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SIXTH SEMI-ANNUAL STATUS REPORT

INSTITUTION | Grambling State University, Grambling, Louisiana 71245.

TITLE OF THE PROJECT | Study of the Extra-ionic electron distributions in semi-metallic structures by Nuclear Quadrupole Resonance Techniques.

Grant | NASA NGR-19-011-016 (suppl. 2) GSU No. 5-5175.

PRINCIPAL INVESTIGATOR* | Dr. A. N. Murty, Professor Department of Physics.

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INTRODUCTION

Estimation of solid state electrostatic potentials, fields and field gradients in ionic solids has been of considerable interest during the past few years. Several methods have been developed starting from a simple point charge model of the solid to an elaborate multipole-model of the lattice[1-6]. The results are of varying degrees of success depending on the accuracy of the a) crystal structure data b) dipole and quadrupole polarizability values and c) the number of ions of the lattice taken into consideration in arriving at the potential. Though there exists considerable controversy regarding the validity of the multipole model of the lattice, and the usefulness of such calculations due to the uncertainties in the parameters (a) and (b) mentioned above, and the appropriateness of allocating a certain charge value to the lattice site, and lastly the uncertainty in the Sternheimer antishielding factor[7,8], the method has yielded satisfactory results in a number of cases[9-12].

The main purpose of our work is to develop a straightforward self-consistent method, that can easily be understood, without presenting serious mathematical conceptual problems, by the senior undergraduate students who are familiar with basic principles of electrostatics. The method will be a direct practical application of basic electrostatics to solid state and also helps in the understanding of the principles of crystal structure. This report presents the necessary mathematical equations derived from first principles and the systematic computational procedure developed to arrive at the solid state EFG (electrostatic field gradients) values. No such calculations have so far been made for the oxides of third and fifth group elements except for Al_2O_3[6] which is used for testing our method and computor program. The program will be applied to estimate the EFG values (or γ_∞ values) in the oxides of gallium, iridium, arsenic, antimony and bismuth.

SEARCH SEQUENCE.

starting with the crystalline co-ordinates of any one of the atoms in the unit cell.
(14th atom) identical atoms in all the next neighbour unit cells are located in the
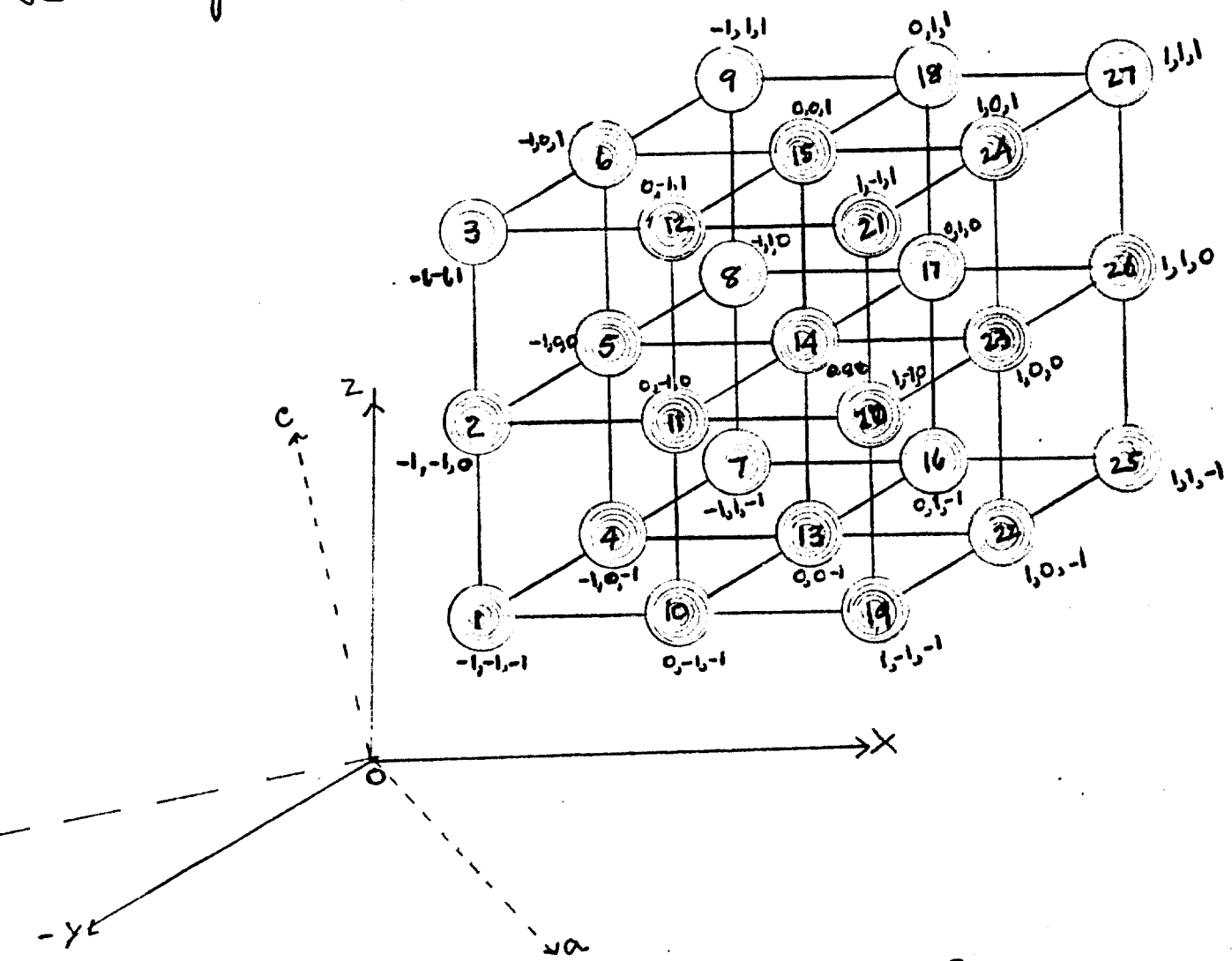following order of sequence.

