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THE OPTIMAL PACKING OF CIRCLES ON A SPHERE

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Abstract

The closest packing of x circles on the surface of a sphere is calculated in the same way that the stereochemical arrangement of atoms around a central atom is determined. A number of improved packings have been discovered for $x = 19$ to 80. A notable feature is that the structures are generally of low symmetry. The packing density p, defined as the fraction of the spherical surface that is enclosed by the circles, increases only very slowly as the number of circles increases and the values remain substantially below that for a close packed plane, or for an octahedron or icosahedron.

1. Introduction

The determination of the closest packing of circles on a plane is a trivial problem, but the closest packing of circles on the surface of a sphere, or other curved surfaces, is more difficult to determine [1]. This problem arises in many different disciplines, but our interest originated in the arrangement of atoms around a central atom, or cluster of atoms.

The problem is to determine the largest diameter that x equal circles may have when packed onto the surface of a sphere of radius r, without any overlapping of the circles. Alternatively, if the centre of each circle is considered as the vertex of a polyhedron, the problem is to find the polyhedron that maximizes the shortest edge lengths. The closeness of packing can be expressed as the shortest edge length of the polyhedron l, which is also the diameter of the circles, or as the packing density p, which is defined as that fraction of the surface of the sphere that is enclosed by the circles.

For $x = 2$ to 12 and for $x = 24$, there are geometric proofs of the best solutions. Relatively high values of the packing density are observed for the tetrahedron ($x = 4$, $p = 0.845299$), octahedron ($x = 6$, $p = 0.878680$), icosahedron ($x = 12$, $p = 0.896095$) and snub cube ($x = 24$, $p = 0.861703$). As x approaches infinity, p is expected to approach the value for a close packed plane, $p = \pi/(2\sqrt{3}) = 0.906900$.

For most values of x, rigorous proofs of the optimum packing are not available, and improved packings are discovered from time to time using a variety of methods.

The best packings for $x = 2$ to 40 known up to 1985 have been described previously [1]. An interesting result from that work is that values of p varied widely, for example $p = 0.814$ to 0.861 for $x = 20$ to 40, and any approach to the limiting value of $p = 0.906900$ is obscured by this variation. The best known packings represent a great variety of structural types. For example, the polyhedra may have pentagonal, square or triangular faces, and each circle may be in contact with five, four or three other circles, or may be in contact with none and allowed to rattle in a hole formed by six or more circles. The structures are generally of low symmetry, although in some cases they may be derived from high-symmetry structures by small distortions. There is no discernable periodicity in symmetry properties or other structural features as x increases.

For $x > 40$, the best values for the packing in the literature have generally been obtained either by imposing some rotational symmetry on the structure, or by imposing very high tetrahedral, octahedral, or icosahedral symmetries, as is often used in the construction of geodesic domes. For these structures, the unexpected result is obtained that the value of the packing density p generally *decreases* as x increases. The most dense packing known for high values of x is for a structure of icosahedral symmetry obtained for $x = 360$, but the value for p of 0.859447 [2] is still inferior to the values obtained for $x = 6$, 12, 24 or 48. The largest structure that has been studied is for $x = 1080$ of icosahedral symmetry, for which p is even lower at 0.854149 [3].

In this paper, results are described for values of x up to 80 in which no symmetry is enforced.

2. Method

In our work, the problem is investigated by numerical techniques. If the distance between the polyhedral vertices i and j, or between the centres of the circles i and j, is d_{ij}, then the repulsive energy between these points is taken to be d_{ij}^{-n}, where n is some positive number. The total energy of the system is then obtained by summing over all such interactions and minimization of the total energy leads to the most favourable arrangement. If $n = 1$, there is a Coulombic interaction between the points, whereas the arrangement of atoms around a central atom is best modelled by $n \sim 6$. As n becomes larger, the energy becomes increasingly dominated by the terms corresponding to the shortest polyhedral edge length, and minimizing the total energy corresponds to maximizing the smallest edge length. As n approaches infinity, the problem becomes one of packing circles on the surface of a sphere. In this work, the energy was minimized as n was progressively increased, usually up to a value of 6144. This generates an approximate polyhedron whose shortest edge lengths vary by only about $0.001r$, which is sufficient to establish the symmetry and connectivity of the structure. Each of these edge lengths is a function of four angular coordinates:

$$d_{ij} = [2 - 2\cos\phi_i \cos\phi_j - 2\sin\phi_i \sin\phi_j \cos(\theta_i - \theta_j)]^{1/2} r.$$

