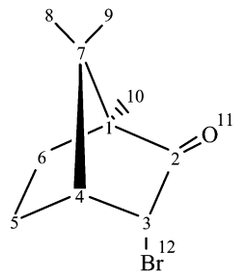


```
data_bromocamphor_2

_molecule_name_common       (+)-3-bromocamphor

_molecule_name_iupac
; 3R-bromo-1R,7,7-trimethyl-4S-bicyclo[2.2.1]heptan-
  2-one
;
    loop_
        _atom_id
        _atom_type
        _atom_attach_h
        _atom_cip
              1  C  0  R    2  C  0  .    3  C  1  R
              4  C  1  S    5  C  2  .    6  C  2  .
              7  C  0  .    8  C  3  .    9  C  3  .
             10  C  3  .   11  O  0  .   12  Br 0  .
```

Fig. 2.4.8.1. CIP stereochemical descriptors for (+)-3-bromocamphor.

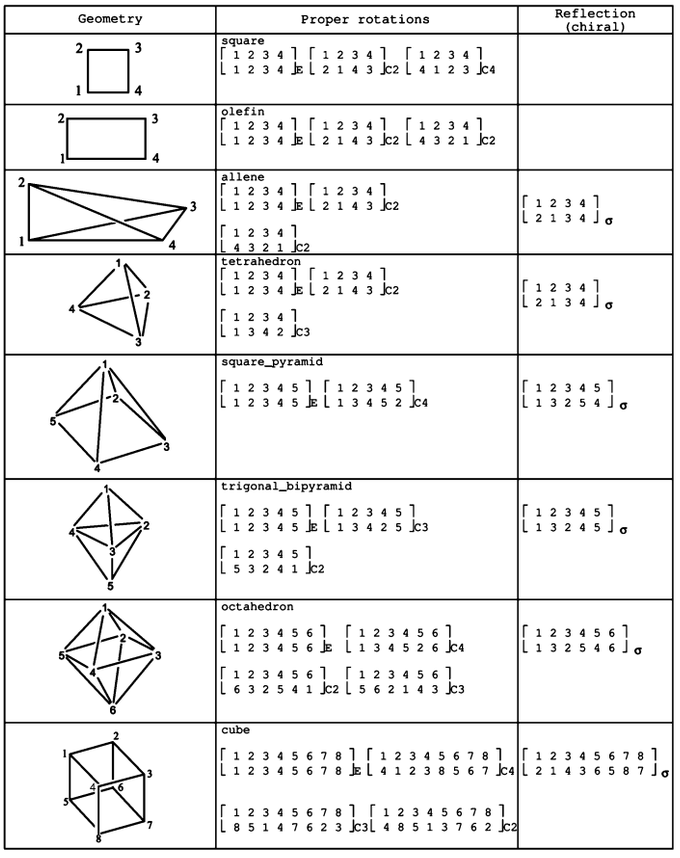

Fig. 2.4.8.2. Archetypal coordination geometries used in stereochemical definition of the MIF data item **_stereo_geometry**.

The stereogenic centre of a stereo group in a molecule has a relationship within that group that is specified by **_define_stereo_relationship**. Descriptions of the standard codes for **_define_stereo_relationship** are as follows.

absolute: The configuration of all stereogenic centres is exactly as described. This represents an enantiomerically pure compound with a known absolute configuration.

relative: The configuration of the stereogenic centres is only relative and the mirror reflection of the centres will also describe the same molecule. Only the configuration described in the MIF, or its mirror image, will be present in the molecule. This represents an enantiomerically pure compound with the described relative configuration.

racemic: The configuration of the stereogenic centres is only relative and the mirror reflection of the centres will also describe the same molecule. Both this configuration and its mirror image are present in a 1:1 ratio. This represents a racemic mixture of the molecule with the described relative configuration.

absolute_excess: The configuration of the stereogenic centres describes the absolute configuration of the excess component of a mixture of this configuration and its mirror reflection. This describes an enantiomeric excess in which the excess component has the described absolute configuration.

relative_excess: The configuration of the stereogenic centres is only relative. A mixture of this configuration and its mirror image is present, with one or other of the components in excess. This describes an enantiomeric excess mixture.

unknown: The configurational relationship between the stereogenic centres is not known.

The geometry of each stereogenic centre is described individually in terms of a prototype geometrical model. The basic principles of this approach have been described elsewhere (Barnard *et al.*, 1990). The eight geometries currently defined for the MIF data item **_stereo_geometry** are given in Fig. 2.4.8.2. They include the organic stereogenic geometries (the tetrahedron, the rectangular description of olefin-related compounds and the anti-rectangle used to describe allene-related systems) and the common archetypal metal coordination geometries (square planar, tetrahedral, trigonal bipyramidal, square pyramidal, octahedral and cubic). This list is non-exclusive and can be extended as required in later versions of the MIF dictionary.

The vertex site of the geometrical model must be occupied by either an atom, an explicit or implicit hydrogen atom, or by an explicitly declared electron pair. In each case, there exist permutations of the enumerated vertices that, if applied, do not change the meaning of the description of the relevant stereo element. Thus, the MIF does not define a canonical ordering for citing geometric vertices and the comparison of two geometries requires the use of the permutation operators. These permutations are also indicated in Fig. 2.4.8.2.

For each stereogenic centre (defined by a **_stereo_atom_id**, or by **_stereo_bond_id_1** and ***_2**), the atom sites forming the stereochemical element specified by a **_stereo_geometry** code are stored as a sequence of **_stereo_vertex_id** values. An example of the specification of absolute stereochemistry, including the ordered enumeration of the tetrahedral vertices for the four stereogenic centres, is given in Fig. 2.4.8.3. In this example, the null symbol (a period) is used to indicate an implicit hydrogen atom or an unshared electron pair.

2.4.9. MIF query applications

A MIF is suitable for interrogating databases because data items are permitted to have a single value, or a 'sequence' of alternative values. This latter option is designated by the dictionary attribute **_type_conditions** which, for MIF applications, is set to