FIG. I

2

Computational procedure

This involves:-

a) Environmental search.determination of the cartesian co-ordinates of all atoms within a chosen distance from the ion at the lattice site of interest.

b) Evaluation of the solid state electrostatic potential (V), field $(V_i = \frac{\partial V}{\partial i}$, i = x. y. z) and field gradient $(V_{ij} = \frac{\partial^2 V}{\partial i \partial j}$, i, j = x, y, z) at the lattice sites of interest.

c) Self consistent evaluation of the induced dipole and quadrupole moments of all polarisable ions of the lattice.

d) Final evaluation of the EFG at the site of interest due to the charge, dipole and quadrupole nature of all the lattice ions.

ENVIRONMENTAL SEARCH

Starting with the crystal structure data consisting of the unit cell dimensions A_0, B_0, C_0 the number of atoms per unit cell No., and their position co-ordinate parameters U. V. W. (Input data for the program), co-ordinates of all atoms within λ(= 1,2,3 .....) unit cells away in the three dimensions are located in the crystalline axis system. The progress of the search sequence is shown in Fig. 1. Starting with the given crystalline co-ordinates $A_0 U$, $B_0 V$, $C_0 W$ of any one of the N_0 atoms in the unit cell, all similar atoms in neighbouring unit cells are located as indicated in figure 1 for λ = 1. There will be 27 identical atoms if the search is confined to one unit cell away, making up the total number of ions included in the computation to 27 N_0. If the search is extended to λ unit cells the total number of ions will be $N_t = (2\lambda + 1)^3 N_0$. The choice of the sphere of influence being in multiples of unit cells is considered as more appropriate than an arbitrary choice of R value as $50 A^0 U$ or $100 A^0 U$, because charge neutrality is preserved in units of crystalline unit cells.

It will be necessary to convert the crystalline co-ordinates into cartesian

co-ordinates if the unit cell symmetry is hexagonal or rhombohedral using the following transformation matrices.

Hexagonal to cartesian :

$$\begin{pmatrix} 1 & 0 & 0 \\ -\frac{1}{2} & \sqrt{3}/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Rhombohedral to cartesian :

$$\begin{pmatrix} \frac{\sin\theta}{2} & \sin\alpha/2 & \cos\theta \\ \frac{\sin\theta}{2} & -\sin\alpha/2 & \cos\theta \\ -\sin\theta & 0 & \cos\theta \end{pmatrix}$$

where α is the rhombohedral angle and θ is the angle between z-axis (axis of symmetry) and the crystalline axes. $\sin\theta = \dfrac{2\sin\alpha/2}{\sqrt{3}}$

The first part of the program computes the cartesian co-ordinates of all the N_t atoms relative to an arbitrary origin and stores them in the X_0, Y_0, Z_0 array.   Then the origin is shifted to one of the nonequivalent sites of interest and the relative co-ordinates and distances of all the ions are computed and stored in another working array XR, YR, ZR, RR for computing the potential, field, and field gradient at that site.

