should be followed by a full search for homometric pairs within the appropriate subset.

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A Method for Calculating Bond Valences in Crystals

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Abstract

A method of calculating the expected bond valences from the connectivity matrix of complex crystals is described. The method is exact (does not require iteration) and is suitable for implementation on a microcomputer.

Introduction

A major advance in inorganic solid-state chemistry has been the development of the bond valence method for predicting and interpreting bond lengths in crystals. In this method valences are assigned to each bond in the crystal and then, from known correlations (Brown & Altermatt, 1985; Brese & O'Keeffe, 1990) between bond valence and bond lengths, the expected bond lengths can be calculated. Alternatively, observed bond lengths can be interpreted in terms of valences. The method, and its historical development, is now well documented (*e.g.* Brown, 1981; O'Keeffe, 1989) and its advantages over other methods (such as using sums of radii) for predicting bond lengths in crystals are well established. This paper is concerned with an algorithm for implementing the method for predicting bond lengths in complex crystals.

The discussion here is restricted to crystals in which there are bonds only between 'cations' and 'anions' (named as such merely for convenience). Let there be m crystallographically distinct cations and n crystallographically distinct anions. Then we recognize the possibility of there being as many as mn kinds of bond, each of which may, in principle have a different valence.

The sum of the individual valences (v) of the bonds from each atom must be equal to the total atom valence (V), so there will be $m+n-1$ independent sums of the sort

$$\sum_j v_{ij} = V_i. \quad (1)$$

However, if we had mn bonds there would be $mn-m-n+1=(m-1)(n-1)$ degrees of freedom remaining. It may be seen then that, for $m, n>1$, in general bond valence sums do not suffice to determine individual bond valences.

A solution to this problem was proposed by Brown (1977) who suggested that individual valences should be made as nearly as possible equal to each other, subject to the bond valence constraints. Brown developed an iterative method to implement this idea and showed that bond lengths predicted were generally in excellent agreement with those observed. Brown (1987) also remarked that it should be profitable to pursue the apparent similarity (Mackay & Finney, 1973) of a bond valence network to electrical circuits to which Kirchhoff's laws may be applied. This analogy is somewhat misleading (O'Keeffe, 1989); nevertheless the idea is very fruitful and leads to an algorithm for direct computation of valences in complex crystals which overcomes the

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difficulties identified by Brown (1987) and which is now described.

Valence constraints from the connectivity matrix

The connectivity matrix as used here is an $m \times n$ matrix in which the entries are the number of bonds between atoms. An example, that of $CaAl_{12}O_{19}$ (Wagner & O'Keeffe, 1988), is given in Fig. 1. From the matrix, reading across one can see that Al(1) is bonded to 2 O(1), 2 O(2), 1 O(3) and 1 O(4), and reading down that O(1) is bonded to 2 Al(1), 1 Al(2) and 1 Al(4) *etc.*

Consider now a general case where cations A and B are both bonded to anions X and Y. The Brown *Ansatz* requires that $v_{AX} - v_{AY}$ and $v_{BX} - v_{BY}$ be as small as possible. It may be shown (O'Keeffe, 1989) that when valence constraints are taken into account, this condition may be written

$$v_{AX} - v_{AY} + v_{BY} - v_{BX} = 0. \qquad (2)$$

Equation (2) is equivalent to setting to zero the sum of valences (taken with alternating signs) around a ring A-X-B-Y in the structure. However such a *ring* need not actually occur in the crystal, but a *circuit* of this type will occur in the connectivity matrix as illustrated below.

Equation (2) is rewritten in the form

$$(v_{AX} - v_{AY}) = (v_{BX} - v_{BY}) \qquad (3)$$

to emphasize that we are requiring the differences in the valences from A to be equal to the differences in valences from B. A better approach (O'Keeffe, 1989) includes weights (discussed below) to take into account that the average valence of bonds from A may be very different from the average valence of bonds from B; *i.e.*

$$(v_{AX} - v_{AY})/s_A = (v_{BX} - v_{BY})/s_B. \qquad (4)$$

	6O(1)	6O(2)	2O(3)	2O(4)	3O(5)
Ca	·	6	·	·	6
6Al(1)	12	12	6	6	·
2Al(2)	6	·	2	·	·
2Al(3)	·	6	·	·	6
Al(4)	6	·	·	·	·
Al(5)	·	·	·	2	3

(*a*)

	O(1)	O(3)	O(2)	O(5)	O(4)
Al(2)	α	β	·	·	·
Al(1)	γ	δ	ε	·	ζ
Al(5)	·	·	·	η	θ
Ca	·	·	ι	κ	·
Al(3)	·	·	λ	μ	·
Al(4)	ν	·	·	·	·

(*b*)

Fig. 1. (*a*) Connectivity matrix for $CaAl_{12}O_{19}$. (*b*) Rearranged connectivity matrix.

