Computation of bond valence parameters with CompBV

- You may register and compute bond valence parameters according to choices you make for the selection of data used in computation and for the optimization algorithm.
- If you agree explicitly your results can be seen by other users of the system.
- It is possible to check optimization results by considering the graph of the function which computes the absolute deviation (alternatively the root mean square) of the bond valence sum from the expected value for a net of r0,b values. This net can be specified by choosing minimal and maximal values for r0 and b as well as the size of steps.

The current basis of computation of parameters is a database with data derived from 31011 structures contained in the ICSD database as of Version 2016 [1].
Data of the ICSD database have been filtered as follows:
- years: 1950-2016
- temperature: 273K-313K
- pressure: 0.095MPa-0.11MPa
- R-value: ≤ 0.15
- minimal occupation: 100%
- maximal bond distance (cutoff distance): 3.6 Å

In case non integer or zero values are given for the oxidation numbers of atoms in crystal structure data, an algorithm described in [2] is used to determine integer oxidation numbers. If this proceeding has no success, data of the corresponding structure are not considered. If integer values are available for all atoms of a structure, coordination polyhedra are looked for using the linear gap method [3][4] and a method using a convex hull algorithm [4]. Results are stored in different databases. We have implemented also other methods such as 'quadratic gap' [4] but in the current version we only offer the two methods just mentioned.
A coordination polyhedron is accepted if it is homogeneous insofar as all ligands are atoms of the same element. No coordinates are stored for the cation and its ligands but only distances.
Bond valence parameters can be computed for a pair of elements and oxidation numbers by creating an appropriate job. After having selected interactively a pair of elements from a representation of the periodic table of elements and appropriate oxidation numbers from a list, filters can be specified restricting the set of polyhedra to be chosen for computation. The user can decide whether polyhedra computed by the linear gap method or by the convex hull algorithm are taken into account. Furthermore, conditions for the form of polyhedra to be used for optimization can be specified. If 'none' is chosen, all polyhedra of the selected database are considered. In case of 'minimum' it is checked whether all ligands of a polyhedron have the same distance to the cation. If 'strict' is claimed by the user, all ligands have to be symmetrically equivalent (this condition is easy to check with an SQL-query but discards a few polyhedra with high symmetry, e.g. the Ba-O polyhedron in CC 180203).
It is possible to ask for parameter values by providing a pair of elements together with oxidation numbers as cation and anion. These data can be filled in arbitrary order. When typing in values corresponding results are shown immediately; hence collections of all available parameter values can be obtained for single elements or elements with oxidation numbers.
In the result, information is given about the user who initiated the computation. Furthermore, the parameters of the optimization method are provided together with some information on the run of the chosen method such as the number of polyhedra involved and the number of iterations in case of the application of simulated annealing.
In the result, a link is included to a page which allows to investigate the graph of the function mentioned at the beginning.

References

[1] Fachinformationszentrum Karlsruhe: ICSD, https://icsd.fiz-karlsruhe.de, 2016

[2] F. Liebau, H.-J. Klein, X. Wang: A crystal chemical approach to superconductivity. I. A bond-valence sum analysis of inorganic compounds, Z. Kristallogr. 226 (2011) 309-318, Oldenbourg Wissenschaftsverlag, München

[3] E. Prince (Ed.): International Tables for Crystallography - Vol. C Part 9, online edition, Springer, 2006

[4] H.-J. Klein, C. Mennerich: Searching similar clusters of polyhedra in crystallographic databases, Int. J. on Advances in Systems and Measurements 2 (2&3), pp. 192-203, 2009