Name

csps - PostScript and EPS structure depiction generator

VERSION

1.13, 2018-6-17

SYNOPYS

csps [-align *none*/*x*/*y*/*diagonal*] [-annotationfontsize pts] [-atomcolor color/*type*] [-atomhighlight 0/1] [-binder *none/left/right/top/bottom*] [-binderwidth mm] [-bondhighlight 0/1] [-bondscale n] [-border mm] [-boxborder pts] [-boxproperty property_name] [-charge 0/1] [-colormode *bow*/*cob/cow/wob*] [-comment comment] [-computestereo 0/1] [-count n] [-csymbol *none/special/all*] [-dashes 0/1] [-eps 0/1] [-feedback] [-fixbridgeheadstereo 0/1] [-footerfontsize pts] [-footerheight pts] [-format *fmt*] [-frame *none/line/shadow*] [-headerfontsize pts] [-headerheight pts] [-highlightcolor color] [-hsymbol *none/special/all*] [-isotope 0/1] [-isotopemapping *none/highlight/invert/boxed/circle/diamond/triangle/cross*] [-linewidth n] [-logotext text] [-matchbondorder 0/1] [-matchfile filename] [-matchisotope 0/1] [-matchmode *first/distinct/unique/nocommon*] [-matchringsystem 0/1] [-matchsmiles SMILES/SMARTS] [-matchstereo *none/absolute/relative*] [-namefontsize pts] [-nameheight pts] [-ncols n] [-nitrostyle *asis/ionic/penta*] [-nrows n] [-offset n] [-orientation *portrait/landscape*] [-outfile filename] [-pagelimit n] [-papersize A7/A6/A5/A4/A3/B6/B5/B4/B3/letter/legal/executive] [-postprocessing 0/1] [-pseudo3d 0/1] [-radical 0/1] [-recalc 0/1] [-resolvearo 0/1] [-shadow mm] [-showcrossedbonds 0/1] [-space mm] [-stereo 0/1] [-symbol *symbol/label/index/box/compact*] [-symbolfontsize pts] [-template SMILES/SMARTS] [-templatealign *none/x/y/diagonal/rotate/redraw/besteffort*] [-templatefile file] [-templatematch *strict/relaxed*] [-title titlestring] [-version] [-wedgepairs *no/all/hydrogen/unconnected*] [-wedgestyle *default/opposite*] [-wedges 0/1] filenames/directories...

Description

csps is a batch-mode structure depiction tool. It will generate structure output formatted as PostScript or EPS files, similar to the well-known Daylight *prado* program, but with an enhanced set of features and superior layout quality.

Structures are laid out in a grid, by default in 2 rows and 3 columns. Above the grid, a title string (option **-title**) can be printed. Below the structure boxes, a footer line with three components is output. The first component, aligned to the left, is a logo text, which can be set with the **-logotext** option. In the center, the running item count of the objects on the page is printed. Finally, the third component, aligned to the right, is the current page count and the total number of pages in the current dataset. The total number of pages is only printed if the input file can be rewound, i.e. it is omitted when the program is reading from standard input or an Internet connection. Each of the structures is centered in a rectangular area. These boxes can be decorated by a line frame or a 3D shadow (option **-frame**). Above each individual structure box, a specific data item associated with the structure can be displayed - usually the compound name (option **-boxproperty**).

The program uses a sophisticated layout algorithm to generate 2D structure coordinates on the fly, if these are not present in the input file, or the **-recalc** option is used to force recomputation. The layout generates stereochemically correct double bonds (even in rings) and will automatically generate a suitable set of wedge bonds if the input data contains stereochemistry in other formats (such as 3D coordinates or parity descriptors) and the **-computestereo** option is set. Implicit hydrogen atoms will be automatically

added.

The program treats each input file as an individual dataset. All page counts etc. are reset when the next dataset is processed. If, instead of a file name, the name of a directory is specified, all readable structure files of known formats in that directory are read as a single virtual datafile. If no file name is specified, or the special file name '-' is used, input is read from the standard input channel.

