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The Distribution of Point Charges on the Surface of a Sphere

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Abstract

The potential, symmetry and Foppl arrangement are given for distributing up to 60 point charges on the surface of a sphere so that the Coulombic potential is a minimum. Some new configurations are described and a general comparison made with the hard-sphere case.

Introduction

The minimization of the potential of N points of unit charge on the surface of a unit sphere can be expressed as

$$V(N, m) = \tfrac{1}{2} \sum_{\substack{i,j=1 \\ i\neq j}}^{N} d_{ij}^{-m}$$

where V is the potential energy, d_{ij} is the distance between points i and j, N is the number of point charges and m is a positive number. When $m = 1$ the Coulombic potential is determined and is known as Thomson's problem. Tammes's problem is where m approaches infinity. These extreme cases are also known as the soft- and hard-sphere cases respectively and are but two of many similar problems that have been posed over the years. For a more detailed account of these other problems see Melnyk, Knop & Smith (1977) and Ashby & Brittin (1986).

Method of calculation

The technique used to calculate the minimum potential was based on the method described by Metropolis, Rosenbluth, Rosenbluth, Teller & Teller (1953) and Kirkpatrick, Gellat & Vecchi (1986) now known as simulated annealing and exemplified by Wille (1986). Each point is examined together with a number of exploratory positions which form a circle around the point. The angle this circle subtends at the centre of the sphere is denoted as θ. The potential is calculated for these exploratory points; if a lower potential is found then the point charge is moved to

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that position. This procedure is repeated for each point. The whole process is iterated until 90% of the points do not change position, at which stage the angle θ is reduced by a constant factor. When the required accuracy is obtained the process is terminated. The annealing process is introduced by occasionally moving a point to an exploratory position even though the potential is greater at that position. The 'temperature', θ, is kept at this particular value for a predetermined number of iterations before reducing it as before. When the temperature is quite low the annealing process is stopped and the minimum potential is determined without any further random moves. The computer programs were written in Fortran using double-precision arithmetic and run on a Prime 9950 and a clone IBM 286.

In order to aid the interpretation of the mimimized configurations, three-dimensional solids were envisaged consisting of triangular facets. Where square facets existed these were considered to be composed of coplanar triangular facets. Each solid consists of N vertices, E edges and F facets.

Results

Table 1 lists the potential, symmetry and Foppl configuration for $N=4$–60 and includes three other configurations of high symmetry. Fig. 1 shows the view looking down the major symmetry axis of the configuration for $N=8$ to $N=31$. The $N=8$ projection is at the bottom left-hand corner. Fig. 2 shows the view looking up the major axis. Figs. 3 and 4 are a similar pair to Figs. 1 and 2 but for $N=32$ to $N=55$.

Table 1. *The Coulombic potential, symmetry group and Foppl configuration for* $N=4$–60

N	E	F	Potential	Group	Foppl
4	6	4	3.67423	T_d	1, 3 or 2, 2
5	9	6	6.47469	D_{3h}	1, 3, 1
6	12	8	9.98528	O_h	3, 3 or 1, 4, 1
7	15	10	14.45298	D_{5h}	1, 5, 1
8	18	12	19.67529	D_{4d}	4, 4
9	21	14	25.75999	D_{3h}	3, 3, 3
10	24	16	32.71695	D_{4d}	1, 4, 4, 1
11	27	18	40.59645	C_{2v}	1, 2, 4, 2, 2
12	30	20	49.16525	I_h	3^4 or $1, 5^2, 1$
13	33	22	58.85323	C_{2v}	1, 2, 2, 4, 2, 2
14	36	24	69.30636	D_{6d}	1, 6, 6, 1
15	39	26	80.67024	D_3	3^5
16	42	28	92.91166	T	$1, 3^5$
17	45	30	106.05040	D_{5h}	$1, 5^3, 1$
18	48	32	120.08447	D_{4d}	$1, 4^4, 1$
19	51	34	135.08947	C_{2v}	$1, 2^9$
20	54	36	150.88157	D_{3h}	$1, 3^2, 6, 3^2, 1$
21	57	38	167.64162	C_{2v}	$1, 2^2, 4, 2^2, 4, 2^2$
22	60	40	185.28754	T_d	1, 3, 3, 6, 3, 3, 3
23	63	42	203.93019	D_3	$1, 3^7, 1$
24	66	44	223.34707	O	4^6
25	69	46	243.81276	C_s	$1^3, 2^7, 1, 2^3, 1$
26	72	48	265.13333	C_2	2^{13}
27	75	50	287.30262	D_{5h}	$1, 5^5, 1$
28	78	52	310.49154	T	$1, 3^9$
29	81	54	334.63444	D_3	$1, 3^9, 1$
30	84	56	359.60395	D_2	$1, 2^{14}, 1$
31	87	58	385.53084	C_{3v}	$1, 3^2, 6, 3^2, 6, 3^2$
32	90	60	412.26127	I_h	$1, 5^6, 1$
33	93	62	440.20406	C_s	$1^2, 2, 1, 2^4, 1, 2^6, 1, 2, 1, 2, 1$
34	96	64	468.90485	D_2	$1, 2^{16}, 1$
35	99	66	498.56987	C_2	$1, 4, 2^{15}$
36	102	68	529.12241	D_2	2^{18}
37	105	70	560.61889	D_{5h}	$1, 5^7, 1$
38	108	72	593.03850	D_{6d}	$1, 6^6, 1$
39	111	74	626.38901	D_{3h}	$3^2, 6, 3, 9, 3, 6, 3^2$
40	114	76	660.67528	T_d	$1, 3^2, 6, 3^2, 6, 3, 6, 3^2$
41	117	78	695.91674	D_{3h}	$1, 3^2, 6, 3, 9, 3, 6, 3^2, 1$
42	120	80	732.07811	D_{5h}	$1, 5^3, 10, 5^3, 1$
43	123	82	769.19085	C_{2v}	$1, 2, 4, 2^3, 4, 2^4, 4^2, 2, 4, 2^2$
44	126	84	807.17426	O_h	$4^3, 8, 4, 8, 4^3$
45	129	86	846.18840	D_3	3^{15}
46	132	88	886.16711	T	$1, 3^{15}$
47	135	90	927.05927	C_s	$1^3, 2^7, 1, 2^2, 1, 2^9, 1, 2^2, 1$
48	138	92	968.71346	O	4^{12}
49	141	94	1011.55718	C_3	$1, 3^{16}$
50	144	96	1055.18231	D_{6d}	$1, 6^8, 1$
51	147	98	1099.81929	D_3	3^{17}
52	150	100	1145.41896	C_3	$1, 3^{17}$
53	153	102	1191.92229	C_{2v}	$1, 4, 2, 4^2, 2, 4^2, 2^2, 4^4, 2^2, 4$
54	156	104	1239.36147	C_2	2^{27}
55	159	106	1287.77703	C_2	$1, 2^{27}$
56	162	108	1337.09535	C_2	2^{28}
57	165	110	1387.38323	D_3	3^{19}
58	168	112	1438.61825	D_2	$1, 2^{11}, 4, 2^2, 4, 2^{11}, 1$
59	171	114	1490.77334	C_2	$1, 2^{29}$
60	174	116	1543.83040	D_3	3^{20}
72	210	140	2255.00119	I	$1, 5^{14}, 1$
92	270	180	3745.61875	I_h	$1, 5^3, 10, 5^2, 10^2, 5^2, 10, 5^3, 1$
100	294	196	4448.35063	T	$1, 3^{33}$

