NAME

InfoPeriodicTableElements.pl - List atomic properties of elements

SYNOPSIS

InfoPeriodicTableElements.pl ElementID(s)...

InfoPeriodicTableElements.pl [-h, --help] [-m, --mode ElementID | AmericanGroupLabel | EuropeanGroupLabel | GroupNumber | GroupName | PeriodNumber | All] [--outdelim comma | tab | semicolon] [--output STDOUT | File] [--outputstyle ElementBlock | ElementRows] [-o, --overwrite] [--precision number] [--propertiesmode Categories | Names | All] [-p, --properties CategoryName,[CategoryName,...] | PropertyName,[PropertyName,...]] [--propertieslinting ByGroup | Alphabetical] [-q, --quote yes | no] [-r, --root rootname] [-w, --workingdir dirname] ElementID(s)...

DESCRIPTION

List atomic properties of elements in the periodic table. A variety of methods are available to specify elements of interest: atomic numbers, element symbols, American or European style group labels, IUPAC group numbers, period numbers, and group names.

Atomic properties data, in addition to basic information about the periodic table elements, is also available for these categories: atomic radii, bulk properties, common valences, electronegativities, electron affinities, historical data, ionization energies, natural isotopes, oxidation states, and thermal properties.

Natural isotopes data include mass number, relative atomic mass and percent natural abundance for each isotope of an element.

PARAMETERS

ElementIDs *ElementSymbol [AtomicNumber...]* | *GroupLabel [GroupLabel...]* | *GroupNumbel [GroupNumber...]* | *PeriodNumber [PeriodNumbe...]*

Command line specification of elements is mode specific. In general, it's a space delimited list of values to identify elements. All element IDs must correspond to a specific mode; mixed specifications is not supported.

For *ElementID* mode, input value format is: *AtomicNumber [ElementSymbol ...]*. Default: *H*. Examples:

```
C
6
C N O P S Cl
6 7 8 15 16 17
C 7 8 15 S 17
```

For *AmericanGroupLabel* mode, input value format is: *GroupLabel [GroupLabel ...]*. Default: *IA*. Possible group label values are: *IA IIA IIIB IVB VB VIB VIIB VIII or VIIIB IB IIB IIIA IVA VA, VIA, VIIA, VIIA*. Examples:

```
IA
IA IVA IIB
```

For *EuropeanGroupLabel* mode, input value format is: *GroupLabel [GroupLabel ...]*. Default: *IA*. Possible group label values are: *IA IIA IIIA IVA VA VIA VIIA VIII or VIIIA IB IIB IIIB IVB VB, VIB VIIB VIIB*. Examples:

```
IA
IA IVB IIB
```

For IUPAC *GroupNumber* mode, input value format is: *GroupNumber [GroupNumber...]*. Default: *1*. Possible group label values are: *1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18*. Examples:

```
1
1 14 12
```

For *GroupName* mode, input value format is: *GroupName [GroupName...]*. Default: *AlkaliMetals*. Possible group name values are: *AlkaliMetals AlkalineEarthMetals Chalcogens CoinageMetals Halogens NobleGases Pnictogens Lanthanides or Lanthanoids, Actinides or Actinoids*. Examples:

```
AlkaliMetals
AlkaliMetals Halogens NobleGases
```

For *PeriodNumber* mode, input value format is: *PeriodNumber [PeriodNumber,...]*. Default: *1*. Possible group label values are: *1 2 3 4 5 6 7*. Examples:

```
1
1 2 3
```

For *All* mode, no input value is needed and atomic properties information is listed for all the elements.

OPTIONS

-h, --help

Print this help message.

-m, --mode *ElementID* | *AmericanGroupLabel* | *EuropeanGroupLabel* | *GroupNumber* | *GroupName* | *PeriodNumber* | *All*

Specify elements for listing atomic properties using one of these methods: atomic numbers and/or element symbols list, American style group labels, European style group labels, IUPAC group number, group names, period numbers, or all elements.

Possible values: *ElementID, AmericanGroupLabel, EuropeanGroupLabel, GroupNumber, GroupName, PeriodNumber, All*. Default: *ElementID*.

--outdelim *comma* | *tab* | *semicolon*

Output text file delimiter. Possible values: *comma, tab, or semicolon* Default value: *comma*.

--output *STDOUT* | *File*

List information at STDOUT or write it to a file. Possible values: *STDOUT or File*. Default: *STDOUT*. -r, --root option is used to generate output file name.

--outputstyle *ElementBlock* | *ElementRows*

Specify how to list element information: add a new line for each property and present it as a block for each element; or include all properties in one line and show it as a single line.

Possible values: *ElementBlock* | *ElementRows*. Default: *ElementBlock*

An example for *ElementBlock* output style:

```
Atomic number: 1
Element symbol: H
Element name: Hydrogen
Atomic weight: 1.00794
... ...
... ...

Atomic number: 6
Element symbol: C
Element name: Carbon
Atomic weight: 12.0107
... ...
... ...
```

An example for *ElementRows* output style:

```
Atomic number, Element symbol, Elemenet name, Atomic weight, ...
1,H,Hydrogen,1.00794,..
6,C,Carbon,12.0107,..
```

-o, --overwrite

Overwrite existing files.

--precision *number*

Precision for listing numerical values. Default: up to *4* decimal places. Valid values: positive integers.

--propertiesmode *Categories* | *Names* | *All*

Specify how property names are specified: use category names; explicit list of property names; or use all available properties. Possible values: *Categories, Names, or All*. Default: *Categories*.