By default, output is generated on the standard output channel, but this can be changed with the **-outfile** option. If PostScript output is generated, all plots are generated as a single data stream. If the **-eps** option is set, every output page is stored instead as an individual EPS file, suitable for import into word processing programs and report generators. The names of these EPS files are constructed from the base name of the input file or directory and a double suffix consisting of the total page number (not reset when a new dataset is processed) and the ending *.eps*. If input is read from standard input, the eps output file name is built using the base file name *stdin*.

The file type of the input files is automatically recognized from their input, with well-known file name suffixes helping in giving precedence to formats which are ambiguous (such as SMILES vs. simple SMARTS). It is also possible to explicitly name the file format via option *-format* in case of format misinterpretation (such as reading SMILES from *stdin*). The format may change from input file to input file. The tool will load all locally available structure file I/O extensions before commencing its operation to cope with the maximum number of file formats. Input files can be processed in compressed or gzip-ed form without prior unpacking. The input file name arguments may each be a local file, an URL (http, ftp, gopher, file) or an email message file containing the structure data in the mail body or as one or more attachments. URL retrieval and compression can be combined. If a file name argument is a directory, all readable files in that directory will be processed, and in this case all files in the directory comprise a virtual data file. Files in a directory can be of different formats.

The supported file formats are listed in the table below.

In case of custom development, additional file formats may be locally available. File formats handler are implemented as dynamically loadable modules.

Format	Comment
441	
AA1	Single-character amino acid sequence
AA3	Three-character amino acid sequence
Alchemy	
ASN	PubChem binary ASN.1
ASNT	PubChem text ASN.1
BDB	This is a native structure database file of the CACTVS toolkit, not the protein database file format "PDB", which is also understood
Cactvs/Binary	

Format	Comment
Cactvs/Scan (CBS)	
CAR	
CDA	
CDX	
CDXML	
Cerius II	
CHAI	
Charmm	
CHEMBL	Text file with CHEMLB IDs
Chiron	
CIF	
CML	
Compass	
Cosmo	
CSV	Text table with structure column
CTX	
EMF/WMF	Retrieves only structures from embedded structure data - no chemical OCR! Indirectly configurable via E_EMF_IMAGE property attributes. Output format may actually be EMF, WMF or placeable WMF.
Gaussian Archives	
Gaussian Cube	
Gaussian Input	
GHEMICAL	
GIF, PNG	Will read only files with embedded structure information - no chemical OCR! Indirectly configurable by E_GIF property attributes.
GROMACS	
Hitlist	
Hyperchem	
IFF	
INCHI	

Format	Comment
Index	This is a special index file format which can be used to select arbitrary subsets of larger files in all of the supported formats
JCAMP/JCP	JCAMP-CS for this application. Most JCAMP files (JCAMP-DX) do not contain structure information.
JME	
KCF	
KNIME	
LINCS	
M3D	
Maestro	The MacroModel format
MDL Molfile	This format covers both plain Molfile and SD-files. Most ISIS query attributes including 3D search and R-groups, are supported.
MMD	
Molconn-Z	
Molgen	
Mopac Input	
Mopac Output	
MRV	
MXYZ	
MYSQL	Virtual access to Mysql table with structure column
NETCDF	
PDB	If no or incomplete connectivity records are present, the program attempts a reconstruction of the bonding information.
PDBCODE	
PDBML	
PDBQT	
PHAR	
RDF	Structure files only. The program currently does not support printing of reactions.
SCF	
SDF	See MDL Molfile

Format	Comment
SDF3000	MDL V3000 format variant. Supports structures, data, collections and simple query constructs, but no R- and S-groups, 3D queries or enhanced stereochemistry yet.
SDDATA	Pure SD data file without structure header
Sharc	
Shel-X	
SID	Text file with PubChem SIDs
SK2	ACD/Labs editor format
SKC	ISIS Draw sketch file format
SLN	
SLNPLUS	
SMARTS	Including recursive SMARTS and many established extensions
SMD 4	
SMD 5	Not a complete implementation. Structures consisting of multiple linked fragments cannot be read.
SMILES	
SPC	
SPL	
STF	
Stigmata/Thor data file (STF)	Daylight format
Sybyl	
Sybyl II	
Table	Standard table formats, separated by comma, semicolon or tab. The program will automatically attempt to detect a SMILES column and use this as structure information.
TGF	ISIS/Draw format
UNII	
VRML	Input only with embedded structure codes, not a scene analysis! Indirectly configurable by E_VRML property attributes.
XBSA	
Xtelplot	
XYZ	