In this work, the angular coordinates are defined relative to the "north pole" at $\phi = 0$ and the "longitude" is given by θ. If each of the distances is set equal to the edge length l of the exact polyhedron, a set of simultaneous equations is obtained which in simple cases is equal to the number of unknowns l, ϕ_i, θ_i, ϕ_j, θ_j, ... (for example, $2x - 2$ unknowns for structures containing no symmetry elements). Solving these equations leads to the desired exact structure. In some cases, the minimization procedure leads to more than the required number of short edge lengths and all combinations of equations must be solved to determine the best packing.

Sometimes, the energy minimization procedure yields an approximate structure in which some circles are not in contact with any of the surrounding circles. These circles and corresponding equations can be deleted from the set of equations to be solved and the circles reinserted later.

Minimization techniques were variants of Fletcher–Powell–Davidon [4]. Equations were solved by Newton–Raphson methods with the approximate structure as the starting point.

3. Results

For values of x from 19–80, a number of packing arrangements have been discovered that are an improvement on the best in the literature, and these are described in turn. A full listing of angular coordinates for all structures may be obtained from the authors and has also been deposited with the Editors. The modified Föppl notation used here to describe structures with axial symmetry provides a list of the number of corners of the succession of planar polygons perpendicular to the principle axis; "a" signifies that the polygon is eclipsed relative to the polygon above it, "$\bar{\text{a}}$" signifies a staggered arrangement, "$\tilde{\text{a}}$" signifies an intermediate arrangement, "a^n" signifies a succession of n such polygons, "(a)" signifies that the polygon is irregular, and "$\frac{2}{2}$" signifies half occupancy of two equivalent sites. For structures containing rattling circles, the angular coordinates, symmetry and Föppl notation correspond to the circles being in the centres of their holes.

$x = 19$

The structure with five points irregularly arranged on a mirror plane and seven on each side as previously proposed [5], $l = 0.808303r$, can be improved [6] by choosing a slightly different set of short edges (by allowing 13 to rattle, and by including edges between 2 and 11 and the symmetry related 3 and 12, see fig. 1 and table 1) to give $l = 0.808558r$.

$x = 21$

The best result in the literature is the D_3 structure, with $l = 0.774344r$ [7]. We have found an improved structure containing no symmetry elements, with $l = 0.775239r$ (fig. 2).

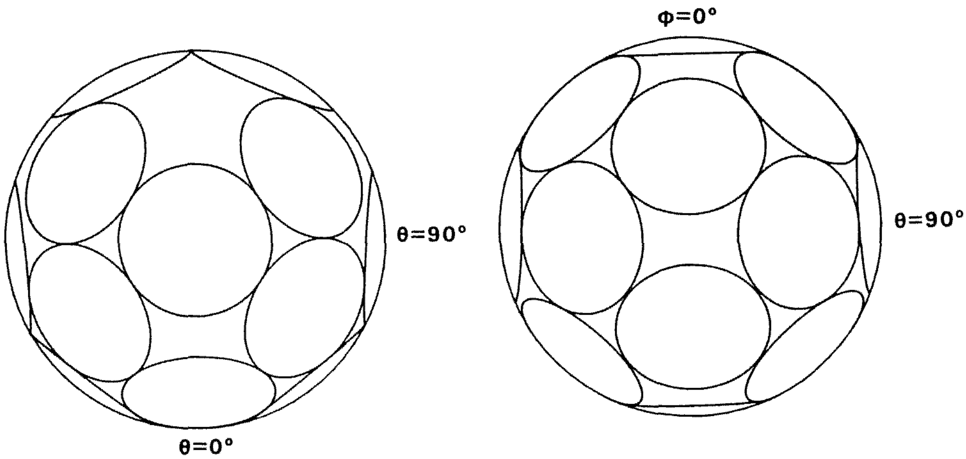

Fig. 1. Packing for $x = 19$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$. A mirror plane passes through $\theta = 0$, 180°.

