To perform the convolution correctly, it is necessary to calculate the reflected intensity in the same way as for the Gaussian function. Fig. 6 describes the results of the calculated reflectivity of a silicon wafer of width 35 mm in the case of a Q_z scan along the ridge. The insert shows on a linear scale how the geometrical correction gives a good estimation at small Q_z of the measured intensity. The computation was performed with the matrix technique (Born & Wolf, 1964) with help of Matlab software (Gibaud & Vignaud, 1993). The electron density depth profile for this silicon wafer can be separated from the calculation, showing the presence of a layer of thickness 17.2 Å at the surface of the bulk silicon. Typical parameters used in the calculation are reported in Table 1. The low electron density of the surface layer reveals that it is probably related more to water deposition than to an oxide deposition. In conclusion, the above corrections strongly depend upon the line shape of the direct beam. When slits and a graphite analyzer (low-resolution mode) are used, the line shape is Gaussian but, in the case of a high-resolution triple-crystal diffractometer (Ge monochromator-crystal-Ge analyzer), the beam line shape is Lorentzian, so a Lorentzian function must be used to perform the corrections. This is illustrated in Fig. 7, which represents the absolute reflectivity of a niobium film on top of a sapphire substrate. The insert shows the observed and corrected calculated reflectivities. In this case, the contamination by the direct beam is not a problem because the FWHM of the direct beam in this high-resolution mode is only 0.01° (*cf.* 0.1° for the low-resolution mode). The geometrical correction is in this case very severe because the sample was only 10 mm wide and the beam 200 μm thick; this is clearly illustrated by the fact that the reflectivity was far less than 1 at $Q = Q_c$.

The authors wish to thank G. Ripault for technical assistance during the measurements and T. Nicolaï for stimulating discussions. One of us (AG) would like to thank R. A. Cowley for helpful discussions and for providing the facilities at the Clarendon Laboratory, where the experiments concerning the Nb-sapphire system were performed and where the system was grown.

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Acta Cryst. (1993). A**49**, 648–654

The Arrangement of Point Charges with Tetrahedral and Octahedral Symmetry on the Surface of a Sphere with Minimum Coulombic Potential Energy

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(*Received 14 September 1992; accepted 27 January 1993*)

Abstract

Up to 100 point charges have been distributed on the surface of a sphere such that the configurations display T and O symmetry as well as being a minimum, global or local, with respect to the Coulombic potential.

Introduction

The symmetry adopted by N point charges on the surface of a sphere such that the Coulombic potential is a minimum has been determined by several investigators: Ashby & Brittin (1986); Edmundson (1992); Erber & Hockney (1991); Frickel & Bronk (1987); Melnyk, Knop & Smith (1977); Rafac, Schiffer, Hangst, Dubin & Wales (1991); Weinrach, Carter, Bennett & McDowell (1990); Wille (1986).

Table 1 lists the values of N when the arrangements display tetrahedral or octahedral symmetry. This paper describes which other values of N can display T and O symmetries and at the same time produce a local minimum in terms of the Coulombic potential.

Tetrahedral configurations

The tetrahedron differs from the other Platonic solids in that it is its own dual and has no centre of

Table 1. *Global minima with T and O symmetry*

N	Symmetry	Föppl configuration	References
4	T_d	1,3	(*a*), (*b*), (*c*)
6	O_h	1, 4, 1	(*a*), (*b*), (*c*)
16	T	$1, 3^5$	(*a*), (*b*), (*c*), (*d*)
22	T_d	$1, 3^2, 6, 3^2$	(*a*), (*b*), (*c*)
24	O	4^6	(*a*), (*b*), (*c*)
28	T	$1, 3^9$	(*a*), (*b*), (*c*)
40	T_d	$1, 3^2, 6, 3^2, 6, 3, 6, 3^2$	(*a*), (*b*)
44	O_h	$4^3, 8, 4, 8, 4$	(*a*), (*b*)
46	T	$1, 3^{15}$	(*a*)
48	O	4^{12}	(*a*), (*b*)

References: (*a*) Edmundson (1992); (*b*) Weinrach *et al.* (1990); (*c*) Frickel & Bronk (1987); (*d*) Ashby & Brittin (1986).

inversion. T symmetry has twelve symmetry operations:

$$3\times C_2,\quad 4\times C_3,\quad 4\times C_3^2 \quad \text{and} \quad 1\times E.$$

T_d symmetry includes six mirror planes, three through each vertex of the tetrahedron, whilst T_h has only three mirror planes together with an inversion centre.

