

Theta series and magic numbers for diamond and certain ionic crystal structures

N. J. A. Sloane

AT&T Bell Laboratories, Murray Hill, New Jersey 07974

(Received 26 September 1986; accepted for publication 25 February 1987)

Two earlier papers by Teo and the author [J. Chem. Phys. **83**, 6520 (1985); Inorg. Chem. **25**, 2315 (1986)] studied circular and spherical clusters in the simplest close-packed structures in two and three dimensions. The present work considers clusters in other fundamental structures (the hexagonal net, diamond), and applies the results to study clusters in related structures (Lonsdaleite, graphite) and in binary arrays with the structure of the idealized ionic crystals NaCl, CsCl, ZnS, CaF₂, TiO₂, O₃Bi₂.

I. INTRODUCTION

In Refs. 1 and 2 Teo and the author investigated circular clusters in the square and hexagonal lattices in two dimensions (2D), and spherical clusters in the simple, face-centered, and body-centered cubic lattices and the hexagonal close-packing in three dimensions (3D), for various choices for the center of the cluster. In these papers we gave the theta series for each cluster, table of the coefficients and their partial sums, which are the nuclearities or magic numbers of the clusters, and coordinates for the atoms in the first few shells of each cluster.

The present paper has two goals: (i) to give the theta series for certain fundamental structures not considered in Refs. 1 and 2 (e.g., the hexagonal net in 2D, the diamond net in 3D); and (ii) to show how these fundamental theta series may be used to study clusters in more complicated structures, including binary and higher-order compounds, and to enumerate the atoms of the individual elements in the clusters. This technique is illustrated by considering the hexagonal diamond (or Lonsdaleite) net, various 3-D nets related to graphite, and binary compounds having the structure of the ionic crystals NaCl, CsCl, ZnS (zinc blende and wurtzite), CaF₂, TiO₂, and O₃Bi₂. For applications of these results see Refs. 1 and 2.

Theta series have been used for almost 100 years in the calculation of numerical sums (such as Madelung's constant) associated with lattices: see, for example, Tosi,³ Glasser and Zucker,⁴ and Borwein *et al.*⁵ However, the present series of papers appears to represent the first application of theta series (at any rate in recent years) to the enumerative or combinatorial study of clusters. For example, the especially simple expressions (17) and (19) for clusters in the diamond structure do not appear to have been published before. On the other hand, it would not be surprising if they were to be found somewhere in the older literature. The author would appreciate hearing of any references that have been overlooked. Computer programs (such as MACSYMA^{6,7}) that are capable of performing algebraic computations now make it particularly easy to manipulate theta series.

Since the methods are similar to those used in Refs. 1 and 2, the treatment here will be brief. Except for diamond we give just an analytic expression for each theta series, and

the number of atoms in the first few shells of the clusters. The nuclearities of the clusters are the partial sums of the latter numbers, and can easily be derived from the information provided, as is illustrated for diamond in Table I.

The same methods may be applied to lattices in spaces of higher dimension; these results are described elsewhere.^{8,9} However, it seems worth giving two particularly appealing examples. The theta series of the E₈ or Gosset lattice in eight dimensions (with respect to a lattice point) is

$$\Theta_{E_8}(X) = \frac{1}{2}(\theta_2(X)^8 + \theta_3(X)^8 + \theta_4(X)^8). \quad (1)$$

Comparison of this expression with Eq. (17) shows that E₈ may be regarded as an eight-dimensional diamond lattice. The theta series of the notorious Leech lattice in 24 dimensions (with respect to a lattice point) is

TABLE I. Clusters in diamond structure, centered at (a) an atom, (b) the midpoint of two neighboring atoms, and (c) the center of a tetrahedral hole. Here S_n is the number of points in the spherical shell of radius √n, and G_n is the magic number of the cluster.

