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Quantifying the Concept of Coordination Number

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Mathematical requirements necessary for the quantification of coordination numbers of irregular coordination polyhedra are listed. A general mathematical formula is given and applied to the case of the CsCl structure using the concept of the polyhedral atomic volume. As a function of the atomic radii difference, the coordination number in this structure varies smoothly from 8 to 14 to 6. The partial coordination numbers of 8 and 6, corresponding to first and second nearest neighbors, are also functionally related to the generalized coordination number.

The determination of the coordination number (CN) of an atom in a structure or molecule is clearly recognized as an important first step in the characterization of that atom's contribution to the bulk material properties. The host of interdependent chemical and physical properties that are known to be CN dependent for various elements include size or radius, atomic valence, bond characteristics (including type, hybridization, ionicity, strength and energy), radical or species stability and reactivity, phonon and electronic spectra, as well as electrical and magnetic properties (Pauling, 1960; Goodenough, 1963). In particular, we note that Templeton (1953, 1955) has developed a simple formula for obtaining a good estimate of the Madelung constant given only the coordination numbers and the stoichiometry. In light of the above, it is not surprising that the set of coordination numbers for a substance constitute some of the principal data sought and reported in structure determinations, whether the material of interest be gaseous (Herzberg, 1960–1966), liquid (Smith, 1964), crystalline (Frank & Kasper, 1958), or amorphous [insulating (Konnert & Karle, 1973), semi-conducting (Renninger & Averbach, 1973), or metallic (Gilman, 1975)].

While the coordination number or ligancy of a central atom is often readily obtained by enumerating the number of neighbors bonded to the central atom, there are numerous cases where the criteria for the enumeration process are indistinct. Consider, for example, the first, second, and third 'shells' of ligands and solvent molecules enclosing transition-metal ions in

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polar liquids or first-, second-, and third-nearest neighbors of metal atoms in intermetallic compounds. Frank & Kasper (1958) defined a 'geometrical coordination number' as the number of faces on an atom's polyhedral 'domain' (termed here 'Voronoi cell'). However, this definition is less than ideal because: (1) it treats all atoms as having the same size; (2) it assigns equal weight to both large and small (unimportant) polyhedral faces; and (3) it makes no distinction as to the kind of bond formed with a neighbor. In view of the fact that modern inorganic chemistry was essentially initiated in the 1890's with Alfred Werner's development of coordination theory and the coordination number (see Bailar, 1956), it is surprising that until now the simple concept of the CN has not been generalized to permit a clear-cut treatment of these more complicated and numerous cases.

The purpose, then, of this communication is to show by reasonable example that quantification of the concept of CN can be accomplished readily. In so doing, suitable criteria for CN quantification are listed, and a mathematical formula for the calculation of CN satisfying these criteria is applied as a function of atomic size to the case of the simple CsCl structure. Finally, suggestions are offered concerning both the ways in which non-integer values of coordination numbers might be employed and the means by which the CN concept might be further extended. At this point, then, it appears desirable to make a distinction between CN and ligancy, reserving the latter term to indicate the number of neighbors bonded to the atom of interest and to mathematically calculate the CN as a function of ligancy.

Current chemical usage of the words 'coordination' and 'coordinate', as in CN and coordinate compound, retains little of the probable original intent referring to equivalence among the ligands as well as an equivalence in their bond formation to the central atom. That such a connotation of equivalence is likely is indicated by both recent and early usage (*Oxford English Dictionary*, 1933); for example, in 1643, the intent is quite clear in the phrase '...working together for common good, not...by subordination, but by coordination of principal causes'. In the development of a mathematical expression for CN as indicated below, we find the connotation of ligand equivalency reasserting itself.

Consider the interaction of a central atom with its *i*th neighbor as being measured by A_i such that the sum of all its interactions is $A_t = \sum_i A_i$ (all neighbors with non-zero A_i), with A_t being finite. Then the CN as a function of all the A_i should satisfy the following restrictions:

(*a*) $\mathrm{CN}(A_i)$ is dimensionless and ≥ 1 if any neighbors with non-zero A_i exist.

(*b*) $\mathrm{CN}(A_i)$ is a continuous function of the A_i but its slope may not be.

(*c*) If N interactions exist such that $A_1 = A_2 = \ldots = A_N$ for all neighbors with non-zero A_i, then $\mathrm{CN}(A_i) = N$.

(*d*) If some of the A_i are unequal, then $\mathrm{CN}(A_i) < N$.

(*e*) If integer m of the A_i are equal and large and $N - m$ are equal and small, then $N > \mathrm{CN}(A_i) > m$.