A brief description is given for each configuration up to $N=50$.

$N=4$

As one would expect the regular tetrahedron is produced. Owing to its symmetry each point is equidistant from every other point and this allows a simple calculation of the potential energy of the system. Thus the potential energy (PE) is due to the interaction of four points with three other points, since each reaction is counted twice, then

$$\mathrm{PE} = 3 \times 4/(2d)$$

where d is the distance between any two points and for a unit sphere is given by

$$d = [\tfrac{8}{3}]^{1/2},$$

hence

$$\mathrm{PE} = [\tfrac{27}{2}]^{1/2} = 3.67423.$$

$N=5$

The trigonal bipyramid, consisting of an equatorial equilateral triangle together with a north and a south pole, is the structure of minimum energy for five points. The polar points are different to the equatorial positions; thus the polar points have a threefold axis whilst each equatorial position has a twofold axis. The mirror planes present give the configuration a D_{3h} symmetry. The polar positions contribute a slight

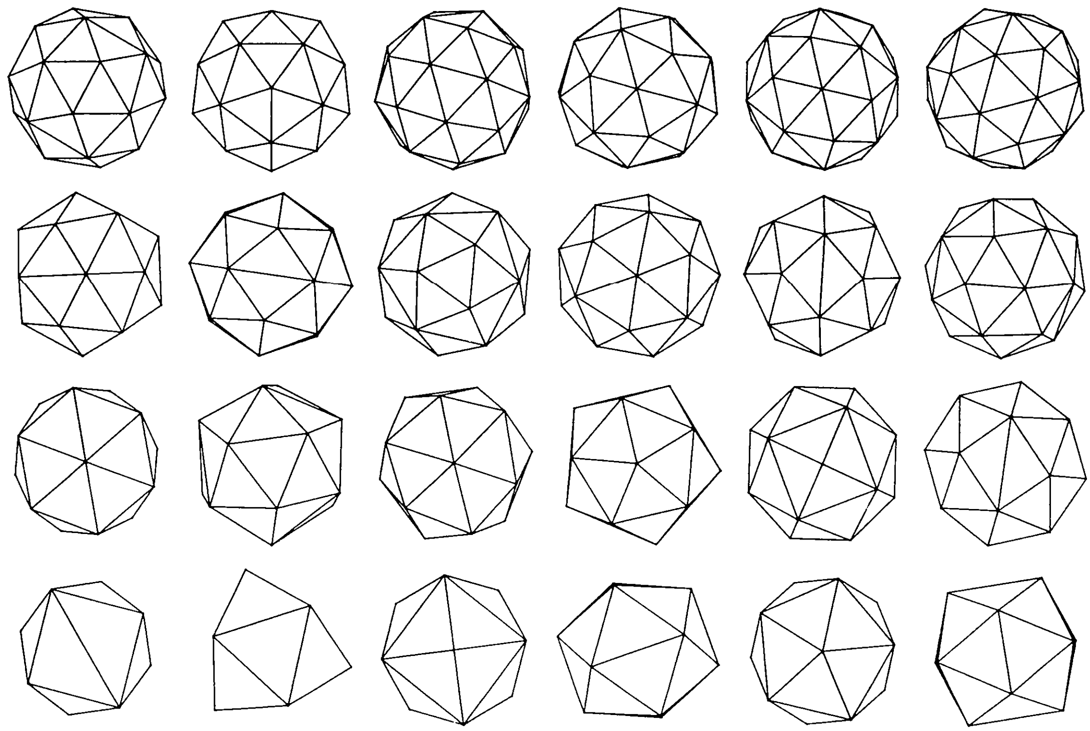

Fig. 1. View down the major axis for $N = 8$ to $N = 31$.

