International Tables for Crystallography (2006). Vol. G, Chapter 4.8, pp. 467–470.

4.8. Molecular Information File dictionary (MIF)

BY F. H. ALLEN, J. M. BARNARD, A. P. F. COOK AND S. R. HALL

This is version 1.2.3 of the molecular information file dictionary (MIF). MIF complements the crystallographic information file with data items describing two-dimensional chemical structure diagrams and bond types in a similar STAR format. Unlike CIF, MIF permits nested looping of data items and data encapsulation in save frames. The MIF format is described in Chapter 2.4.

_atom_attach_all
_atom_attach_ring
_atom_attach_nh
_atom_attach_h (*numb*)

The number of atom sites considered to be attached (*i.e.* chemically bonded) to this site. The extensions are:

`all`	all sites,
`ring`	all sites forming rings,
`nh`	all sites excluding hydrogens and unshared electron pairs,
`h`	hydrogen-atom sites.

Appears in list containing **_atom_id**.
The permitted range is $0 \rightarrow \infty$. **[atom]**

_atom_charge (*numb*)

Specifies the formal electronic charge on the atom for the different atomic representation conventions. The convention for charge is specified by **_define_bonding_convention**.
Appears in list containing **_atom_id**.
The permitted range is $-99 \rightarrow 99$. **[atom]**

_atom_cip (*char*)

Specifies the Cahn–Ingold–Prelog designation for the atom. The designators are by Prelog & Helmchen (1982).

Reference: Prelog, V. & Helmchen, G. (1982). *Angew. Chem. Int. Ed. Engl.* **21**, 567–583.

Appears in list containing **_atom_id**. **[atom]**

_atom_coord_x
_atom_coord_y
_atom_coord_z (*numb*)

Specifies the Cartesian coordinates for the atom with an arbitrary origin and arbitrary orthogonal axes.
Appears in list containing **_atom_id**. **[atom]**

_atom_environment (*char*)

Environment of the atom site.
Appears in list containing **_atom_id**.
The data value must be one of the following:

`atom`	a single atom site
`frag`	atom site in molecular fragment

Where no value is given, the assumed value is '`atom`'. **[atom]**

_atom_frag_id (*numb*)

ID of atom site within the molecular fragment.
Appears in list containing **_atom_id**. **[atom]**

_atom_frag_key (*char*)

Name of save frame containing atom data on molecular fragment.
Appears in list containing **_atom_id**. **[atom]**

_atom_id (*char*)

This specifies a unique code for an 'atom site' in a molecule or fragment. A designated atom site may be occupied by a 'dummy' atom (see **_atom_type**). A special syntax exists for this code which permits a template molecular fragment to be referred to as an 'atom site', and for the atom within that template to be identified. The syntax is $m > n$ where m is the code identifying the template fragment (contained within a save frame) and n is the code matching an **_atom_id** value stored within the save frame.
Appears in list as essential element of loop structure. May match child data name(s):
_bond_id_1, **_bond_id_2**, **_stereo_vertex_id**. **[atom]**

_atom_label (*char*)

The code providing unique identification of the atom site for display purposes. See also **_atom_type**.
Appears in list containing **_atom_id**. **[atom]**

_atom_mass_number (*numb*)

Specifies the mass number or the isotopic state of the atom. The default is the 'most abundant naturally occurring' value.
Appears in list containing **_atom_id**.
The permitted range is $1 \rightarrow \infty$. **[atom]**

_atom_radical_count (*numb*)

Specifies the formal radical state of the atom site identified by **_atom_id**. This is the number of unpaired electrons associated with the atom, *e.g.* the value of 1 specifies one singly occupied orbital on the atom that is not involved in bonding.
Appears in list containing **_atom_id**.
The permitted range is $0 \rightarrow \infty$. **[atom]**

_atom_spin_multiplicity (*numb*)

The spin multiplicity applies only if the **_atom_radical_count** value is nonzero, and is derived from the formula $2S + 1$, where S is the absolute value of the sum of the electron spins ($+\frac{1}{2}$ or $-\frac{1}{2}$) on the atom. Thus, a biradical atom may have the values 1 or 3 [$2(\frac{1}{2} - \frac{1}{2}) + 1$ or $2(\frac{1}{2} + \frac{1}{2}) + 1$] to represent a singlet or a triplet biradical.
Appears in list containing **_atom_id**.
The permitted range is $1 \rightarrow \infty$. **[atom]**

_atom_type (*char*)

Specifies the type of atom site identified by **_atom_id**. Hydrogen atoms will usually not be assigned to sites except where they are connected to more than one other atom, or where it is necessary to reference them, for example, in describing stereochemistry.

