Supplementary Materials: Charge Distribution and Bond Valence Sum Analysis of Sulfosalts. The ECoN21 computer program.

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The Code Units Used by the ECoN21 Program

ECoN21.pas

The main body of the program. It contains the reaction to mouse and keyboard events in the main window and handles the calls of procedures and functions for specific calculations by other units. What it does:

- retrieves and displays data read from the chosen CIF file
- sorts and groups the atoms
- merges atoms in   isomorphic   positions and calculates the site populations
- generates atoms by symmetry
- builds the atom records
- sets the calculation stages
- handles the options for calculation and for listing of results

This unit builds the main window of the interface:
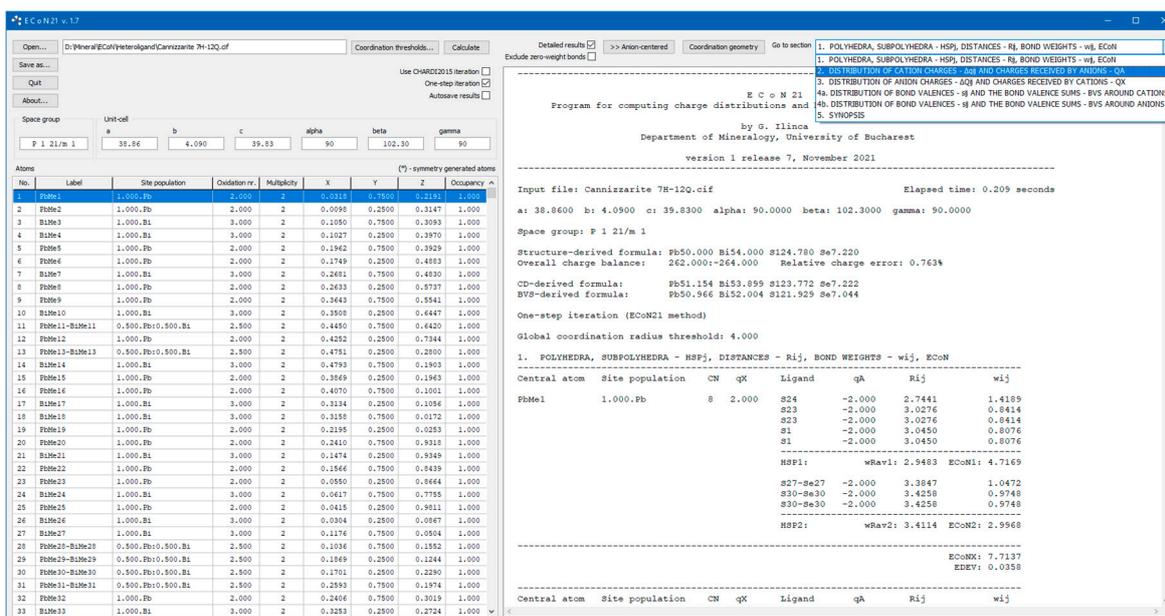
The main unit invokes calculation routines located in the units described further on (not included in the supplementary materials).

MainCalc.pas

The unit containing the bulk of the charge distribution and bond valence sum computation. Contains procedures for sorting arrays, string handling, string-number conversion and back, formatting of numbers etc. The unit includes initialization routines and the calculation of :

- bond lengths and coordination numbers
- homoligand subpolyhedra
- orthogonalization matrix and orthogonal coordinates
- iterated weighted bond averages

- bond weights and ECoN
- bond valence sums
- deviation of ECoN from CNR
- Baur and Brown distortion indexes
- (iterated) charge distribution
- structure-derived formula
- charge balance
- charge distribution- and BVS-derived formulas
- mean average percentage deviations of computed charges and BVS
- global stability index

Poly.pas

The unit contains the procedures and functions for the analysis of coordination geometry. The following calculations are made by this unit:

- number of coordination polyhedra faces
- standard deviations of bond lengths
- polyhedral volumes
- coordinates of the centroids
- displacements of centroids from central atoms
- components of the vector defined by the central atom and the centroid
- radii and volumes of least-squares fitted spheres
- standard deviations of distances between centroids and ligands
- linear and volume-based eccentricities
- linear and volume-based sphericities
- volumes of ideal coordination polyhedra
- volume distortions of the coordination polyhedra

CalcExpress.pas (version 1.7, freeware by AidAim software:
https://www.aidaim.com/products/download.php)

Mathematical expression parser used for generating atom coordinates from symmetry operations.