Table 1

Angular parameters (i degrees) for structure with $x = 19$

Vertex	ϕ	θ
1	0	–
2	47.691914	55.770194
4	47.691914	123.047331
6	62.101913	0
7	85.302713	156.068667
9	87.688130	85.821687
11	92.376778	38.347394
13	125.154230	0
14	120.368721	122.264027
16	127.476486	180
17	134.620587	63.450826
19	175.168400	180

$x = 22$

The best value quoted in the literature is incorrect [8]. Our optimization procedure produces a structure which to a first approximation can be considered to be based on a tetrahedron with one circle at each vertex, one above each edge, and an equilateral triangular arrangement of three above each triangular face, with triangular edges parallel. The exact structure (fig. 3 and table 2) is significantly distorted from tetrahedral and contains no symmetry elements. An almost identical

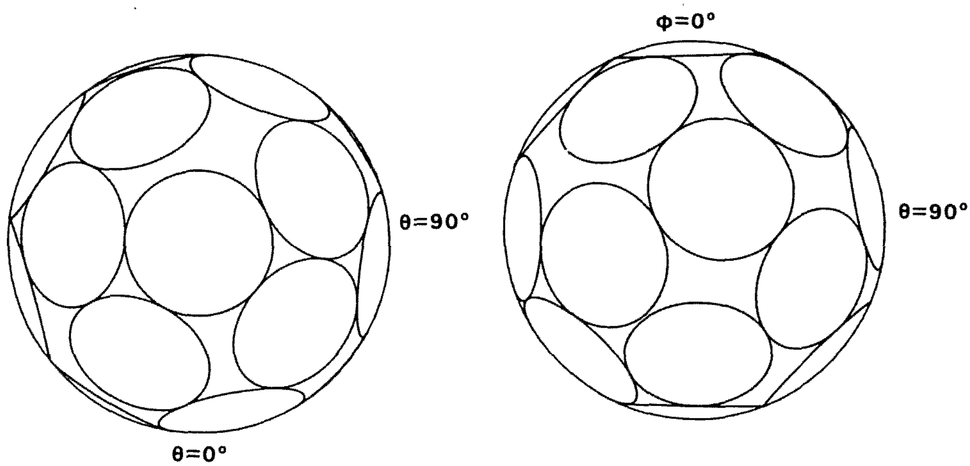

Fig. 2. Packing for $x = 21$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$.

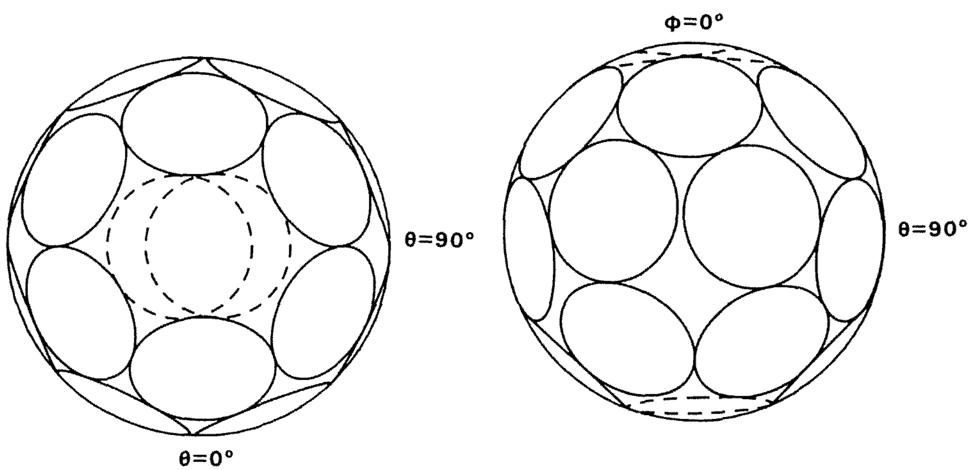

Fig. 3. Packing for $x = 22$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$. A pseudo-S_4 axis passes through $\phi = 0, 180°$. Alternative sites for circles 1 and 2 are shown by broken lines.

Table 2

Angular parameters (in degrees) for structure with $x = 22$

Vertex	ϕ	θ
1	6.236991	90.000000
3	44.394849	0
7	50.173569	118.052241
11	52.884727	59.975977
15	82.449089	152.722749
19	85.790424	19.459660

structure has been found by Lazić et al. [6]. There are 42 edge lengths of $0.761175r$, but rather remarkably the next four longer edges are identical, $0.790924r$. These four edges are related by an S_4 axis through $\phi = 0, 180°$, as are all circles with the exception of 1 and 2. Circles 1 and 2 are displaced from this axis and have two alternative sites, 1, 1′ and 2, 2′, which are related by the S_4 axis and are shown by the broken lines in fig. 3. It should be noted that 1 and 2 are not free to rattle, the two alternative sites forming rigid structures. Disorder of this type is common in crystal structures where an atom, or group of atoms, may occupy one of two symmetry-related sites in the unit cell which, when summed over the entire crystal, leads to the observation of partial occupancy of each site, but this appears to be the only known case of such "disorder" for the current problem of packing circles on a sphere.