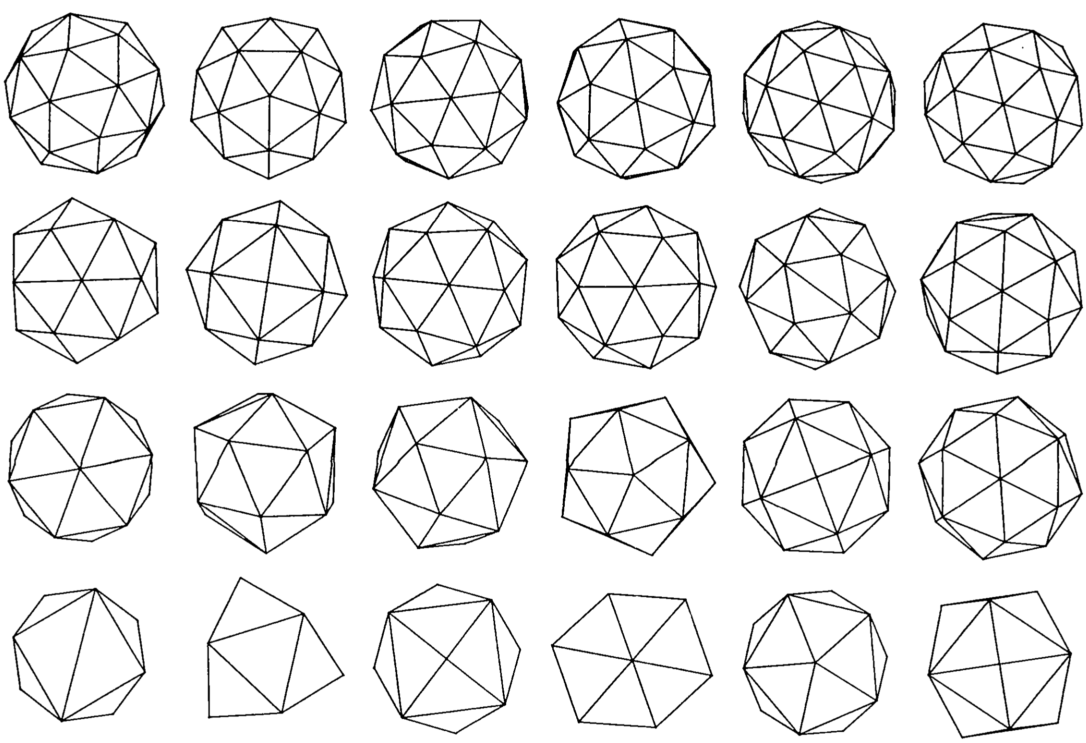

Fig. 2. View up the major axis for $N = 8$ to $N = 31$.

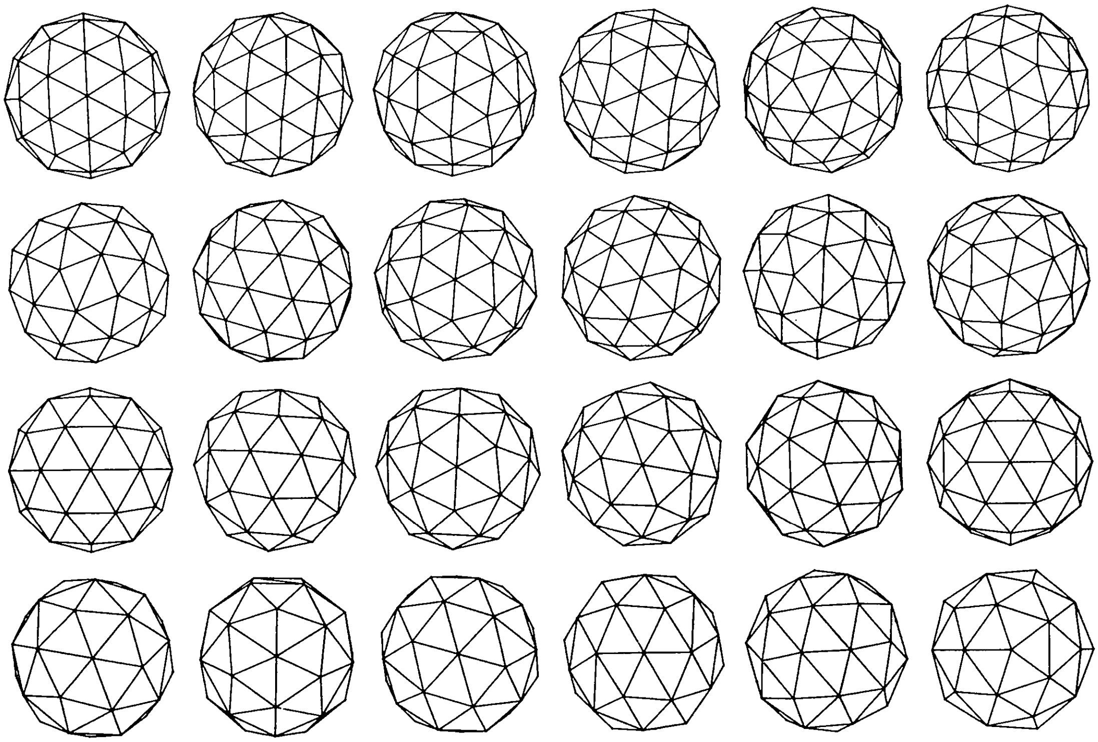

Fig. 3. View down the major axis for $N = 32$ to $N = 55$.