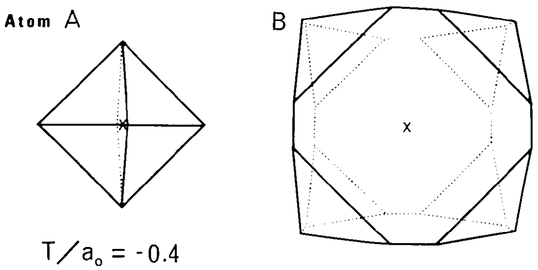
The formulae proposed here for the quantification of CN within the above restrictions are given as equations (1) and (2),

$$\frac{1}{\mathrm{CN}} = \sum_{1}^{N} \left(\frac{A_i}{A_t}\right)^2 \tag{1}$$

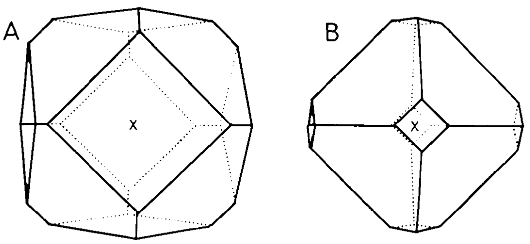
$$\frac{1}{\mathrm{CN}_w} = \sum_{1}^{N} \left[w_i A_i \Big/ \sum_{1}^{N} w_j A_j \right]^2 \tag{2}$$

where w_i in equation (2) are finite weighting factors.

Reasonable measures, A_i, of bond formation might include bond strengths, bond energies, force constants for the bond-stretching motion, overlap integrals, or bond orders. The corresponding CN for each kind of A_i might be expected to differ in minor ways. As an example of the application of the proposed formula equation (1) and minor differences between CN for different kinds of A_i, we will use a geometric approach involving the construction of a polyhedral cell about atoms of different sizes in the simple CsCl structure. If planes perpendicular to the bond axis are placed midway between the outside spherical surfaces of the bonded atoms of different radii, one may construct



(*a*) $T/a_0 = -0.4$



(*b*) $T/a_0 = 0.154$

Fig. 1. Scaled, space-filling PAV cells for the CsCl structure. They have coordination numbers $\mathrm{CN}_{\mathrm{area}}$ of 8·0 and 10·04 for the upper *A* and *B* atoms, and of 14·00 and 9·62 for the lower pair, while their ligancies or 'geometrical' CN are 8, 14, 14, and 14, respectively.

what has been described elsewhere as polyhedral atomic volume (PAV) cells (Carter, 1974, 1976). These cells are the smallest polyhedra formed by the planes about the atoms and are often space-filling for simple structures. We note that this construction does not require the spherical atoms to be in contact and generally they will not be. Even if the spheres overlap, the position of planes perpendicular to the internuclear axis depends only on the radii difference. Fig. 1 illustrates such PAV polyhedra for the CsCl structure for two values of $T = r_A - r_B$, where r_A and r_B are the respective radii of the atoms *A* and *B*. In Fig. 1(*a*), the smaller *A* atom ($T/a_0 = -0{\cdot}4$) has an octahedral cell, while the *B* atom has 14 faces, eight of them triangular corresponding to weak *A–B* interactions; six of them have octagonal faces corresponding to strong *B–B* interactions in the $\langle 100 \rangle$ directions (a_0 = crystal cell edge). For $T/a_0 = 0{\cdot}154$, Fig. 1(*b*), we find that the now larger *A* atom has 14 faces of equal area, while the *B* atom has also 14 faces of rather different areas with the *A–B* interactions predominating. In the last case, $T/a_0 = 0{\cdot}154$, the former usage of the CN concept would assign the same CN to both atoms *A* and *B*.

The new results of this communication are suggested in Fig. 2, where the CN(*T*) are plotted for both atoms in the CsCl structure as a function of their normalized radii difference T/a_0. (The coefficient, f_{A-B}, for a 'partial' CN, discussed below, is also plotted.) For the *A* atom, the coordination number $\mathrm{CN}_{\mathrm{vol}}$ based on the pyramidal volume associated with each face is plotted as a solid line. Here the face is the base and the atom location is the pyramidal apex. The dashed line often slightly below $\mathrm{CN}_{\mathrm{vol}}$ corresponds to $\mathrm{CN}_{\mathrm{area}}$ and is based on the cell-face areas ($= A_i$). The dotted line is the mirror image of $\mathrm{CN}_{\mathrm{vol}}$ and corresponds to $\mathrm{CN}_{\mathrm{vol}}$ for the *B* atom. For the *A* atom we note that $\mathrm{CN}_{\mathrm{vol}}$ changes smoothly from the octahedral value of 8 and $T/a_0 \le -0{\cdot}2886$, to a maximum of 14 at $T/a_0 = 0{\cdot}1581$ (or $0{\cdot}1540$ for $\mathrm{CN}_{\mathrm{area}}$), and then finally decreases to a limiting value of 6 at $T/a_0 = 0{\cdot}866$. In the CsCl structure we note that $\mathrm{CN}_{\mathrm{vol}} = 6$ is unreal for finite atoms since it corresponds to an imbedding of the small atom in the large one as $|T/a_0| \to \sqrt{3}/2 = 0{\cdot}866$.

