Users' manual for molecule generator `surge`

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VERSION 2.0

Abstract

This is the manual for the molecule generator `surge`.

1 Introduction

`Surge` is a command-line generator of chemical structures. It is written in a portable subset of the `C` language and runs on any computer that can run `nauty`.

- See Appendix A for installation instructions.
- See [2] for a description of how `surge` works.

`Surge` is open-source software released under the permissive Apache 2.0 license. Please see the file `README.txt` for more information.

2 Basic usage

The only compulsory input is a chemical formula and the default action is to count the molecules without writing them. For example:

```
surge C8H11NO
>Z generated 17379 -> 500039 -> 2123287 in 0.10 sec
```

Here `surge` has reported that it found 2,123,287 molecules in 0.10 seconds. Some of the molecules are shown in Figure 1.

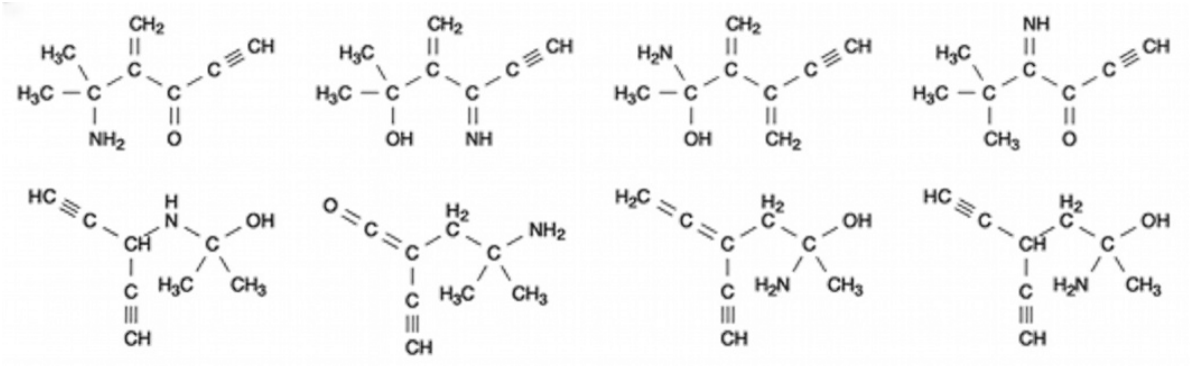


Figure 1: Some of the 2,123,287 molecules produced by `surge C8H11NO`.

The other numbers, 17,379 and 500,039, reported by `surge` give a glimpse of its inner workings. `Surge` first generates simple graphs (graphs with no vertex labels and all edges simple), then it assigns elements to the vertices, then finally it assigns bond type (single, double or triple) to each edge.

For example, Agrocybyne B, found in the edible brown mushroom *agrocybe praecox*, is made in three stages as shown in Figure 2.

The output "`17379 -> 500039 -> 2123287`" from `surge` means that 17,379 simple graphs were generated, elements were assigned to the vertices in 500,039 ways, then bond multiplicities were assigned to make 2,123,287 molecules.

Execution of `surge` with no arguments, or with the single argument `-help` produces a brief usage description. Next we will describe the available options in detail.

Options are indicated by a hyphen in the Unix style, such as `-u`. They can be concatenated or written separately: `-u -t0` is the same as `-ut0`. The single exception is the option `-oFILE` (specify output file) where the file name is everything from the "`-o`" to the end of the option.

If options have values, they must be written against the option name and not separately: "`-t2`" is valid but "`-t 2`" is not.

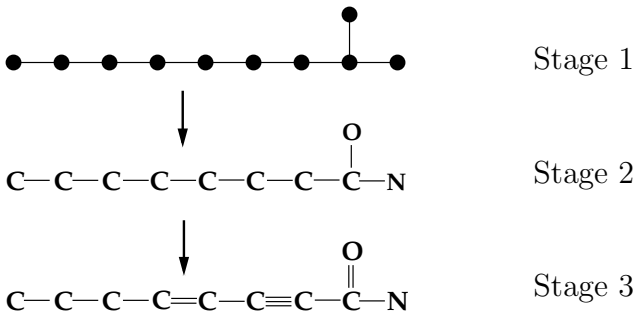


Figure 2: The three stages of generating Agrocybyne B.

3 Specifying the molecular formula

The molecular formula is specified by a string of symbols and numbers, without punctuation. Elements are given by the "input symbol" as shown in Table 1.

Note that some elements can have multiple valences, for example phosphorus can have valence 3 or 5. Following the table, writing `P` indicates phosphorus at valence 3, while `Px` indicates phosphorus at valence 5. With one exception that will be noted later, output uses the standard chemical symbol; the "input symbol" is only for input. For example,

```
surge C3Sx2H4
```

specifies 3 carbon atoms, 2 sulphur atoms at valence 4, and 4 hydrogen atoms.

The value "max-coord" shown in Table 1 is the maximum coordination number of that element; that is, the maximum number of distinct neighbouring atoms including hydrogen (ignoring bond multiplicities). `Surge` imposes two restrictions for chemical reasons:

(a) If an atom has 5 or more neighbours, none of the neighbours are hydrogen.

(b) Nitrogen atoms can have at most 4 neighbours.

Note that you need the `-c` and/or `-d` options to allow more than 4 neighbours, see Section 7.