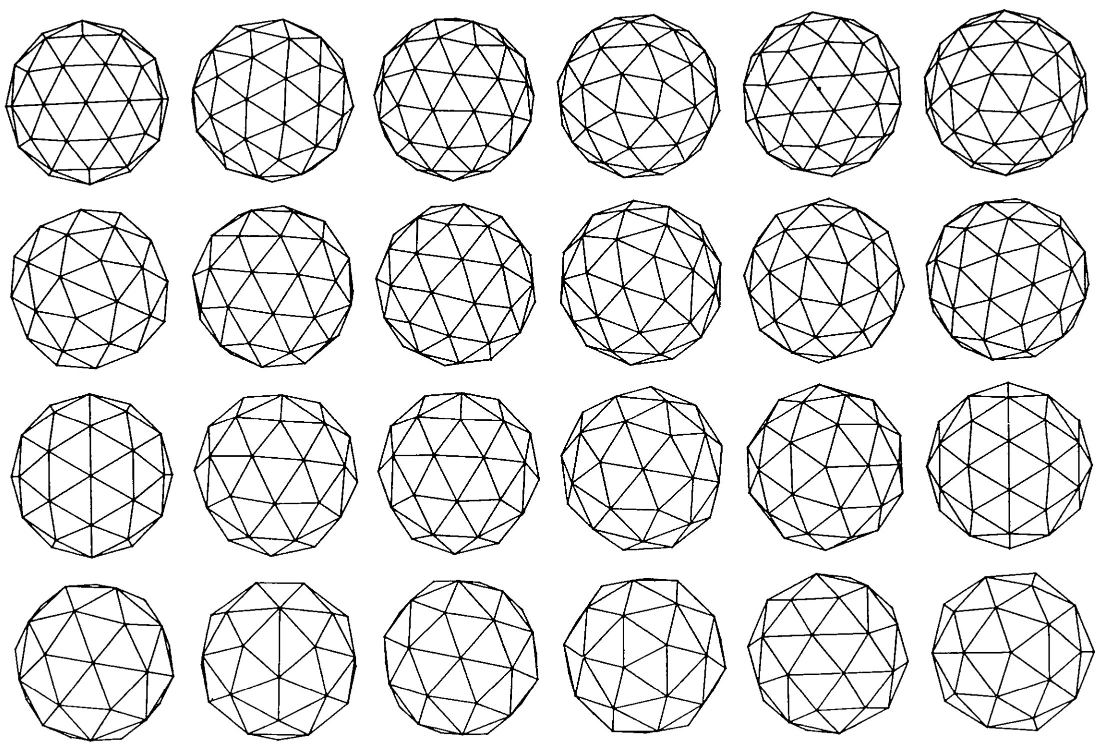

Fig. 4. View up the major axis for $N = 32$ to $N = 55$.

excess of 1.214% to the total potential whilst each equatorial point is 0.809% lower. The nearest-neighbour distances (NND) for the equatorial–equatorial positions is 1.7320508 which is identical to the theoretical value of $\{3\}^{1/2}$. The NND for the equatorial–polar position is 1.4142135 which again is identical to the theoretical value of $\{2\}^{1/2}$.

$N=6$

Like four points, six points produced a Platonic solid configuration, the octahedron. It can also be described as a square bipyramid where the polar and the equatorial positions are identical or as a trigonal antiprism. The Foppl configurations are 1,4,1 or 3,3 respectively. The total PE can be calculated by assuming for each point four near neighbours at a distance d_1 and a more distant neighbour at d_2 where

$$d_1=[2]^{1/2}$$

and

$$d_2=2.$$

Thus the potential is given by

$$\mathrm{PE}=\tfrac{6}{2}\{4/[2]^{1/2}+\tfrac{1}{2}\}=9.985281.$$

The NND is $\{2\}^{1/2}$ which is the same as for $N=5$ and $N=7$ since the same equator-to-pole distance is specified in both cases.

$N=7$

This configuration follows on from five and six to produce a pentagonal bipyramid, like five the two polar points differ from the equatorial ones which have an excess of 0.909% of the average potential energy. The polar points have fivefold symmetry whilst the equatorial positions have twofold, together with the mirror planes the configuration has the D_{5h} point group. The Foppl configuration is 1,5,1.

The NND for the equatorial positions is 1.1755705 whilst the equatorial–polar distance is, as expected, 1.4142136.

