

Chapter 9.1

GEOM

P.R. MALLINSON AND K.W. MUIR,
DEPARTMENT OF CHEMISTRY,
UNIVERSITY OF GLASGOW,
GLASGOW G12 8QQ

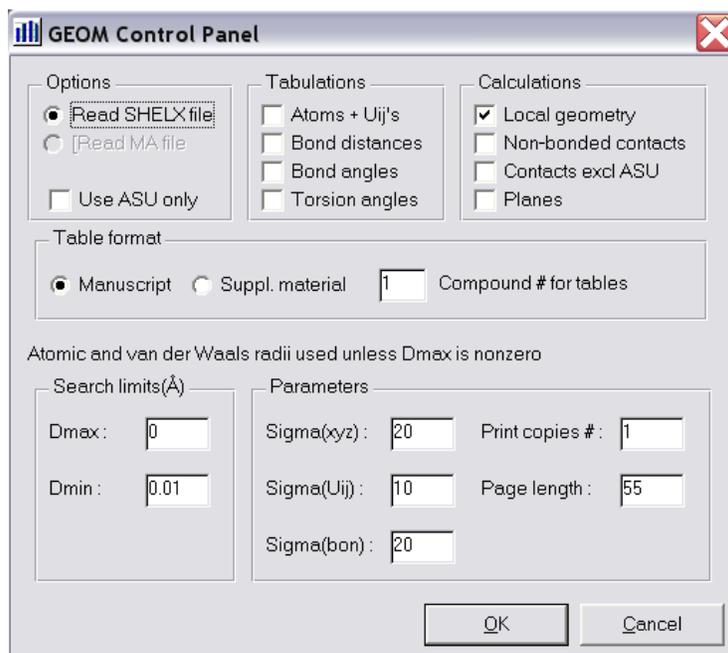
This program is designed to produce easily-readable listings of the local geometry at each atom, intermolecular contacts, and mean planes, with tabulation of atomic parameters, bond lengths, angles and torsion angles (all with e.s.d.'s) in appropriate form for report generation. The tables are written to a file TABLES.LST, which may be edited before printing. Complete bond and angle tables are obtained, even when molecular symmetry is present. In this case, the asymmetric unit should be a connected set of atoms (use Model-Assemble Residues in SXGRAPH) to ensure that all torsion angles are generated.

Crystallographic data are obtained from the WinGX system's crystal model file (name.INS or name.RES), or preferably from the file SHELXL.LST which contains the least squares errors.

The available options are:

- Tables with ATOMS, BONDS, ANGLES, TORSION_ANGLES
- Listings of LOCAL_GEOMETRY, NON-BONDED_DISTANCES, CONTACTS
- Least squares PLANES

The commands are entered via a GUI shown below



Clicking the **OK** button starts execution of the program. The results are in the files GEOM.LST (which is automatically opened) and optionally TABLES.LST. The meaning of the parameters and options are given below :

9.1.1 ATOMS sig(xyz) limit sig(Uij) limit

Makes a publication listing of atomic coordinates and temperature factors, e.s.d.'s in the least significant digits in parentheses. Temperature factors for isotropic atoms appear alongside the coordinates, also the equivalent isotropic temperature factor for anisotropic atoms. Anisotropic temperature factors are always tabulated separately from the coordinates. The two parameters control the the automatic rounding of coordinated and thermal parameters respectively, according to their precision. The desired upper limit of the e.s.d. in the least significant digit is given, default limits being 20 for coordinate e.s.d. and 10 for temperature factors e.s.d.

9.1.2 BONDS sig(bond length) limit dmax dmin

Makes a publication listing of bond lengths, with e.s.d. in the least significant digits in parentheses. The first parameter is the desired upper limit of the e.s.d. for controlling the automatic rounding of the bond lengths according to precision, the default limit being 10. Bonds are defined as distances up to the sum of the covalent radii (obtained from the crystal model file or system databank file), unless *dmax* is given. In that case bonds are distances up to *dmax*, or between *dmin* and *dmax* if *dmin* is given.

9.1.3 ANGLES dmax dmin

Makes a publication listing of bond angles, with e.s.d. in the least significant digits in parentheses. The parameters *dmax* and *dmin* have the same significance as in the BONDS command, covalent radii being used by default

9.1.4 TORSION_ANGLES dmax dmin

Makes a publication listing of torsion angles, with e.s.d. in the least significant digits in parentheses. The parameters *dmax* and *dmin* have the same significance as in the BONDS command, covalent radii being used by default. The e.s.d. are computed from the formula of Huber-Buser and Dunitz, 1961 and Stanford and Waser, 1972.

9.1.5 LOCAL_GEOMETRY dmax dmin

Makes an atom-by-atom listing of bond lengths and angles with e.s.d., showing the symmetry transformations, lattice translations and equivalent position coordinates for bonded atoms in different asymmetric units. The parameters *dmax* and *dmin* have the same significance as in the BONDS command, covalent radii being use by default.

9.1.6 NON-BONDED_DISTANCES dmax dmin

Makes a listing of unique interatomic distances with e.s.d. (excluding bonds) up to the sum of the van der Waals radii, showing symmetry transformations, lattice translations and equivalent position coordinates. Contacts are defined by the covalent and van der Waals radii, unless *dmax* is nonzero. In that case contacts are distances between the sum of the covalent radii and *dmax*, or between *dmin* and *dmax* if *dmin* is also given. The search algorithm is described by Rollett, 1965.

9.1.7 CONTACTS dmax dmin

Same as NON-BONDED CONTACTS but excludes distances between atoms in the same asymmetric unit, i.e. those related by the identity symmetry operation and zero lattice translations.

9.1.8 PLANES

Computes mean planes of groups of up to 20 atoms. The program prompts the user to type the atom labels, and asks whether the atoms are to be weighted according to the precision of their positions or whether unit weights are required. There follows a prompt for the option to include in the mean plane atoms related by a center of symmetry at the crystallographic origin, in which case only the atoms in the asymmetric unit need to be specified. In groups with any other symmetry, all equivalent positions of the atoms must be present in the model file and explicitly referenced in the groups contents. Also, all atoms in a group must be in the same asymmetric unit, since no symmetry transformations or lattice translations are applied. The mean plane is defined as the plane at right angles to the groups axis of highest moment of inertia, which is the eigenvector of the tensor of inertia. The weighted sum of squared deviations of the atoms from the plane is minimised. If only two atom labels are given, the angle between the line so defined and all other lines and plane normals are calculated.

9.1.9 PAGE_LENGTH

Controls the number of lines per page in the publication listing of atom parameters, bond lengths, bond angles and torsion angles

9.1.10 ASYMMETRIC

This forces bonds *etc* for the complete molecule to be calculated, if the asymmetric unit does not describe a complete molecule.

9.1.11 Use MA file

This allows the user to open a GX style file, *name.MA* which contains the coordinate su's.

9.1.12 Correlations

This has no effect in WinGX.

9.1.13 Sig(xyz), Sig(Uij), Sig(Bon)

These parameters control the automatic rounding of values and their su's.

9.1.14 DMAX, DMIN

These set the limits of searching for bonds, angles *etc* ; if DMAX is set to zero (the default action), then the atomic and Van der Waals radii held internally by WinGX are used - these may be modified *for the current session only* by using the Model-Database menu item for a particular element(s).