(a) Diamond, atom			(b) Diamond, edge			(c) Diamond, hole		
n	S _n	G _n	n - 3/16	S _n	G _n	n	S _n	G _n
0	1	1	0	2	2	3/4	4	4
3/4	4	5	1	6	8	1	6	10
2	12	17	2	12	20	2 3/4	12	22
2 3/4	12	29	3	12	32	3	8	30
4	6	35	4	6	38	4 3/4	12	42
4 3/4	12	47	5	18	56	5	24	66
6	24	71	6	18	74	6 3/4	16	82
6 3/4	16	87	7	12	86	8 3/4	24	106
8	12	99	8	30	116	9	30	136
8 3/4	24	123	9	14	130	10 3/4	12	148
10	24	147	10	6	136	11	24	172
10 3/4	12	159	11	30	166	12 3/4	24	196
12	8	167	12	24	190	13	24	220
12 3/4	24	191	13	18	208	14 3/4	36	256
14	48	239	14	30	238	16 3/4	12	268
14 3/4	36	275	15	26	264	17	48	316
16	6	281	16	24	288	18 3/4	28	344
16 3/4	12	293	17	30	318	19	24	368
18	36	329	18	24	342	20 3/4	36	404
18 3/4	28	357	19	18	360	21	48	452
20	24	381	20	24	384	22 3/4	24	476
20 3/4	36	417	21	36	420	24 3/4	36	512
22	24	441	22	24	444	25	30	542
22 3/4	24	465	23	48	492	26 3/4	36	578
24	24	489	24	30	522	27	32	610

5925 5926 5927

$$\Theta_{\text{Leech}}(X) = \frac{1}{2}(\theta_2(X)^{24} + \theta_3(X)^{24} + \theta_4(X)^{24}) - \frac{69}{16}(\theta_2(X)\theta_3(X)\theta_4(X))^8. \quad (2)$$

There is no 3-D analog of this lattice.

II. THETA SERIES

Let T be an array of points (or *atoms*) in Euclidean space (of any numbers of dimensions). The *norm* s 's of a vector s is its squared length. The *theta series* of T with respect to an arbitrary point P is the formal power series

$$\Theta_{T,P}(X) = \sum_{t \in T} X^{(t-P) \cdot (t-P)}. \quad (3)$$

The subscript P may be omitted if it is clear from the context. The coefficient of X^n in $\Theta_{T,P}(X)$, S_n say, is therefore the number of atoms in T at squared distance n from P , i.e., the number of atoms on the spherical shell of radius \sqrt{n} around P . The partial sum

$$G_n = \sum_{m < n} S_m \quad (4)$$

is the total number of atoms in the *spherical cluster* of radius \sqrt{n} centered at P , i.e., the *nuclearity* or *magic number* of that cluster.

If T is a *binary* array, consisting of two types of atoms, say

$$T = T_X \cup T_Y,$$

where T_X (resp. T_Y) is the set of atoms of type X (resp. Y), then the bivariate theta series of T with respect to an arbitrary point P is defined to be

$$\Theta_{T,P}(X,Y) = \Theta_{T_X,P}(X) + \Theta_{T_Y,P}(Y). \quad (5)$$

For greater emphasis we sometimes replace X and Y by the symbols for the corresponding elements, as is illustrated in Eqs. (27)–(29).

The symbols Z , Z^2 , Z^3 denote the *integer points* along a line, the *square lattice* of points with integer coordinates in 2D, and the *simple cubic lattice* in 3D, respectively. The *hexagonal lattice* in 2D (with coordination number 6, and scaled so that neighboring atoms are at unit distance apart) is denoted by A_2 .

The theta series of the structures considered in this paper may be conveniently expressed in terms of the seven fundamental functions given in Eqs. (6)–(12). These are

$$\eta_a(X) = \sum_{m=-\infty}^{\infty} X^{(m+a)^2} = \Theta_{Z+a}(X), \quad (6)$$

for any real number a , which is the theta series with respect to the origin of the 1-D array

