```
data_BAWGEL
_audit_creation_date              93-05-24
_audit_creation_method            manual_conversion_of_ccdc_file
_audit_update_record
;  82-07-05  CCDC entry created from journal data
                      A.L.Spek,A.J.M.Duisenberg (1981) 189,10,1531
   93-05-21  Received file from Owen Johnson, CCDC.
   93-05-24  Initial conversion of the file to CIF/MIF format.
;
_chemical_name_systematic         'bis(Benzene)-chromium bromide'
_chemical_formula_moiety          'C12 H12 Cr1 1+,Br1 1-'

_cell_length_a                    9.735(6)
_cell_length_b                    9.316(3)
_cell_length_c                    11.941(8)
_cell_angle_alpha                 90
_cell_angle_beta                  90
_cell_angle_gamma                 90
_cell_formula_units_Z             4

_symmetry_space_group_name_H-M    Fmmm

loop_
    _symmetry_equiv_pos_as_xyz
        x,y,z x,1/2+y,1/2+z 1/2+x,y,1/2+z 1/2+x,1/2+y,z -x,y,z -x,1/2+y,1/2+z
        1/2-x,y,1/2+z 1/2-x,1/2+y,z  x,-y,z x,1/2-y,1/2+z 1/2+x,-y,1/2+z
        1/2+x,1/2-y,z -x,-y,z -x,1/2-y,1/2+z 1/2-x,-y,1/2+z 1/2-x,1/2-y,z

loop_
    _atom_type_symbol
    _atom_type_radius_bond
                           C 0.68   H 0.23   Br 1.21   Cr 1.35

_exptl_crystal_density_meas       1.764
_refine_ls_R_factor_obs           0.0540
_reflns_observed_criterion        3sigma(I)

loop_
    _atom_site_label
    _atom_site_fract_x
    _atom_site_fract_y
    _atom_site_fract_z
                      Cr1 0.0     0.0     0.0
                      Br1 0.0     0.0     0.50000
                      C1  0.06900 0.12800 0.13400
                      C2  0.13900 0.0     0.13400
                      H1  0.09300 0.20400 0.12500
                      H2  0.19800 0.0     0.13000
loop_
    _geom_bond_atom_site_label_1
    _geom_bond_atom_site_label_2
    _geom_bond_distance
    _geom_bond_site_symmetry_1
    _geom_bond_site_symmetry_2

                         Cr1 C1 2.100  .   .
                         Cr1 C2 2.090  .   .
                         C1  C1 1.340  .   5_555
                         C1  C2 1.370  .   .
                         C1  H1 0.760  .   .
                         C2  H2 0.580  .   .
```

Fig. 1.1.6.2. Example 2 of a CIF (using the same data as shown in Fig.1.1.3.2).

### 1.1.7. The Crystallographic Information File

As outlined in Section 1.1.6, the working group commissioned by the WPCI set out to establish an exchange protocol suitable for submitting crystallographic data to journals and databases, and this resulted in the development of the CIF syntax. At the same time, the group was also asked to form a list of those data items considered to be essential in a manuscript submitted to *Acta Crystallographica*. The data items originally recommended are listed in Fig. 1.1.7.1.

The syntax of a CIF (a detailed description is given in Chapter 2.2) was intentionally a simple subset of the STAR File syntax (see Chapter 2.1 for details). This simplification was considered important for its easy implementation in existing crystallographic software packages – clearly a primary goal for any format that was to be widely available for submitting data to journals and databases.

A compilation of data names referring to specific quantities or concepts in a crystal-structure determination was drawn up. This compilation included the items already identified as necessary for publication and many more besides. As a list of standard tags intended for unambiguous use, the collection was known from the outset as a *dictionary* of data names.

```
# The following CIF data names encompass the IUCr Journals Commission
# requirements for the reporting of a small-molecule structure in Acta
# Crystallographica, Section C

_chemical_compound_source
_chemical_formula_sum
_chemical_formula_moiety
_chemical_formula_weight
_symmetry_cell_setting
_symmetry_space_group_name_H-M
_cell_length_a
_cell_length_b
_cell_length_c
_cell_angle_alpha
_cell_angle_beta
_cell_angle_gamma
_cell_volume
_cell_formula_units_Z
_exptl_crystal_density_diffrn
_exptl_crystal_density_meas
_exptl_crystal_density_method
_diffrn_radiation_type
_diffrn_radiation_wavelength
_cell_measurement_reflns_used
_cell_measurement_theta_min
_cell_measurement_theta_max
_exptl_absorpt_coefficient_mu
_cell_measurement_temperature
_exptl_crystal_description
_exptl_crystal_colour
_exptl_crystal_size_max
_exptl_crystal_size_mid
_exptl_crystal_size_min
_exptl_crystal_size_rad
_diffrn_measurement_device
_diffrn_measurement_method
_exptl_absorpt_correction_type
_exptl_absorpt_correction_T_min
_exptl_absorpt_correction_T_max
_diffrn_reflns_number
_reflns_number_total
_reflns_number_observed
_reflns_observed_criterion
_diffrn_reflns_av_R_equivalents
_diffrn_reflns_theta_max
_diffrn_reflns_limit_h_min
_diffrn_reflns_limit_h_max
_diffrn_reflns_limit_k_min
_diffrn_reflns_limit_k_max
_diffrn_reflns_limit_l_min
_diffrn_reflns_limit_l_max
_diffrn_standards_number
_diffrn_standards_interval_count
_diffrn_standards_interval_time
_diffrn_standards_decay_%
_refine_ls_structure_factor_coef
_refine_ls_R_factor_obs
_refine_ls_wR_factor_obs
_refine_ls_goodness_of_fit_obs
_refine_ls_number_reflns
_refine_ls_number_parameters
_refine_ls_hydrogen_treatment
_refine_ls_weighting_scheme
_refine_ls_shift/esd_max
_refine_diff_density_max
_refine_diff_density_min
_refine_ls_extinction_method
_refine_ls_extinction_coef
_atom_type_scat_source
_refine_ls_abs_structure_details
_computing_data_collection
_computing_cell_refinement
_computing_data_reduction
_computing_structure_solution
_computing_structure_refinement
_computing_molecular_graphics
_computing_publication_material
_publ_section_experimental
```

Fig. 1.1.7.1. Initial set of data items considered to be essential in a structure report submitted to *Acta Crystallographica Section C*.

The WPCI proposed the CIF format as a standard exchange protocol at the open meetings of the IUCr Commissions on Crystallographic Data and Computing at the 1990 XVth IUCr Congress in Bordeaux. The proposal was accepted and the CIF format was subsequently adopted by the IUCr as the preferred format for data exchange (Hall *et al.*, 1991).

The administration of the CIF standard, including the approval of new data items, is the responsibility of the IUCr Committee for the Maintenance of the CIF Standard (COMCIFS). This committee plays a central role in the coordination of CIF activities, such as the creation of new dictionaries for defining crystallographic data items and the updating of data definitions in existing dictionaries. Chapter 3.1 describes relevant aspects of its role in the