Bonds.pas

Builds and handles the dialog for setting global, bond- and polyhedron-specific coordination radius thresholds.
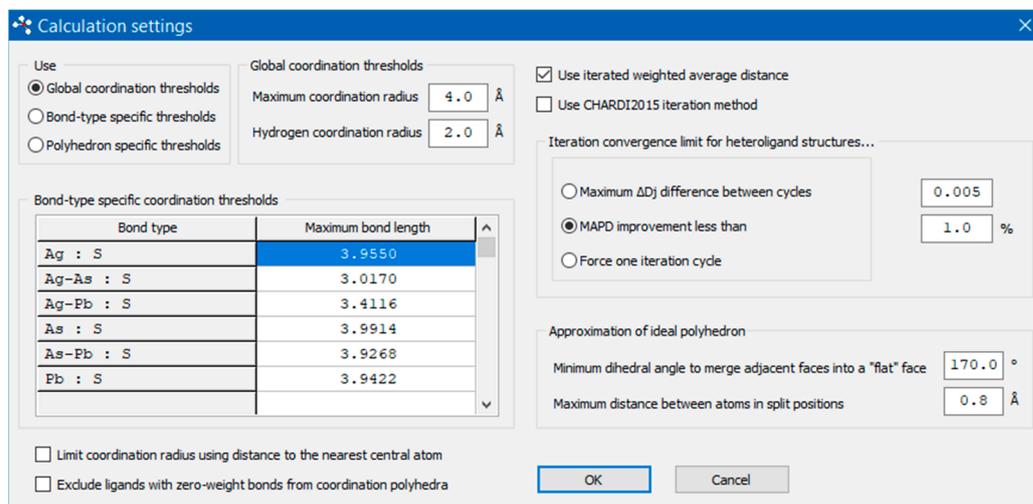
The dialog handles options for limiting the coordination sphere using the distance to the nearest neighboring central atom and for excluding zero-weight bonds from the

coordination polyhedra. Contains an option for adjusting the minimum dihedral angle between adjacent faces of the coordination polyhedra as well as the maximum distance between atoms in binary split positions. These options determine the approximation of ideal coordination polyhedra.

ManCoord.pas

　　　Contains the dialog and procedures for the manual setting of coordination. The dialog opens when the 'Polyhedron specific threshold' radio button in the Coordination thresholds dialog is checked. For each central atom, a list of distances to nearest ligands and neighboring central atoms is displayed. The coordination limit is set by double-clicking on what is to be considered most distant ligand in the coordination polyhedron.
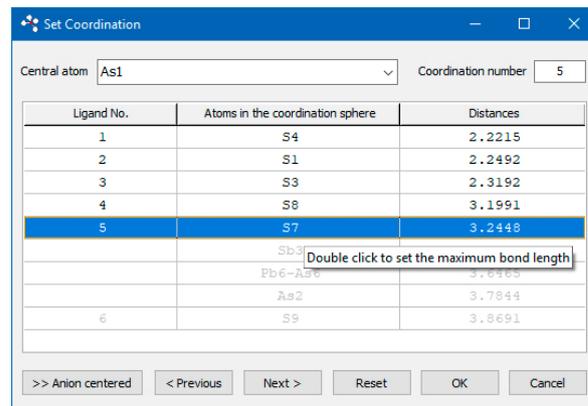
Results.pas

　　　The unit controls the formatting of tables listing various types of results: detailed or summary lists of charge distribution and bond valence sums or detailed or summary lists of quantities describing the coordination geometry.

About.pas

　　　Displays program version and authorship information.