..., $a-1, a, a+1, a+2, a+3, \dots$;

$$\begin{aligned} \theta_2(X) &= \eta_{1/2}(X) = \Theta_{Z+1/2}(X) \\ &= 2X^{1/4} + 2X^{9/4} + 2X^{25/4} + 2X^{49/4} + \dots, \end{aligned} \quad (7)$$

$$\begin{aligned} \theta_3(X) &= \eta_0(X) = \Theta_Z(X) \\ &= 1 + 2X + 2X^4 + 2X^9 + 2X^{16} + 2X^{25} + \dots, \end{aligned} \quad (8)$$

$$\begin{aligned} \theta_4(X) &= \theta_3(-X) \\ &= 1 - 2X + 2X^4 - 2X^9 + 2X^{16} - 2X^{25} + \dots \end{aligned} \quad (9)$$

(θ_2 , θ_3 , and θ_4 are particular examples of Jacobi theta series¹⁰); and the theta series of the hexagonal lattice with respect to an atom, the midpoint of an edge joining two neighboring atoms, and the center of a triangular hole, respectively, which are

$$\begin{aligned} \phi_0(X) &= \Theta_{A_2, \text{atom}}(X) \\ &= \theta_2(X)\theta_2(X^3) + \theta_3(X)\theta_3(X^3) \\ &= 1 + 6X + 6X^3 + 6X^4 \\ &\quad + 12X^7 + 6X^9 + 6X^{12} + \dots, \end{aligned} \quad (10)$$

$$\begin{aligned} \phi_1(X) &= \Theta_{A_2, \text{edge}}(X) \\ &= \frac{1}{2}\theta_2(X^{1/4})\theta_2(X^{3/4}) \\ &= 2X^{1/4} + 2X^{3/4} + 4X^{7/4} + 2X^{9/4} + 4X^{13/4} + \dots, \end{aligned} \quad (11)$$

$$\begin{aligned} \phi_2(X) &= \Theta_{A_2, \text{hole}}(X) \\ &= \theta_2(X)\eta_{1/6}(X^3) + \theta_3(X)\eta_{1/3}(X^3) \\ &= \frac{1}{2}(\phi_0(X^{1/3}) - \phi_0(X)) \\ &= 3X^{1/3} + 3X^{4/3} + 6X^{7/3} + 6X^{13/3} \\ &\quad + 3X^{16/3} + \dots. \end{aligned} \quad (12)$$

Tables 4–6 of Ref. 1 give the first 80 terms in (10)–(12). The Jacobi theta series $\theta_2, \theta_3, \theta_4$ satisfy numerous identities^{1,4,10}; these have been used to simplify later formulas whenever possible.

III. TWO-DIMENSIONAL NETS

Two-dimensional nets have been extensively studied; see, for example, Wells^{11,12} and O'Keeffe and Hyde.¹³ There are three regular nets, two of which (the square lattice $4^4 = Z^2$ and the hexagonal lattice $3^6 = A_2$) we investigated in Refs. 1, 2, and 14.

We now consider the third regular net, the *hexagonal net* $6^3 = H_2$ (Fig. 1). This may be regarded as the union of A_2 and a reflected copy of A_2 . Let neighboring atoms be at unit distance apart. Then, using the results in Ref. 1, it follows that the theta series of H_2 with respect to an atom, the midpoint of an edge joining neighboring atoms, and the center of a hexagonal hole are, respectively,

$$\begin{aligned} \Theta_{H_2, \text{atom}}(X) &= \phi_0(X^3) + \phi_2(X^3) \\ &= \frac{1}{2}(\phi_0(X) + \phi_0(X^3)) \\ &= 1 + 3X + 6X^3 + 3X^4 + 6X^7 + 6X^9 \\ &\quad + 6X^{12} + 6X^{13} + 3X^{16} + 6X^{19} + \dots, \end{aligned} \quad (13)$$

$$\begin{aligned} \Theta_{H_2, \text{edge}}(X) &= \phi_1(X) - \phi_1(X^3) \\ &= \theta_2(X^{3/4})\eta_{1/6}(X^{9/4}) \\ &= 2X^{1/4} + 4X^{7/4} + 4X^{13/4} + 4X^{19/4} \\ &\quad + 2X^{25/4} + 4X^{31/4} + 4X^{37/4} + 4X^{43/4} \\ &\quad + 6X^{49/4} + 4X^{61/4} + \dots, \end{aligned} \quad (14)$$