The data value must be one of the following:

H	1	He	2	Li	3	Be	4	B	5	C	6
N	7	O	8	F	9	Ne	10	Na	11	Mg	12
Al	13	Si	14	P	15	S	16	Cl	17	Ar	18
K	19	Ca	20	Sc	21	Ti	22	V	23	Cr	24
Mn	25	Fe	26	Co	27	Ni	28	Cu	29	Zn	30
Ga	31	Ge	32	As	33	Se	34	Br	35	Kr	36
Rb	37	Sr	38	Y	39	Zr	40	Nb	41	Mo	42
Tc	43	Ru	44	Rh	45	Pd	46	Ag	47	Cd	48
In	49	Sn	50	Sb	51	Te	52	I	53	Xe	54
Cs	55	Ba	56	La	57	Ce	58	Pr	59	Nd	60
Pm	61	Sm	62	Eu	63	Gd	64	Tb	65	Dy	66
Ho	67	Er	68	Tm	69	Yb	70	Lu	71	Hf	72
Ta	73	W	74	Re	75	Os	76	Ir	77	Pt	78
Au	79	Hg	80	Tl	81	Pb	82	Bi	83	Po	84
At	85	Rn	86	Fr	87	Ra	88	Ac	89	Th	90

Affiliations: FRANK H. ALLEN, Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, CB2 1EZ, England; JOHN M. BARNARD and ANTHONY P. F. COOK, BCI Ltd, 46 Uppergate Road, Stannington, Sheffield S6 6BX, England; SYDNEY R. HALL, School of Biomedical and Chemical Sciences, University of Western Australia, Crawley, Perth, WA 6009, Australia.

Pa	91	U	92	Np	93	Pu	94	Am	95	Cm	96
Bk	97	Cf	98	Es	99	Fm	100	Md	101	No	102
Lr	103	usp	'unshared electron pair'			dum	'dummy atom'				

Appears in list containing **_atom_id**. **[atom]**

_atom_valency (*numb*)

Specifies the valency state of the atom site identified by **_atom_id**.

Appears in list containing **_atom_id**.

The permitted range is $-99 \rightarrow 99$. **[atom]**

_bond_cip (*char*)

Specifies the Cahn–Ingold–Prelog designation for the bond. The designators are by Prelog & Helmchen (1982).

Reference: Prelog, V. & Helmchen, G. (1982). *Angew. Chem. Int. Ed. Engl.* **21**, 567–583.

Appears in list containing **_bond_id_1**, **_bond_id_2**. **[bond]**

_bond_environment (*char*)

Specifies the connection environment of the bond.

Appears in list containing **_bond_id_1**, **_bond_id_2**.

The data value must be one of the following:

ring	in a ring
chain	in a chain

[bond]

_bond_id_1
_bond_id_2 (*char*)

Specify the atom-site codes of 'chemically connected' sites. The atom ID codes may appear in either order except for asymmetric bonds. Each 'bond' pair may be represented only once. The special syntax for representing atom sites within molecular templates is described in the **_atom_id** definition.

Appears in list as essential element of loop structure. **Must** match parent data name **_atom_id**. **[bond]**

_bond_type_casreg3 (*char*)

Code indicating the nature of the bond according to the *Chemical Abstracts* Service Registry III bonding convention. The convention is specified with **_define_bonding_convention**.

Reference: Mockus, J. & Stobaugh, R. E. (1980). *J. Chem. Inf. Comput. Sci.* **20**, 18–22.

Appears in list containing **_bond_id_1**, **_bond_id_2**.

Related items:

_bond_type_mif (convention),
_bond_type_ccdc (convention).

The data value must be one of the following:

S	single exact bond
D	double exact bond
T	triple exact bond
A	ring alternating normalized bond
U	tautomer normalized bond

[bond]

_bond_type_ccdc (*char*)

Code indicating the nature of the bond according to the Cambridge Crystallographic Data Centre (CCDC) bonding convention. The convention is specified with **_define_bonding_convention**.

Reference: Allen, F. H., Davies, J. E., Galloy, J. J., Johnson, O., Kennard, O., Macrae, C. F., Mitchell, E. M., Mitchell, G. F., Smith, J. M. & Watson, D. G. (1991). *J. Chem. Inf. Comput. Sci.* **31**, 187–204.

