

5. APPLICATIONS

```

data_mumbo_jumbo

_audit_creation_date          91-03-20
_audit_creation_method        from_xtal_archive_file_using_CIFIO
_audit_update_record
; 91-04-09                    text and data added by Tony Willis.
 91-04-15                    rec'd by co-editor with diagram as manuscript HL7
;
_dummy_test                   "rubbish to see what dict_ says"

_chemical_name_systematic
  trans-3-Benzoyl-2-(tert-butyl)-4-(iso-butyl)-1,3-oxazolidin-5-one
_chemical_formula_moiety      'C18 H25 N O3'
_chemical_formula_weight      303.40
_chemical_melting_point       ?

####_cell_length_a           5.959(1)
_cell_length_b                14.956(1)
_cell_length_c                19.737(3)
_cell_measurement_theta_min   25
_cell_measurement_theta_max   31
_symmetry_cell_setting        orthorhombic

loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_thermal_displace_type
_atom_site_calc_flag
  s .20200 .79800 .91667 .030(3) Uij ?
  o .49800 .49800 .66667 .02520 Uiso ?
  c1 .48800 .09600 .03800 .03170 Uiso ?

loop__blat1__blat2 1 2 3 4 5 6 a b c d 7 8 9 0

```

Fig. 5.4.9.2. Example CIF read by the sample program *CIF_IN* shown in Fig. 5.4.9.1.

```

CIFtbx warning: test.cif data_mumbo_jumbo line:      8
Data name _dummy_test not in dictionary!
CIFtbx warning: test.cif data_mumbo_jumbo line:     35
Data name _blat1 not in dictionary!
CIFtbx warning: test.cif data_mumbo_jumbo line:     35
Data name _blat2 not in dictionary!

Access items in data block  mumbo_jumbo

Cell dimension(s) missing!
Cell      0.0000  14.9560  19.7370  0.0000  0.0010  0.0030
Cell setting  orthorhombic

Next data name in CIF is  _atom_type_symbol

Audit record
 91-04-09                    text and data added by Tony Willis.
 91-04-15                    rec'd by co-editor with diagram as manuscript HL7

Atom sites
s      0.2020  0.7980  0.9167  0.0300
o      0.4980  0.4980  0.6667  0.0252
c1     0.4880  0.0960  0.0380  0.0317

```

Fig. 5.4.9.3. Printout from the example program *CIF_IN* run on the test file of Fig. 5.4.9.2.

CIFtbx error messages are in four parts: 'warning' or 'error' header line, the name of the file being processed, the current data block or save frame, and the line number. Another line contains the text of the message.

5.4.11.1. Fatal errors: array bounds

The following fatal messages are issued if the *CIFtbx* array bounds are exceeded. Operation terminates immediately. Array bounds can be adjusted by changing the *PARAMETER* values in

cifbx.sys. If the value of *MAXBUF* needs to be changed, the file *cifbx.cmv* must also be updated.

```

Input line_value > MAXBUF
Number of categories > NUMBLOCK
Number of data names > NUMBLOCK
Cifdic names > NUMDICT
Dictionary category names > NUMDICT
Items per loop packet > NUMITEM
Number of loop_s > NUMLOOP

```