Format	Comment
XYZR	Since this file format only contains atomic radii and no element information, input is reliable only if the file uses the same VDW radii table as CACTVS, or the radius table has been adapted by a script modification.

EXAMPLES

csps -bonds 8 -binder top -pagelimit 3 -orientation landscape file1.sdf - <file2.sdf | lp -dpsprinter

OPTIONS

-align *none/x/y/diagonal*

Change the alignment of the 2D structure layout. By default, structure coordinates are generated in a layout where common ring systems are in their familiar orientations. In case of rectangular image sizes, a rotation of the structure so that the largest coordinate extent is aligned with the X or Y axis, or the diagonal, can sometimes improve the visual appearance. This option can be used both for newly computed 2D plot coordinates or coordinates read from file.

-annotationfontsize pts

This parameter controls the font size for atom annotations, such as formal charges or isotope labels. If the value is negative (the default), the font size is automatically derived from the element symbol size. If it is set to zero, no atom annotations are printed.

-atomcolor color/*type/empty_string*

This parameter controls the default coloring of atoms which are displayed as symbols. If this parameter is omitted, or set to an empty string, the atom coloring scheme is implicitly defined by the selected color mode (**-colormode** option). If the parameter is set to *type*, atoms will be colored according to the built-in element table. This is the same scheme which is applied in the absence of this option and the colormode is *cow* or *cob*. Alternatively, a color name such as *white* (default in colormode *wob*), *black* (default in colormode *bow*), or a hexadecimal RGB notation such as #2040F0 may be used to select a uniform color for all plotted atom symbols.

-atomhighlight 0/1

This flag controls whether atoms which are matched by a highlighting substructure (options **-matchfile**, **-matchsmiles**) will be drawn in the highlight color (option **-highlightcolor**). By default this flag is off, meaning that only matched substructure bonds will be highlighted (option -bondhighlight), but not atom symbols or nodes.

-binder *none/top/right/bottom/left*

If this parameter is set to anything but *none*, extra space will be inserted on the selected edge of the paper. The width of the binder region can be controlled with the **-binderwidth** option. The default is to omit the extra space for a binder region.

-binderwidth mm

Control the width or height of the extra space allocated as a binder region. The default is 30 mm. If the **-binder** option is set to *none*, this parameter does not have any effect.

-bondhighlight 0/1

This flag controls whether bonds which are matched by a highlighting substructure

(options -**matchfile**, -**matchsmiles**) will be drawn in the highlight color (option -**highlightcolor**). By default this flag is on, meaning that matched substructure bonds will be highlighted, but not atom symbols or nodes (option -**atomhighlight**).

-**bondscale** n
Specify the number of bonds in x-direction which can drawn into a structure box without re-scaling the structure drawing. The default value is 12. structures with an x extent of 12 standard bond lengths just fit into the structure box in horizontal direction. Smaller structures will be drawn centered and have extra space to the left and right. Larger structures are automatically shrunk so that they still fit into their boxes without overspill. This mechanism ensures that structures of normal (up to the scale parameter) size will all be drawn with the same bond lengths and thus appear graphically consistent, without having larger compounds break out of their boxes or cutting off part of their graph. Re-scaling of structures fitting horizontally may still occur if the structure exceeds the height of the structure box. Re-scaling is always uniform in order to avoid distortions. Setting this parameter to a smaller value lets small structures make better use of the area of their boxes, but increases the likelihood of enforced size adjustment for the larger compounds in a structure set.