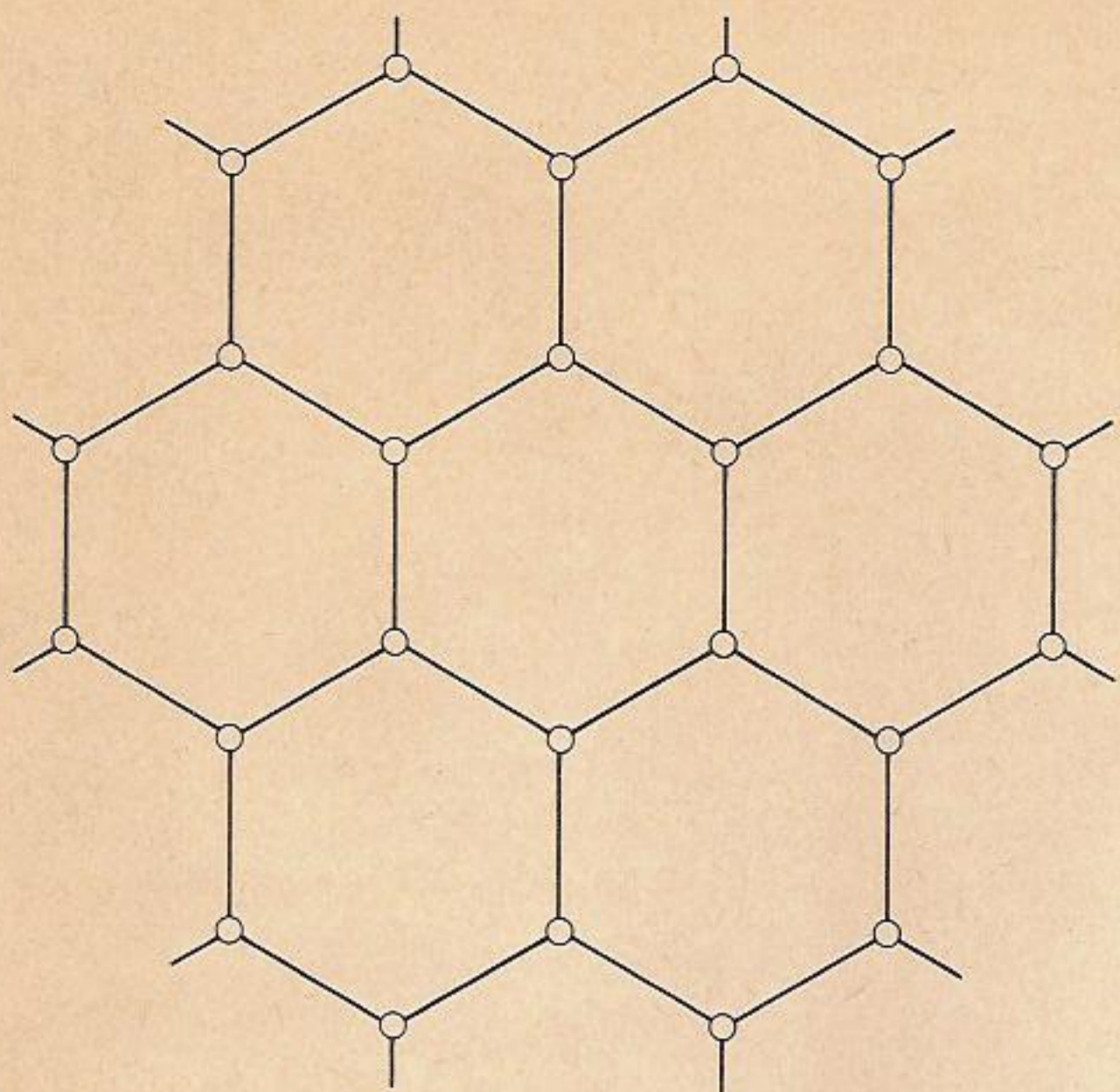


FIG. 1. Two-dimensional hexagonal net H_2 .