Additional elements can added at run time, see Section 9.

4 Output options

`-u` Don't write any molecules; just generate them and report the number. This is the default.

element	symbol	input symbol	valence	max-coord	index
carbon	C	C	4	4	0
nitrogen	N	N	3	3	1
		Nx	5	4	10
oxygen	O	O	2	2	2
phosphorus	P	P	3	3	3
		Px	5	5	13
sulfur	S	S	2	2	4
		Sx	4	4	11
		Sy	6	6	12
fluorine	F	F	1	1	5
chlorine	Cl	Cl	1	1	6
bromine	Br	Br	1	1	7
iodine	I	I	1	1	8
boron	B	B	2	2	9
silicon	Si	Si	4	4	14
hydrogen	H	H	1	1	–

Table 1: List of elements known to `surge` by default.

`-oFILE` Specify a file name for output, to be used instead of the standard output. You can specify names with spaces or special characters by using quotes, for example `-o'Very Many Molecules.smi'`

`-v` Write some additional statistics to standard error.

`-z` Except for the cases of `-u` and `-O1`, the output is gzipped. This option is only available if `surge` has been built with the `zlib` library (see Appendix A).

`-m#/#` (where each `#` is a number) This option tells `surge` to do only a part of the generation. If the two numbers are *res* and *mod*, respectively, it must be that $0 \leq res \leq mod - 1$. For example, to split the generation into four parts which can be run independently, use `-m0/4`, `-m1/4`, `-m2/4` and `-m3/4` respectively on the parts. The overhead in this splitting is very low. However, if the number of parts is large some of the parts may be a lot bigger than others.

The output formats available are illustrated in Figure 3. Note that hydrogen is not explicitly represented in any of the formats.

`-F` Output in SDfile format [1] like in Figure 3(a). Note that the valence column of the atom block is always filled in.

(a) `surge C8H11NO` — SDfile output format.

```
 Surge 2.0

  10  9  0  0  0  0            999 V2000
     0.0000    0.0000    0.0000 C   0  0  0  0  0  4  0  0  0  0  0  0
     0.0000    0.0000    0.0000 C   0  0  0  0  0  4  0  0  0  0  0  0
     0.0000    0.0000    0.0000 C   0  0  0  0  0  4  0  0  0  0  0  0
     0.0000    0.0000    0.0000 C   0  0  0  0  0  4  0  0  0  0  0  0
     0.0000    0.0000    0.0000 O   0  0  0  0  0  2  0  0  0  0  0  0
     0.0000    0.0000    0.0000 N   0  0  0  0  0  3  0  0  0  0  0  0
     0.0000    0.0000    0.0000 C   0  0  0  0  0  4  0  0  0  0  0  0
     0.0000    0.0000    0.0000 C   0  0  0  0  0  4  0  0  0  0  0  0
     0.0000    0.0000    0.0000 C   0  0  0  0  0  4  0  0  0  0  0  0
     0.0000    0.0000    0.0000 C   0  0  0  0  0  4  0  0  0  0  0  0
   1  5  2  0  0  0  0
   1  6  1  0  0  0  0
   1  8  1  0  0  0  0
   2  7  1  0  0  0  0
   2  9  1  0  0  0  0
   3  8  3  0  0  0  0
   3 10  1  0  0  0  0
   4  9  1  0  0  0  0
   4 10  2  0  0  0  0
 M  END
 $$$$
```

(b) `surge -S C8H11NO` — SMILES output format.

```
 CCCC=CC#CC(=O)N
```

(c) `surge -A C8H11NO` — Alphabetic output format.

```
 10 9 C8NOH11 0=9 0-8 0-5 1-4 1-6 2#5 2-7 3-6 3=7
```

(d) `surge -O3 C8H11NO` — Numeric output format.

```
 10 9 0 0 0 0 2 1 0 0 0 0  0 4 1 0 5 0 0 7 0 1 6 0 1 8 0 2 7 2 2 9 0 3 8 0 3 9 1
```

Figure 3: Output formats for Agrocybyne B, C8H11NO

`-S` Output in SMILES format compatible with the OpenSMILES specification [6]. See Figure 3(b).

`-A` Output in "alphabetic format", which is unique to `surge`. The example in Figure 3(c) starts "`10 9`" which means 10 atoms and 9 bonds (not counting hydrogen in either case). Then follows the chemical formula `C8NOH11`, which may have the elements in a different order from what you gave. This is the sole output format where the input symbols are used in place of standard symbols, in order to show the valence. The non-hydrogen atoms are numbered in the order they appear in the formula starting with 0: atoms 0–7 are `C`, atom 8 is `N` and atom 9 is `O`. Then the bonds are listed using the atom numbers with `-` for single, `=` for double and `#` for triple.

`-O#` (where `#` is 1, 2 or 3). This is intended mostly for debugging purposes, but `-O3` is probably the simplest output to read with a program. For `-O1` and `-O2`, the generation only goes as far as stages 1 and 2, respectively (recall Figure 2).

For `-O1`, unlabelled simple graphs are written in `nauty`'s `graph6` format.