-**border** mm
Control the width of the border of the structure boxes and annotations to the edge of the paper. The default are 10 mm.

-**boxborder** pts
This is the space left between the coordinates of the maximum or minimum structure parts and the border of the structure box, if the structure fits tightly or is scaled down (see -**bondscale** parameter). Note that atom symbols need extra space around the center of the atomic coordinates, so it is not recommended to set this parameter to zero. Since the optimum value for this parameter is dependent on the atom symbol font size, it is specified in pts, not mm.

-**boxproperty** property_name
Select the name of a structure property which is displayed above the structure boxes. By default, the property is E_NAME, the default name property, which is automatically set when files with a defined name field are processed. Other useful properties are, for example, E_WEIGHT (molecular weight), E_IDENT (ident string), E_COMMENT (comment field), E_FORMULA (formula) or any property which is defined in an SD file data field. Note that only properties associated with a molecular ensemble can be used, but no atom/molecule/bond/etc. properties. In case of externally defined properties (such as SD file data fields), both the original name as specified in the file and the internal CACTVS nomenclature can be used. If CACTVS knows about a computational method to derive the requested information from the data it read from the input file, it is not required that the data is already present. This means that you can use E_FORMULA with any file, but E_IDENT only with files which contain data which is mapped to this property, since it is not computable. If this parameter is set to an empty string, no property data is output, and the space it would occupy is reclaimed for the structure drawing.

-**charge** 0/1
If this parameter is set to 0, atom symbols will not be annotated by formal charges. The default is 1.

-**colormode** *bow/cob/cow/wob*
Select the color scheme. The four supported styles are black on white (*bow*), color on

black (*cob*), color on white (*cow*) and white on black (*wob*). The first part of these styles describes the coloring of atom symbols, the second part the background of the structure boxes. The color of bonds is either white (on black background) or back (on white background), if the input file does not contain explicit bond coloring information. If the input file does not contain explicit atom colors, they will be chosen as white, black, or a color depending on the element type. The default element color scheme is adjusted to the background - the colors are chosen brighter on black background than on white background.

-comment string
Specify a comment, such as a copyright notice, which is embedded in the PostScript files in a PostScript language comment field. It is not printed.

-computestereo 0/1
If set, the program will try to compute stereo descriptors from the input data. Secondary, indirect sources of stereo information can be 3D coordinates, various stereo descriptors already present in the input (such as parity), wedge attributes on bonds, and 2D coordinates for stereo bonds. If the computation fails, for example because no suitable secondary data source was present, no error is reported.

-count n
Convert a maximum of *n* records from each file or virtual directory file set. The *-offset* option can be used to position the file before the count begins and thus convert only a region of a large file.

-csymbol *all/special/none*
Control the display of carbon atom symbols. The default is *special*, meaning that certain carbon atoms such as those with a triple bond or a formal charge, will be printed with a C symbol. Other carbon atoms are displayed as nodes only. The *all* mode will print all carbons as C, while the *none* mode will always suppress the output of an element symbol.

-dashes 0/1
If this flag is set to 0, the dash attribute on wedges and simple bond lines will be ignored. In order to avoid wrong display of stereochemistry, it should only set to 0 in combination with a **-wedges** 0 option. The default is 1.

-eps 0/1
If set to 1, this option changes the output mode to generate individual EPS files for all pages, instead of a single PostScript output stream. Please refer to the introduction section for a more detailed explanation. By default this flag is off.

-feedback
If set, a dot is printed on the standard error channel for every page written.Only structures which are actually written out are counted.

-fixbridgeheadstereo 0/1
If this flag is set, the program tries to detect problematic stereo center displays at bridgehead atoms. In case of a bicyclic ring system, the bridgehead atom to the front will always have a solid up wedge, and the rear atom a dashed wedge. If necessary, the structure will be flipped vertically - which may result in a drawing which will appear to be drawn with a flipped template in case templates are used. This flag has an effect only if new 2D coordinates are computed. By default it is not set. In any case, the local stereochemistry at all atoms will be correct - but if these atoms are part of a complex ring system with bridges, the overall geometry may be questionable.