$$\begin{aligned} \Theta_{H_2, \text{hole}}(X) &= \phi_0(X) - \phi_0(X^3) = 2\phi_2(X^3) \\ &= 6X + 6X^4 + 12X^7 + 12X^{13} + 6X^{16} + 12X^{19} \\ &\quad + 6X^{25} + 12X^{28} + 12X^{31} + 12X^{37} + \dots \end{aligned} \quad (15)$$

Remarks: In principal there is no difficulty in calculating the theta series of any 2-D or 3-D structure (as illustrated in Sec. IX of Ref. 1). The interesting question is to find as simple an expression as possible. Using Refs. 1 and 2 and the above formulas simple expressions may be obtained for many other 2-D nets. For example the theta series of the *Kagomé net* (Fig. 8 of Ref. 13) with respect to an atom and the center of a hexagonal hole are

$$\phi_0(z) - \phi_1(4z) \quad \text{and} \quad \phi_0(z) - \phi_0(4z), \quad (16)$$

respectively.

IV. THE DIAMOND NET

The *diamond net* (p. 117 of Ref. 11, p. 121 of Ref. 12, p. 26 of Ref. 15) may be regarded as the union of a face-centered cubic (fcc) lattice [in which the 12 neighbors of the origin have coordinates of the form $(\pm 1, \pm 1, 0)$] and a translation of this fcc lattice by $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. The minimal distance between atoms is $\sqrt{3}/2$. Then using the results in Ref. 1 we find that the theta series of diamond with respect to an atom [e.g., the point $(0,0,0)$], the midpoint of an edge [e.g., $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$], and the center of a tetrahedral hole [e.g., $(0,0,1)$] are, respectively,

$$\begin{aligned} \Theta_{\text{diamond,atom}}(X) &= \frac{1}{2}(\theta_2(X)^3 + \theta_3(X)^3 + \theta_4(X)^3) \\ &= 1 + 4X^{3/4} + 12X^2 + 12X^{11/4} + \dots, \end{aligned} \quad (17)$$

$$\begin{aligned} \Theta_{\text{diamond,edge}}(X) &= \theta_2(\sqrt{X})\{\theta_2(X^2)\eta_{3/8}(X^4) + \theta_3(X^2)\eta_{1/8}(X^4)\} \\ &= 2X^{3/16} + 6X^{19/16} + 12X^{35/16} + 12X^{51/16} + \dots, \end{aligned} \quad (18)$$

$$\begin{aligned} \Theta_{\text{diamond,hole}}(X) &= \frac{1}{2}(\theta_2(X)^3 + \theta_3(X)^3 - \theta_4(X)^3) \\ &= 4X^{3/4} + 6X + 12X^{11/4} + 8X^3 + \dots \end{aligned} \quad (19)$$

Table I displays the first 50 coefficients S_n in (17)–(19) and their partial sums G_n [see Eq. (4)]. The first column agrees with and extends a small table given by Prins and Petersen¹⁶ (reprinted on p. 1039 of Ref. 17).

For the closely related *hexagonal diamond* or *Lonsdaleite net* (Fig. 3.35c of Ref. 12) we give just the theta series with respect to an atom, which on the same scale is

$$\begin{aligned} &\{\theta_2(X^{16/3})\phi_2(X^2) + \theta_3(X^{16/3})\phi_0(X^2)\} + \{\eta_{1/8}(X^{16/3}) \\ &\quad \times \phi_2(X^2) + (\frac{1}{2}\theta_2(X^{4/3}) - \eta_{1/8}(X^{16/3}))\phi_0(X^2)\} \\ &= 1 + 4X^{3/4} + 12X^2 + X^{25/12} + 9X^{11/4} + 6X^4 \\ &\quad + 6X^{49/12} + 9X^{19/4} + 2X^{16/3} + 18X^6 + \dots \end{aligned} \quad (20)$$

(using Tables 16 and 22 of Ref. 1).