If an extra point is added randomly to one of the equilateral-triangular facets of the tetrahedron then two more points are required to conserve the threefold rotation axis of that facet; because there are four such facets, the total number of extra points added is twelve. Thus,

$$N=4+12a, \quad \text{series } T_1,$$

describes the number of apices that can have T symmetry of the form where there are the four original tetrahedral positions and where 'a' describes the number of unique apices in the configuration. The series 4, 16, 28, 40 is very noticeable in Table 1.

One can envisage a second series, created by adding apices at the mid-points of each edge of the basic tetrahedron or two points such that the twofold rotation about the mid-point is retained. Thus,

$$N=4+12a+6b, \quad \text{series } T_2,$$

where b is the number of points along each edge. If $b=1$ and $a=1$ and 3, then one obtains $N=22$ and 46, which are also in Table 1.

When the original four points of the basic tetrahedron are removed, the above two series become

$$N=12a, \qquad \text{series } T_3;$$

$$N=12a+6b, \quad \text{series } T_4.$$

If the inverses of the original apices are included, then the two equations are

$$N=8+12a, \qquad \text{series } T_5,$$

$$N=8+12a+6b, \quad \text{series } T_6.$$

Thus, the general equation becomes

$$N=12a+6b+4c,$$

where $c=0$, 1 or 2.

To include T_h symmetry, it was expected that the factor of twelve would be increased to 24 to include the inverse apices and c would be made equal to two.

Octahedral configurations

The simple O group has 24 operations:

$$3\times C_4,\quad 3\times C_4^2,\quad 3\times C_4^3,\quad 4\times C_3,$$

$$4\times C_3^2,\quad 6\times C_2 \quad \text{and} \quad 1\times E,$$

whilst the O_h group includes nine mirror planes. The configurations can be formulated from either an octahedron or a cube. For the case of a cube, each square facet has a fourfold axis and so four points are required to conserve the symmetry of the facet. The six facets of the cube require a total of 24 points. For the case of an octahedron, each equilateral triangle requires three points, again making 24, for the eight facets. Thus,

$$N=24a, \quad \text{series } O_1.$$

By including the original points of the octahedron and cube, respectively, two additional series are produced:

$$N=24a+6, \quad \text{series } O_2;$$

$$N=24a+8, \quad \text{series } O_3.$$

Two further series can be produced if the mid-point of each edge of the original figure is used:

$$N=24a+6+12b, \quad \text{series } O_4;$$

$$N=24a+8+12b, \quad \text{series } O_5.$$

Other combinations can be used to produce three more series:

$$N=6+8+12b+24a, \quad \text{series } O_6;$$

$$N=24a+12b, \qquad \text{series } O_7;$$

$$N=6+8+24a, \qquad \text{series } O_8;$$

the general equation becoming

$$N=24a+12b+6c+8c',$$

where c and c' are either 0 or 1, depending on whether apices occur at the corners of the basic cube or of the octahedron.

Method

In a previous paper (Edmundson, 1992), the minimum potential was located by making exploratory moves for each point in an iterative process. In the forcing of the system to retain T symmetry, groups of twelve points are moved simultaneously, whilst, with O symmetry, each group consists of 24 points. Thus, for $N=34$, with T symmetry, one requires $a=2$, $b=1$ and $c=1$. This means that the four

Table 2. *The basic tetrahedral coordinates*

Apex number	x	y	z
1	0	1	0
2	$8^{1/2}/3$	$-1/3$	0
3	$-8^{1/2}/6$	$-1/3$	$(2/3)^{1/2}$
4	$-8^{1/2}/6$	$-1/3$	$-(2/3)^{1/2}$