-footerfontsize pts
Select the font size of the annotations on the page footer line (logo text, item count and page count). The default point size is 12.

-footerheight pts
Set the height of the footer. By default it is 14 pts. The value is automatically adjusted not to be smaller than the footer font size (**-footerfontsize** option).

-format *fmt*
Explicitly set the format of the input file. This can be helpful if it cannot be determined unambiguously by automatic analysis. The most common use case is the distinction between SMILES and simple SMARTS when reading from *stdin*, or files without a standard suffix.

-frame *none/line/shadow*
Select the decoration of the structure boxes. The default is *line*, meaning that the boxes are enclosed by a thin line. Other styles are *none* (no decoration) and *shadow* (add a drop shadow to the boxes in addition to the enclosing line).

-headerfontsize pts
Select the font size of the header line (**-title** option). The default is 12 points.

-headerheight pts
Set the height of the header area. By default it is 14 pts. The value is automatically adjusted not to be smaller than the header font size (**-headerfontsize** option).

-highlightcolor color
Specify the color by which bonds matching a substructure fragment should be highlighted. This parameter has no effect if neither substructure matching is selected (**-matchsmiles**, **-matchfile** options), or the input data contains already bonds with the *highlight* attribute. The default color is red. Color names can be given either as a name in the X11 color database, or in hex notation (#FF0000 for red). If the colormode (**-colormode**) is *bow* or *wob*, the highlight color is not used. Instead, highlighted bonds are drawn with fat lines.

-hsymbol *none/special/all*
Control the rendering of hydrogens. By default, in the *special* mode, only hydrogen atoms which are traditionally plotted (such as on hetero atoms and aldehydes) are printed. Mode *all* will display all hydrogen atoms, which mode *none* suppresses them all.

-isotope 0/1
If this flag is unset, isotope labels will not be displayed. Note that the **-isotopemapping** flag operates independently. If that display option is active, it will often be combined with a **-isotope** 0 flag setting. By default isotope labels are displayed.

-isotopemapping *none/highlight/invert/boxed/circle/diamond/triangle/cross*
If this option is not set to *none* (the default), atoms with explicit isotope labelling will be shown with additional display flags, such as with an atom symbol rendered in the highlight color (**-highlightcolor**), or surrounded by a circle marker. Note that the display or suppression of the isotope label as atom symbol annotation, which is controlled by the **-isotope** flag, operates independently. Usually, the option **-isotope** 0 is combined with this flag if the isotope label is just used a a marker to identify specific atoms and does not stand for a real isotopic element.

-linewidth pts
Set the width of a standard (non-fat) bond line. The default are 1.4 pts. The width of fat bond lines is derived from this base value.

-logotext string
Set the text which is printed in the bottom left corner of the paper sheets. By default it is the name of the licensing company.

-matchbondorder 0/1
If this flag is set to 0, substructure matching with the **-matchsmiles** and **-matchfile** options does no longer take the bond order into account. The default setting is 1, meaning that bond oder is significant.

-matchfile filename
Set the name of a file with substructure fragments. The file can be in any of the formats the program recognizes, and it may contain multiple records. All records are read from this file and, possibly in combination with the fragment specified by the **-matchsmiles** option, are matched against the structures which are plotted on the output pages. Bonds in the display structures, that match any of the substructure fragments, subject to the setting of the **-matchmode** parameter, are marked with the *highlight* bond attribute. Bonds with this attribute are rendered in the color defined by the **-highlightcolor** option instead of their standard appearance. File formats which allow the explicit specification of substructure match features, such as SMARTS and MDL query molfile, can be used. MDL query syntax is, with the exception of some complex R-group queries, fully supported, while the SMARTS parser is currently limited to simpler cases, such as atom lists and standard atom attributes, but does not support and/or dependencies or bond queries. Implicit hydrogen addition is suppressed while reading the substructure fragment file.

-matchisotope 0/1
If this flag is set to 1, isotope labelling in the substructure fragments (options **-matchsmiles** and **-matchfile**) must match where specified. By default, this option is not active.