V. GRAPHITE AND RELATED 3-D NETS

The hexagonal net H_2 contains twice as many atoms as hexagonal holes, and many different 3-D nets may be formed by stacking appropriately displaced layers of H_2 (p. 922 of Ref. 12). By stacking identical layers, i.e., using the sequence $AAA \dots$ we obtain the *primitive hexagonal array* (p. 596 of Ref. 13). If the distance between layers is a , and the distance between atoms in the same layer is 1, the theta series of the primitive hexagonal array with respect to an atom is, from (13),

$$\frac{1}{2}\theta_3(X^{a^2})(\phi_0(X^{1/2}) + \phi_0(X^{3/2})). \quad (21)$$

By stacking layers in the sequence $ABAB \dots$ we obtain the ordinary *graphite net* (p. 922 of Ref. 12), in which there are two geometrically distinct types of atoms. With respect to an atom which is opposite *atoms* in the two adjacent layers, the theta series of graphite is also given by (21). With respect to an atom which is opposite *holes* in the two adjacent layers, the theta series of graphite is

$$\theta_3(X^{4a^2})(\phi_0(X^{3/2}) + \phi_2(X^{3/2})) + 2\theta_2(X^{4a^2})\phi_2(X^{3/2}). \quad (22)$$

By stacking layers in the order $ABCABC \dots$ we obtain the *rhomboidal graphite net* (p. 923 of Ref. 12), in which all atoms are geometrically equivalent. The theta series with respect to any atom is

$$\begin{aligned} &\frac{1}{4}\phi_0(X^2)(3\theta_3(X^{9a^2}) - \theta_3(X^{a^2})) \\ &\quad + \frac{1}{4}\phi_0(X^{2/3})(3\theta_3(X^{a^2}) - \theta_3(X^{9a^2})). \end{aligned} \quad (23)$$

VI. IONIC CRYSTAL STRUCTURES

To illustrate the application of theta series to binary compounds we consider seven of the most regular ionic crystal structures. The first six are pictured on p. 15 of Ref. 18. We use the most symmetrical (idealized) versions of these

structures, in which the parameters of the unit cell are such as to give the highest coordination number. The same techniques may be applied to more general structures, but the resulting theta series are not as simple.

The first four examples all follow the same pattern. We begin with the simplest.

(i) The idealized *rock salt* (NaCl) structure consists of two types of atoms (Na and Cl, or more generally X and Y) placed alternately at the points of the simple cubic lattice. The theta series with respect to an X -type atom is [from (45) and (53) of Ref. 1]

$$\begin{aligned} \Theta_{\text{rock salt}, X}(X, Y) &= \Theta_{\text{fcc, atom}}(X) + \Theta_{\text{fcc, oct. hole}}(Y) \\ &= \frac{1}{2}(\theta_3(X)^3 + \theta_4(X)^3) + \frac{1}{2}(\theta_3(Y)^3 - \theta_4(Y)^3) \\ &= X^0 + 6Y + 12X^2 + 8Y^3 + 6X^4 + 24Y^5 \\ &\quad + 24X^6 + 12X^8 + 30Y^9 + 24X^{10} + \dots \end{aligned} \quad (24)$$

The X - and Y -type atoms are geometrically equivalent, so the theta series with respect to a Y -type atom is obtained by interchanging X and Y in (24).

(ii) The *cesium chloride* (CsCl) structure similarly consists of two types of atoms placed alternately at the points of the body-centered cubic (bcc) lattice. The theta series with respect to an X -type atom is [from (37), (43) of Ref. 1]

$$\begin{aligned} \Theta_{\text{CsCl}, X}(X, Y) &= \Theta_{Z^3, \text{atom}}(X) + \Theta_{Z^3, \text{hole}}(Y) \\ &= \theta_3(X)^3 + \theta_2(Y)^3 \\ &= X^0 + 8Y^{3/4} + 6X + 12X^2 + 24Y^{11/4} + 8X^3 \\ &\quad + 6X^4 + 24Y^{19/4} + 24X^5 + 24X^6 + \dots \end{aligned} \quad (25)$$