If atom A is bonded to X and Y, atom B is bonded to X and Z and atom C is bonded to Y and Z, the equation corresponding to (2) is

$$v_{AX} - v_{AY} + v_{CY} - v_{CZ} + v_{BZ} - v_{BX} = 0. \qquad (5)$$

This corresponds to a vector sum now around a ring X-A-Y-C-Z-B but again such a ring need not occur in the crystal structure, although a corresponding circuit will appear in the connectivity matrix. With weights, (5) becomes by analogy with (4)

$$(v_{AX} - v_{AY})/s_A + (v_{CY} - v_{CZ})/s_c + (v_{BZ} - v_{BX})/s_B = 0. \qquad (6)$$

One can continue with equations involving $2r$-rings ($r = 4, 5, \ldots$) but in practice I have rarely come across a crystal structure which required consideration of equations with $r > 3$. Equations of the type (4) and (6) are here called circuit equations.

An important point is that the bond valence constraints [(1)] taken with the circuit equations [*e.g.* (4) and (6)] always constitute a set of linear equations that have a unique set of solutions for the bond valences for a structure (O'Keeffe, 1989). This paper is concerned with developing a procedure to identify rapidly the circuit equations - the bond valence sums are of course trivially written down - and then solving for the valences. I first illustrate the procedure for $CaAl_{12}O_{19}$.

For convenience in exposition, the connectivity matrix is rearranged as in Fig. 1(*b*), with the entries being symbols for the magnitudes of the bond valences [thus $\alpha = v_{Al(2)O(1)}$]. It may be seen that $CaAl_{12}O_{19}$ contains 11 different kinds of atom and 13 kinds of bond (valences α–ν). There are ten independent valence sums so three *independent* equations of the type (3) and (5) are needed. These can be read off the connectivity matrix in Fig. 1(*b*) as follows. The four-membered circuits are $\alpha\beta\delta\gamma$ and $\iota\kappa\mu\lambda$. The six-membered circuits are $\varepsilon\zeta\theta\eta\kappa\iota$ and $\varepsilon\zeta\theta\eta\mu\lambda$. From these we have [with s_1 to s_5 being weights associated with bonds from Al(2), Al(1), Al(5), Ca and Al(3) respectively]

$$(\alpha - \beta)/s_1 + (\delta - \gamma)/s_2 = 0 \qquad (a)$$

$$(\iota - \kappa)/s_4 + (\mu - \lambda)/s_5 = 0 \qquad (b)$$

$$(\varepsilon - \zeta)/s_2 + (\theta - \eta)/s_3 + (\kappa - \iota)/s_4 = 0 \qquad (c)$$

$$(\varepsilon - \zeta)/s_2 + (\theta - \eta)/s_3 + (\mu - \lambda)/s_5 = 0. \qquad (d)$$

It should be clear that $(d) = (b) + (c)$ so we have three independent equations. These three, combined with the ten independent valence-sum equations, provide a set of 13 linear equations for the 13 valences.

A computational strategy for complex crystals

The equations in the above example were readily obtained by inspection, and the resulting equations can be solved by hand, but the problem becomes more suitable for computer methods for more complex crystals.

In a matrix of size $m \times n$ one has the possibility of as many as mn non-zero entries. If there are no non-zero entries it may be fairly easily (but not simply) shown that the number of $2r$ circuits that do not contain $2(r-1)$ or smaller circuits is

$$N_r = m!n!/[2r(m-r)!(n-r)!]. \qquad (7)$$

This number is much greater than the number of independent equations needed which is $(m-1) \times (n-1)$ in the case of all non-zero entries. In a real crystal structure, coordination numbers are usually rather small (say 2-12) so the number of non-zero entries in the connectivity matrix of a complex crystal is much less than the possible number. The number of circuits is correspondingly drastically reduced.

As an example of a complex crystal I use the structure of $BaGe_2O_5$ II (Ozima, 1985) for which $m = 13$ and $n = 20$. Thus there are 33 crystallographically distinct atoms in the structure. If every cation were bonded to every anion there would be $13 \times 20 = 260$ bonds and $13 \times 12 \times 20 \times 19/4 = 14\,820$ four-membered circuits and $13 \times 12 \times 11 \times 20 \times 19 \times 18/6 = 1\,956\,240$ six-membered circuits. In fact the number of distinct bonds is 76. Thus one needs $76 - 32 = 44$ circuit equations. It transpires that there are 74 four-membered circuits, but these do not yield 44 independent equations, so one must include six-membered circuits of which there are 695. One then has $33 + 74 + 695 = 802$ equations which in fact have a unique solution for the 76 individual bond valences.