Table 3. *The basic octahedral coordinates*

Apex number	x	y	z
1	0	1	0
2	1	0	0
3	0	0	1
4	-1	0	0
5	0	0	-1
6	0	-1	0

Table 4. *Data for tetrahedral configurations*

N	a	b	c	Potential	S	Δ	MP	Föppl arrangement
4	0	0	1	3.674235	T_d	1	2	1, 3
6	0	1	0	9.985281	O_h	1	0, 4	3, 3
8	0	0	2	19.740774	O_h	1	0, 4	$1, 3^2, 1$
10	0	1	1	33.467677	T_d		4	$1, 3^3$
12	1	0	0	49.165253	I_h	1	4	$1, 5^2, 1$ or 3^4
14	0	1	2	69.342378	O_h	1	4, 6	$1, 3^4, 1$
16	1	0	1	92.911655	T	3		$1, 3^5$
18	1	1	0	120.643750	O_h	2	4, 8	$3^2, 6, 3^2$
20	1	0	2	151.798621	I_h	1	4	5^4 or $1, 3, 6^2, 3, 1$
22	1	1	1	185.287536	T_d	3	6	$1, 3^2, 6, 3^3$
24	2	0	0	223.347074	O	3		3^8
26	1	1	2	266.149838	O_h	1	8, 8	$1, 3^3, 6, 3^3, 1$
28	2	0	1	310.491542	T	5		$1, 3^9$
30	2	1	0	359.831047	O	3		3^{10}
32	2	0	2	412.261275	I_h	1	8	$1, 5^6, 1$ or $[1, 3^2, 6, 3]_2$
34	2	1	1	470.157371	T			$1, 3^{11}$
36	3	0	0	529.282064	T	7		3^{12}
38	2	1	2	594.276246	O	3		$1, 3^{12}, 1$
40	3	0	1	660.675279	T_d	5	8	$1, 3^2, 6, 3^2, 6, 3, 6, 3^2$
42	3	1	0	732.256241	I_h	2	8	$3^2, 6, 3^2, 6, 3^2, 6, 3^2$
44	3	0	2	807.174263	O_h	3	4, 10	$4^3, 8, 4, 8, 4^3$
46	3	1	1	886.167114	T	8		$1, 3^{15}$
48	4	0	0	968.713455	O	5		3^{16}
48	3	2	0	970.043142	T	9		$3^{11}, 6, 3^3$
50	3	1	2	1055.854669	T_h	5	8	$1, 3^{16}, 1$
52	4	0	1	1145.447334	T	9		$1, 3^{17}$
54	4	1	0	1239.794851	O	5		3^{18}
56	4	0	2	1338.453609	T	9		$1, 3^{18}, 1$
58	4	1	1	1439.105779	T_d	8	8	$1, 6, 3^2, 6^3, 3, 6, 3^2, 6, 3^2$
60	5	0	0	1543.844655	T	11		3^{20}
62	4	1	2	1653.410295	O	5		$1, 3^{20}, 1$
64	5	0	1	1765.823383	T	11		$1, 3^{21}$
66	5	1	0	1884.045965	T	12		3^{22}
68	5	0	2	2003.232343	T	11		$1, 3^{22}$
70	5	1	1	2127.128180	T_d	8	10	$1, 3^2, 6, 3^2, 6^2, 3, 6^2, 3, 6, 3^2, 6, 3$
72	6	0	0	2255.131117	O	7		3^{24}
72	5	2	0	2255.001521	T_d	10	8	$3, 6, 3^2, 6, 3, 6^2, 3^2, 6^4, 3^2$
74	5	1	2	2388.572067	T	12		$1, 3^{24}, 1$
76	6	0	1	2523.113188	T	13		$1, 3^{25}$
78	6	1	0	2662.046475	T_h	8	12	3^{26}
80	6	0	2	2805.577601	O	7		$1, 3^{26}, 1$
82	6	1	1	2952.996155	T_d	9	12	$1, 3^3, 6, 3, 6^2, 3, 6, 3, 6^2, 3, 6, 3^2, 6, 3^2$
84	7	0	0	3104.331188	T_h	8	12	3^{28}
86	6	1	2	3258.492973	O_h	5	12, 14	$[1, 3^2, 6, 3^2, 6, 3, 6^2, 3]_2$
88	7	0	1	3416.736916	T	15		$1, 3^{29}$
90	7	1	0	3579.519192	O	8		$3^{14}, 6, 3^{14}$
92	7	0	2	3745.618739	I_h	3	12	$[1, 5^3, 10, 5^2, 10]_2$
94	7	1	1	3916.229550	T	16		$1, 3^{31}$
96	8	0	0	4089.190491	T_h	11	8	3^{32}
96	7	2	0	4091.323078	T	17		$3^{24}, 6, 3^6$
98	7	1	2	4269.274356	T	16		$1, 3^{32}, 1$
100	8	0	1	4448.350634	T	17		$1, 3^{33}$

original apices of the tetrahedron, together with the six mid-points, are not moved, whilst two separate apices, together with their accompanying eleven apices, are moved in an exploratory manner.