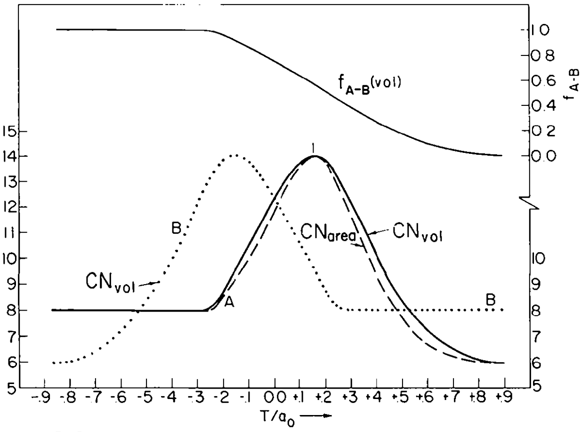


Fig. 2. $\mathrm{CN}_{\mathrm{vol}}$ and the corresponding f_{A-B} for atom *A* illustrated as a function of increasing *A* atom size; the dotted line indicates the *B* atom $\mathrm{CN}_{\mathrm{vol}}$. The dashed line gives the *A* atom $\mathrm{CN}_{\mathrm{area}}$ which is based on the areas of its polyhedra faces. For the *A* atom the partial coordination numbers CN_{A-B} and CN_{A-A} are 8 and 6, respectively, for $T/a_0 > 0{\cdot}2886$.

While the formula for CN, equation (1), was derived primarily intuitively from the past usage [restriction (*c*) above], we note in Fig. 2 that all other expectations and restrictions are also satisfied. As further support for its correctness, let us consider the case where the bond interaction terms are identified as the bond orders between the central atom and its ligands, *i.e.* $A_i = m_i$. The chemical valence of the central atom is then the sum of the bond orders, $V = \sum n_i$, so that we have equation (3):

$$\frac{1}{\mathrm{CN}_{\mathrm{val}}} = \sum_i^N \left(\frac{n_i}{V^2}\right)^2 = \frac{1}{V}\sum_i^N n_i \left(\frac{n_i}{V}\right). \tag{3}$$

We may calculate the average ligand bond order $\bar{n}$ then as the valence divided by $\mathrm{CN}_{\mathrm{val}}$, equation (4):

$$\bar{n} = \frac{V}{\mathrm{CN}_{\mathrm{val}}} = \sum_i^N n_i \frac{n_i}{V}. \tag{4}$$

Thus $\bar{n}$ corresponds to a weighted average of the n_i with the normalized weighting factors (n_i/V).

The concept of a 'partial coordination number' is useful when there are different kinds of the A_i interactions. The different kinds might correspond to a grouping of the *N* interactions on the basis of (1) bond type, ionic or covalent; (2) neighbors, metal or nonmetal; or (3) shells, ligand distance from the central atom. For an atom with *L* different kinds of neighbors, a 'partial' coordination number CN_l can be usefully defined as

$$\frac{1}{\mathrm{CN}_l} = \sum_{i=1}^{N_l} (A_i^2) \Bigg/ \left(\sum_{i=1}^{N_l} A_i\right)^2 \tag{5}$$

where both sums, $\sum_{i=1}^{N_l}$, are only over the *l*th kind of neighbors and

