 (03.11.2020)	61
9.13	v0.6.0 (10.04.2020)	62
9.14	v0.5.2 (29.01.2020)	62
9.15	v0.5.1 (26.08.2019)	62
9.16	v0.5.0 (25.08.2019)	62
9.17	v0.4.5 (17.03.2018)	62
9.18	v0.4.4 (10.12.2018)	62
9.19	v0.4.3 (16-07-2018)	63
9.20	v0.4.2 (26-12-2018)	63
9.21	v0.4.1 (03-12-2017)	63
9.22	v0.4.0 (22-11-2017)	63
9.23	v0.3.6 (17-09-2017)	63
9.24	v0.3.5 (07-09-2017)	63
9.25	v0.3.4 (28-06-2017)	64
9.26	v0.3.3 (16-05-2017)	64
9.27	v0.3.2 (01-05-2017)	64
9.28	v0.3.1 (25-01-2017)	64
9.29	v0.3.0 (09-01-2017)	64
9.30	v0.2.17 (08-01-2017)	65
9.31	v0.2.16 (06-01-2017)	65
9.32	v0.2.15 (02-01-2017)	65
9.33	v0.2.14 (02-01-2017)	65

9.34	v0.2.13 (01-01-2017)	65
9.35	v0.2.12 (21-12-2016)	65
9.36	v0.2.11 (10-11-2016)	65
9.37	v0.2.10 (18-10-2016)	66
9.38	v0.2.9 (16-10-2016)	66
9.39	v0.2.8 (29-08-2016)	66
9.40	v0.2.7 (02-04-2016)	66
9.41	v0.2.6 (02-04-2016)	66
9.42	v0.2.5 (02-04-2016)	66
9.43	v0.2.4 (05-02-2016)	67
9.44	v0.2.3 (27-01-2016)	67
9.45	v0.2.2 (29-11-2015)	67
9.46	v0.2.1 (26-10-2015)	68
9.47	v0.2.0 (22-10-2015)	68
9.48	v0.1.0 (11-07-2015)	69
10	License	71
11	Indices and tables	73
	Bibliography	75
	Python Module Index	81
	Index	83

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 H Hydrogen 1.008																	2 He Helium 4.00260
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
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
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
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 [87.90721]	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
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]
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 140.90768	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{mendeleeev2014,  
  auhor = {Mentel, Łukasz},  
  title = {mendeleeev} -- A Python resource for properties of chemical elements, ions,  
↪ and isotopes, ver. 0.15.0},  
  howpublished = {\url{https://github.com/lmmentel/mendeleeev}},  
  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 `mendelev` package

```
[2]: from mendelev 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,
```

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```

        evaporation_heat=383.0,
        fusion_heat=50.6,
        gas_basicity=814.1,
        geochemical_class='major',
        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)>],

```

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```

        jmol_color='#f0c8a0',
        lattice_constant=5.43,
        lattice_structure='DIA',
        mendelev_number=88,
        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_m3=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

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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
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 mendelev 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]: # calculate 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]: 12.2487640000000001
```

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 mendeleev

- 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 `mendeleev` 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 `mendeleev.fetch`

```
[1]: from mendeleev.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
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
```

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```

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
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 mendeleeev_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
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
```

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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_radius")
     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 NaN
3           1       NaN    NaN    NaN    NaN   59.0    NaN    NaN NaN NaN
4           2       NaN    NaN   16.0    NaN   27.0    NaN    NaN NaN NaN
5           3       NaN    NaN    1.0    NaN   11.0    NaN    NaN NaN NaN
6           4       NaN    NaN   -8.0    NaN   15.0    NaN    NaN NaN NaN
7           -3       NaN    NaN    NaN    NaN  146.0    NaN    NaN NaN NaN
              3       NaN    NaN    NaN    NaN    NaN    NaN    NaN NaN NaN
              5       NaN    NaN  -10.4    NaN    NaN    NaN    NaN NaN NaN
8           -2       NaN  135.0  136.0    NaN  138.0    NaN    NaN NaN NaN
9           -1       NaN  128.5  130.0    NaN  131.0    NaN    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
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 mendelev.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	

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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', ' '): -3.540721753312244, ('II', ' '): -2...
2	{}
3	{('IV', ' '): 1.7160634314550876, ('VI', ' '): 1...
4	{}
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 mendelev 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 mendeleeev.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 mendeleeev.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,
```