For `-O2`, simple graphs with elements assigned to vertices are written. At this stage, bond multiplicities have not been chosen. The output line for Agrocybyne B is

```
10 9 0 0 0 0 2 1 0 0 0 0  0 4 0 5 0 7 1 6 1 8 2 7 2 9 3 8 3 9
```

which means 10 vertices arbitrarily numbered 0–9, 9 edges, the elements assigned to the vertices (using the "index" column from Table 1), then a list of 9 edges (0–4, etc.). This format is compatible with the `-T` output of the `nauty` utility `vcolg`.

For `-O3`, complete generation of molecules is performed and they are written in the format shown in Figure 3(d). It is the same as `-O2` except that each edge is followed by a bond multiplicity indicator: 0 means single, 1 means double, 2 means triple. This format is compatible with the `-T` output of the `nauty` utility `multig`.

Default. If none of `-F`, `-S`, `-A` or `-O` are given, `-u` is assumed.

Although `surge` has an optional aromaticity filter (see Section 6), none of the output formats indicate aromatic bonds.

The choice of output format can make a large difference to the running time, because `surge` generates molecules much faster than they can be written. Here are representative times for `C8N2O2H12`, for which there are 377,394,455 isomers. We are writing to a fast pipe on a MacBook M3 pro, and the times would be even greater if we wrote to a physical device. The deciding factor is the number of bytes that must be written, which is the main reason why SDfile output is comparatively slow.

`-u` (no output) 9 seconds
`-S` (SMILES) 8.3 GB in 37 seconds
`-A` (alphabetic) 25.7 GB in 46 seconds

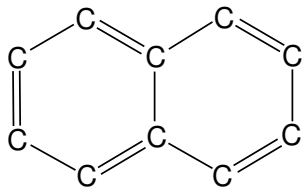
`-O3` (numeric) 41.1 GB in 54 seconds
`-F` (SDfile) 422 GB in 1097 seconds.

If you are looking for a needle in a haystack—a few special molecules in a vast collection—the most efficient approach is to test before writing, as explained in Section 10.

5 Rings and cycles

Our description of `surge` options takes care to distinguish two types of closed path, which we call rings and cycles.

A *cycle* is a closed path that does not repeat any atom except that it finishes on the same atom it started on. A *ring* is a cycle with the additional restriction that there is no bond between any of its atoms apart from the bonds forming the cycle. (In graph theory language, a ring is a *chord-free cycle*, also known as an *induced cycle*.) Every ring is a cycle, but a cycle may or may not be a ring.



Naphthalene has two rings of length 6, but three cycles (the two rings, plus a cycle of length 10). The cycle of length 10 is not a ring because of the extra bond between two of its atoms.

Five `surge` options restrict the cycles of the molecule.

`-t#` or `-t#:#` (where each `#` is a number). Specify the allowed number of cycles of length 3. For example, `-t0` or `-t1:3`. Recall that option values have to written against the option letter; you can't write `-t 0` with a space.

`-f#` or `-f#:#` (where each `#` is a number). Specify the allowed number of cycles of length 4. For example, `-f0` or `-f1:3`.

`-p#` or `-p#:#` (where each `#` is a number). Specify the allowed number of cycles of length 5. For example, `-p0` or `-p1:3`.

`-h#` or `-h#:#` (where each `#` is a number). Specify the allowed number of cycles of length 6. For example, `-h0` or `-h1:3`.

`-b` Specify that no cycles of odd length are permitted. A simple exercise is that there is a cycle of odd length if and only if there is a ring of odd length, so an equivalent description is that no rings of odd length are permitted. (In graph theory language, the graph is *bipartite*.)

All of the above pay no attention to which atoms belong to the cycle. However, one additional option allows only carbon atoms.

`-C#` or `-C#:#` (where each `#` is a number). Specify the number of 6-rings (chord-free cycles of length 6) composed entirely of carbon atoms.

6 Aromaticity

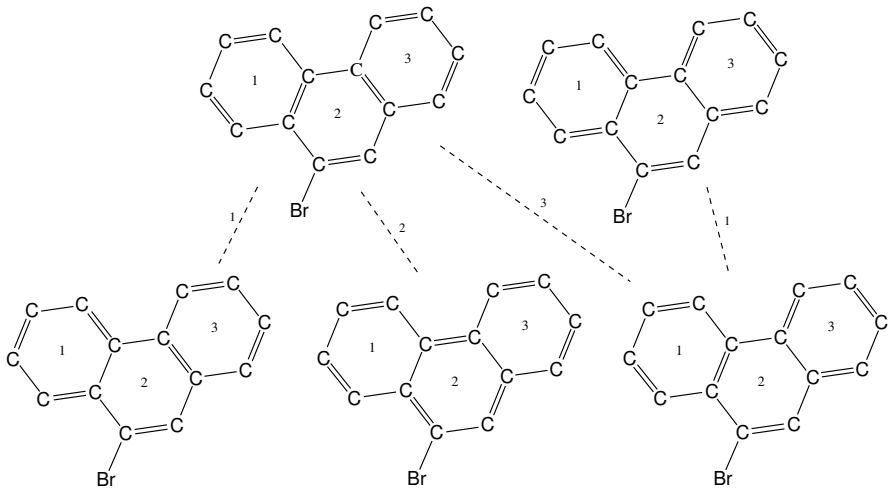


Figure 4: The five aromatically equivalent Kekulé structures for 9-bromophenantrene. The dashed lines indicate which aromatic cycle is rotated. Note that the two forms in the top row are not related by a single rotation.