(iii) The *zinc blende* (ZnS) structure is obtained in the same way from the diamond net. The theta series with respect to an X -type atom is [compare Eq. (17)]

$$\begin{aligned} \Theta_{\text{zinc blende}, X}(X, Y) &= \frac{1}{2}(\theta_2(Y)^3 + \theta_3(X)^3 + \theta_4(X)^3) \\ &= X^0 + 4Y^{3/4} + 12X^2 + 12Y^{11/4} + 6X^4 + 12Y^{19/4} \\ &\quad + 24X^6 + 16Y^{27/4} + 12X^8 + 24Y^{35/4} + \dots \end{aligned} \quad (26)$$

(iv) The *wurtzite* (ZnS) structure¹⁹ is similarly obtained from hexagonal diamond. The theta series with respect to an X -type atom is obtained by replacing X by Y in the second bracketed expression in (20).

(v) In the idealized *fluorite* (CaF₂) structure the two types of atoms are not geometrically equivalent, and so it seems clearest to replace X and Y by the appropriate chemical symbols. With respect to a calcium atom we have [using (45) and (51) of Ref. 1]

$$\begin{aligned} \Theta_{\text{CaF}_2, \text{Ca}}(\text{Ca}, \text{F}) &= \Theta_{\text{fcc, atom}}(\text{Ca}) + 2\Theta_{\text{fcc, tet. hole}}(\text{F}) \\ &= \frac{1}{2}(\theta_3(\text{Ca})^3 + \theta_4(\text{Ca})^3) + \theta_2(\text{F})^3 \\ &= \text{Ca}^0 + 8\text{F}^{3/4} + 12\text{Ca}^2 + 24\text{F}^{11/4} \\ &\quad + 6\text{Ca}^4 + 24\text{F}^{19/4} + 24\text{Ca}^6 + 32\text{F}^{27/4} \\ &\quad + 12\text{Ca}^8 + 48\text{F}^{35/4} + \dots \end{aligned} \quad (27)$$

[compare (26)]. The fluorite structure may also be regard-

ed as a simple cubic lattice of F atoms with half the holes filled by Ca atoms. Therefore, with respect to a fluorine atom, we have

$$\begin{aligned} \Theta_{\text{CaF}_2, \text{F}}(\text{Ca}, \text{F}) &= \Theta_{Z^3, \text{atom}}(\text{F}) + \frac{1}{2}\Theta_{Z^3, \text{hole}}(\text{Ca}) \\ &= \theta_3(\text{F})^3 + \frac{1}{2}\theta_2(\text{Ca})^3 \\ &= \text{F}^0 + 4\text{Ca}^{3/4} + 6\text{F} + 12\text{F}^2 + 12\text{Ca}^{11/4} + 8\text{F}^3 \\ &\quad + 6\text{F}^4 + 12\text{Ca}^{19/4} + 24\text{F}^5 + 24\text{F}^6 + \dots \end{aligned} \quad (28)$$

For *antifluorite* (p. 161 of Ref. 12) we interchange Ca and F in (27) and (28).

(vi) The *rutile* (TiO₂) structure illustrates how less regular structures may be handled. Rutile consists of Ti atoms at the positions of the bcc lattice and O atoms at four translates of the simple cubic lattice Z^3 by the amounts

$$\pm(u, u, 0), \pm(\frac{1}{2} + u, \frac{1}{2} - u, 0),$$

where $u \approx 0.30$. The theta series of the translate $Z^3 + (u, v, w)$ is $\eta_u(X)\eta_v(X)\eta_w(X)$. It follows using (71) of Ref. 1 that

$$\begin{aligned} \Theta_{\text{TiO}_2, \text{Ti}}(\text{Ti}, \text{O}) &= \theta_2(\text{Ti})^3 + \theta_3(\text{Ti})^3 \\ &\quad + 2\eta_u(\text{O})^2\theta_3(\text{O}) + 2\eta_{u+1/2}(\text{O})^2\theta_2(\text{O}). \end{aligned} \quad (29)$$