Potential, Field and Field Gradient

The expressions for fields ($V_i = \frac{\partial V}{\partial i}$, (i = x, y, z) and field gradients ($V_{ij} = \frac{\partial^2 V}{\partial i \partial j}$, i, j, = x, y, z) at a point P (x, y, z) in space due to a multipole situated at the origin having a point charge C_p, dipole moment $\vec{D}$ (= i D_x + j D_y + k D_z) and quadrupole moment

$$Q = \begin{pmatrix} Q_{xx} & Q_{xy} & Q_{zx} \\ Q_{xy} & Q_{yy} & Q_{yz} \\ Q_{zx} & Q_{yz} & Q_{zz} \end{pmatrix}$$

are obtained by direct differentiation of the potential expressions for the monopole (V^M), dipole (V^D), and quadrupole (V^Q) .

Since the general expressions derived in cartesian co-ordinates could not be reduced into a very compact form they are presented in an analytical form indicating the individual contributions of each dipole component and quadrupole tensor element to the field and field gradient.

MONOPOLE
(charge C_p)

Potential: $\qquad V^m = C_p/r$

Field:

$$V_x^m = -\frac{x}{r^3} C_p . \qquad V_y^m = -\frac{y}{r^3} C_p .$$

$$V_z^m = -\frac{z}{r^3} C_p .$$

Field gradient:

$$V_{xx}^m = -r^{-5}(r^2 - 3x^2) C_p$$

$$V_{yy}^m = -r^{-5}(r^2 - 3y^2) C_p$$

$$V_{zz}^m = -r^{-5}(r^2 - 3z^2) C_p$$

$$V_{xy}^m = 3r^{-5} xy C_p$$

$$V_{yz}^m = 3r^{-5} . yz C_p$$

$$V_{zx}^m = 3r^{-5} . zx C_p .$$

DIPOLE.

$$(\text{moment } \vec{D} = (\hat{\imath}\, D_x + \hat{\jmath}\, D_y + \hat{k}\, D_z)$$

Potential :

$$V^D = r^{-3}(x\,D_x + y\,D_y + z\,D_z)$$

Field :

$$V_x^D = r^{-5}\left[(r^2 - 3x^2)D_x - 3xy\,D_y - 3xz\,D_z\right]$$

$$V_y^D = r^{-5}\left[-3xy\,D_x + (r^2 - 3y^2)D_y - 3yz\,D_z\right]$$

$$V_z^D = r^{-5}\left[-3zx\,D_x - 3yz\,D_y + (r^2 - 3z^2)D_z\right]$$

Field gradient :

$$V_{xx}^D = -3r^{-7}\left[(3r^2 - 5x^2)x\,D_x + (r^2 - 5x^2)y\,D_y + (r^2 - 5x^2)z\,D_z\right]$$

$$V_{yy}^D = -3r^{-7}\left[(r^2 - 5y^2)x\,D_x + (3r^2 - 5y^2)y\,D_y + (r^2 - 5y^2)z\,D_z\right]$$

$$V_{zz}^D = -3r^{-7}\left[(r^2 - 5z^2)x\,D_x + (r^2 - 5z^2)y\,D_y + (3r^2 - 5z^2)z\,D_z\right]$$

$$V_{xy}^D = -3r^{-7}\left[(r^2 - 5x^2)y\,D_x + (r^2 - 5y^2)x\,D_y - 5xyz\,D_z\right]$$

$$V_{yz}^D = -3r^{-7}\left[-5xyz\,D_x + (r^2 - 5y^2)z\,D_y + (r^2 - 5z^2)y\,D_z\right]$$

$$V_{zx}^D = -3r^{-7}\left[(r^2 - 5x^2)z\,D_x - 5xyz\,D_y + (r^2 - 5z^2)x\,D_z\right]$$

QUADRUPOLE

$$\text{Moment } Q = \begin{pmatrix} Q_{xx} & Q_{xy} & Q_{zx} \\ Q_{xy} & Q_{yy} & Q_{yz} \\ Q_{zx} & Q_{yz} & Q_{zz} \end{pmatrix}$$