When the `-R` is given to `surge`, a filter is applied to remove all but one molecule in each aromatic equivalence class. In the present version, only carbon-cycle aromaticity is detected. Since there is no single agreed definition of aromaticity [3], we give a precise description of our implementation.

By an *aromatic cycle* we mean a simple cycle of carbon atoms, with the number of atoms being congruent to 2 modulo 4 and the bonds alternating single and double. (Note that the cycle does not need to be chord-free.) To *rotate* an aromatic cycle means to replace single bonds by double bonds and vice-versa. Now we can define two molecules to be *aromatically equivalent* if (up to isomorphism) one can be obtained from the other by a sequence of rotations of aromatic cycles.

The example of 9-bromophenantrene is shown in Figure 4.

The current version of `surge` does not indicate aromaticity in the output. It just outputs an arbitrary single member of each equivalence class. When `-R` is given, the

summary line has an extra count showing the number of molecules after aromaticity filtering. Compare:

```
surge C8H11NO
>Z generated 17379 -> 500039 -> 2123287 in 0.10 sec

surge -R C8H11NO
>Z generated 17379 -> 500039 -> 2123287 -> 2123169 in 0.15 sec
```

7 Other global structural restrictions

`-e#` or `-e#:#` (where each `#` is a number). Specify the allowed number of bonds (ignoring attached hydrogens). Bonds are counted without regard to their multiplicity. Examples: `-e15` or `-e12:13`. If the number of atoms is n and the number of bonds is e, then $e - n + 1$ is the minimum number of bonds that need to be broken to reach an acyclic structure.

`-d#` Specify an upper bound on the number of distinct neighbours that are not hydrogen atoms. The default is 4.

`-c#` Specify an upper bound on the number of distinct neighbours including hydrogen atoms. The default is 4.

`-T` Forbid triple bonds.

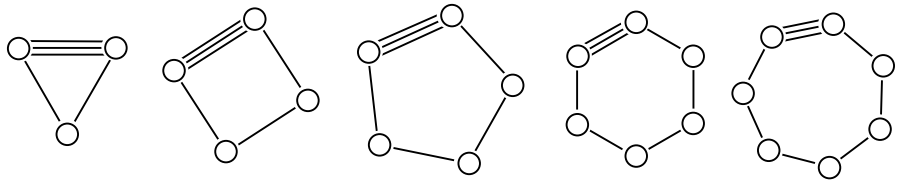
`-P` Require that the molecule be planar. That is, it can be drawn in the plane with no bonds crossing.

8 Forbidden substructures

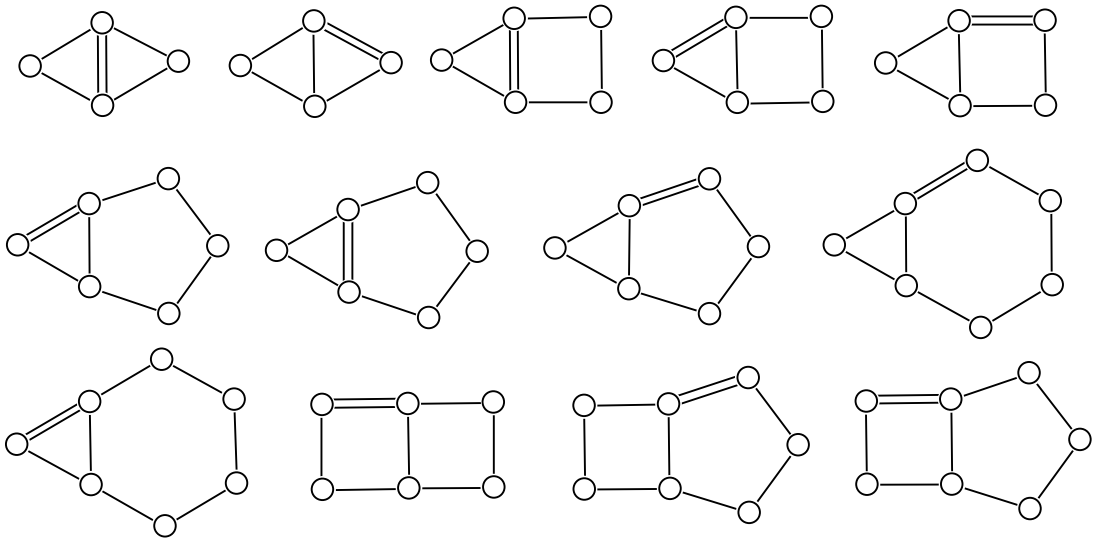
`Surge` has the facility to remove molecules which contain certain substructures using the `-B` option. The argument of `-B` is a list of numbers separated by commas without spaces. For example, `-B2,3,8`. Each number indicates a set of substructures that are forbidden. You can use `-B` more than once, for example `-B2,4,6` is the same as `-B4 -B6,2`. We will describe the meaning of each number separately. In some cases it is necessary to understand the distinction between rings and cycles, as explained in Section 5.

In the pictures, a circle represents any type of atom, a simple join matches any bond, a double join matches a double or triple bond, and a triple join matches only a triple bond. Many of the families below were inspired by MOLGEN [4].