(vii) The final example illustrates how close-packed tetrahedral structures (such as are described on pp. 161 and 162 of Ref. 12) may be handled. The idealized O₃Bi₂ structure consists of Bi atoms at the points of an fcc lattice in which three-quarters of the tetrahedral holes are occupied by O atoms. The theta series with respect to a Bi atom is [using (45) and (51) of Ref. 1, and counting the holes with the correct multiplicity]

$$\begin{aligned} \Theta_{\text{O}_3\text{Bi}_2, \text{Bi}}(\text{O}, \text{Bi}) &= \Theta_{\text{fcc, atom}}(\text{Bi}) + \frac{3}{4} \cdot 2\Theta_{\text{fcc, tet. hole}}(\text{O}) \\ &= \frac{1}{2}(\theta_2(\text{Bi})^3 + \theta_3(\text{Bi})^3) + \frac{3}{2}\theta_2(\text{O})^3 \\ &= \text{Bi}^0 + 6\text{O}^{3/4} + 12\text{Bi}^2 + 18\text{O}^{11/4} + 6\text{Bi}^4 \\ &\quad + 18\text{O}^{19/4} + 24\text{Bi}^6 + 16\text{O}^{27/4} + 12\text{Bi}^8 \\ &\quad + 24\text{O}^{35/4} + \dots \end{aligned} \quad (30)$$

The coordination number of 6 agrees with Table 4.5 of Ref. 12.

Erratum of Ref. 1: In Eq. (10) of Ref. 1, the second + sign should be omitted.

ACKNOWLEDGMENT

This project was proposed by my former colleague Boon K. Teo, and I thank him for his suggestions. I regret that circumstances have interrupted our collaboration.

¹N. J. A. Sloane and B. K. Teo, *J. Chem. Phys.* **83**, 6520 (1985).

²B. K. Teo and N. J. A. Sloane, *Inorg. Chem.* **25**, 2315 (1986).

³M. P. Tosi, *Solid State Phys.* **16**, 1 (1964).

⁴M. L. Glasser and I. J. Zucker, *Theor. Chem. Adv. Perspect.* **5**, 67 (1980).

⁵D. Borwein, J. M. Borwein, and K. F. Taylor, *J. Math. Phys.* **26**, 2999 (1985).

⁶Mathlab Group, *MACSYMA Reference Manual* (M.I.T., Laboratory for

- Computer Science, Cambridge, MA, 1983), Version 10.
- ⁷N. J. A. Sloane, *Not. Am. Math. Soc.* **33**, 40, 318 (1986).
- ⁸N. J. A. Sloane, *IEEE Trans. Inf. Theory* **27**, 327 (1981).
- ⁹J. H. Conway and N. J. A. Sloane, *Sphere-Packings, Lattices and Groups* (Springer, New York, 1987).
- ¹⁰E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (Cambridge U. P., Cambridge, 1963), 4th ed.
- ¹¹A. F. Wells, *Three-Dimensional Nets and Polyhedra* (Wiley, New York, 1977).
- ¹²A. F. Wells, *Structural Inorganic Chemistry* (Oxford U. P., Oxford, 1984), 5th ed.
- ¹³M. O'Keeffe and B. G. Hyde, *Philos. Trans. R. Soc. Ser. A* **295**, 553 (1980).
- ¹⁴B. K. Teo and N. J. A. Sloane, *Inorg. Chem.* **24**, 4545 (1985).
- ¹⁵R. W. G. Wyckoff, *Crystal Structures* (Wiley, New York, 1963), 2nd ed., Vol. 1.
- ¹⁶J. A. Prins and H. Petersen, *Physica* **3**, 147 (1936).
- ¹⁷J. O. Hirschfelder, C. F. Curtis, and R. B. Bird, *Molecular Theory of Gases and Liquids* (Wiley, New York, 1954).
- ¹⁸F. A. Cotton and G. Wilkinson, *Advanced Inorganic Chemistry* (Wiley, New York, 1980), 4th ed.
- ¹⁹M. L. Glasser, *J. Phys. Chem. Solids* **10**, 229 (1959).