Appears in list containing **_bond_id_1**, **_bond_id_2**.

Related items:

_bond_type_casreg3 (convention),
_bond_type_mif (convention).

The data value must be one of the following:

S	single (two-electron) bond or σ bond to metal
D	double (four-electron) bond
T	triple (six-electron) bond
Q	quadruple (eight-electron, metal–metal) bond
A	alternating normalized ring bond (aromatic)
C	catena-forming bond in crystal structure
E	equivalent (delocalized double) bond
P	π bond (metal–ligand π interaction)

[bond]

_bond_type_mif (*char*)

Code indicating the nature of the bond according to the MIF bonding convention. Aromatic and normalized tautomeric bonds cannot be shown. The convention is specified with **_define_bonding_convention**.

Appears in list containing **_bond_id_1**, **_bond_id_2**.

Related items:

_bond_type_casreg3 (convention),
_bond_type_ccdc (convention).

The data value must be one of the following:

S	single (two-electron) bond
D	double (four-electron) bond
T	triple (six-electron) bond
O	other (*e.g.* coordination) bond

[bond]

_define_bonding_convention (*char*)

Specifies the convention used for the values of the items **_atom_charge**, **_atom_radical_count**, **_atom_spin_multiplicity** and **_atom_valency**.

The data value must be one of the following:

casreg3	*Chemical Abstracts* Service Registry III
ccdc	Cambridge Crystallographic Data Centre
mif	basic MIF

Where no value is given, the assumed value is 'mif'. **[define]**

_define_stereo_relationship (*char*)

Defines the enantiomorphic relationship of the stereo geometry in the data cell (data block or save frame). The descriptions of independently defined stereo regions, whose centres all have the same inter-centre relationship, may be grouped together. For each such group, the inter-centre relationship is specified by **_define_stereo_relationship**. Where there is only one such group, all the relevant data may be included in the data block or save frame for the molecule as a whole. Where there are several different such groups, each should be shown in a separate save frame and **_reference_stereo_group** should be used to reference the different save frames. For each stereo group, a two-level loop structure will be used to define the stereocentres it contains. Each stereogenic atom site is defined by **_stereo_atom_id** and **_stereo_geometry** at the first loop level, and by **_stereo_vertex_id** at the second. Each stereogenic bond is defined by **_stereo_bond_id_1**, **_stereo_bond_id_2** and **_stereo_geometry** at the first level, and by **_stereo_vertex_id** at the second level.

The data value must be one of the following:

absolute	configuration is as shown
relative	configuration is relative
unknown	configuration is unknown
racemic	two stereoisomers: equal mix of D and L
absolute_excess	two stereoisomers; excess as shown
relative_excess	two stereoisomers; excess unknown

Where no value is given, the assumed value is 'unknown'. **[define]**

_display_colour (*char*)

The colour code specifying the colour of the object identified by **_display_symbol**. The permitted colour codes are stored with the RGB ratios as a separate validation file 'mif_core_colours.val'.

The data value must be one of the following:

black	000:000:000_RGB	white	255:255:255_RGB
white_snow	255:250:250_RGB	white_smoke	245:245:245_RGB
white_ivory	255:255:240_RGB	white_azure	240:255:255_RGB
white_lavender	230:230:250_RGB	white_rose	255:228:225_RGB
grey	192:192:192_RGB	grey_light	211:211:211_RGB