Potential:

$$V^Q = 0.5\, r^{-5}\left[(3x^2-r^2)Q_{xx} + (3y^2-r^2)Q_{yy} + (3z^2-r^2)Q_{zz} \right.$$
$$\left. + 6xy\, Q_{xy} + 6yz\, Q_{yz} + 6zx\, Q_{zx}\right]$$

Field

$$V_x^Q = 1.5\, r^{-7}\left[(3r^2-5x^2)x\,Q_{xx} + (r^2-5y^2)x\,Q_{yy} + (r^2-5z^2)x\,Q_{zz} \right.$$
$$\left. + 2(r^2-5x^2)y\,Q_{xy} - 10xyz\, Q_{yz} + 2(r^2-5x^2)z\,Q_{zx}\right]$$

$$V_y^Q = 1.5\, r^{-7}\left[(r^2-5x^2)y\,Q_{xx} + (3r^2-5y^2)y\,Q_{yy} + (r^2-5z^2)y\,Q_{zz} \right.$$
$$\left. + 2(r^2-5y^2)x\,Q_{xy} + 2(r^2-5y^2)z\,Q_{yz} - 10xyz\,Q_{zx}\right]$$

$$V_z^Q = 1.5\, r^{-7}\left[(r^2-5x^2)z\,Q_{xx} + (r^2-5y^2)z\,Q_{yy} + (3r^2-5z^2)z\,Q_{zz} \right.$$
$$\left. - 10xyz\, Q_{xy} + 2(r^2-5z^2)y\,Q_{yz} + 2(r^2-5z^2)x\,Q_{zx}\right]$$

FIELD GRADIENTS DUE TO QUADRUPOLES.

$$V^q_{xx} = \left[3\frac{(r^2-7x^2)(3r^2-5x^2)}{2r^9} - \frac{6x^2}{r^7} \right] Q_{xx} +$$

$$\left[\frac{3(r^2-7x^2)(r^2-5y^2)}{2r^9} + \frac{3x^2}{r^7} \right] Q_{yy} + \left[\frac{3(r^2-7x^2)(r^2-5z^2)}{2r^9} + \frac{3x^2}{r^7} \right] Q_{zz} -$$

$$\frac{15xy(3r^2-7x^2)}{r^9} Q_{xy} - \frac{15yz(r^2-7x^2)}{r^9} Q_{yz} + \frac{15zx(3r^2-7x^2)}{r^9} Q_{zx}.$$

$$V^q_{yy} = \left[\frac{3(r^2-7y^2)(r^2-5x^2)}{2r^7} + \frac{3y^2}{r^7} \right] Q_{xx} +$$

$$\left[\frac{3(r^2-7y^2)(3r^2-5y^2)}{2r^9} - \frac{6y^2}{r^7} \right] Q_{yy} + \left[\frac{3(r^2-7y^2)(r^2-5z^2)}{2r^9} + \frac{3y^2}{r^7} \right] Q_{zz} -$$

$$\frac{15xy(3r^2-7y^2)}{r^9} Q_{xy} - \frac{15yz(3r^2-7y^2)}{r^9} Q_{yz} - \frac{15zx(r^2-7y^2)}{r^9} Q_{zx}.$$

$$V^q_{zz} = \left[\frac{3(r^2-7z^2)(r^2-5x^2)}{2r^9} + \frac{3z^2}{r^7} \right] Q_{xx} +$$

$$\left[\frac{3\,(r^2-7z^2)(r^2-5y^2)}{2r^9} + \frac{3z^2}{r^7} \right] Q_{yy} + \left[\frac{3(r^2-7z^2)(3r^2-5z^2)}{2r^9} - \frac{6z^2}{r^7} \right] Q_{zz} -$$

$$\frac{15xy\,(r^2-7z^2)}{r^9}\,Q_{xy} - \frac{15yz\,(3r^2-7z^2)}{r^9}\,Q_{yz} - \frac{15zx\,(3r^2-7z^2)}{r^9}\,Q_{zx}.$$

$$V^Q_{xy} = \frac{-15xy\,(3r^2-7x^2)}{2r^9}\,Q_{xx} + \frac{15xy\,(3r^2-7y^2)}{2r^9}\,Q_{yy} - \frac{15xy\,(r^2-7z^2)\,Q_{zz}}{2r^9} +$$