$$\sum_{l=1}^{L} N_l = N.$$

The partial CN_l are related to the total CN by

$$\frac{1}{\mathrm{CN}} = \sum_{l=1}^{L} f_l^2/\mathrm{CN}_l \tag{6}$$

where the partial coefficients are

$$f_l = \left(\sum_{i=1}^{N_l} A_i\right) \Bigg/ A_t \tag{7}$$

with

$$\sum_{l=1}^{L} f_l = 1.$$

Clearly, these coefficients must satisfy the condition that $0 \leq f_l \leq 1$. As an example, we have plotted at the top of Fig. 2 for the A atom, the f_{A-B} based on pyramidal volume which corresponds to only the A–B bonds. Thus when $T/a_0 \leq -0{\cdot}2886$, the A atom has only B neighbors (CN = 8) and $f_{A-B} = 1$. Thereafter for increasing T/a_0, f decreases, eventually to zero at $T/a_0 = +0{\cdot}866$. When the A and B atoms have equal radii, at $T/a_0 = 0$, the A–B interactions must predominate, since $f_{A-B} = 0{\cdot}750$ and there are 8 A–B interactions compared to 6 A–A interactions. We also note that in the region of $-0{\cdot}2886 \leq T/a_0 \leq 0{\cdot}866$, the partial coordination numbers for those interactions are just what our crystal–chemical sense indicates they should be, namely, $\mathrm{CN}_{A-B} = 8$ and $\mathrm{CN}_{A-A} = 6$. This general approach has been utilized to study the boron PAV in the transition-metal borides as a function of coefficients f (B–metal interactions) (Carter, 1976).

Mackay (1971, 1974) has discussed crystal structures also on a geometric basis using the polyhedra of Voronoi (1908), which corresponds to the case of equal (or zero) radii, *i.e.* $T = r_A - r_B = 0$. He has employed the solid angle (as a fraction of a sphere) subtended by the mutual polyhedral face of two atoms as a measure of their interaction. Using his results for $Ba_3V_2O_8$, and taking these solid angles as the A_i in equation (1), we immediately calculate the coordination number of Ba_I as CN = 10·704 with partial coordination numbers $\mathrm{CN(Ba_I–O_I)} = \mathrm{CN(Ba_I–O_{II})} = 6{\cdot}0$. In the case of the CsCl structure, we note that the results will be very similar to those of Fig. 1 if the solid angle is employed as the A_i of equation (1). Thus we find that the CN maxima (= 14) occur at $T/a_0 = 0{\cdot}1482$, 0·1540, and 0·1581 for the A_i based on subtended solid angles, polygon face areas, and pyramidal volumes, respectively. Finally, we note that while Mackay (1971, 1974) introduced a connectivity matrix C_{ij} the sum of whose rows (or columns) gave the CN for atom i (or j), the resultant CN is identical to that proposed by Frank & Kasper (1958).

Two possible uses for a quantified non-integer CN might be in the refinement of the empirical relation (Templeton, 1953, 1955) for a reduced Madelung constant α and in the classification of compounds and structure types by an average CN. In equation (8), the 'reduced Madelung constant, α'

$$\alpha = 1{\cdot}89 - 1{\cdot}00/m \tag{8}$$

is given in terms of m, a weighted-harmonic-mean CN defined as equation (9), where

$$\frac{1}{m} = (\textstyle\sum k_i/p_i)/(\sum k_i). \tag{9}$$

k_i atoms of one kind had the usual integral coordination number p_i, and the sum is over the contents of the crystal unit cell (or over a stoichiometric formula). Explicitly, then, the first suggestion would entail the use of a quantified CN, as per this communication, to refine Templeton's empirical relation, equation (8), for the reduced Madelung constant. This might entail the weighted CN of equation (2) where the weights w_i might be employed to account for the usual change in electronic charge between the first and second shell of ions. The second related use might employ a weighted-mean coordination number like m of equation (9) to characterize and catalog both compounds and crystalline-structure types. Since a CN based on the PAV cell is a function of both atomic position parameters and atomic size, it constitutes an appropriate measure for replacing the p_i in the case of individual compounds. In the case of structure types with the atoms in symmetry-fixed positions, the Voronoi cell (Smith, 1964; Frank & Kasper, 1958; Voronoi, 1908), where all atoms have the same size, provides a suitable base for calculating the CN's required for a structure-characterizing mean CN [equation (9)].

As a final suggestion, we note that in the calculation of radial distribution functions for glassy materials, the coordination number $N_{ij}(r_{ij})$ is defined (Konnert & Karle, 1973) as the number of neighbors of kind j the i atom has at distance r_{ij}. The extension of the present CN [equations (1) or (2)] suggests the use of a moving window of width d centered at r_{ij} with the weights being a function of position s within the window, *i.e.*

$$|r_{ij} - d/2| \leq |s| \leq |r_{ij} + d/2|. \tag{10}$$

On a geometric cell basis, a moving-window approach could produce in real space PAV-like cells of increasing volume corresponding to the *unreduced* Brillouin zones of increasing zone number in reciprocal space.