grey_slate	112:128:144_RGB	grey_slate_dark	047:079:079_RGB
grey_slate_light	119:136:153_RGB	blue	000:000:255_RGB
blue_light	176:224:230_RGB	blue_medium	000:000:205_RGB
blue_dark	025:025:112_RGB	blue_navy	000:000:128_RGB
blue_slate_dark	072:061:139_RGB	blue_slate	106:090:205_RGB
blue_royal	065:105:225_RGB	blue_sky	135:206:235_RGB
blue_sky_deep	000:191:255_RGB	blue_sky_light	135:206:250_RGB
blue_steel	070:130:180_RGB	turquoise	064:224:208_RGB
turquoise_light	175:238:238_RGB	turquoise_dark	000:206:209_RGB
turquoise_medium	072:209:204_RGB	cyan	000:255:255_RGB
cyan_light	224:255:255_RGB	green	000:255:000_RGB
green_light	152:251:152_RGB	green_dark	000:100:000_RGB
green_sea	046:139:087_RGB	green_sea_dark	143:188:143_RGB
green_sea_medium	060:179:113_RGB	green_sea_light	032:178:170_RGB
green_spring	000:255:127_RGB	green_lawn	124:252:000_RGB
green_aquamarine	127:255:212_RGB	green_chartreuse	127:255:000_RGB
green_yellow	173:255:047_RGB	green_lime	050:205:050_RGB
green_forest	034:139:034_RGB	green_olive	107:142:035_RGB
green_khaki	240:230:140_RGB	yellow	255:255:000_RGB
yellow_light	255:255:224_RGB	yellow_gold	255:215:000_RGB
yellow_goldenrod	218:165:032_RGB	yellow_goldenrod_pale	238:232:170_RGB
yellow_goldenrod_light	238:221:130_RGB	yellow_goldenrod_dark	184:134:011_RGB
yellow_green	154:205:050_RGB	brown	165:042:042_RGB
brown_rosy	188:143:143_RGB	brown_indian_red	205:092:092_RGB
brown_saddle	139:069:019_RGB	brown_sienna	160:082:045_RGB
brown_peru	205:133:063_RGB	brown_burlywood	222:184:135_RGB
brown_beige	245:245:220_RGB	brown_wheat	245:222:179_RGB
brown_sandy	244:164:096_RGB	brown_tan	210:180:140_RGB
brown_chocolate	210:105:030_RGB	salmon	250:128:114_RGB
salmon_light	255:160:122_RGB	salmon_dark	233:150:122_RGB
orange	255:165:000_RGB	orange_dark	255:140:000_RGB
red	255:000:000_RGB	red_coral	255:127:080_RGB
red_tomato	255:099:071_RGB	red_orange	255:069:000_RGB
red_violet	219:112:147_RGB	red_maroon	176:048:096_RGB
pink	255:192:203_RGB	pink_light	255:182:193_RGB
pink_deep	255:020:147_RGB	pink_hot	255:105:180_RGB
violet	238:130:238_RGB	violet_red_medium	199:021:133_RGB
violet_red	208:032:144_RGB	violet_magenta	255:000:255_RGB
violet_plum	221:160:221_RGB	violet_orchid	218:112:214_RGB
violet_dark	148:000:211_RGB	violet_blue	138:043:226_RGB
violet_purple	160:032:240_RGB	violet_thistle	216:191:216_RGB

Appears in list containing **_display_id**. Where no value is given, the assumed value is 'black'. **[display]**

_display_conn_colour (*char*)

The colour code specifying the colour of the object identified by **_display_conn_symbol**. The permitted colour codes are stored with the RGB ratios as a separate validation file 'mif_core_colours.val'.

The data value must be one of the following:

black	000:000:000_RGB	white	255:255:255_RGB
white_snow	255:250:250_RGB	white_smoke	245:245:245_RGB
white_ivory	255:255:240_RGB	white_azure	240:255:255_RGB
white_lavender	230:230:250_RGB	white_rose	255:228:225_RGB
grey	192:192:192_RGB	grey_light	211:211:211_RGB
grey_slate	112:128:144_RGB	grey_slate_dark	047:079:079_RGB
grey_slate_light	119:136:153_RGB	blue	000:000:255_RGB
blue_light	176:224:230_RGB	blue_medium	000:000:205_RGB
blue_dark	025:025:112_RGB	blue_navy	000:000:128_RGB
blue_slate_dark	072:061:139_RGB	blue_slate	106:090:205_RGB
blue_royal	065:105:225_RGB	blue_sky	135:206:235_RGB
blue_sky_deep	000:191:255_RGB	blue_sky_light	135:206:250_RGB
blue_steel	070:130:180_RGB	turquoise	064:224:208_RGB
turquoise_light	175:238:238_RGB	turquoise_dark	000:206:209_RGB
turquoise_medium	072:209:204_RGB	cyan	000:255:255_RGB
cyan_light	224:255:255_RGB	green	000:255:000_RGB
green_light	152:251:152_RGB	green_dark	000:100:000_RGB
green_sea	046:139:087_RGB	green_sea_dark	143:188:143_RGB
green_sea_medium	060:179:113_RGB	green_sea_light	032:178:170_RGB
green_spring	000:255:127_RGB	green_lawn	124:252:000_RGB
green_aquamarine	127:255:212_RGB	green_chartreuse	127:255:000_RGB
green_yellow	173:255:047_RGB	green_lime	050:205:050_RGB
green_forest	034:139:034_RGB	green_olive	107:142:035_RGB
green_khaki	240:230:140_RGB	yellow	255:255:000_RGB
yellow_light	255:255:224_RGB	yellow_gold	255:215:000_RGB
yellow_goldenrod	218:165:032_RGB	yellow_goldenrod_pale	238:232:170_RGB
yellow_goldenrod_light	238:221:130_RGB	yellow_goldenrod_dark	184:134:011_RGB
yellow_green	154:205:050_RGB	brown	165:042:042_RGB
brown_rosy	188:143:143_RGB	brown_indian_red	205:092:092_RGB
brown_saddle	139:069:019_RGB	brown_sienna	160:082:045_RGB
brown_peru	205:133:063_RGB	brown_burlywood	222:184:135_RGB
brown_beige	245:245:220_RGB	brown_wheat	245:222:179_RGB
brown_sandy	244:164:096_RGB	brown_tan	210:180:140_RGB
brown_chocolate	210:105:030_RGB	salmon	250:128:114_RGB
salmon_light	255:160:122_RGB	salmon_dark	233:150:122_RGB
orange	255:165:000_RGB	orange_dark	255:140:000_RGB
red	255:000:000_RGB	red_coral	255:127:080_RGB
red_tomato	255:099:071_RGB	red_orange	255:069:000_RGB
red_violet	219:112:147_RGB	red_maroon	176:048:096_RGB
pink	255:192:203_RGB	pink_light	255:182:193_RGB
pink_deep	255:020:147_RGB	pink_hot	255:105:180_RGB
violet	238:130:238_RGB	violet_red_medium	199:021:133_RGB
violet_red	208:032:144_RGB	violet_magenta	255:000:255_RGB
violet_plum	221:160:221_RGB	violet_orchid	218:112:214_RGB
violet_dark	148:000:211_RGB	violet_blue	138:043:226_RGB
violet_purple	160:032:240_RGB	violet_thistle	216:191:216_RGB

Appears in list at level 2 containing **_display_conn_id**. Where no value is given, the assumed value is 'black'. **[display_conn]**

_display_conn_id (*numb*)

The identifying number of a display object which is connected to another display object in level 1 of the loop packet which is designated as **_display_id**. The ID number appearing as the **_display_conn_id** *must* appear elsewhere in the loop structure as a value for **_display_id**.

Appears in list at level 2 as essential element of loop structure. **Must** match parent data name **_display_id**. **[display_conn]**

_display_conn_symbol (*char*)

The symbol code for the bond connection to the displayed objects identified by **_display_id** and **_display_conn_id**. The symbol codes and descriptions are stored in the validation file 'mif_core_bonds.val'.

The data value must be one of the following:

.c	dotted line to object centres
-c	dashed line to object centres
1c	solid line to object centres
2c	double solid line to object centres
3c	triple solid line to object centres
.b	dotted line to object boundary
-b	dashed line to object boundary
1b	solid line to object boundary
2b	double solid line to object boundary
3b	triple solid line to object boundary
>b	wedge with apex at **_display_conn_id**
<b	wedge with apex at **_display_id**

Appears in list at level 2 containing **_display_conn_id**. **[display_conn]**

_display_coord_x
_display_coord_y (*numb*)

The projected coordinates of the display object identified in **_display_object** and **_display_symbol**. A display diagram has the *y* axis from bottom to top and the *x* axis from bottom left to right. The display origin is defined with **_display_origin**. Coordinate values can be scaled using **_display_scale** and **_display_span_**.

Appears in list containing **_display_id**. **[display]**

_display_define_origin (*char*)

A code signaling where the origin of the **_display_coord_** values should be placed.

The data value must be one of the following:

centre	at centre of diagram
bottom	at the bottom left corner
top	at the top left corner

Where no value is given, the assumed value is 'bottom'. **[display_define]**

_display_define_scale (*numb*)

The multiplication scale needed to convert **_display_coord_** pixels to centimetres.

The permitted range is 0. $\rightarrow \infty$. **[display_define]**

_display_define_span_x
_display_define_span_y (*numb*)

The maximum dimensions of the display diagram. **_display_define_span_x** is the horizontal dimension and **_display_define_span_y** is the vertical dimension.

The permitted range is 0. → ∞. **[display_define]**

_display_id (*numb*)

The identifying number of the display object described by the combination of **_display_object** and **_display_symbol**.