The numbers given above suggest an appropriate strategy for computing. First the connectivity matrix is derived (for the purpose of this paper that may be taken as given) and the bond valence sum equations set out. The connectivity matrix is then scanned for four-membered circuits (this will take of the order of N_2 loops) and the circuit equations tested for a unique solution. This is most conveniently done *via* a singular value decomposition (SVD) of the matrix of coefficients. I use the algorithms *SVDCMP* and *SVBKSB* presented by Press, Flannery, Teukolsky & Vetterling (1986) which appear to be very stable. If there is a unique solution (it should be stressed that the problem is never overdetermined) then the problem is finished as the SVD leads directly to the required bond valences. If there is not a unique solution then the connectivity matrix is scanned for six-membered circuits (now requiring the much larger number of N_3 loops) and again a SVD is used to search for a unique solution. I have not yet found a non-trivial crystal structure which requires eight-membered circuits (it would require that the structure contain at least eight-membered rings in which every atom were of a different kind, and at the same time the absence of smaller rings involving all these atoms*).

This method, which however requires a lot of storage for a large problem, appears to be much more efficient in time than any procedure that culls redundant equations before attempting their solution.

The example of $BaGe_2O_5$ given above is probably as complex as one is likely to meet in practice. Using a microcomputer (Macintosh II) it takes approximately 20 min to find the six-membered circuits and 20 min for the SVD of the 802×76 matrix and obtaining the valences. As the time required scales roughly as $(mn)^3$, this size of problem is near the practical limit for the present generation of microcomputers. Problems of a more usual size, such as that of $CaAl_{12}O_{19}$ or Na_2PO_3F (discussed below), take a few seconds.

The use of weights

It is my experience that the best weight s to use in the circuit equations is the Pauling bond strength which is the same as the average valence of the bonds from the atom in question (*i.e.* atom valence/coordination number). If the weights are set equal to unity, one finds sometimes when there is a very large range of bond valence [as in the example of Na_2PO_3F considered by Brown (1977)] that the valences of the weakest bonds can actually become negative.

In fact use of weights equal to the Pauling bond strength gives results very similar to those originally reported by Brown (1977) for Na_2PO_3F (Durand, Cot & Galigné, 1974). Table 1 shows a comparison of valences calculated by the present method (with and without weights) with those calculated by Brown's iterative method. The agreement when weights are used is remarkably close.

In most instances the results are not very sensitive to the weights used. In the example of $CaAl_{12}O_{19}$, the bond lengths predicted using no weights differ by only ~0·002 Å from those predicted using weights equal to the Pauling bond strength [which ranges from 1/6 for Ca–O bonds to 3/4 for Al(2)–O bonds].

Cu^{II}, Cu^{III} and related oxides

One may also use weights in the bond valence sums. An example of the possible utility of such a procedure is provided by the oxides of copper which are currently of considerable interest. As is well known, in such compounds Cu^{II} or Cu^{III} have a primary coordination of four coplanar O atoms and often one or two additional coordinating atoms further away. The bonds to the further atoms have a strong antibonding component and are consequently much weaker than

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* A simple example (there is no simpler) of a structure with only an eight-membered circuit is that of the 8*H* (*ccch*) modification of SiC for which the connectivity matrix is (3100/0310/0031/1003), but here the valences can be found by inspection.

Table 1. *Comparison of valences calculated by the present method with those calculated by Brown* (1977) *for* Na_2PO_3F

'Calc.1' refers to calculations without weights and 'Calc.2' refers to calculations using weights as described in the text.