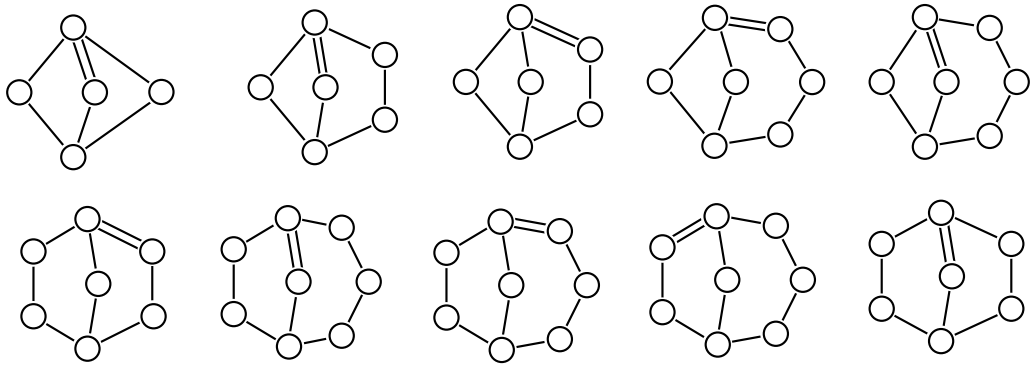
`-B1` Rings of length up to 7 have no triple bonds. This is equivalent to cycles of length up to 7 having no triple bonds.



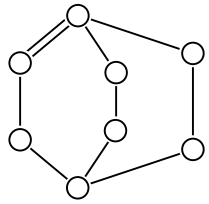
`-B2` Consider rings of length r and s which share one bond (i.e. fused rings). Let e be the common bond and let f be any bond belonging to one of the rings and sharing exactly one atom with e. In the cases $\{r, s\} = \{3, 3\}$, $\{3, 4\}$ and $\{3, 5\}$, both e and f must be single bonds. In the cases $\{r, s\} = \{3, 6\}$, $\{4, 4\}$ and $\{4, 5\}$, f must be a single bond.



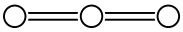
`-B3` Consider rings of length r and s which share two bonds. Let e be one of the shared bonds and let f be a bond belonging to one of the rings and sharing exactly one atom with e. In the cases $\{r, s\} = \{4, 4\}$, $\{4, 5\}$, $\{4, 6\}$, $\{5, 5\}$ and $\{5, 6\}$, both e and f must be single bonds.



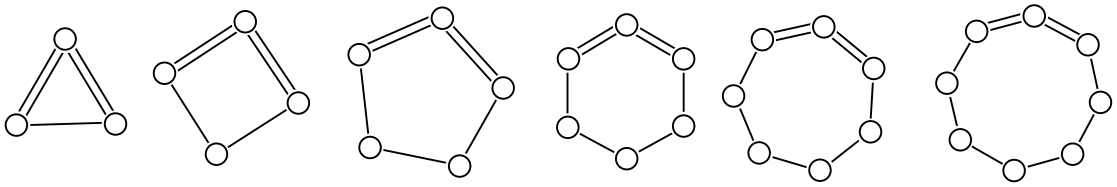
`-B4` Consider two rings of length 6 that share three bonds. Then any bond which lies in one of the rings and has exactly one atom in the other ring must be a single bond.



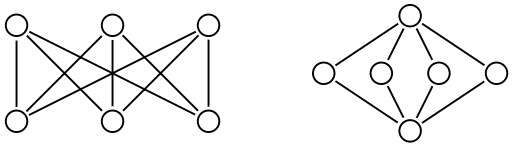
`-B5` No atom has two double or triple bonds unless it is also bonded to some other non-hydrogen atom.



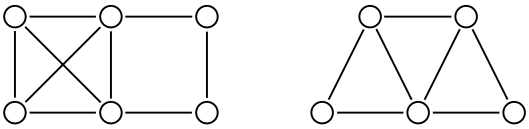
`-B6` No atom in a ring of length up to 8 has two double bonds unless it is also bonded to some other non-hydrogen atom.



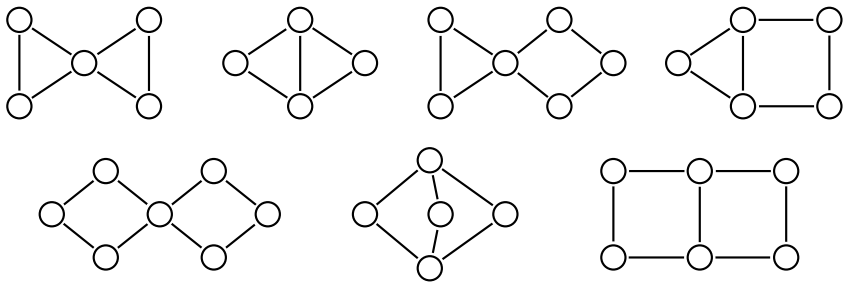
`-B7` These are forbidden: two atoms with four common neighbours, and three atoms with three common neighbours.



`-B8` These are forbidden: a cycle of length 5 having an atom bonded to each of the other 4 atoms, a set of 4 atoms all bonded to each other sharing one bond with a cycle of length 4.



`-B9` Every atom lies on at most one ring of length 3 or 4. Equivalently, every atom lies on at most one cycle of length 3 or 4.