$N=8$

One configuration for eight points is the cube. A simple calculation reveals there are three nearest neighbours, three next neighbours and one far neighbour giving

$$\mathrm{PE}=\tfrac{8}{2}\{2.59808+1.83712+\tfrac{1}{2}\}=19.74077$$

whereas the minimum energy found is 19.67529. Further examination of the structure shows it to be a square antiprism. This is a cube with the top face rotated through 45° so that the four points are now offset (in the staggered form) so that there is a lower potential compared to the eclipsed form of the cube. The staggered arrangement of consecutive rings is very common in more complicated configurations. It is the first arrangement where square facets are encountered. The Foppl configuration is 4,4, whilst the arrangement displays the D_{4h} point group.

The NND for the square facets are 1.172477 whilst the longer sides of the isosceles triangular facets are 1.2876935 in length.

$N=9$

The nine points are arranged in three rings with each ring containing three points. The middle ring is positioned at the equator and the other two are equally displaced in the northern and southern hemispheres but in the staggered position relative to the equatorial ring. The three equatorial points have a 0.596% excess of the potential. The N- and S-polar equilateral triangular facets differ from the remaining facets resulting in a D_{3h} symmetry. Another description of this arrangement is of a trigonal prism with the three oblong facets capped. The equatorial vertices are not nearest neighbours, the N- and S-polar rings are nearest neighbours at a distance of 1.40729 rather than 1.41421 if the equator were such. The equilateral triangles are of length 1.2307058 whilst the capped positions have the polar rings as nearest neighbours at 1.1355403.

$N=10$

This configuration is best described as the square antiprism of eight points which has the two square facets capped. These two points have an excess of 0.771% of the charge. The nearest neighbour for the polar positions is at 1.07453, the original square facet is of length 1.28167 whilst the equatorial triangular facets are of length 1.09352.

$N=11$

As one might expect eleven has a low symmetry, C_{2v}, and has six different types of triangular facets. It is the first to contain a hexavalent vertex or hexamer. There are five different potential values; one at −0.826% of the average value, two at −0.486%, two at −0.216%, four at 0.017% and two at 1.081%.

$N=12$

The expected icosahedron is produced. The minimum configurations for $V=4$, 6 and 12 are those of the Platonic solids which consist of equilateral triangles.

$N=13$

Like $N=11$, 13 has the low C_{2v} symmetry with seven different types of triangular facets. It is one of the few configurations with more than 12 points which does not contain 12 pentamers.

$N = 14$

14 is a highly symmetrical figure of D_{6d}; it is composed of twelve pentamers and two hexamers which are positioned at the poles. The twelve pentamers have an excess of 0.228% whilst the two polar hexamers have a 1.365% lower potential than the average. The polar nearest-neighbour distance is 1.04368 whilst the near polar rings are separated by the distance 0.89030. The third distance is 1.02070.

$N = 15$

The previous configurations differ from $N = 15$ in that they all contain a mirror plane and hence their mirror images are identical. This configuration does not contain a mirror plane and therefore its mirror image is not superimpossible; this property is known as stereoisomerism or enantiomorphism. The system consists of five rings with each ring containing three points giving a Foppl configuration of 3^5 with D_3 symmetry. If the rings are simply staggered then the total potential is 80.67221 which is higher than the minimum of 80.67024. This lower potential is obtained by imparting a twist to successive rings thus removing the mirror plane. Since the twist can be made in a clockwise or anticlockwise direction then there are two forms. There are as expected twelve pentavalent vertices and three hexavalent ones which are situated in the third, equatorial, ring. The top and bottom rings form an equilateral facet of length 0.973199. There are five different sized triangles.

$N = 16$

This configuration has a Foppl nomenclature of $1,3^5$, which is typical of tetrahedral symmetry. It can best be described as a truncated tetrahedron (12 vertices) with each original tetrahedral facet, now a hexagon, capped adding a further four points to make 16 vertices. The equilateral triangular facets produced by the truncation are rotated so deforming the hexagonal caps. This twisting imparts enantiomorphism to the structure. The four capped positions are hexamers and occupy the tetrahedral points. There are only three different types of triangular facets present. The equilateral triangles are of length 0.885285, whilst the facets directly attached to these are of size 0.885285, 0.918199 and 1.027089. The third facet has dimensions 0.918199, 1.027089 and 0.828373.

$N = 17$

This system is highly symmetrical having a D_{5h} structure with a Foppl configuration of $1,5^3,1$. The three rings are staggered with the equatorial ring containing the five hexamers. There are only three types of faces; polar, tropic and equatorial facets. The polar ones have dimensions 0.883677, 0.883677 and 0.931924 whilst the equatorial one are 0.846946, 0.846946, and 1.175570.

$N = 18$

This structure has the Foppl configuration of $1,4^4,1$; it has tetravalent vertices at the poles with eight pentamers and eight hexamers. The four rings are staggered to one another without a twist giving it a D_{4d} symmetry.

$N = 19$

The Foppl arrangement of this system is $1,4,2,4,2^2,4$ and as such has a four-sided facet at the S pole. Examination of the distances shows it to be a rectangle of sides 0.84061 and 0.76391. As is the case usually with C-type symmetry prolonged iteration is required to reach a minimum value which eventually produced a value of 1.13586 as the diagonal. The N-pole point is not a tetramer since the next ring of two points is sufficiently close to produce a hexamer.

$N = 20$

The dodecahedron is not obtained as the minimum-energy configuration; instead a Foppl arrangement of $1,3^2,6,3^2,1$ with D_{3h} symmetry is obtained. The configuration contains three rhombus-shaped facets which are situated symmetrically around the equator such that two diagonally opposed points of each facet lie on the equator. These six points are all pentamers. The length of the side of the rhombus is 0.78949.