This option is used in conjunction with -p, --properties option to specify properties of interest.

-p, --properties *CategoryName,[CategoryName,...]* | *PropertyName,[PropertyName,...]*

This option is --propertiesmode specific. In general, it's a list of comma separated category or property names.

Specify which atomic properties information to list for the elements specified using command line parameters: list basic and/or isotope information; list all available information; or specify a comma separated list of atomic property names.

Possible values: *Basic*| *BasicAndNaturalIsotope* | *NaturalIsotope* | *PropertyName,[PropertyName,...]*. Default: *Basic*.

Basic includes: *AtomicNumber, ElementSymbol, ElementName, AtomicWeight, GroundStateConfiguration,*

GroupNumber, PeriodNumber, FirstIonizationEnergy.

NaturalIsotope includes: *AtomicNumber, ElementSymbol, ElementName, MassNumber, RelativeAtomicMass, NaturalAbundance*.

Here is a complete list of available properties: AllenElectronegativity, AllredRochowElectronegativity, AtomicNumber, AtomicRadiusCalculated, AtomicRadiusEmpirical, AtomicWeight, Block, BoilingPoint, BondLength, BrinellHardness, BulkModulus, Classification, CoefficientOfLinearExpansion, Color, CommonValences, LowestCommonValence, HighestCommonValence, CommonOxidationNumbers, LowestCommonOxidationNumber, HighestCommonOxidationNumber, CovalentRadiusEmpirical, CriticalTemperature, DensityOfSolid, DiscoveredAt, DiscoveredBy, DiscoveredWhen, ElectricalResistivity, ElectronAffinity, ElementName, ElementSymbol, EnthalpyOfAtmization, EnthalpyOfFusion, EnthalpyOfVaporization, FirstIonizationEnergy, GroundStateConfiguration, GroundStateLevel, GroupName, GroupNumber, NaturalIsotopeData, MeltingPoint, MineralHardness, MolarVolume, MullikenJaffeElectronegativity, OriginOfName, PaulingElectronegativity, PeriodNumber, PoissonsRatio, Reflectivity, RefractiveIndex, RigidityModulus, SandersonElectronegativity, StandardState, SuperconductionTemperature, ThermalConductivity, VanderWaalsRadius, VelocityOfSound, VickersHardness, YoungsModulus.

--propertieslisting *ByGroup* | *Alphabetical*

Specify how to list properties for elements: group by category or an alphabetical by property names. Possible values: *ByGroup or Alphabetical*. Default: *ByGroup*. During *Alphabetical* listing, element identification data - *AtomicNumber, ElementSymbol, ElementName* - is show first, and natural isotope data - *MassNumber, RelativeAtomicMass, NaturalAbundance* - is listed in the end.

-q, --quote *yes* | *no*

Put quotes around column values in output text file. Possible values: *yes or no*. Default value: *yes*.

-r, --root *rootname*

New text file name is generated using the root: <Root>.<Ext>. File name is only used during *File* value of -o, --output option.

Default file name: PeriodicTableElementsInfo<mode>.<Ext>. The csv, and tsv <Ext> values are used for comma/semicolon, and tab delimited text files respectively.

-w, --workingdir *dirname*

Location of working directory. Default: current directory.

EXAMPLES

To list basic atomic properties information for element H, type:

```
% InfoPeriodicTableElements.pl
```

To list basic atomic properties information for elements C,N,O and F, type:

```
% InfoPeriodicTableElements.pl C N O F
```

To list all available atomic properties information for elements C,N,O and F, type:

```
% InfoPeriodicTableElements.pl --propertiesmode all 6 N O 9
```

To list basic and natural isotope information for elements C,N,O and F, type:

```
% InfoPeriodicTableElements.pl --propertiesmode Categories
  --properties BasicAndNaturalIsotope  C N O F
```

To list AtomicNumber, ElementName, AtomicWeight and CommonValences information for elements C,N,O and F, type:

```
% InfoPeriodicTableElements.pl --propertiesmode Names
  --properties AtomicNumber,ElementName,AtomicWeight,CommonValences
  C N O F
```

To alphabetically list basic and natural isotope information for elements C,N,O and F in rows instead of element blocks with quotes around the values, type:

```
% InfoPeriodicTableElements.pl --propertiesmode Categories
  --properties BasicAndNaturalIsotope --propertieslisting alphabetical
  --outdelim comma --outputstyle ElementRows --quote yes C N O F
```

To alphabetically list all available atomic information for elements C,N,O and F in rows instead of element blocks with quotes around the values and write them into a file ElementProperties.csv, type:

```
% InfoPeriodicTableElements.pl --propertiesmode Categories
  --properties BasicAndNaturalIsotope --propertieslisting alphabetical
  --outdelim comma --outputstyle ElementRows --quote yes
  --output File -r ElementsProperties -o -m All
```

To list basic atomic properties information for elements in groups IA and VIA using American style group labels, type:

```
% InfoPeriodicTableElements.pl -m AmericanGroupLabel IA VIA
```

To list basic atomic properties information for elements in groups IA and VB using European style group labels, type:

```
% InfoPeriodicTableElements.pl -m AmericanGroupLabel IA VB
```

To list basic atomic properties information for elements in groups Halogens and NobleGases, type:

```
% InfoPeriodicTableElements.pl -m GroupName Halogens NobleGases
```

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SEE ALSO

InfoAminoAcids.pl InfoNucleicAcids.pl

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