	Calc.1	Calc.2	Brown
Na(1)–O(2)	0·22	0·17	0·17
Na(1)–O(4)	0·13	0·12	0·09
Na(1)–O(5)	0·16	0·13	0·16
Na(1)–O(6)	0·13	0·12	0·11
Na(1)–F(2)	−0·08	0·08	0·09
Na(2)–O(1)	0·24	0·20	0·20
Na(2)–O(2)	0·25	0·20	0·21
Na(2)–O(3)	0·24	0·20	0·20
Na(2)–O(4)	0·16	0·14	0·13
Na(2)–O(6)	0·16	0·14	0·15
Na(2)–F(1)	−0·03	0·11	0·10
Na(3)–O(1)	0·20	0·19	0·18
Na(3)–O(2)	0·21	0·20	0·20
Na(3)–O(3)	0·20	0·19	0·18
Na(3)–O(4)	0·12	0·14	0·12
Na(3)–O(5)	0·15	0·15	0·19
Na(3)–O(6)	0·12	0·14	0·13
Na(4)–O(1)	0·25	0·21	0·21
Na(4)–O(3)	0·25	0·21	0·21
Na(4)–O(4)	0·17	0·15	0·15
Na(4)–O(5)	0·20	0·16	0·15
Na(4)–O(6)	0·17	0·15	0·16
Na(4)–F(1)	−0·02	0·12	0·12
P(1)–O(1)	1·32	1·40	1·40
P(1)–O(2)	1·32	1·43	1·43
P(1)–O(3)	1·32	1·40	1·40
P(1)–F(1)	1·05	0·76	0·78
P(2)–O(4)	1·30	1·33	1·27
P(2)–O(5)	1·33	1·43	1·48
P(2)–O(6)	1·30	1·33	1·33
P(2)–F(2)	1·08	0·92	0·91

Table 2. *Observed and calculated bond lengths* (Å) *for* $Ba_2YCu_3O_7$

Both the Cu atoms are assumed to have the same valence (7/3) and $R_{CuO} = 1{\cdot}70$ Å. Calc.1 is without weights in the valence sums, Calc.2 is with a weight of 1/4 taken for the Cu(2)–O(4) bond.

	Obs.	Calc.1	Calc.2
Ba–O(1)	2·89	2·86	2·82
Ba–O(2)	2·98	2·93	3·14
Ba–O(3)	2·96	2·93	3·14
Ba–O(4)	2·75	2·85	2·76
Cu(1)–O(1)	1·94	1·90	1·94
Cu(1)–O(4)	1·86	1·90	1·86
Cu(2)–O(2)	1·93	2·00	1·94
Cu(2)–O(3)	1·96	2·00	1·94
Cu(2)–O(4)	2·31	1·93	2·24

the primary bonds. Such an effect can be mimicked by reducing the contribution to the bond valence sums of the weaker bond. A weight factor of 1/4 has been arbitrarily chosen. To implement this correction in practice, the number of the weaker bonds in the bond valence sum is reduced by a factor of 1/4 (so that this number may now not be an integer) and the subsequently calculated valences of these bonds is reduced by the same factor.

An example of the effect of such a procedure on the calculated bond lengths in $Ba_2YCu_3O_7$ [in which the valence of all Cu atoms has been set equal to 2·33; compare O'Keeffe & Hansen (1988)] is shown in Table 2. It is satisfying that the effect of weighting is to model more accurately the rest of the Cu–O bonds in the structure.

Further work is necessary to see whether a scheme can be developed to apply universally to bonds from these and other cations such as Mn^{III}. The empirical nature of the applied weight is not really at odds with the spirit of the bond valence method which so far has a strong empirical component [but compare Burdett (1988)]. The alternative, which I find less satisfactory, is simply to fix the valence of the 'weak' bonds at a value consistent with their observed bond lengths (Brown, 1989).

Comments

The method outlined above requires as input only the connectivity matrix and atomic valences. When comparing predictions with known structures I generate the connectivity matrix using as input only the space group, lattice parameters and atomic coordinates. A criterion is needed to determine the existence of a bond (Altermatt & Brown, 1985), but in practice the method is not likely to work well when there is a real ambiguity about the existence of a bond.

A weakness of the method (but one that suggests avenues for further development) is that it assumes that all bonds from a given atom to crystallographically equivalent neighbors have the same valence and, by implication, the same length. In general this is not the case. Thus in the corundum form of Al_2O_3 (which should be sufficiently familiar) there is only one kind of Al and one kind of O atom but two kinds of Al–O bond that have significantly different bond lengths. The connectivity matrix does not distinguish between these two kinds of bond. A possible solution to this problem is to use the predicted bond lengths as a starting point in the application of a further procedure, along the lines of molecular mechanics, that allows the crystal to relax subject to the constraints of interatomic forces.