$N = 21$

The Foppl configuration is $1,2^2,4,2^2,4,2^2$ and not $1,2^{20}$ as was originally thought; in fact it is nearly $1,4^5$. Like $N = 19$ it has a four-sided facet at the S pole, however, this is a rhombus with sides 0.77681 and diagonal distances of 1.05804 and 1.26222.

$N = 22$

This like $N = 16$ is tetrahedral but has mirror planes giving it T_d symmetry. It consists of the four basic tetrahedral positions each at the centre of a hexagon which is composed of a single type of scalene triangle, thus producing a threefold rotational axis. These hexagons touch each other at alternating apices. The gaps left consist of a large triangle which is triangulated to produce four smaller ones. There are only three kinds of triangles.

$N = 23$

This configuration is enantiomorphic like $N = 15$ and $N = 16$. However, after this system diastereomers occur quite often. It has a Foppl arrangement of $1,3^7,1$ with D_3 symmetry since although the rings are staggered a twist is imparted to them thus removing the mirror plane.

$N = 24$

At first sight this system appears to produce the snub cube, one of the Archimedian solids. The true snub cube has 32 equilateral triangular facets and six square facets which are distributed in an octahedral arrangement. If the points are on a unit sphere then each nearest-neighbour distance is the same at 0.74420. Although each vertex is identical the triangular facets are divided into two kinds. 24 that are directly attached to the square facets and eight that are not. The potential for the semiregular solid is 223.45508 whilst a value of 223.24709 is obtained for the distorted configuration. The square facets are of dimension 0.71780; the eight non-attached triangular facets are equilateral of length 0.76601 whist the remaining 24 triangles are of length 0.71780, 0.76601 and 0.77680.

$N = 25$

This is the first arrangement which has no rotational symmetry, only a mirror plane which passes through five of the vertices. The single positions in the Foppl configuration are the apices in the mirror plane.

$N = 26$

The Foppl configuration of 2^{13} together with a C_2 symmetry produces 24 differently shaped triangles.

$N = 27$

There are only four differently shaped facets each occurring in concentric rings. The five rings each of five apices are staggered.

$N = 28$

This has T symmetry with only five differently shaped triangles.

$N = 29$

The D_3 structure has nine differently shaped triangles with three lozenge-shaped facets around the equator.

$N = 30$

The Foppl configuration is $1,2^{14},1$. However, the first three rings of two apices are sufficiently close together so as to make the N-pole vertex a hexamer. The distorted hexagon produced has only a twofold rotational axis. There are 13 differently shaped triangles.

$N = 31$

The Foppl configuration shows that there is an N-polar apex with an equilateral triangle in the S-pole region thus conserving the threefold rotational axis.

$N = 32$

This as expected has I_h symmetry with each facet consisting of an isosceles triangle of dimensions 0.640852, 0.640852 and 0.713644. It is the dual of the Archimedian solid, the truncated icosahedron, the popular pattern nowadays described on footballs.

$N = 33$

The figure contains two four-sided facets both of which straddle the mirror plane.

$N = 34$

Although the Foppl arrangement is $1,2^{16},1$ the first three rings of two apices are sufficiently close so as to produce a hexamer as a N and a S pole with twofold symmetry. There are 16 differently shaped triangles.

$N = 35$

The two top rings in the Foppl arrangement of $1,4,2^{15}$ are sufficiently close so as to make the N pole a hexamer with a twofold rotational axis.

$N = 36$

This has a Foppl configuration of 2^{18} which requires a twist so that vertices in the alternating rings are more distant thus reducing the potential.

$N = 37$

There is a local minimum of 560.62798 with C_2 symmetry compared to the global minimum of 560.61889 with D_{5h} symmetry. There are five differently shaped triangles arranged in concentric rings.

$N = 38$

The D_{6h} arrangement consists of four differently shaped triangles arranged in rings each with six vertices.

$N = 39$

This arrangement has nine points around the equator with a Foppl configuration of $3^2,6,3,9,3,6,3^2$. It consists of equilateral triangles at the N and S poles and has a total of nine differently shaped triangles.

$N = 40$

This has T_d symmetry with only five differently shaped triangles.

$N = 41$

This can be considered to be the $N = 39$ arrangement with the N and S poles added.

$N = 42$

It was expected that the I_h configuration would be the global minimum but this was not the case. A potential of 732.25624 is higher than the minimum of 732.07811 found with D_{5h} symmetry having ten vertices around the equator. The configuration is best described as being derived from the icosidodecahedron which consists of 30 vertices, 20 triangular and 12 pentagonal facets which occur in an icosahedral arrangement of 1,5,5,1. The nothern hemisphere is rotated so that the pentagons are in the eclipsed rather than the staggered position in relation to their southern counterparts. Each pentagon is then capped bringing the total number of vertices to $30 + 12 = 42$.

$N = 43$

The iteration procedure took a long time for this configuration to converge but eventually it produced C_{2v} symmetry. There are nine apices in one mirror plane and seven in the other giving 21 differently shaped triangles.

$N = 44$

The O_h symmetry is very obvious consisting of capped regular hexagons of which there are eight. The hexagons meet at alternating positions whilst the other positions form the corners of a square facet. Triangles emanate from the edges of the square to close the structure. There are only three differently shaped triangles.

