

## 5. APPLICATIONS

```

star_arc_qtest.cif
star_out_qtest.out

data_   #<< wild-card block name - accepts first

# request all fractional coord items
  _atom_site_fract_
  _atom_site_label
# capitals to test case insensitivity
  _atom_site_aniso_LABEL
# request something that is not in the CIF
  _dummy
  _atom_site_aniso_U_11

data_P6122
_       #<< this requests all data in this block

```

Fig. 5.3.5.1. An example request list for *QUASAR*.

```

data_P6122

loop_
  _atom_type_symbol
  _atom_type_oxidation_number
  _atom_type_number_in_cell
  # capitals to test case insensitivity
  _atom_type_scatter_dispersion_REAL
  _atom_type_scatter_dispersion_imag
  _atom_type_scatter_source
  S 0 6 .319 .557
      Int_Tab_Vol_III_p202_Tab._3.3.1a
  O 0 6 .047 .032
      Cromer,D.T. & Mann,J.B._1968_AC_A24,321.
  C 0 20 .017 .009
      Cromer,D.T. & Mann,J.B._1968_AC_A24,321.
  RU 0 1 -.105 3.296
      Cromer,D.T. & Mann,J.B._1968_AC_A24,321.

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
  _atom_site_calc_attached_atom
  _atom_site_type_symbol
  s .20200 .79800 .91667 .030(3) Uij ? ? s
  o .49800 .49800 .66667 .02520 Uiso ? ? o
  c1 .48800 .09600 .03800 .03170 Uiso ? ? c

loop_
  _atom_site_aniso_label
  _atom_site_aniso_U_11
  _atom_site_aniso_U_22
  _atom_site_aniso_U_33
  _atom_site_aniso_U_12
  _atom_site_aniso_U_13
  _atom_site_aniso_U_23
  _atom_site_aniso_type_symbol
  s .035(4) .025(3) .025(3) .013(1) .000 .000 s

```

Fig. 5.3.5.2. Example CIF for demonstrating the use of *QUASAR*.

The request list must specify the data block from which the requested data are to be extracted. Multiple data blocks may be requested in the same file. An entry 'data\_' operates as a wild

```

data_P6122

loop_
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_label
  .20200 .79800 .91667 s
  .49800 .49800 .66667 o
  .48800 .09600 .03800 c1

loop_
  _atom_site_aniso_label
  _dummy # requested item not present
  _atom_site_aniso_U_11
  s ? .035(4)

# -----end-of-data-block-----

data_P6122

loop_
  _atom_type_symbol
  _atom_type_oxidation_number
  _atom_type_number_in_cell
  _atom_type_scatter_dispersion_REAL
  _atom_type_scatter_dispersion_imag
  _atom_type_scatter_source
  S 0 6 .319 .557
      Int_Tab_Vol_III_p202_Tab._3.3.1a
  O 0 6 .047 .032
      Cromer,D.T. & Mann,J.B._1968_AC_A24,321.
  C 0 20 .017 .009
      Cromer,D.T. & Mann,J.B._1968_AC_A24,321.
  RU 0 1 -.105 3.296
      Cromer,D.T. & Mann,J.B._1968_AC_A24,321.

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
  _atom_site_calc_attached_atom
  _atom_site_type_symbol
  s .20200 .79800 .91667 .030(3) Uij ? ? s
  o .49800 .49800 .66667 .02520 Uiso ? ? o
  c1 .48800 .09600 .03800 .03170 Uiso ? ? c

loop_
  _atom_site_aniso_label
  _atom_site_aniso_U_11
  _atom_site_aniso_U_22
  _atom_site_aniso_U_33
  _atom_site_aniso_U_12
  _atom_site_aniso_U_13
  _atom_site_aniso_U_23
  _atom_site_aniso_type_symbol
  s .035(4) .025(3) .025(3) .013(1) .000 .000 s

# -----end-of-data-block-----

```

Fig. 5.3.5.3. Result of running *QUASAR* with the example request list of Fig. 5.3.5.1 on the CIF listed in Fig. 5.3.5.2.

card and indicates that requests should be served from the next data block encountered. In the example above, the first group of requests will be met from the first data block in the CIF; the second set from the data block named 'P6122' (if present).