```
data_cyclohexane

_molecule_name_common            cyclohexane

    loop_
        _atom_id
        _atom_type
        _atom_attach_h          1  C  2   2  C  2   3
                  C  2   4  C  2   5  C  2   6  C  2
loop_
    _bond_id_1
    _bond_id_2
    _bond_type_mif
           1 2 S  2 3 S  3 4 S  4 5 S  5 6 S  6 1 S

loop_
    _reference_conformation
                      $chair   $boat   $twisted_boat

save_chair
    loop_
        _atom_id
        _atom_coord_x
        _atom_coord_y
        _atom_coord_z     1   1.579  0.159  0.263
                          2   0.756  0.507 -0.986
                          3   0.825  0.493  1.541
                          4  -0.549 -0.131  1.590
                          5  -1.377  0.222  0.347
                          6  -0.626 -0.158 -0.937
save_

save_boat
    loop_
        _atom_id
        _atom_coord_x
        _atom_coord_y
        _atom_coord_z     1   1.657 -0.426  0.356
                          2   1.031  0.133 -0.927
                          3   0.960  0.133  1.602
                          4  -0.568 -0.040  1.558
                          5  -1.051 -0.738  0.279
                          6  -0.499 -0.028 -0.964
save_

save_twisted_boat
    loop_
        _atom_id
        _atom_coord_x
        _atom_coord_y
        _atom_coord_z     1   0.933  0.922  0.971
                          2   1.186  0.220 -0.368
                          3  -0.119  0.161  1.796
                          4  -1.135 -0.581  0.911
                          5  -1.371  0.181 -0.397
                          6  -0.083  0.236 -1.238
save_
```

Fig. 2.4.4.3. Atom and bond properties for cyclohexane, together with 3D coordinate representations of three alternative conformations: chair, boat and twisted boat.

2.4.4.5. Global blocks

A global block is similar to a data block except that it is opened with a `global_` statement and contains data that are common or 'default' to all subsequent data blocks in a file. Global data items remain active until re-specified in a subsequent data block or global block.

In some applications it may be efficient to place data that are common to all data blocks within a global block. In particular, save frames may be defined within global blocks and then referenced in subsequent data blocks [this statement corrects an error in Hall & Spadaccini (1994)]. Examples of global data are shown in Figs. 2.4.7.1 and 2.4.7.2, in which a variety of frequently referenced structural units are encapsulated within save frames specified in global blocks.

2.4.5. Atoms, bonds and molecular representations

The MIF dictionary (see Chapter 4.8) contains definitions of the principal data items needed to specify molecular connectivity and spatial representations. These definitions are grouped according to purpose or, as referred to in the DDL dictionary language (Hall & Cook, 1995), by category. Categories are formally specified in the MIF dictionary using the data attribute `_category` but they may also be identified from the data-name construction '`_<category>_<subcategory>_<descriptor>`'. Note that data items appearing in the same looped list must belong to the same category.

The values of some data items are restricted, by definition in the MIF dictionary, to standard codes or states. For example, the item `_bond_type_mif` can only have values `S`, `D`, `T` or `O` as in its dictionary definitions:

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

The MIF dictionary plays the important additional role of validating and standardizing data values. This is illustrated with the data item `_display_colour`, which identifies the colours of 'atom' and 'bond' graphical objects. The colour codes or states for this item are specified in its dictionary definitions as a set of permitted red/green/blue (RGB) ratios, and no other colours may be used in a MIF. This has the technical advantage of making colour states searchable for chemical applications.

Fig. 2.4.4.2 shows MIF data for the molecule (+)-3-bromocamphor. The 'atom' list contains the items `_atom_id`, `_atom_type` and `_atom_attach_h`, which identify the chemical properties of the atoms, plus the items `_atom_coord_x`, `*_y` and `*_z`, which specify the 3D molecular structure in Cartesian coordinates [these are taken from diffraction results (Allen & Rogers, 1970)]. The item `_atom_label` is also used with any graphical depiction of the 3D model. The 'bond' loop in this example uses the simple `_bond_type_mif` conventions described above. The data names needed to depict stereochemistry are discussed with examples (Figs. 2.4.8.1, 2.4.8.2 and 2.4.8.3) in Section 2.4.8.

The MIF approach to representing 2D chemical structure separates the specification of chemical atom and bond properties. This provides additional flexibility in the description of the graphical objects, such as atomic nodes and bonded connections. The MIF data required to generate a 2D chemical diagram are shown in Fig. 2.4.4.2. The diagram generated from this data will be in a display area of 500 × 500 coordinate units at a scale of 50 units per cm (the 2D chemical diagram shown in Fig. 2.4.4.2 is not to this scale). The default origin (the bottom left corner of the display area) can be specified with the item `_display_define_origin`. The data used to depict a 2D structure form a two-level loop with the 'atomic' graphical objects at level 1 and the 'bond' graphical objects at level 2. The item `_display_object` has the values '.' (null or no object), 'text' (an element or number string) or 'icon'. The size and colour of the atom site are specified with `_display_size` and `_display_colour`. The bonds connected to each atom site are specified as a sequence of `_display_conn_id` numbers (in loop level 2). These numbers must match one of the