

anacal calculation of chemical composition from elemental analysis results

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bash script, version=1.00

Synopsis

```
anacal [options] file [max_dev]
```

Options:

- s use the short format
- w in the short format, report weight instead of mole fractions
- h prints this help

Description

Given, for a chemical composition:

- the elemental percentages for (some of the) elements and
- a set of bruto formulae, one for each possible component

anacal calculates compositions with one or more of the formula's resulting in a good (i.e. better than a certain standard deviation) fit between calculated and experimental element percentages.

Input is taken from `file.ea`, output is written to `stdout`. The extension `.ea` is automatically appended to the input file.

Run without parameters for help.

Input

The input file should have the following structure (numbers are line numbers):

- 1 a title line
- 2 elementsymbol followed by percentage for each element determined
- 3+ bruto formula's of the possible components, one per line;
comments may be added with the `#`-character;
remaining characters up to end-of-line are skipped.

Sample input file (case sensitive):

```
6718 DEBO 145
C54.53 H6.31 N8.10 S14.48
C15 H20 N2 O3 S
C11 H16 N2 O S
C4 H12 N2 S2
C2 H4 O S
S      #sulphur
H Cl   #hydrochloric acid
H2 O   #water
```

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