

5.4. CIFTBX: FORTRAN TOOLS FOR MANIPULATING CIFS

```

C..... Open a new CIF
400   if(pfile_('test.new')) goto 450
      write(6,'(//a/)' ) ' Output CIF by this name exists already!'
      goto 500
C..... Request dictionary validation check
450   if(dict_('cif_core.dic','valid')) goto 460
      write(6,'(//a/)' ) ' Requested Core dictionary not present'
C..... Insert a data block code
460   f1 = pdata_('whoops_a_daisy')
C..... Enter various single data items to show how
      f1 = pchar_(' _audit_creation_method','using CIFTbx')
      f1 = pchar_(' _audit_creation_extra2','Terry O'Connell')
      f1 = pchar_(' _audit_creation_extra3','Terry O"Connell')
      f1 = ptext_(' _audit_creation_record',' Text data may be ')
      f1 = ptext_(' _audit_creation_record',' entered like this')
      f1 = ptext_(' _audit_creation_record',' or in a loop.')
      f1 = pnumb_(' _cell_measurement_temperature', 293., 0.)
      f1 = pnumb_(' _cell_volume', 1759.0, 13.)
      f1 = pnumb_(' _cell_length_b', 8.7535353524313,0.)
      f1 = pnumb_(' _cell_length_c', 19.737, .003)
C..... Enter some looped data
      f1 = ploop_(' _atom_type_symbol')
      f1 = ploop_(' _atom_type_oxidation_number')
      f1 = ploop_(' _atom_type_number_in_cell')
      do 470 i=1,3
        f1 = pchar_(' ',alpha(1:i))
        f1 = pnumb_(' ',float(i),float(i)*0.1)
470   f1 = pnumb_(' ',float(i)*8.64523,0.)
C..... Do it again but as contiguous data with text data
      f1 = ploop_(' _atom_site_label')
      f1 = ploop_(' _atom_site_occupancy')
      f1 = ploop_(' _some_silly_text')
      do 480 i=1,2
        f1 = pchar_(' ',alpha(1:i))
        f1 = pnumb_(' ',float(i),float(i)*0.1)
480   f1 = ptext_(' ',' Hi Ho the diddly oh!')
500   call close_

```

Fig. 5.4.10.1. Sample program to create a CIF.

```

data_whoops_a_daisy
_audit_creation_method      'using CIFTbx'
_audit_creation_extra2      'Terry O'Connell'      #< not in dictionary
_audit_creation_extra3      'Terry O"Connell'      #< not in dictionary
_audit_creation_record
;Text data may be
entered like this
or in a loop.
;
_cell_measurement_temperature 293
_cell_volume                  1759(13)
_cell_length_b                8.75354
_cell_length_c                19.737(3)
loop_
  _atom_type_symbol
  _atom_type_oxidation_number
  _atom_type_number_in_cell
    a          1.00(10)      8.64523
    ab         2.0(2)       17.2905
    abc        3.0(3)       25.9357
loop_
  _atom_site_label
  _atom_site_occupancy
  _some_silly_text           #< not in dictionary
    a          1.00(10)
;Hi Ho the diddly oh!
;
    ab         2.0(2)
;Hi Ho the diddly oh!
;

```

Fig. 5.4.10.2. Sample CIF created by the example program of Fig. 5.4.10.1.