

2. CONCEPTS AND SPECIFICATIONS

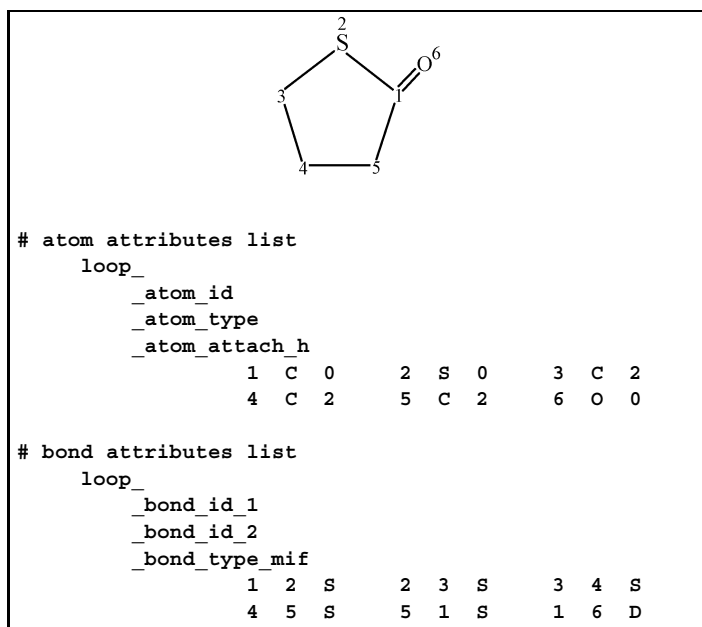


Fig. 2.4.4.1. MIF coding of atom and bond properties for thiabutylactone.

connections to atom sites 1 and 4 (the other connections to site 7 appear in the next two packets). Data items that appear in looped lists are identified in the MIF dictionary (see Chapter 4.8) as having the attribute `_list` set to either 'yes' or 'both'. Other relationships between looped data items are also specified in the dictionary.

2.4.4.3. Save frames

Save frames are employed in a MIF to encapsulate grouped data for efficient cross-referencing. If a set of data needs to appear repeatedly in a data application, it is efficient to place this data into an addressable save frame. Molecular fragments, such as amino-acid units, are a case in point. A save frame is bounded by the statement `save_framecode` and terminated by a `save_` statement. It can be referenced within the parent data block using the value `$framecode` where the `framecode` matches the string in the `save_framecode`. Note that all data names must be unique within a save frame, but the same data names may appear in other save frames or in the parent data block. Save frames may not contain other save frames but save-frame references (`$framecode`) may appear in other save frames.

Save frames can be used in a MIF for many purposes. A simple application, the storage of alternative 3D conformational representations describing cyclohexane, is illustrated in Fig. 2.4.4.3. Within the STAR syntax, save-frame references (`$framecode`) may occur before or after the save-frame definition within any data block. MIF preserves this basic STAR syntax. Save frames are particularly useful for defining commonly referenced structural templates and examples of this facility are discussed and illustrated (Figs. 2.4.7.1 and 2.4.7.2) in Section 2.4.7.

2.4.4.4. Data blocks

A data block is a sequence of unique data items or save frames. It is opened with a `data_blockcode` statement and closed by another data-block statement or a `global_` statement (see below). The `blockcode` string identifies the block within the file. Examples of data blocks are shown in Figs. 2.4.4.2, 2.4.4.3 and 2.4.6.1. Each data block in a file must have a unique `blockcode`.

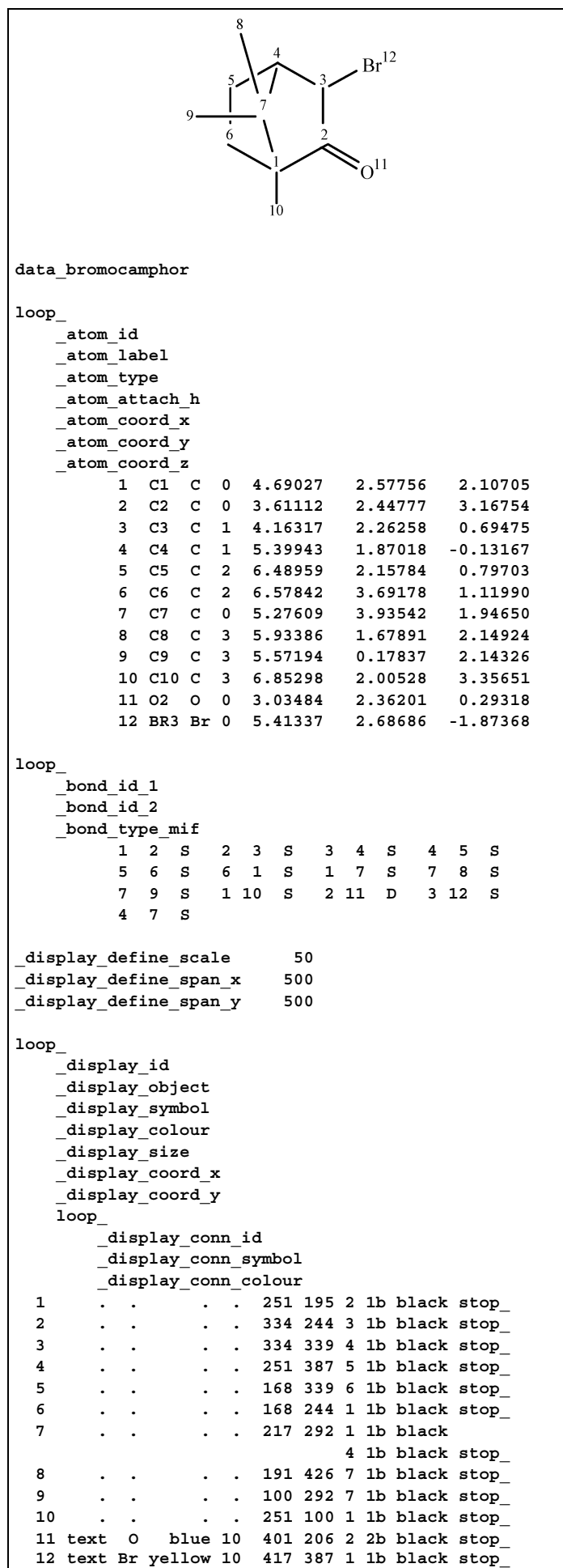


Fig. 2.4.4.2. MIF coding of atom properties (including 3D coordinates), bond properties and display information for (+)-3-bromocamphor.