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The Crystal and Molecular Structure of 1-Phenyl-1,3-butanedionato(1,6-dichloro-1,5-cyclooctadiene)rhodium(I)

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$C_{18}H_{19}O_2Cl_2Rh$, monoclinic, $P2_1/c$, $Z = 8$, FW 441·2, $a = 17{\cdot}390$ (3), $b = 12{\cdot}816$ (2), $c = 16{\cdot}523$ (4) Å, $\beta = 109{\cdot}41$ (1)°, $V = 3473$ (1) Å^3, $D_x = 1{\cdot}69$, $D_m = 1{\cdot}65$ (1) g cm^{-3} (flotation), λ(Cu $K\bar{\alpha}$) = 1·5418 Å (graphite monochromator), μ(Cu $K\bar{\alpha}$) = 108·0 cm^{-1}, final $R = 0{\cdot}030$ for 3522 observed reflexions $[F_o^2 > 3\sigma(F_o^2)]$ in the range $0 < 2\theta \leq 108°$.

Introduction

In a complex study of the chemical and physical properties of 1,3-substituted rhodium chelates (Bouchal, Škramovská, Čoupek, Pokorný & Hrabák, 1972; Ryska, Bouchal & Hrabák, 1973), the determination of the crystal and molecular structure of the symmetrically substituted 1,3-diphenyl-1,3-propanedionato(1,6-dichloro-1,5-cyclooctadiene)rhodium(I) (Ječný & Huml, 1974) was followed by a study of the structure of the asymmetrically substituted title compound.

The lattice parameters were determined by the least-squares method using 15 reflexions from the angle

Table 1. *Final fractional coordinates of non*-H *atoms and their e.s.d.'s* (× 10^4)

	x	*y*	*z*		*x*	*y*	*z*
Rh(1)	1308·7 (2)	3806·2 (3)	5087·8 (2)	Rh(2)	4482·9 (2)	1047·6 (3)	3436·1 (2)
Cl(11)	−358 (1)	3557 (1)	5474 (1)	Cl(21)	6149 (1)	2342 (1)	4186 (1)
Cl(12)	2378 (1)	5901 (1)	5830 (1)	Cl(22)	4537 (1)	−1311 (1)	4142 (1)
O(11)	411 (2)	3194 (2)	4051 (2)	O(21)	4277 (2)	2548 (2)	3739 (2)
O(12)	1746 (2)	4574 (2)	4259 (1)	O(22)	3463 (2)	596 (2)	3710 (2)
C(101)	1800 (3)	5466 (4)	3039 (3)	C(201)	2302 (3)	608 (4)	4122 (3)
C(102)	2371 (4)	6133 (4)	3578 (4)	C(202)	2369 (3)	−466 (4)	4244 (4)
C(103)	2753 (4)	6887 (4)	3247 (4)	C(203)	1737 (4)	−1032 (5)	4378 (4)
C(104)	2580 (4)	6961 (4)	2377 (4)	C(204)	1043 (4)	−531 (5)	4376 (4)
C(105)	2010 (4)	6327 (5)	1839 (4)	C(205)	967 (4)	528 (5)	4232 (4)
C(106)	1619 (4)	5567 (4)	2162 (4)	C(206)	1591 (3)	1092 (4)	4108 (4)
C(107)	724 (3)	4115 (4)	2947 (3)	C(207)	3108 (3)	2237 (4)	4143 (3)
C(108)	1402 (3)	4668 (4)	3448 (3)	C(208)	3007 (3)	1175 (4)	3984 (3)
C(109)	292 (3)	3396 (4)	3268 (3)	C(209)	3726 (3)	2854 (4)	4034 (3)
C(110)	−399 (4)	2788 (5)	2644 (4)	C(210)	3766 (4)	3995 (4)	4258 (4)
C(111)	1090 (3)	2568 (4)	5813 (3)	C(211)	5092 (3)	1663 (4)	2657 (3)
C(112)	1893 (4)	2137 (5)	6425 (4)	C(212)	4894 (4)	1082 (5)	1829 (4)
C(113)	2592 (4)	2869 (5)	6636 (4)	C(213)	4674 (4)	−58 (4)	1900 (4)
C(114)	2459 (3)	3808 (4)	6031 (3)	C(214)	4376 (3)	−269 (4)	2654 (3)
C(115)	2038 (3)	4701 (4)	6126 (3)	C(215)	4908 (3)	−493 (4)	3478 (3)
C(116)	1614 (4)	4912 (5)	6774 (4)	C(216)	5824 (3)	−536 (4)	3785 (4)
C(117)	1018 (4)	4086 (6)	6792 (4)	C(217)	6192 (3)	389 (4)	3509 (4)
C(118)	724 (3)	3462 (4)	5976 (3)	C(218)	5670 (3)	1362 (4)	3429 (3)