$x = 25$

The minimization of the repulsion between points using our optimization procedures leads to a number of different structures, all of which have relatively low packing densities. The best of these contains a threefold axis and has also been obtained by Lazić et al. [6]: $l = 0.710776r$ (fig. 4 and table 3).

$x = 26$

A reasonably good solution to packing 27 circles on a sphere is the D_{5h} $1\bar{5}^51$ structure of Székely [9], and our optimization procedure for $x = 26$ leads to structures that are superficially related but with one circle missing. There are a number of valid structures that are similar and related to each other by a small reorganization of the shortest edge lengths and those that are only 0.1–0.5% longer. All structures contain at least one rattling circle. Our best solution is $l = 0.700983r$ (fig. 5). A related structure has been obtained by Lazić [6].

$x = 29$

The previous best result was obtained by removing one circle from the D_3 $x = 30$ structure: $l = 0.660981r$. We have obtained a better structure, $l = 0.661981r$, that contains no symmetry, but further improvements are likely [10].

$x = 33$

The optimization procedure yields a structure which to a very good approximation has D_3 symmetry [11]. Based on this symmetry, the (revised) angular coordinates are given in table 4. Kottwitz [12] has pointed out that this structure can be improved by removal of the three twofold axes through $\phi = 90°$, $\theta = 0, 60°, 120°$ and the addition of three new polyhedral edges, 7–13, 8–14 and 9–15. These new edges indirectly pull the circles 1 to 9 down to increasing ϕ and circles 25 to 33 up to decreasing ϕ (fig. 6 and table 4). These changes also lift circles 16, 17 and 18 from $\phi = 90°$ to $\phi = 89.996143°$, and the value of l increases from $0.622257505r$ to

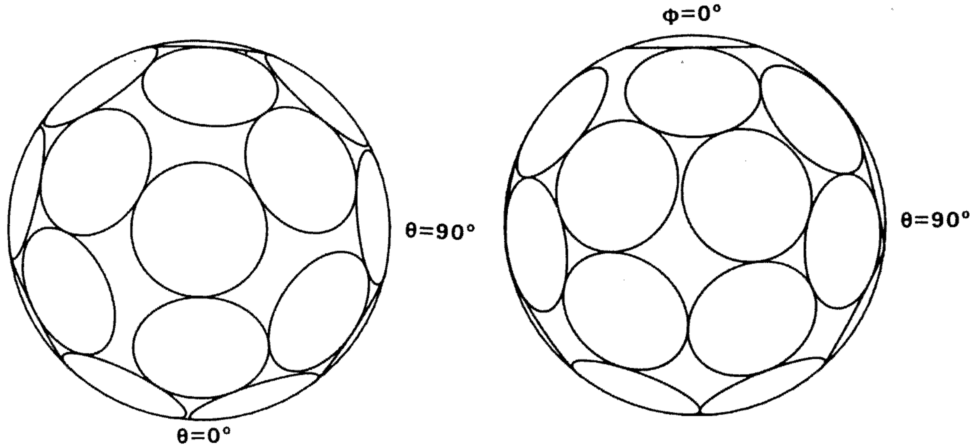

Fig. 4. Packing for $x = 25$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$. A C_3 axis passes through $\phi = 0, 180°$.

Table 3

Angular parameters (in degrees) for structure with $x = 25$

Vertex	ϕ	θ
1	0	–
2	41.634461	0
5	54.230207	54.827000
8	77.056343	93.603622
11	80.639519	17.310622
14	95.844565	56.203937
17	118.687162	93.034144
20	122.077147	21.541143
23	155.772121	62.368132