Table 5. *Data for octahedral configurations*

N	a	b	c	c'	Potential	S	Δ	MP	Föppl Arrangement
6	0	0	1	0	9.985281	O_h	1	2, 4	1, 4, 1
8	0	0	0	1	19.740774	O_h	1	0, 4	4^2
12	0	1	0	0	49.341688	O_h	2	2, 4	4^3
14	0	0	1	1	69.342378	O_h	1	4, 6	$1, 4^3, 1$
18	0	1	1	0	120.643750	O_h	2	4, 8	1, 4, 8, 4, 1
20	0	1	0	1	155.231453	O_h		4, 6	4^5
24	1	0	0	0	223.347074	O	3		4^6
26	0	1	1	1	266.149838	O_h	1	8, 8	$1, 4^2, 8, 4^2, 1$
30	1	0	1	0	359.831047	O	3		$1, 4^7, 1$
32	1	0	0	1	412.312762	O_h	3	8, 8	$4^3, 8, 4^3$
36	1	1	0	0	531.911333	O_h	4	4, 6	$4^2, 8, 4, 8, 4^2$
38	1	0	1	1	594.276246	O	3		$1, 4^9, 1$
42	1	1	1	0	733.022273	O_h	3	8, 8	$1, 4^2, 8^3, 4^2, 1$
44	1	1	0	1	807.174263	O_h	3	4, 10	$4^3, 8, 4, 8, 4^3$
48	2	0	0	0	968.713455	O	5		4^{12}
50	1	1	1	1	1056.089367	O_h	3	8, 12	$1, 4^3, 8^3, 4^3, 1$
54	2	0	1	0	1239.794851	O	5		$1, 4^{13}, 1$
56	2	0	0	1	1338.466334	O	5		4^{14}
60	2	1	0	0	1543.902037	O_h	5	6, 12	$4^3, 8, 4, 12, 4, 8, 4^3$
62	2	0	1	1	1653.410295	O	5		$1, 4^{15}, 1$
66	2	1	1	0	1884.526276	O	6		$1, 4^7, 8, 4^7, 1$
68	2	1	0	1	2006.704671	O	6		4^{17}
72	3	0	0	0	2255.131117	O	7		4^{18}
74	2	1	1	1	2390.845398	O			$1, 4^8, 8, 4^8, 1$
78	3	0	1	0	2665.518404	O_h	6	10, 12	$[1, 4^2, 8^2, 4^2]_2 12$
80	3	0	0	1	2805.577601	O	7		4^{20}
84	3	1	0	0	3105.565051	O	8		4^{21}
86	3	0	1	1	3258.492973	O_h	5	12, 14	$[1, 4^2, 8, 4^2, 8, 4]_2 12$
90	3	1	1	0	3579.519192	O	8		$1, 4^{10}, 8, 4^{10}, 1$
92	3	1	0	1	3747.353918	O	8		4^{23}
96	4	0	0	0	4089.893493	O_h	7	8, 16	$[4^3, 8, 4^2, 8, 4]_2 16$
98	3	1	1	1	4269.167832	O	8		$1, 4^{11}, 8, 4^{11}, 1$

Generation of the twelve tetrahedral apices

The coordinates of the basic tetrahedron were set up as shown in Table 2. If an extra point (x, y, z) is now added, then, to conserve the threefold symmetry around apex 1, the following matrix will generate the two aditional points:

$$\begin{vmatrix} \cos\alpha & 0 & \sin\alpha \\ 0 & 1 & 0 \\ -\sin\alpha & 0 & \cos\alpha \end{vmatrix} \quad \text{matrix } \mathbf{A},$$

with $\alpha = 2\pi/3$ and $4\pi/3$. The three points are now rotated in such a way that apex 1 is transposed to apex 2; this is done by a combination of two rotations about the major axes. First, a rotation using matrix **A** with $\alpha = \pi/3$ about the y axis; second, a rotation about the z axis using the matrix

$$\begin{vmatrix} \cos\beta & \sin\beta & 0 \\ -\sin\beta & \cos\beta & 0 \\ 0 & 0 & 1 \end{vmatrix} \quad \text{matrix } \mathbf{B},$$

with $\cos\beta = -1/3$, the angle subtended at the centre by any two of the tetrahedral points. The three transformed points are now rotated using matrix **A**, with $\alpha = 2\pi/3$ and $4\pi/3$, to generate the remaining six points.

Generation of the 24 octahedral apices

The coordinates of the basic octahedron were set up as shown in Table 3. The additional new point is rotated about the fourfold y axis using matrix **A**, to produce four points. These points are then rotated around the fourfold x axis using

$$\begin{vmatrix} 1 & 0 & 0 \\ 0 & \cos\gamma & \sin\gamma \\ 0 & -\sin\gamma & \cos\gamma \end{vmatrix}, \quad \text{matrix } \mathbf{C}.$$

The last eight points are generated by rotating four suitable coordinates around the z axis using matrix **B**. The calculations were performed using Fortran with double-precision arithmetic on an IBM-clone 286 computer.