9 Adding extra elements

Extra elements/valences can be added temporarily using the `-E` option. Any reasonable number of -E options can be given. The syntax is one of these:

`-EXv -EXYv -EXvc -EXYvc`

`X` is the input name of the element (what you must use in the command line molecular formula). `Y` is the standard chemical symbol for this element. If `Y` is omitted, it is assumed the same as `X`.

Both `X` and `Y` must be a single uppercase letter, or an uppercase letter followed by a lowercase letter.

`v` and `c` are respectively the valence and the maximum coordination number (the maximum number of distinct neighbours including hydrogen). If `c` is not given, it is the same as `v`. Both `v` and `c` must consist of a single digit.

Example: To add arsenic as As with valence 3, and as Az with valence 5, you can do this: `-EAs3 -EAzAs5`.
The standard chemical formats SMILES (`-S`) and SDfile (default) will use As for both cases, but the distinct input names serve to tell the program which valences to use.

If you want to add elements more permanently, you can do it using the PLUGIN facility (Section 10) and it is also quite easy to add them to the program.

10 PLUGIN facility

By compiling code into `surge` , additional features can be efficiently incorporated. To use this feature, create a C file which contains any or all of these:

(1) variable and function definitions

(2) a macro definition for `SURGEPLUGIN_INIT`

(3) a macro definition for `SURGEPLUGIN_STEP0`

(4) a macro definition for `SURGEPLUGIN_STEP1`

(5) a macro definition for `SURGEPLUGIN_STEP2`

(6) a macro definition for `SURGEPLUGIN_STEP3`

(7) a macro definition for `SURGEPLUGIN_SWITCHES`

(8) a macro definition for `SURGEPLUGIN_SUMMARY`

The package contains these examples:

`plugin0.c` : Remove molecules containing $K_{2,3}$, that is, two atoms having three or more common neighbours. Also add arsenic (As) with valence 3 to the table of known elements.

`plugin1.c` : Specify the number of atoms with exactly 4 neighbours that are not hydrogen atoms. The required number is given by a new option `-V#` or `-V#:#`.

`plugin2.c` : Add an option `-Y` that forbids adjacent oxygens.

`plugin3.c` : Count the number of hydrogen atoms attached to carbon atoms, and write the values at the end.

To compile a plugin into the program, include an option like
`-DSURGEPLUGIN='"plugin1.c"'` on the compile command. Note that the plugin code is inserted directly into the `surge` code, not just linked to it. This means that `surge`'s internal variables are visible to the plugin.

(1) variable and function definitions – These are placed at the outer program level, before any `surge` functions are defined. Using `static` is recommended.

If you define a string as the value of `HELPTEXT2`, it will appear as extra text when the program is run with argument `-help`.

(2) `SURGEPLUGIN_INIT` — This is placed right at the beginning of the execution. It can be used for adding extra elements to the table of elements. To do this, call the function

```
addelement(char *inputname, char *name, int valence, int maxcoord)
```

Here, *`inputname`* is the symbol for the element as used on the command line. All input symbols must be unique, even for the the same element at different valences, *`name`* is the usual chemical symbol for the element, *`valence`* is the valence, and *`maxcoord`* is the maximum number of distinct neighbours including hydrogen. Example: To add arsenic as As at valence 3 and as Az at valence 5:

```
addelement("As","As",3,3); addelement("Az","As",5,5);
```

SMILES and SDfile output will use “As” for both.

You can also use SURGEPLUGIN_INIT for initialising global variables used by the plugin.

(3) SURGEPLUGIN_STEP0 — This is placed at intermediate levels in the generation of simple graphs (corresponding to PRUNE in geng). Variables available are:

graph *g = the graph so far (nauty format)

int n = the number of vertices so far

int maxn = the target number of vertices, equal to the number of non-hydrogen atoms

It can be useful to know that the last vertex added by the program was vertex $n-1$ and the subgraph without that vertex was the most recently seen graph with $n-1$ vertices. If you want to discard this graph and all its extensions, just return the value 1. If not, don't return.

(4) SURGEPLUGIN_STEP1 — This is placed after simple graphs have been generated and before elements have been assigned to the vertices. That is, at Stage 1. All the -B options have already been imposed except -B5,6. Also -t, -f, -p, -b and -P have been imposed. Variables available are:

graph *g = the simple graph for the non-hydrogen atoms

int n = the number of vertices in g

int deg[0..n-1] = the degrees of g

If you want to discard this graph, just return.

(5) SURGEPLUGIN_STEP2 — This is placed after elements have been assigned to vertices. That is, at Stage 2. Variables available are:

graph *g = the simple graph for the non-hydrogen atoms

int n = the number of vertices in g

int ne = the number of edges in g

int deg[0..n-1] = the degrees of g

edge[0..n-1] = a list of edges. This is a structured type of which the fields x, y give the vertices for this edge. (Here and everywhere in the program except for some output formats, vertices and edges are numbered starting at 0.) Don't assume any other fields are set. So far, multiplicities of edges have not been decided.

int vcol[0..n-1] = the elements assigned to the vertices. The value is an index into the table element[] that lists all the available elements. See the program text for the fields of element[]. The function elementindex(s) gives the index of the element with input name s, for example elementindex("Sx"). If you want to discard this assignment of elements to vertices, just return.