$N = 45$

There are two configurations of close potential, a C_{2v} at 846.18865 and the global minimum, D_3, at 846.18840 which has 15 differently shaped triangles.

$N = 46$

This is a good example of where there are two local minima each close in potential to the global minimum. Thus,

$V = 886.17146$ C_2 2^{23}
$V = 886.17022$ C_{2v} $1,4,2^2,4^2,2^2,4^2,2,4^2,2,4,1$
$V = 886.16711$ T $1,3^{15}$.

$N = 47$

There are two configurations quite close in potential at 927.06227 and 927.05927 both with C_s symmetry. There are seven apices in the mirror plane defined by the Foppl nomenclature of $1^3,2^7,1,2^2,1,2^9,1,2^2,1$.

$N = 48$

This configuration contains six square facets of length 0.72465. There are five differently shaped triangles but just two types of vertices. One consists of the apices of the square facets ($4 \times 6 = 24$) whilst the other consists of the apex of the triangle whose base is the side of the square facets ($4 \times 6 = 24$).

$N = 49$

This structure has a threefold vertex at the N pole with an equilateral triangle at the S pole. There are 32 differently shaped triangles.

$N = 50$

The D_{6d} configuration consists of five differently shaped triangles arranged in rings around the sixfold axis.

Discussion

Most earlier workers proposed the basic arrangement then calculated the potential by varying certain parameters which usually specified various angles. Lin & Williams (1973) show very clearly how the minimum configuration varies with the Coulombic power. When the number of vertices is large and the configuration is of low symmetry then the computational time is extremely long due to the large number of parameters required to specify the particular configuration. This method will obviously fail if the minimum arrangement has not been considered as a possibility. King (1970) lists what may seem an exhaustive set of arrangements for N up to 16 but fails to include the correct configurations for $N = 11$, 13, 15 and 16. Similarly, Munera (1986) examines only certain arrangements and thus has higher potentials for $N = 11$, 13, 15, 16, 19 and 20. Melnyk, Knop & Smith (1977) give a comprehensive review for N up to 16. However, the Foppl arrangement for $N = 14$ of $1,6^2,1$ is the optimal configuration with potential 69.30636 rather than that proposed by Melnyk, Knop & Smith (1977) of $1,4^3,1$. According to the present calculations the latter has a local minimum of 69.34238 although Wille (1986) quotes Melnyk *et al.* as finding 69.496 for this arrangement. More recently, Weinrach, Carter, Bennett & McDowell (1990) have listed the symmetry for up to 50 points using a Monte

Table 2. *Combined mean residuals for systems with C symmetry*

N	Combined mean residual	Symmetry
11	0.001202	C_{2v}
13	0.000679	C_{2v}
19	0.000007	C_{2v}
21	0.000067	C_{2v}
25	0.000041	C_s
26	0.000074	C_2
31	0.000103	C_{3v}
33	0.000132	C_3
35	0.000012	C_2
43	0.000009	C_{2v}
47	0.000052	C_s
49	0.000031	C_3

Carlo random-walk method. Their data are in agreement except for $N = 18$, 30, 37, 38, 43, 46 and 49. However, comparison of potentials (Weinrach, Carter, Bennett & McDowell, 1991) shows that differences only exist for $N = 37$, 38, 46 and 49. The other configurations differ in assignment of the symmetry elements; they used a semivisual approach and might have missed some rotational axes.

In most instances, for a particular arrangement the x coordinate values sum to zero, and likewise for the y and x coordinates. However, with the configurations having C-type symmetry these sums are nonzero. Table 2 lists the arrangements with C-type symmetry and their corresponding combined mean residuals. Ashby & Brittin (1986) point this out for the case of $N = 11$ but give no reason. If the residual sums of the x, y and z coordinates are denoted as dx, dy and dz for an N-particle configuration then the mean residuals are given as

$$MR_x = \mathrm{d}x/N$$

$$MR_y = \mathrm{d}y/N$$

$$MR_z = \mathrm{d}z/N.$$

The combined mean residual is defined as

$$\mathrm{CMR} = \{MR_x^2 + MR_y^2 + MR_z^2\}^{0.5}.$$

This is a constant for each configuration and independent of the orientation of the system or initial coordinates in the iteration process.

Tetrahedral symmetry, T_d, has been found for $N =$ 4, 22 and 40 whilst T is produced by $N = 16$, 28, 46 and 100. The latter would form a series if only $N = 70$ was present. Performing calculations whereby T symmetry is forced on the arrangement produces a potential of 2130.76887 which is higher than the minimum found of 2127.10090 for D_2 symmetry. Configurations having T symmetry can be produced for values of N which conform to the formula

$$N = 4 + 12a$$

where a is a positive integer. The first term corresponds to the four original tetrahedral positions whilst the factor of 12 in the second term shows that for every unique point added a further 11 points are needed to conserve the T-group symmetry. The minimum potential for $N = 52$ is 1145.41896 with C_3 symmetry whilst the T configuration has a value of 1145.44733 although both have a Foppl arrangement of $1,3^{17}$.

Icosahedral symmetry, I_h, occurs for $N = 12$, 32 and 92 whilst I symmetry occurs for $N = 72$. Surprisingly, for $N = 42$ a D_{5h} configuration of potential 732.07811 is obtained which is lower than the icosahedral arrangement of potential 732.25624.