Results

The results of the calculations are shown in Table 4 for the tetrahedral arrangements and in Table 5 for the octahedral arrangements. S denotes the symmetry of the configuration, Δ denotes the number of differently shaped triangles in the arrangement and MP is the number of apices in the mirror plane. For O_h symmetry, the two numbers refer to the two kinds of mirror planes. Where O symmetry occurs in Table 4, the Föppl arrangement is given with respect to the threefold axis. Square brackets are sometimes used in the Föppl description as a shorthand. Thus, a configuration of $A.B.A'$ is reduced to $[A]_2B$, where A and B can be a string of numbers several elements in length and A' is the reverse of A. Fig. 1 shows the view down the threefold axis for the tetrahedral configurations of Table 4 for $N=22$ to 70. The $N=34$ system is not included because it is not possible to determine a unique set of triangular facets. Fig. 2 is the same as Fig. 1, except the view is up the threefold axis. Fig. 3 shows both views for the tetrahedral arrangements for $N=72$ to 98, with $N=74$ and 96 not shown. Fig. 4 shows the octahedral configurations from Table 5 for $N=26$ to 98, with $N=74$ not shown.

Discussion

T_1 series

This series produces the basic T symmetry, except for $N=4$ and 40, which are T_d; the first four members are global minima. The number of differently shaped triangles, Δ, for the T members of the series, is given by

$$\Delta = 2a + 1.$$

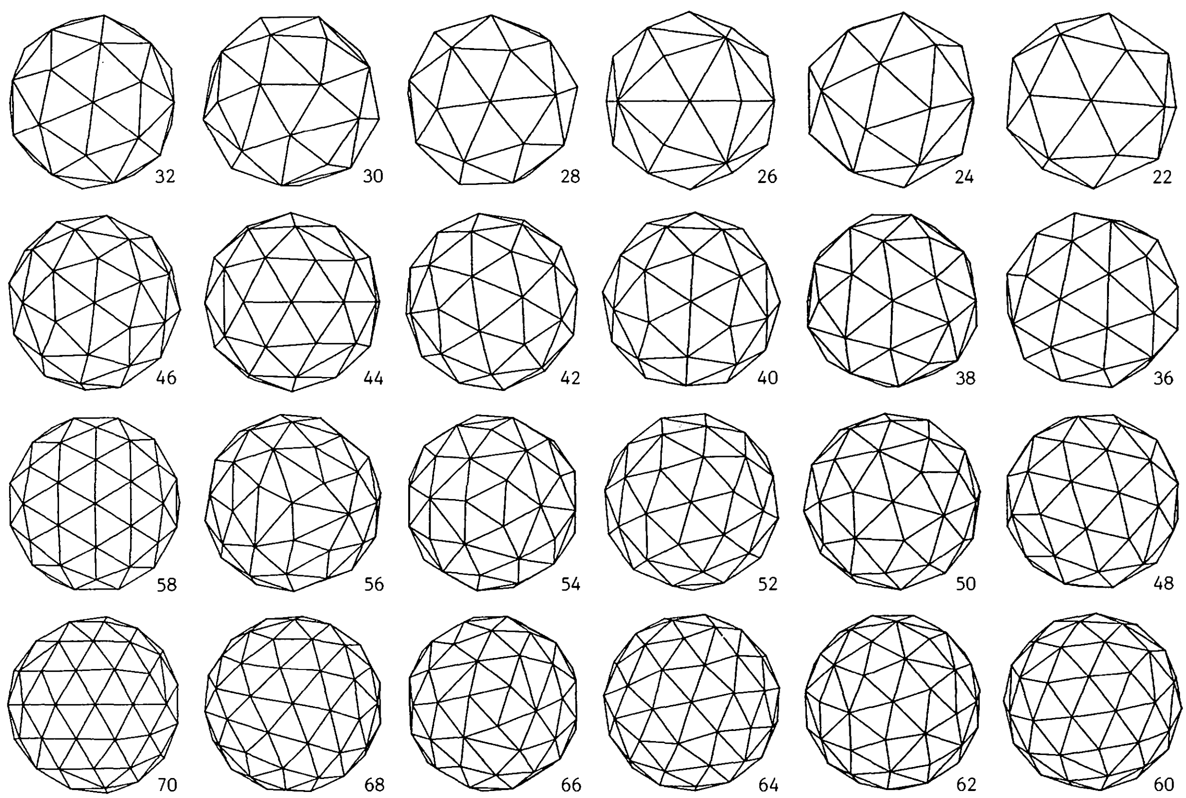

Fig. 1. Tetrahedral configurations for $N=22$ to 70, with $N=34$ not shown. View down the threefold axis.

A similar expression for the T_d series is complicated by the number of facets in the mirror planes.