$$\left[\frac{3(r^2-5x^2)(r^2-5y^2)}{r^9} + \frac{30x^2y^2}{r^9} \right] Q_{xy} - \frac{15xz\,(r^2-7y^2)}{r^9}\,Q_{yz} - \frac{15yz\,(r^2-7x^2)}{r^9}\,Q_{zx}$$

$$V^Q_{yz} = -\frac{15yz\,(r^2-7x^2)}{2r^9}\,Q_{xx} - \frac{15yz\,(3r^2-7y^2)}{2r^9}\,Q_{yy} - \frac{15yz\,(3r^2-7z^2)}{2r^9}\,Q_{zz} +$$

$$-\frac{15zx\,(r^2-7y^2)}{r^9}\,Q_{xy} + \left[\frac{3(r^2-5y^2)(r^2-5z^2)+30y^2z^2}{r^9} \right] Q_{yz} - \frac{15xy\,(r^2-7z^2)}{r^9}\,Q_{zx}$$

$$V^Q_{zx} = -\frac{15zx\,(3r^2-7x^2)}{2r^9}\,Q_{xx} - \frac{15zx\,(r^2-7y^2)}{2r^9}\,Q_{yy} - \frac{15zx\,(3r^2-7z^2)}{2r^9}\,Q_{zz} +$$

$$-\frac{15yz\,(r^2-7x^2)}{r^9}\,Q_{xy} - \frac{15xy\,(r^2-7z^2)}{r^9}\,Q_{yz} + \left[\frac{3(r^2-5x^2)(r^2-5z^2)+30z^2x^2}{r^9} \right] Q_{zx}$$

The total potential (V) and hence the field (V_i) and field gradient (V_{ij}) at any ion site s is

$$V(s) = \sum_{n=1}^{N_t} V_n^M + V_n^D + V_n^Q$$

where n includes all of the ions of the lattice. But they cannot be computed without the knowledge of the multipole moments (C_p, D_i, Q_{ij}) which are, in turn, dependent on V_i and V_{ij}.

$$D_i = \alpha_D V_i \quad \text{and} \quad Q_{ij} = \alpha_Q V_{ij}$$

$$V(s) = \sum f(C_p, D_i, Q_{ij}, x, y, z)$$

V(s) and hence V_i and V_{ij} is a function of the multipole moments and co-ordinates

of the lattice ~~charges~~ sites as given by the equations above. As such, a self-consistent solution is sought for the estimation of the E.F.G's. As can be seen from the detailed expressions, the coefficients of the multipole moments of the lattice charge are entirely determined by their position co-ordinates only. Knowing the crystal structure data, the environmental search part of the program computes the cartesian co-ordinates of all the lattice charges relative to the chosen ion site and stores them in the XR, YR, ZR, RR array. Hence the coefficients can be computed independently.

For computational convenience the detailed expressions given above are expressed in terms of a set of S_i and P_i functions. By using these functions the development of the computor program has become considerably simpler since many of the coefficients repeat themselves. To save the computational time on the computer the coefficients are presented in the form of a matrix (C_{ij}).

The number of computations needed for each ion considered are reduced by 50% by this method. The S and P functions and the C matrix in terms of S and P functions are given below. Only the elements given by the S functions need to be computed. If an element C_{ij} (CIJ) occurs in a subsequent column as C_{kl} (CKL element) it is given as CIJ.

S and P functions

$$f_1, f_2 = x, y, z$$

1. $S_1(f_1) = -f_1/r^3$

2. $S_2(f_1, f_2) = -3f_1 f_2/r^5$

3. $S_3(f_1) = (r^2 - 3f_1^2)/r^5$

4. $S_4(f_1, f_2) = \dfrac{3f_1}{r^7}(r^2 - 5f_2^2)$

5. $S_5(f_1, f_2) = \dfrac{3f_1}{r^7}(3r^2 - 5f_2^2)$

6. $S_6(f_1) = 5f_1/r^2$

7. $S_7(f_1) = (r^2 - 7f_1^2)/r^2$

8. $S_8(f_1) = 3f_1^2/r^7$

9. $S_9(f_1) = (3r^2 - 7f_1^2)/r^2$

10. $S_{10}(f_1, f_2) = 3r^{-9}\left[(r^2 - 5f_1^2)(r^2 - 5f_2^2) + 10f_1^2 f_2^2\right]$