Comparison between the hard- and soft-sphere models shows that generally the soft approach produces a range of near-neighbour distances unlike the single-valued hard case. In doing so the soft model produces lower potentials. Table 3 compares the near-

Table 3. *Angular separation for the hard and soft models*

N	Thomson's angle (°)	Tammes's angle (°)
4	109.47122	109.47122
5	90.00000	90.00000
6	90.00000	90.00000
7	72.00000	77.86954
8	71.69415	74.85861
9	69.18975	70.52878
10	64.99563	66.14682
11	58.53956	63.43495
12	63.43495	63.43495
13	52.31691	57.13670
14	52.86609	55.67057
15	49.22487	53.65783
16	48.93622	52.24439
17	50.10807	51.09033
18	47.53442	49.55667
19	44.90971	47.69191
20	46.09332	47.43111
21	44.32044	45.61322
22	43.30200	44.74016
23	41.48111	43.70996
24	42.06531	43.69077
25	39.60726	41.63446
26	38.99162	41.03766
27	39.93995	40.67761
28	37.82374	39.35514
29	36.39129	38.71365
30	36.94193	38.59712
31	36.37312	37.70981
32	37.37737	37.47522

Table 4. *Convergence of distances from the soft to the hard sphere*

m	d_1	d_2	d_3
1	0.7178000	0.7660127	0.7768037
2	0.7198987	0.7646470	0.7733341
4	0.7238918	0.7617696	0.7674000
8	0.7300616	0.7566854	0.7593555
16	0.7362291	0.7515417	0.7522690
32	0.7401096	0.7480303	0.7482113
64	0.7421356	0.7461527	0.7461979
128	0.7431653	0.7451883	0.7451994
256	0.7436845	0.7446995	0.7447023
512	0.7439451	0.7444534	0.7444541
1024	0.7440756	0.7443300	0.7443302
2048	0.7441409	0.7442683	0.7442683

neighbour distances in terms of the angle subtended at the centre of the sphere for the hard and soft cases. The hard data are a compilation from Clare & Kepert (1986), Kottwitz (1991), Lazic, Senk & Seskar (1987), Mackay, Finney & Gotoh (1977), Szekely (1974) and Tarnai & Gaspar (1983, 1991).

The case of $N=24$ for $m=1$ produces a distorted snub cube which has three near-neighbour distances. As m is increased the three separate values converge to a single value approaching 0.74420 for the true snub cube. Table 4 shows the convergence of the distances with increasing power of m.

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SHORT COMMUNICATIONS

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Acta Cryst. (1992). **A48**, 69-70

Improvement of the tangent formula by constraints based on additional information. II.

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Abstract

Recently, Rius & Miravitlles [*Acta Cryst.* (1991). **A47**, 567-571] have shown the viability of simultaneously refining the phases of the largest structure factors by least-squares minimization of the quantity $R=\sum_{\mathbf{H}} w(\mathbf{H})[F(\mathbf{H})^2-F_{\text{calc}}(\mathbf{H})^2]^2$ where the $\mathbf{H}$ summation extends over all measured reflections and $w(\mathbf{H})$ is a weighting factor. Here, an alternative method of minimizing R by sequentially refining the phases $\varphi_{\mathbf{h}}$ of the largest structure factors is suggested that takes advantage of the possibility of expressing $\partial R/\partial\varphi_{\mathbf{h}}=0$ as an explicit function of $\varphi_{\mathbf{h}}$.

Let the residual R be defined according to the expression

$$R_1(\Phi)=\sum_{\mathbf{H}} w(\mathbf{H})m(\mathbf{H})[E(\mathbf{H})^2-\mathbf{E}_c^*(\mathbf{H})\mathbf{E}_c(\mathbf{H})]^2, \quad (1)$$

or, alternatively,

$$R_2(\Phi)=\sum_{\mathbf{H}} w(\mathbf{H})m(\mathbf{H})[E(\mathbf{H})-E_c(\mathbf{H})]^2, \quad (2)$$

where Φ represents the collectivity of phases $\varphi_{\mathbf{h}}$ of the strong normalized structure factors $\mathbf{E}(\mathbf{H})$ and $\mathbf{H}$ denotes the measured reflections in one asymmetrical unit of the reciprocal space. The factor $m(\mathbf{H})$ is the multiplicity of $\mathbf{H}$ and $w(\mathbf{H})$ is the inverse of the variance associated with the difference $E(\mathbf{H})^2-E_c(\mathbf{H})^2$ [or $E(\mathbf{H})-E_c(\mathbf{H})$]. Applying Sayre's equation (Sayre, 1952), $\mathbf{E}_c(\mathbf{H})$ may be approximated by

$$\mathbf{E}_c(\mathbf{H})=E_c(\mathbf{H})\exp i\varphi_{\mathbf{H}}=\theta(\mathbf{H})\sum_{\mathbf{h}'}\mathbf{E}(\mathbf{h}')\mathbf{E}(\mathbf{H}-\mathbf{h}') \quad (3)$$

with $\mathbf{E}(\mathbf{h}')$ and $\mathbf{E}(\mathbf{H}-\mathbf{h}')$ belonging to the set of strong E's and $\theta(\mathbf{H})$ a scaling factor. Obviously, the residual R will

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