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```

        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, ',
        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

`mendeleev` 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 mendeleev 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 `mendeleev.vis.plotly`
- `periodic_table_bokeh` in `mendeleev.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
```

Matplotlib is building the font cache; this may take a moment.

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",
```

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```
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 38, 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 co- valent 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 polarizabil- ity	a.u.	[51]
dipole_polarizability_	float	Dipole polarizabil- ity uncertainty	a.u.	[51]
discoverers	str	The discoverers of the element		
discovery_location	str	The location where the element was dis- covered		
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 elec- tronegativity ⁽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 elec- tron 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 classi- fication		[59]
glawe_number	int	Glawe's number (scale)		[19]
goldschmidt_class	str	Goldschmidt classi- fication		[59, 60]
group	int	Group in periodic ta- ble		
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	β^- n	β^- -delayed neutron emission
B-2n	β^- 2n	β^- -delayed 2-neutron emission
B-3n	β^- 3n	β^- -delayed 3-neutron emission
B+p	β^+ p	β^+ -delayed proton emission
B+2p	β^+ 2p	β^+ -delayed 2-proton emission
B+3p	β^+ 3p	β^+ -delayed 3-proton emission
B-A	$\beta^- \alpha$	β^- -delayed α emission
B+A	$\beta^+ \alpha$	β^+ -delayed α emission
B-d	β^- d	β^- -delayed deuteron emission
B-t	β^- t	β^- -delayed triton emission
IT	IT	internal transition
SF	SF	spontaneous fission
B+SF	β^+ SF	β^+ -delayed fission
B-SF	β^- 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 *mendelev*. 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 *mendelev*:

- *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 mendelev 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>	param abundance Abundance of the isotope
<code>IsotopeDecayMode(**kwargs)</code>	param mode ASCII symbol for the decay mode
<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`, [52](#)
- `mendelev.db`, [51](#)
- `mendelev.econf`, [52](#)
- `mendelev.electronegativity`, [52](#)
- `mendelev.fetch`, [53](#)
- `mendelev.ion`, [55](#)
- `mendelev.mendelev`, [54](#)
- `mendelev.models`, [54](#)

F

`fetch_electronegativities()` (in module `mendeleev.fetch`), 42
`fetch_ionic_radii()` (in module `mendeleev.fetch`), 42
`fetch_ionization_energies()` (in module `mendeleev.fetch`), 42
`fetch_table()` (in module `mendeleev.fetch`), 41

G

`get_engine()` (in module `mendeleev.db`), 43
`get_session()` (in module `mendeleev.db`), 43

M

`mendeleev.cli`
 module, 52
`mendeleev.db`
 module, 51
`mendeleev.econf`
 module, 52
`mendeleev.electronegativity`
 module, 52
`mendeleev.fetch`
 module, 53
`mendeleev.ion`
 module, 55
`mendeleev.mendeleev`
 module, 54
`mendeleev.models`
 module, 54
`mendeleev.utils`
 module, 56
`mendeleev.vis.bokeh`
 module, 55
`mendeleev.vis.periodictable`
 module, 55
`mendeleev.vis.plotly`
 module, 56
`mendeleev.vis.seaborn`
 module, 56
`mendeleev.vis.utils`
 module, 56
 module

`mendeleev.cli`, 52
`mendeleev.db`, 51
`mendeleev.econf`, 52
`mendeleev.electronegativity`, 52
`mendeleev.fetch`, 53
`mendeleev.ion`, 55
`mendeleev.mendeleev`, 54
`mendeleev.models`, 54
`mendeleev.utils`, 56
`mendeleev.vis.bokeh`, 55
`mendeleev.vis.periodictable`, 55
`mendeleev.vis.plotly`, 56
`mendeleev.vis.seaborn`, 56
`mendeleev.vis.utils`, 56