(6) SURGEPLUGIN_STEP3 — This is executed for each completed molecule. All the command-line restrictions have now been applied. Variables available are:

n, ne, edge, vcol = as for SURGEPLUGIN_STEP2

int mult[0..ne-1] = one less than the multiplicity of the bond (ie. 0=single, 1=double,

2=triple)
  `int` ***hyd***[0..***n***-1] = number of attached hydrogen atoms.
If you want to discard this molecule, just return.

Since `surge` generates molecules much faster than it can write them, using this facility to perform strong pruning tests can significantly decrease the total time.

(7) `SURGEPLUGIN_SWITCHES` — You can use this to define extra command-line options. See `plugin1.c` and `plugin2.c` for examples.

To define a new option, you need to have a `boolean` variable and if the option takes a value or a range you need variables to hold those values. You can define these variables at step (1) above. The `boolean` variable should be initialised to `FALSE`.

Examples:
`SWBOOLEAN('H',`***Hswitch***`)` defines ***Hswitch***=`TRUE` for `-H`
`SWINT('H',`***Hswitch***`,`***Hval***`,"surge -H")` specifies an integer parameter. For example, `-H6` defines ***Hswitch***=`TRUE` and sets ***Hval***=6. `"surge -H"` appears in an error message if there is any. ***Hval*** has type `int`.
`SWRANGE('H',":-",`***Hswitch***`,`***Hmin***`,`***Hmax***`,"surge -H")` defines an interval. `-H5:7` and `-H5-7` both set ***Hswitch***=`TRUE`, ***Hmin***=5 and ***Hmax***=7. The ends of the interval can be omitted: `-H5:` sets ***Hswitch***=`TRUE`, ***Hmin***=5, ***Hmax***=∞. ***Hmin*** and ***Hmax*** are `long int` variables. To define more than one switch, separate them by `else`. Example:

```
SWBOOLEAN('H',Hswitch) else SWINT('J',Jswitch,Jval,"surge -J")
```

with no semicolons.

(8) `SURGEPLUGIN_SUMMARY` — You can use this to write information that the plugin code has collected. Write to stderr. It is placed at the end of execution just before `surge`'s summary `>Z` line is written. See `plugin3.c` for an example.

The source code for the plugin examples is in Appendix B.

A Installation

`Surge` is written in a portable subset of the language `C`. The package is available from [8] and [7]. The first site also has some precompiled versions for Mac, Linux and Windows.

Your first task is to install `nauty` if it isn't installed already [5]. At least `nauty 2.8` is recommended for best performance.

In addition to the include files and library of `nauty`, you need these source files from `nauty` that are also included in the `surge` package for convenience:

```
geng.c
planarity.c
```

If you want `surge` to be able to `gzip` its output (`-z` option), you also need to install `zlib` [9] if you don't have it already. On most systems you need the development tools as well as the library.

If you have the utility `make`, as you probably will if you are working on Linux, MacOSX, `wsl` or Cygwin, start by editing the definitions of `CC`, `CCOPT`, `NAUTY`, `NAUTYLIB`, `ZLIB` and `LZ` that are explained near the start of the file `makefile`.

Then you just need to type "`make surge`" and it will be done.

If you don't have `make`, you can compile `surge` manually. In the following, replace `CC`, `CCOPT`, `NAUTY`, `NAUTYLIB`, `ZLIB` and `LZ` by their meanings as defined in `makefile`:

```
CC -o surge -g -I NAUTY -DWORDSIZE=64 -DMAXN=WORDSIZE \
   -DOUTPROC=surgeproc CCOPT -DPREPRUNE=surgepreprune ZLIB \
   -DPRUNE=surgeprune -DGENG_MAIN=geng_main surge.c geng.c \
    planarity.c NAUTYLIB/nautyL1.a LZ
```

When compiled in this manner, the limits on molecule size are 64 for both the number of vertices and the number of bonds (ignoring both hydrogens and bond multiplicity.)

B Sample plugins

In this appendix we give some examples of plugins that use the features described in Section 10.

Example of SURGEPLUGIN_STEP0: plugin0.c

```
/* This is a plugin for surge that removes molecules with
   two atoms having three or more common neighbours.
   Also, arsenic at valence 3 and 5 is added. */

#define HELPTEXT2 " This version removes molecules with K(2,3).\n"

#define SURGEPLUGIN_INIT \
   addelement("As","As",3,3); addelement("Az","As",5,5);

#define SURGEPLUGIN_STEP0 \
 { int ii,jj; \
   for (jj = n; --jj >= 1; ) \
   for (ii = jj; --ii >= 0; ) \
       if (POPCOUNT(g[ii] & g[jj]) >= 3) return 1; }
```

Substructures that only rely on the simple graph structure can be detected at the initial stage. In the special case of removing cases that contain a given simple graph, the most efficient place is during the generation of the simple graphs.

SURGEPLUGIN_STEP0 is called by geng at each level of the simple graph generation. Returning a non-zero value causes this graph and all its descendants to be discarded.

Note that POPCOUNT is a nauty macro that counts the 1-bits in a word. We enclosed the code in braces { } to avoid possible conflict with surge variables.

