Structure validation: CIF

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CIF Data Items: Core Dictionary

_cell_measurement_pressure
pressure in kilopascals at which unit cell parameters were measured

_diffrn_ambient_pressure
mean hydrostatic pressure in kilopascals at which diffraction
intensities were measured

_diffrn_ambient_pressure_gt; _diffrn_ambient_pressure_lt
mean hydrostatic pressure in kilopascals above which (*_gt) or
below which (*_lt) the intensities were measured

_exptl_crystal_pressure history
relevant details concerning the pressure history of a sample

Powder CIF-Dictionary

_pd_prep_pressure
  preparation pressure of the sample in kilopascals

Modulated Structures CIF- Dictionary

_cell_wave_vectors_pressure_max
_cell_wave_vectors_pressure_min
  maximum and minimum values of the pressure in kilopascals
  defining the interval within which the modulation wave vector(s)
  were measured

Cif data items: Macromolecular Cif-Dictionary

_cell_measurement.pressure
_diffrn.ambient_pressure
_diffrn.ambient_pressure_gt
_diffrn.ambient_pressure_lt

_cell_measurement.pressure_esd
standard deviation of _cell_measurement.pressure

_diffrn.ambient_pressure_esd
standard deviation of diffrn.ambient_pressure

_exptl_crystal_grow.pressure
ambient pressure in kilopascals at which the crystal was grown

_exptl_crystal_grow.pressure_esd
standard deviation of exptl_crystal_grow.pressure

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Alerts of level A   (they have to be answered…)

PROBLEM: _diffrn_reflns_theta_full (too) Low ....   12.64 Deg.
RESPONSE: Due to limited opening angle of the diamond anvil cell.

PROBLEM: _diffrn_measured_fraction_theta_full Low 0.43
RESPONSE: Due to limited opening angle of the diamond anvil cell.

ALERT C, G   (warning messages)

- The value of R(int) is greater than 0.12
  R(int) given 0.131

- Expected hkl max differ from CIF values
  From the CIF: _diffrn_reflns_theta_max 28.29
  From the CIF: _reflns_number_total 461
  From the CIF: _diffrn_reflns_limit_ max hkl 6. 9. 9.
  From the CIF: _diffrn_reflns_limit_ min hkl -7. -9. -9.
  TEST1: Expected hkl limits for theta max
  Calculated maximum hkl 9. 11. 9.
  Calculated minimum hkl -9. -11. -9.