T_2 series

This series again produces T or T_d configurations with global minima for $N = 22$ and 46. Δ for the T symmetry is given by

$$\Delta = 2a + 2.$$

T_3 series

O arrangements are produced for $N = 24$ and 48, which are global minima with square facets. The $N = 72$ arrangement has square facets but it is only a local minimum. For most of the tetrahedral series, it is possible to produce different tetrahedral arrangements by describing the 'a' value in the general equation and increasing the 'b' value correspondingly. Thus, for $N = 24$ with $a = 2$, $b = 0$ and $c = 0$, a potential of 223.347074 is produced; whilst with $a = 1$, $b = 2$ and $c = 0$, a potential of 224.062223, which has T_d symmetry, is obtained. This rearrangement is equivalent to forcing two points to reside along each edge of the basic tetrahedron but still retaining the twofold rotation axis about the mid-point of the edge. For $N = 72$, a lower potential of 2255.001521 with T_d symmetry is obtained using this technique. T_h symmetries are obtained for both $N = 84$ and 96. Forcing the T_3 series into $N = 24a$ produces a further arrangement having O_h symmetry with a Föppl configuration of $[3, 6, 3, 6^3, 3, 6, 3, 6]_2$ and a potential of 4093.321826.

T_4 series

This series in the main produces O symmetry, where it occurs,

$$\Delta = a + 1.$$

The $N = 18$ member is essentially the cuboctahedron with the six square faces capped. Similarly, the $N = 30$ configuration is basically the snub cube with its six square faces capped, whilst the $N = 42$ member is the icosidodecahedron with the twelve pentagons capped.

The $N = 78$ member has apices at the intersection of the three T_h mirror planes. There are eight other apices per mirror plane, making a total of 30 altogether. The remainder, $78 - 30 = 48$, consists of two unique apices together with their accompanying points and inverses. This T_h configuration is probably a global minimum; a D_3 system has a potential of 2662.04721 (Edmundson, 1991).

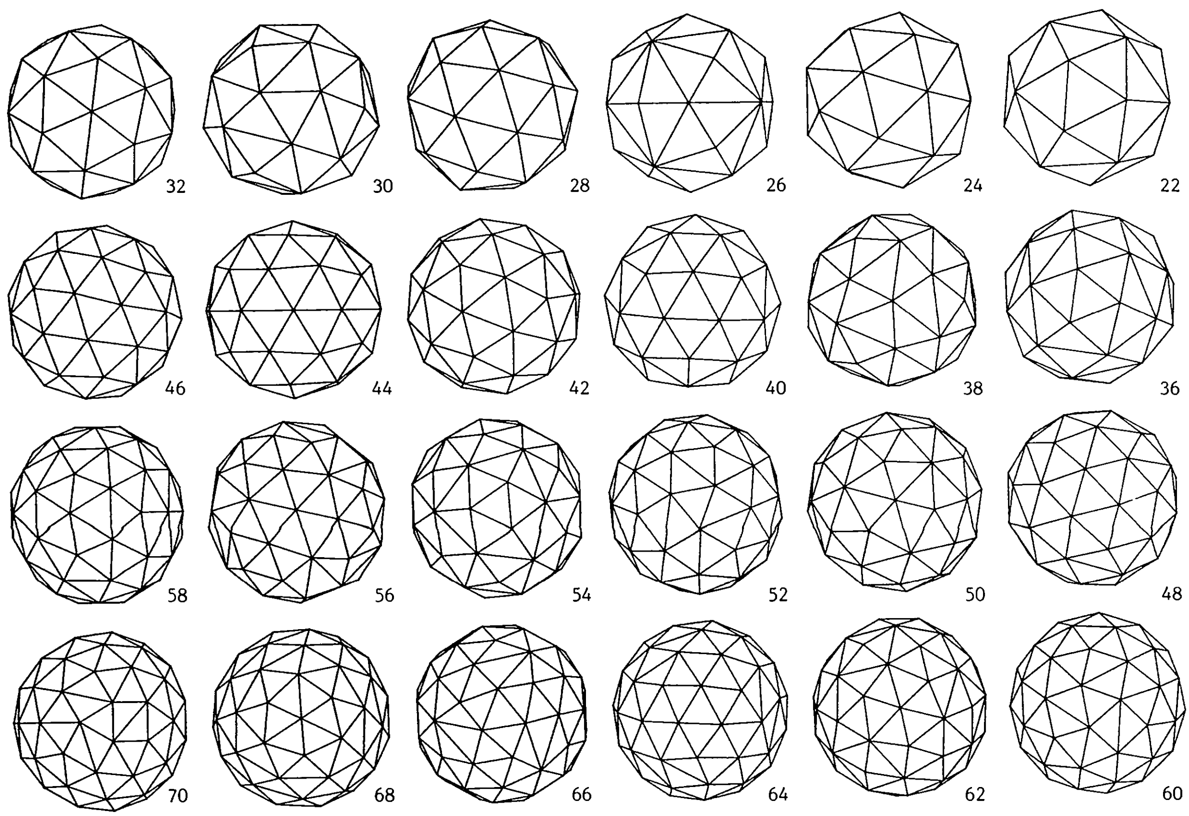

Fig. 2. Tetrahedral configurations for $N = 22$ to 70, with $N = 34$ not shown. View up the threefold axis.