-matchmode *first/distinct/nocommon/unique*
This parameter controls the handling of multiple substructure matches of the display molecules by the fragments specified by the **-matchfile** and **-matchsmiles** options. In mode *first* (the default) only the first match of each fragment is evaluated. Mode *distinct* allows multiple matches (potentially overlapping), while mode *nocommon* will also allow overlaps, but only if the match locations do not overlap. Mode *unique* finally is similar to mode *distinct*, but will only display matches which are not topologically equivalent. The match mode applies to each individual fragment only, matches of multiple fragments do not interact. The bonds selected for matches in the modes *first* and *nocommon* are dependent on the atom numbering and not generally predictable.

-matchringsystem 0/1
If this option is active, ring systems must match. A benzene fragment will not match a naphthalene molecule. By default is option is off, meaning that benzene *will* match naphthalene.

-matchsmiles SMILES/SMARTS-string
Specify a substructure fragment as a SMILES/SMARTS string. The program will attempt to match this fragment, possibly in combination with additional fragments read via the **-matchfile** parameter, on all structures which are displayed. Bonds in the

display structures, that match any of the substructure fragments, subject to the setting of the -**matchmode** parameter, are marked with the *highlight* bond attribute. Bonds with this attribute are rendered in the color defined by the -**highlightcolor** option instead of their standard appearance. The SMARTS parser currently supports only a limited set of SMARTS features, such as atom lists and simple atom attributes. And/or logic or bond attributes are currently not supported. Note that most SMARTS query strings require quoting to protect them from interpretation by the shell.

-**matchstereo** *no/absolute/relative*
Choose the handling of stereochemistry in substructure matching. By default, stereochemistry is ignored (mode *no*). Alternatively, stereo centers and stereo bonds in the substructures can be required to match exactly (mode *absolute*). Relative stereochemistry matching is useful only for atom stereochemistry: a +,+ (in pseudo 3D coordinates, not R/S stereo descriptors) substructure center combination will match a +,+ or -,- structure feature, but the diastereomers +,- and -,+ will not. This scheme can be expanded to more than two stereo centers. Stereochemistry matching is only supported for tetrahedral centers (including those with an electron pair), double bonds and allenes. Higher geometries such as octahedral centers are currently not checked in the matching algorithm.

-**namefontsize** pts
Specify the font size of the naming area of the structure boxes, which is filled by the -**boxproperty** option. By default a 10 point font is used.

-**nameheight** pts
Set the height of the name/property data area of the structure boxes. It is automatically adjusted not to be smaller than the name font size (-**namefontsize** option)

-**ncols** n
Specify the number of structure box columns in the output. The default is 2. When output is rotated (-**orientation** parameter), the meaning of rows and columns is exchanged - it always assumes you are looking at the page with the title on top.

-**nitrostyle** *ionic/asis/penta*
This option controls the encoding of nitro groups and similar functional groups in the graphical output. If the option is not set, or set to *asis*, no processing takes place. Otherwise, all nitro groups and similar functional units are re-coded as charge pairs (with a tetravalent, positively charged nitro etc. atom, and a negatively charged ligand) or alternatively as the uncharged variant with an octet expansion on the nitrogen (or similar atom).

-**nrows** n
Specify the number of structure box rows in the output. The default is 3. When output is rotated (-**orientation** parameter), the meaning of rows and columns is exchanged - it always assumes you are looking at the page with the title on top.

-**offset** n
This parameter specifies a record offset into each individual file or virtual directory file set which is processed. The default offset is 0. If used in combination with the *-count* option, sections of larger files can be processed.

-**orientation** *portrait/landscape*
Select whether the output should be rotated or not. Note that the meaning of the -**ncols** and -**nrows** parameter is adjusted - these parameters always assume that you are looking at a properly oriented page with the title on top.

-**outfile** filename
This parameter defines the name of the output file. The default output is to standard output. The output file name can be an anonymous ftp URL. Please refer to the introductory section to learn about the naming conventions if EPS style output is selected.