Example of SURGEPLUGIN_STEP1: plugin1.c

```
/* This is a plugin for surge that implements an extra option
   -V# or -V#:# for the number of atoms with exactly 4 distinct
   non-H neighbours. */

#define HELPTEXT2 \
" -V# -V#:# Specify number of atoms with exactly 4 non-H neighbours\n"

static boolean Vswitch = FALSE;
static long Vmin,Vmax;

#define SURGEPLUGIN_STEP1 \
 { int ii,Vval; Vval=0; \
   for (ii = 0; ii < n; ++ii) if (deg[ii] == 4) ++Vval; \
   if (Vswitch && (Vval < Vmin || Vval > Vmax)) return; }

#define SURGEPLUGIN_SWITCHES \
  SWRANGE('V',":-",Vswitch,Vmin,Vmax,"surge -V")
```

SURGEPLUGIN_STEP1 is placed at the point where generation of simple graphs is complete. This code counts the number of vertices of the simple graph that have degree 4 and executes `return` to discard the graph if the count isn't within the bounds given by the `-V` option.

Example of SURGEPLUGIN_STEP2: plugin2.c

```
/* This is a plugin for surge that optionally forbids
   adjacent oxygen atoms. */

#define HELPTEXT2 \
" This version forbids adjacent oxygen atoms if -Y is given.\n"

static boolean Yswitch = FALSE;
#define SURGEPLUGIN_SWITCHES  SWBOOLEAN('Y',Yswitch)

static int oxygenindex = -1;
#define SURGEPLUGIN_STEP2 \
 if (oxygenindex < 0) oxygenindex = elementindex("O"); \
 if (Yswitch) { int ii; for (ii = 0; ii < ne; ++ii) \
   if (vcol[edge[ii].x] == oxygenindex \
    && vcol[edge[ii].y] == oxygenindex) return; }
```

SURGEPLUGIN_STEP2 is placed at the point where elements have been assigned to vertices but bond multiplicities have not been chosen.

The number of edges is *ne* and the array *edge* lists edge information. Namely, for edge *ii*, *edge*[*ii*].*x* and *edge*[*ii*].*y* are the two vertex numbers for that edge.

Also, for vertex *v*, *vcol*[*v*] is the element for that vertex, given as an index into an internal table of elements. The call `elementindex("O")` finds the index for oxygen, which we remember in the variable *oxygenindex* so that we don't have to call `elementindex("O")` repeatedly.

Executing `return` when an edge has oxygen at both ends discards this family of molecules.

Example of SURGEPLUGIN_STEP3: plugin3.c

```
/* This is a plugin for surge that counts how many hydrogen atoms
   are attached to carbon atoms. */

#define HELPTEXT2 \
" This version counts the hydrogen atoms attached to carbon atoms.\n"

static long long CHcount[5*MAXN+1]={0};

#define SURGEPLUGIN_STEP3 \
 { int ii,CHval; CHval=0; for (ii = 0; ii < n; ++ii) \
      if (vcol[ii] == carbonindex) CHval += hyd[ii]; \
   ++CHcount[CHval]; }

#define SURGEPLUGIN_SUMMARY \
 fprintf(stderr,"Counts by the number of hydrogens attached to carbons:\n"); \
 { int ii; for (ii = 0; ii <= 5*MAXN; ++ii) \
     if (CHcount[ii] > 0) fprintf(stderr," %2d : %lld\n",ii,CHcount[ii]); }
```

SURGEPLUGIN_STEP3 is placed where complete molecules are available. At this point, n is the number of vertices, $vcol[v]$ is the element assigned to vertex v, and $hyd[v]$ is the number of attached hydrogens.

carbonindex is set during program start-up to be the index of carbon in the internal table of elements. For each molecule we find the total number of hydrogens attached to carbons and increment the appropriate entry of *CHcount*[].

SURGEPLUGIN_SUMMARY is called at the end of execution and used to display the results.

C Change log

Dec 3, 2021. Initial release (version 1.0)

Mar 30, 2022. Now `-u` (no output) is default and `-F` is needed to get SDfile output.

Sep 29, 2024. Add `-h` for counting 6-cycles. Making version 1.1.

Jan 16, 2026. Add `-R` for aromaticity filtering. Add `-C` for counting 6-rings of carbon. Making version 2.0.

References

[1] BIOVIA, CTfile Formats (2016). https://help.accelrysonline.com/ulm/onelab/1.0/content/ulm_pdfs/direct/reference/ctfileformats2016.pdf

[2] B. D. McKay, M. Aziz Yirik and C. Steinbeck, Surge—a fast open-source chemical graph generator. *J. Cheminformatics*, **14** (2022), article 24.

[3] Various authors, Aromaticity. https://en.wikipedia.org/wiki/Aromaticity

[4] R. Gugisch, A. Kerber, A. Kohnert, R. Laue, M. Meringer, C. Rücker and A. Wassermann, MOLGEN Molecular Structure Generation. https://www.molgen.de

[5] B. D. McKay and A. Piperno, Nauty & Traces graph isomorphism software. https://users.cecs.anu.edu.au/~bdm/nauty/

[6] OpenSMILES specification. https://opensmiles.org

[7] `Surge` molecular generator. https://users.cecs.anu.edu.au/~bdm/surge/

[8] `Surge` molecular generator (GitHub). https://structuregenerator.github.io

[9] J-l. Gailly and M. Adler, Zlib compression library. https://www.zlib.net