T_5 series

Both the T_3 and T_4 series have produced T_h symmetry for $N=78$, 84 and 96, without the need for taking into account the number of apices in the mirror planes or whether two mirror planes share common apices. In this series, the inverses are included to aid in forcing T_h symmetry. However, no T_h configurations are produced. The dodecahedron is produced for $N=20$, whilst the arrangements for $N=32$, 44 (Edmundson, 1992; Weinrach *et al.*, 1990; Erber & Hockney, 1991) and 92 (Edmundson, 1991) are all global minima.

T_6 series

The $N=26$ arrangement is the dual of the truncated cuboctahedron, the hexakis octahedron, distorted so the apices fit on the sphere. The internal angles of the triangular facets of the true dual are 55.025, 37.775 and 87.200, whilst those of the distorted figure are 55.776, 40.880 and 83.344.

The lowest number of apices that produces T_h symmetry occurs with $N=50$; again, there are six points common to the mirror planes with four further points per mirror plane. These 18, together with the basic eight points, leave 24 points, equating to one unique apex with T_h symmetry.

Octahedral series

The octahedral configurations were generally higher in energy than the tetrahedral arrangements with the same number of points. Systems with square facets ($C=0$) would be expected to be energetically unfavourable; however, these prove to be global minima for both $N=24$ and $N=48$ but not for $N=72$. The global minimum for $N=72$ is the I arrangement of potential 2255.00119, thus there are three configurations (Tarnai, 1990). The other icosahedral arrangements, *i.e.* $N=32$, 42 and 92, can be forced into possessing tetrahedral symmetry by alteration of the 'a' and 'b' values as mentioned earlier. Together with the O arrangements in Table 5, these systems also display the three configurations; in fact, for $N=42$ the global minimum has a D_{5h} symmetry (Edmundson, 1992; Weinrach *et al.*, 1990).

The three systems, $N=38$, 52 and 76, visually form a well defined progression. The $N=38$ has distorted