-**pagelimit** n
Set the maximum number of pages produced from each data source (file or virtual directory set). The default is 100.

-**papersize** *A7/A6/A5/A4/A3/B6/B5/B4/B3/letter/legal/executive*
Specify the size of the paper. This default for this parameter is *letter* for US customers, A4 for the rest of the world.

-**postprocessing** 0/1
If this parameter is set (it is on by default), a minimum level of sanity checks and attempts to correct various common structure coding problems are performed. If this option is set to zero, structures are strictly encoded and displayed as they were in the input files.

-**pseudo3d** 0/1
This is a parameter which controls the layout algorithms for 2D structure plot coordinates. It has no effect if 2D data is already present in the file. Essentially, if set, the longest central carbon chain in the input structure is depicted in a pseudo-3D projection. It does not have an effect on compounds without central chains of at least three carbon atoms.

-**radical** 0/1
Select whether to display a radical mark on radical centers or not. By default this option is active.

-**recalc** 0/1
If set, 2D coordinates found in the input file are discarded and recomputed when required during file writing. By default, this option is not active and information will be preserved where possible.

-**resolvearo** 0/1
The usage of aromatic bonds (type 4) in MDL Molfiles is frequently incorrect. Type 4 is a query attribute and must not occur in standard structure data files. This type of bond in a substructure does not define an aromatic bond, but instead requires the presence of such a bond on the corresponding matched structure bond. This program reads this data correctly as a special bond type which is exempt from electron counting, etc. However, in case a file which such bonds must be processed as structure file, a Kekulé representation of the structure can be generated from the bond data if the -**resolvearo** flag is set.

-**shadow** mm
Set the size of the drop shadow on structure display boxes. This option has only an effect if the -**frame** attribute is set to *shadow*. The default is 3 mm.

-**showcrossedbonds** 0/1
If set, which is the default, mark stereogenic double bonds which do not possess expicit stereochemistry as stereochemically undefined, e.g. draw them as crossed bonds. If the flag is unset, such annotations are suppressed.

-space mm

Set the space between the structure boxes on the output pages. The default is 5 mm.

-stereo 0/1

This option controls the annotation of atoms by stereo descriptors (R/S,P/M,D/L). By default, this option is not set. Note that the display of bonds as wedges and dashes is *not* controlled by this attribute. Use the **-dashes** and **-wedges** flags for this purpose.

-symbol *symbol/label/index/box/compact*

By default (mode *symbol*) atoms are displayed with their element symbols (refer to the **-csymbol** and **-hsymbol** options for further methods to control the display of atoms). Alternatively, atoms can be displayed as their label (mode *label*) or atom table index (mode *index*). If the structures are read from a file encoded in a format which does not allow the storage of specific atom labelling, both index and label are equivalent and integers, beginning with 1, which indicate the position of the atom in the internal atom table. The mode *box* will suppress the display of atom symbols and use colored boxes for hetero atoms instead. The *compact* mode merges hydrogen atoms at hetero atoms (such as in NH_2) into the primary atom symbol. The layout of the structure is also taken into account, so that an HO- symbol is used if the connection point of an OH group is to the right. The hydrogen atoms which are merged into the primary symbol and their bonds are no longer displayed.

-symbolfontsize pts

Specify the size of element symbols or labels in the structure displays. The default is -1, meaning that the program should automatically choose a suitable standard font size, which may be scaled down if a structure is shrunk (see **-bondscale** option).

-template SMILES/SMARTS

A substructure template in SMILES or SMARTS notation. This option is used in combination with the **-templatealign** option.