Appears in list as essential element of loop structure. May match child data name(s): **_display_conn_id**. **[display]**

_display_object (*char*)

Signals how the object identified by **_display_id** is to be displayed. The value 'text' signals that **_display_symbol** contains a character string for display; the value 'icon' signals that **_display_symbol** is a code which identifies the molecular symbol to be displayed; and the value 'null' signals that no object will be shown at this site.

Appears in list containing **_display_id**.

The data value must be one of the following:

text	character string specified as **_display_symbol**
icon	icon specified as a **_display_symbol** code
.	no object is displayed

Where no value is given, the assumed value is '.'. **[display]**

_display_size (*numb*)

This value specifies the maximum *y* dimension of the object identified by **_display_symbol** in pixels.

Appears in list containing **_display_id**.

The permitted range is 0. → ∞. **[display]**

_display_symbol (*char*)

The interpretation of this item is dependent on the value of the item **_display_object**. If **_display_object** is 'text', then the **_display_symbol** is assumed to be a literal character string that should be displayed. If **_display_object** is 'icon', then the **_display_symbol** is a code that specifies the molecular symbol or icon to be displayed. The permitted code enumerations for **_display_symbol** and their descriptions are stored in the separate validation file 'mif_core_molecules.val'.

Appears in list containing **_display_id**, **_display_object**.

The data value must be one of the following:

3s	unsaturated three-membered ring with circle
4s	unsaturated four-membered ring with circle
5s	unsaturated five-membered ring with circle
6s	unsaturated six-membered ring with circle
7s	unsaturated seven-membered ring with circle
8s	unsaturated eight-membered ring with circle
lp	lone pair symbol
*	any text string (when **_display_object** is 'text')

[display]

_molecule_name_common
_molecule_name_iupac
_molecule_name_cas_8ci
_molecule_name_cas_9ci
_molecule_name_cas_10ci (*char*)

Specifies the short and systematic names for the molecule described within the data block or save frame. Data names can have the extensions

iupac	IUPAC name (IUPAC, 1971, 1979)
cas_8ci	*Chemical Abstracts 8th Collective Index*
cas_9ci	*Chemical Abstracts 9th Collective Index*
cas_10ci	*Chemical Abstracts 10th Collective Index*

References: IUPAC (1971). *Pure Appl. Chem.* **28**, 1–110; IUPAC (1979). *The Notation of Organic Chemistry.* Oxford: Pergamon.

[molecule]

_reference_conformation
_reference_stereo_group (*char*)

The frame-code pointer strings (starting with a $ character) which identify save frames containing specific categories of data which have been specified with a **_define_** data value.

Appears in list as essential element of loop structure. **[reference]**

_stereo_atom_id (*char*)

Specifies the identity of the stereogenic centre to which the sites defined under **_stereo_vertex_id** are attached.

Appears in list as essential element of loop structure. **Must** match parent data name **_atom_id**. **[stereo]**

_stereo_bond_id_1
_stereo_bond_id_2 (*char*)

Specifies the atom-site identifiers of the connected atoms that form the stereogenic bond. These atom sites are connected to the atom sites defined under **_stereo_vertex_id** and which define the stereochemistry of the cited bond.

Appears in list as essential element of loop structure. **Must** match parent data name **_atom_id**. **[stereo]**

_stereo_geometry (*char*)

Specifies the geometry of the stereocentre being described. Note that the enumeration values are not descriptions of the chemical entities, only the stereo geometry. Thus, the stereochemistry of hindered biphenyls may conform to the *allene* geometry, although they are not chemically allenes. The order of the associated **_stereo_vertex_id** values is determined by the geometry. The first site is selected as that closest to the axis of highest symmetry for the described geometry. Subsequent sites are selected sequentially by right-hand rotations about this axis; otherwise by selecting a site closest to the initial site.

Appears in list as essential element of loop structure.

The data value must be one of the following:

square	four sites
olefin	four sites in a rectangle
allene	four sites in a distorted tetrahedron
tetrahedron	four sites
square_pyramid	five sites
trigonal_bipyramid	five sites
octahedron	six sites
cube	eight sites

[stereo]

_stereo_vertex_id (*char*)

Specifies the identity of atom sites at the vertices of the stereogenic centre. The order of the selected vertex sites for each geometry is described in **_stereo_geometry**. Where one or more of the vertices in the specified geometry corresponds to an implicit hydrogen atom or unshared electron pair, the value '.' may be used. The special syntax for representing atom sites within molecular templates is described in the **_atom_id** definition.

Appears in list at level 2 as essential element of loop structure. **Must** match parent data name **_atom_id**. **[stereo]**