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APPENDIX

Fortran code to find circuits

The following fragment of code, written in a dialect of Fortran (in which statements are separated by semicolons for economy) will find the coordinates (row, column) of entries in a connectivity matrix of dimensions $B(m, n)$ that form four-circuits and six-circuits. m and n are the numbers of cations and anions respectively. It uses for auxiliary storage an integer array (initially of zeros) of dimensions $NP[m, n(n-1)/2, 2]$ which stores the coordinates of all pairs of non-zero entries in each row. In practice, at the points (C) where the circuits are identified, appropriate entries are made in a matrix of coefficients of the circuit and sum equations.

```
      NN=(N*(N-1))/2
      DO(I=1,M);L=0;DO(J=1,N-1);DO(K=J+1,N);L=L+1
          IF(B(I,J).NE.0.0.AND.B(I,K).NE.0.0) THEN
            NP(I,L,1)=J;NP(I,L,2)=K
          ENDIF
      ENDDO;ENDDO;ENDDO
      N4=0                                           ! find 4-circuits
      DO(I=1,M-1);DO(J=I+1,M);DO(K=1,NN)
        IF(NP(J,K,1)=0) CYCLE
        IF(NP(I,K,1)=NP(J,K,1).AND.NP(I,K,2)=NP(J,K,2)) THEN
          N4=N4+1;N1=NP(I,K,1);N2=NP(I,K,2)
C              4-circuit in rows I,J and columns N1,N2
        ENDIF
      ENDDO;ENDDO;ENDDO                          ! found N4 4-circuits
      N6=0                                           ! find 6-circuits
      DO(I=1,M-2);DO(J=I+1,M-1);DO(KI=1,NN);DO(LI=1,NN)
      DO(K1=1,2);DO(K2=1,2)
        J1=2-K1/2;J2=2-K2/2
        IF(NP(I,KI,K1)=NP(J,LI,K2).AND.NP(I,KI,J1).NE.NP(J,LI,J2))THEN
          DO(K=J+1,M);DO(L=1,NN);DO(K3=1,2)
            J3=2-K3/2
            IF(NP(I,KI,J1)=NP(K,L,K3).AND.NP(J,LI,J2)=NP(K,L,J3)) THEN
              N6=N6+1;N1=NP(I,KI,K1);N2=NP(I,KI,J1);N3=NP(J,LI,J2)
C               6-circuit: row 1 = I  cols N1 and N2
C                          row 2 = J  cols N1 and N3
C                          row 3 = K  cols N2 and N3
            ENDIF
          ENDDO;ENDDO;ENDDO
        ENDIF
      ENDDO;ENDDO;ENDDO;ENDDO;ENDDO;ENDDO        ! found N6 6-circuits
```

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A Simple Approach to Quasicrystal Structure and Phason Defect Formulation*

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Abstract

The advantages of the cut or section method in describing quasicrystal structures and phason defects are given. The real and reciprocal quasilattice formulation is derived straightforwardly. It is shown that the linear phason strain which leads to the quasilattice distortion is equivalent to a rotation of physical space relative to the high-dimensional space. A continuous rotation of the physical space will make the quasilattice deviate from its idealized form and turn gradually into a periodic lattice. The derivation of a geometrical relationship between the icosahedral quasilattice and the corresponding b.c.c. lattice becomes simple and clear. This will be beneficial to the construction of a quasicrystal structure model by reference to the corresponding b.c.c. crystal structure.

1. Introduction

Soon after the discovery of icosahedral quasicrystals in rapidly solidified Al–Mn alloys (Shechtman, Blech, Gratias & Cahn, 1984), great attention was paid to the description of quasicrystal structure which has a long-range quasiperiodic translational order and long-range orientational order. The quasicrystal structure offers a new kind of incommensurate crystal structure. Its Fourier transform consists of a δ function as for periodic crystals but the point symmetries are incompatible with traditional crystallography. Some authors proposed a density wave description of quasicrystal structures (Kalugin, Kitaev & Levitov, 1985; Bak, 1985*a*, *b*; Levine, Lubensky, Ostlund, Ramaswamy, Steinhardt & Toner, 1985; Lubensky, Ramaswamy & Toner, 1985; Jaric, 1985; Nelson & Sachdev, 1985; Sachdev & Nelson, 1985). Others described the quasicrystal structure by a technique based on projection from a high-dimensional lattice to obtain the quasicrystalline lattice (Kramer & Neri, 1984; Kalugin, Kitaev & Levitov, 1985; Duneau & Katz, 1985; Elser, 1985, 1986). It was shown that the analytical formulation of quasicrystal structures derived from the projection method is identical with the density wave description (Li & Wang, 1988). The quasicrystalline lattice can also be obtained by the generalized dual method (Socolar, Steinhardt & Levine, 1985; Levine & Steinhardt, 1986; Socolar & Steinhardt, 1986) or the multigrid method (de Brujin,

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