```
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', 8.75353553524313,0.)
         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.