11. $S_{11}(f_1, f_2) = 1.5r^{-9}\left[(r^2 - 7f_1^2)(r^2 - 5f_2^2)/r^2 + 2f_1^2\right]$

12. $S_{12}(f_1) = 1.5r^{-7}\left[(r^2 - 7f_1^2)(3r^2 - 5f_1^2) - 4f_1^2\right]$

13. $P_1 = 2.5/r^2$

14. $P_2 = P_1 \cdot S_7(x)$, $\quad P_3 = P_1 \cdot S_7(y)$, $\quad P_4 = P_1 \cdot S_7(z)$

15. $P_5 = P_1 \cdot S_9(x)$, $\quad P_6 = P_1 \cdot S_9(y)$, $\quad P_7 = P_1 \cdot S_9(z)$

FIELDS & FIELD GRADIENTS	CHARGE	DIPOLES			QUADRUPOLES					
	CP	DX	DY	DZ	Q_{xx}	Q_{yy}	Q_{zz}	Q_{xy}	Q_{yz}	Q_{zx}
V_x	$S1(x)$	$-C41$	$-C71$	$-C91$	$-C42/2$	$-C52/2$	$-C62/2$	$-C72$	$-C82$	$-C92$
V_y	$S1(y)$	$-C71$	$-C51$	$-C81$	$-C72/2$	$-C53/2$	$-C63/2$	$-C52$	$-C83$	$-C82$
V_z	$S1(z)$	$-C91$	$-C81$	$-C61$	$-C92/2$	$-C83/2$	$-C64/2$	$-C82$	$-C63$	$-C62$
V_{xx}	$S3(x)$	$-S5(x,x)$	$C72$	$C92$	$S15(x)$	$S14(x,y)$	$S14(x,z)$	$2C75$	$C98$	$2C95$
V_{yy}	$S3(y)$	$-S4(x,y)$	$-S5(y,y)$	$C83$	$S14(y,x)$	$S15(y)$	$S14(y,z)$	$2C76$	$2C86$	$C88$
V_{zz}	$S3(z)$	$S4(x,z)$	$-S4(y,z)$	$-S5(z,z)$	$S14(z,x)$	$S14(z,y)$	$S15(z)$	$2C77$	$2C87$	$2C97$
V_{xy}	$S2(x,y)$	$-S4(y,z)$	$C52$	$C82$	$-C71 \cdot P5$	$-C71 \cdot P6$	$-C71 \cdot P4$	$S13(x,y)$	$C88$	$C98$
V_{yz}	$S2(y,z)$	$-S6(z) \cdot C22$	$-S4(z,y)$	$C63$	$-C81 \cdot P2$	$-C81 \cdot P6$	$-C81 \cdot P7$	$2C96$	$S13(y,z)$	$C68$
V_{zx}	$S2(z,x)$	$-S4(z,x)$	$C82$	$C62$	$-C91 \cdot P5$	$-C91 \cdot P3$	$-C91 \cdot P7$	$2C85$	$C68$	$S13(z,x)$

Self consistent solutions of multipole moments

Taking one by one, each of the N_t atoms chosen to be included in the computation the 90 C_{ij} elements are computed for each atom and the final sum is stored in the term matrix T_{ij}

$$T_{ij} = \sum_{n=1}^{N_t} C_{ij}^n$$

The first three rows of the T-matrix represent the contribution of the lattice to the electrostatic field at the ion site(s) when summed along the row after multiplication by the corresponding multipole moment D_i (i = 1, 10 - D_i monopole moment or charge C_p; D_2, D_3, D_4 = D_x, D_y, D_z components of the induced dipole moment; D_5, D_6, D_7, D_8, D_9, D_{10} = Q_{xx}, Q_{yy}, Q_{zz}, Q_{xy}, Q_{yz}, Q_{zx} induced quadrupole moment tensor elements respectively) and the last six rows the electrostatic field gradient. Thus the rows of the C/T matrix give

$$V_i = \sum_{j=1}^{10} T_{ij} \cdot D_j$$

$$
\begin{array}{lll}
V_x \text{ for } i = 1 & V_{xx} \text{ for } i = 4 & V_{xy} \text{ for } i = 7 \\
V_y \text{ for } i = 2 & V_{yy} \text{ for } i = 5 & V_{yz} \text{ for } i = 8 \\
V_z \text{ for } i = 3 & V_{zz} \text{ for } i = 6 & V_{zx} \text{ for } i = 9
\end{array}
$$