-templatealign *none/x/y/diagonal/rotate/redraw/besteffort*

Align the layout of the image according to a substructure template, which was specified by the **-template** or **-templatefile** options. If no substructure is present, this parameter is ignored. The substructure is matched on all structures. If is does not match, no error is generated and processing continues as if this parameter had not been specified or set to *none*. The *redraw* option implicitly sets additional substructure flags which will allow matching of substructure *ring* atoms and bonds only on corresponding structure atoms and bonds which are in the same class of ring system. With this option, a ring system must be matched completely, so for example a phenyl ring in the template will not match a naphthalene ring in a structure. Non-ring parts of the structure may be matched in any style. The only exception is that it is also allowable for a terminal chain atom in the template substructure to match a ring atom in the structure. The other template match variants do not have the ring system match limitations. If the template substructure does not possess 2D coordinates of its own and the *rotate* or *redraw* modes are selected, coordinates for the template will be computed by the standard 2D layout procedure. The first of potentially multiple different matches of the template substructure is used a the starting point for structure coordinate updates. The simple *x*, *y*, and *diagonal* modes will align the major axis of the matched atoms of the structure to the x and y axis or on a 30 degrees angle to the x axis, respectively. For these options, no substructure 2D layout coordinates are used. The *rotate* variant will rotate the structure by multiples of 30 degrees with and without a coordinate flip. From among those 24 orientations, the one with the best similarity to the substructure

coordinates is chosen. Finally, the *redraw* variant will regenerate the 2D layout coordinates, using the matched fragment with its coordinates transferred from the substructure as the nucleus for the layout. In this style, all matched structure coordinates will have exactly the same relative coordinates as the substructure atoms, but the standard bond length will be scaled to one. The *besteffort* combined mode will first try to match the template with the redraw option. If the template does not match in this mode, a second attempt will be made with a *rotate* mode.

-templatefile filename
The name a file which contains a substructure template. This option is used in combination with the **-templatealign** option. Only the first record of the file is read. If the file does not contain 2D coordinates, and these are needed for the selected **-templatealign** option, coordinates will be generated.

-templatematch *strict/relaxed*
This flag influences the match operation of fragments on structures. In mode *strict*, aliphatic fragment atoms will not match aromatic structure parts. In *relaxed* mode, the default, aliphatic fragment atoms will also match aromatic systems. This setting applies only to atoms without further query attributes. If any atom bears an explicit *aromatic* or *aliphatic* query attribute, this attribute has precedence. If a template is specified as SMARTS strings, uppercase atoms are decoded without an explicit *aliphatic* query attribute and will this match aromatic systems. This option can be used to counter this convention.

-title string
This is an arbitrary string which is printed above the structure boxes on each page. If it is empty (the default), no text is printed and the space is reclaimed for the layout of the structure boxes.

-version
Print version and licensing information and then exit.

-wedges 0/1
This parameter controls whether wedge bonds are displayed as such or not. If this parameter is set to 0, but the **-dashes** parameter is still switched on, full wedges will be printed as a bold bond and dashed wedges as simple dashed bond. If the **-dashes** option is also inactive, the display of bond stereo attributes is completely suppressed. The default value for this parameter is 1.

-wedgepairs *no/all/hydrogen/unconnected*
Add extra wedges when generating 2D coordinates. By default (option value *no*), only a single wedge is used to determine the stereochemistry at atomic centers. In modes *all, unconnected* and *hydrogen*, a second wedge is attached to a bond extending from the stereo center to further disambiguate the stereochemical relationships. The second wedge will be preferably attached to a bond leading to a hydrogen ligand, if such neighbor exists. In mode *hydrogen*, only bonds to hydrogen will be used, if no such bond exists, no second wedge is drawn. Mode *unconnected* is the same as *all*, with the exception that the extra wedge to the preferred ligand will not be drawn in case this ligand already participates in a wedge bond, regardless whether it is located at the tip or the bottom of such a wedge bond. In any case, the wedge is never drawn to a ring atom - if no chain neighbor without a wedge bond exists, the second wedge is omitted in all modes.

-wedgestyle *default/opposite*

If the mode *opposite* is selected, the drawing of the environment of atoms which are located at the tip of two or more wedge bonds of the same class (solid or dashed) is changed. If any of the offending ligands is a single atom, it will be moved into another gap of the neighbor sphere in such a way that the wedge style is changed to the opposite, and the stereochemistry of the center retained. While this feature is useful to meet specific drawing style demands, the graphical quality of the structure layout will usually suffer.

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