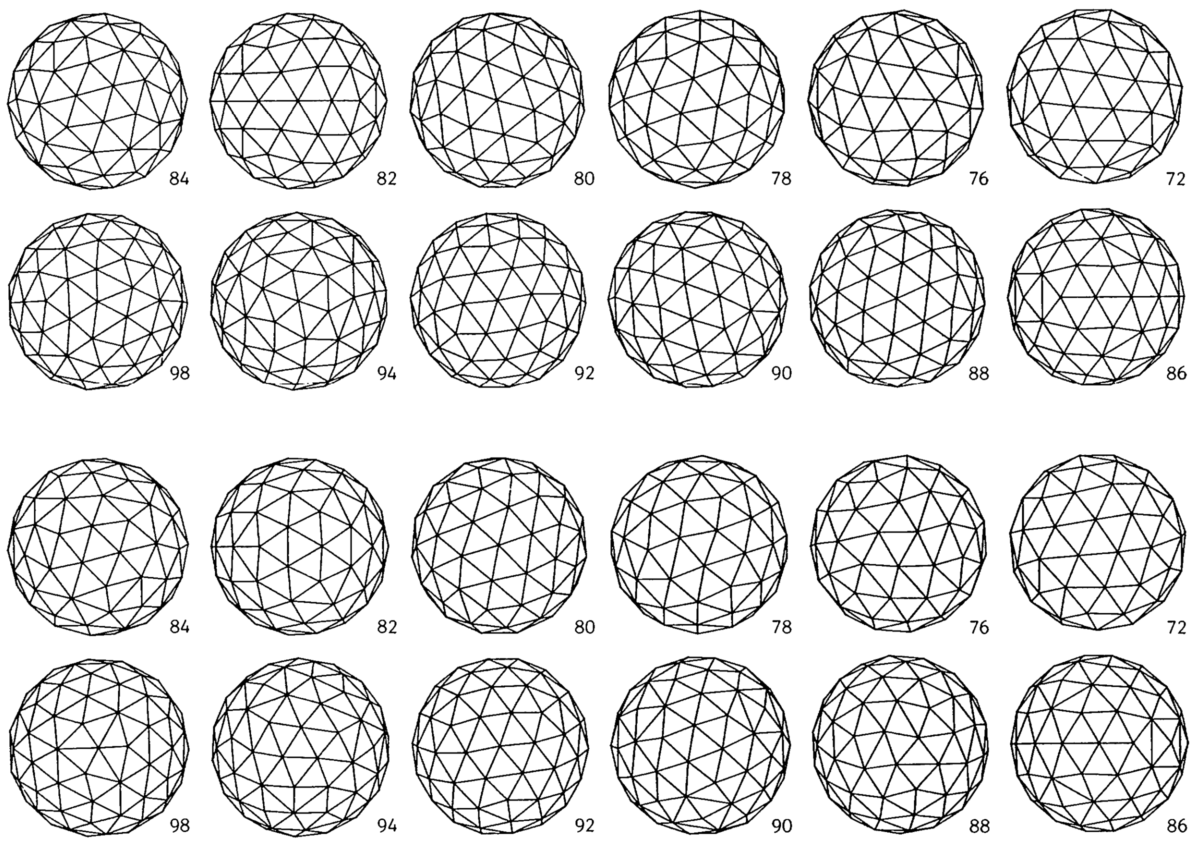

Fig. 3. Tetrahedral configurations for $N=72$ to 98, with $N=74$ and 96 not shown. The top two rows are views up the threefold axis whilst the bottom two rows are views down the threefold axis.

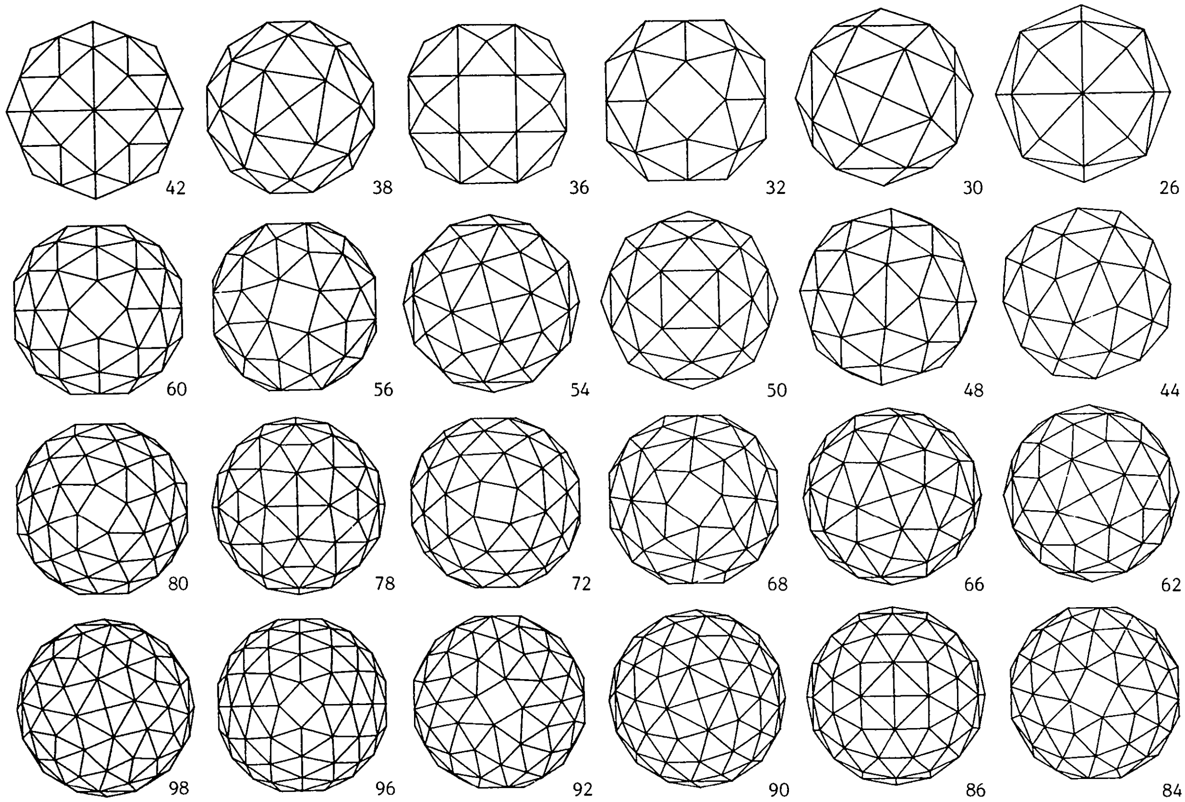

Fig. 4. Octahedral configurations for $N = 26$ to 98, with $N = 74$ not shown.

capped hexagons with alternate edges having capped squares completely attached. For $N = 52$, the hexagons and squares are now joined only *via* an apex, whilst, for $N = 76$, the two are no longer in contact.

I thank the University of East London for the use of their HP7580B plotter.

Note added in proof: Erber & Hockney in a private communication have shown that the I_h configuration for $N3 = 92$ is not a global minimum.

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