To start with an arbitrary set of D-values (charge, dipole and quadrupole moments) is assigned and provided as input data to the computor along with the values of dipole and quadrupole polarisabilities α_D and α_Q. Following the Gauss-Zillard iteration process the self consistent Dipole and Quadrupole moments are obtained. Since there are only 9 independent equations, three for the fields V_x, V_y, V_z and six for the field gradients V_{xx}, V_{yy}, V_{zz}, V_{xy}, V_{yz}, V_{zx} one can solve for D_x, D_y, D_z and Q_{xx}, Q_{yy}, Q_{zz}, Q_{xy}, Q_{yz}, and Q_{zx}. The charge value (C_p-D_1) should be assigned based on the ionic nature of the solid or one can determine the best possible value so as to be consistent with the experimental value of field gradients when they are known. The 9 equations are represented by two sets

$$D_{i+1} = \alpha_D V_i = \alpha_D \sum_{j=1}^{10} T_{ij} D_j \quad \text{for } i = 1 \text{ to } 3$$

$$D_{i+1} = \alpha_Q V_i = \alpha_Q \sum_{j=1}^{10} T_{ij} D_j \quad \text{for } i = 4 \text{ to } 9$$

Note D_1 is eliminated from the equations by incrementing the index on the left by one. Inserting the assigned values for D_i's in the first equation ($i = 1$) a new value is obtained for D_2, i.e. D_x. This value of D_x is used in solving the second equation ($i = 2$) for D_3 i.e. D_y. In the third equation ($i = 3$) new values of D_x and D_y are used and D_3 i.e. D_z is obtained and the process continues using improved values progressively until the 9-D values are obtained. After completing the first cycle the new D-values are compared with the old values and the cycle is repeated using the new values until the total difference between successive iterations is ≤ 0.0001.

$$\triangle = \sum_{i=1}^{10} \left| D_i^{n+1} - D_i^n \right| \leq 0.0001$$

In a typical case this accuracy was achieved in eight iterations. If the lattice consists of more than one inequivalent ions, either due to their chemical or physical nature the number of unknowns becomes 9S, where S is the number of inequivalent lattice sites where polarisable charge distribution exists. In general metallic atoms are treated merely as point charges, since their polarisability values are negligible compared with non-metallic atoms. The T-matrix should be evaluated at each of the S-sites to render the 9S simultaneous equations.

EVALUATION OF THE EFG AT THE QUADRUPOLE NUCLEUS

The final phase of the program consists almost of a repetition of the above computation up to the evaluation of the T-matrix, starting with the lattice site of interest, where the quadrupole nucleus is located, as origin.   Using the original array XO, YO, ZO of the position co-ordinates, the cartesian co-ordinates of all atoms relative to the quadrupole nucleus of interest are computed:-

XR = XO(Q) - XO(n) etc. and so on and the program proceeds until the term matrix T_{ij} is obtained.   Using the self consistent multipole moments evaluated in the previous phase, the electrostatic fields and field gradients are readily obtained from

$$V_i = \sum_{j=1}^{10} T_{ij} D_j$$

i = 1 - 3 Fields and i = 4 - 9 Field gradients.

The final output is obtained in the form of 9 x 13 matrix.   The 1st column indicates the contribution due to the lattice charges only V_c 2nd, 3rd and 4th due to individual dipole/components V_{DX}, V_{DY}, V_{DZ},   5th column total contribution due to the dipoles V_D, 6 - 11th individual contributions due to the six quadrupole tensor elements

$V_{Q_{xx}}$, $V_{Q_{yy}}$, $V_{Q_{zz}}$, $V_{Q_{xy}}$, $V_{Q_{yz}}$, $V_{Q_{zx}}$;   12th column the total contribution of quadrupoles V_Q and finally the 13th column is the total contribution due to all multipoles V_T.   The program is tested by computing the EFG values for Al_2O_3 for which data is available[6], and is presently being extended to study the oxides of arsenic, antimony, bismuth, iridium and gallium.

Experimental nuclear quadrupole resonance data is available for the V group oxides (As, Sb and Bi).   Search for NQR signals in the oxides of iridium and gallium has so far not yielded any results at room temperature.   These will be re-investigated at liquid nitrogen temperatures at the Queen Elizabeth College NQR laboratories.

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