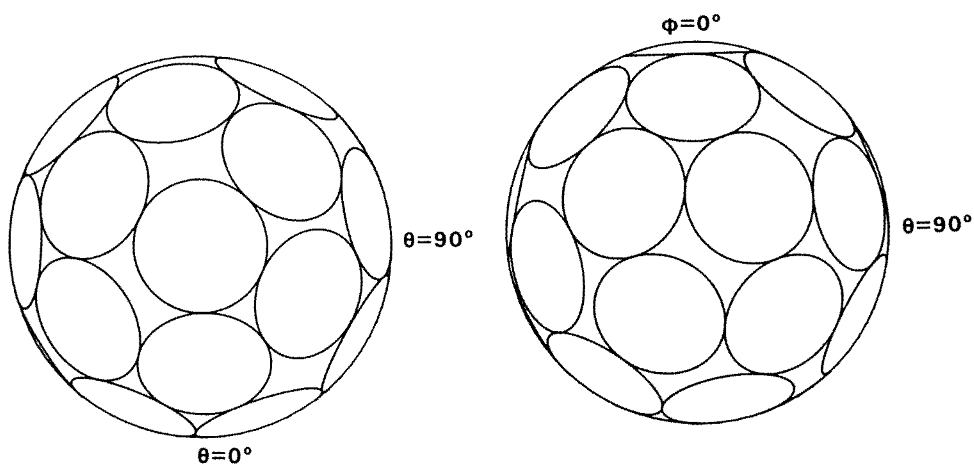

Fig. 5. Packing for $x = 26$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$.

Table 4

Angular parameters (in degrees) for structure $x = 33$

	D_3 structure		C_3 structure	
Vertex	ϕ	θ	ϕ	θ
1	21.054790	119.333347	21.054801	119.333475
4	42.844974	59.333347	42.844996	59.333475
7	56.317183	14.283276	56.317212	14.283398
10	69.805143	89.229021	69.819919	89.206686
13	77.523119	46.743999	77.494512	46.631326
16	90.000000	0.000000	89.996143	- 0.010420
19	(102.476881)	(- 46.743999)	102.448482	- 46.856838
22	(110.194857)	(- 89.229021)	110.209214	- 89.251070
25	(123.682817)	(- 14.283276)	123.682788	- 14.283398
28	(137.155026)	(- 59.333347)	137.155004	- 59.333475
31	(158.945210)	(- 119.333347)	158.945199	- 119.333475

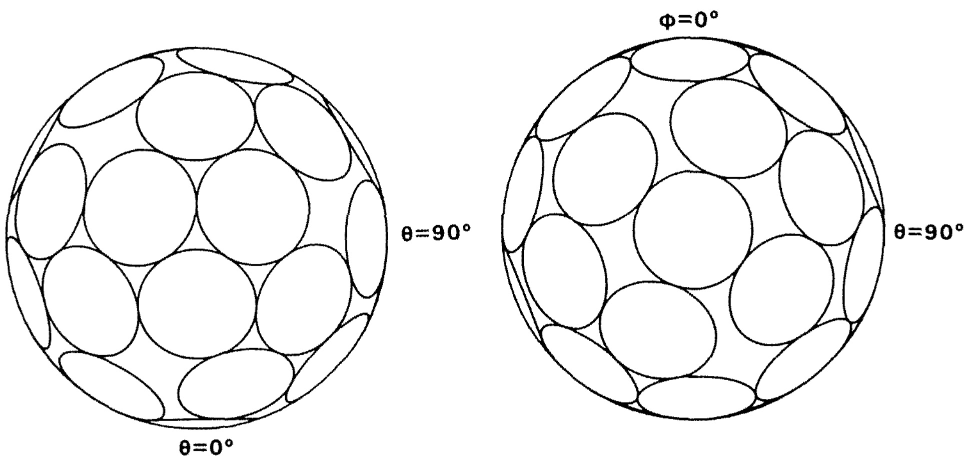

Fig. 6. Packing for x = 33, viewed from ϕ = 0 and ϕ = 90°, θ = 0. A C_3 axis passes through ϕ = 0, 180°.

$0.622257802r$. These changes are remarkably small. It is notable that circles 1 to 9 are related to circles 25 to 33 by D_3 symmetry, whereas circles 10 to 24 are related to each other by only C_3 symmetry.

$x = 41$

In this work, a structure with C_2 symmetry was obtained, $l = 0.563219r$, which is an improvement on the previous best structure with fivefold symmetry [9]: $l = 0.562052r$. A value of $l = 0.563488r$ has recently been claimed, but no details are available [10].

$x = 43$

The structure obtained in this work contains no symmetry elements and has quite an irregular appearance (fig. 7), and further improvements are likely.

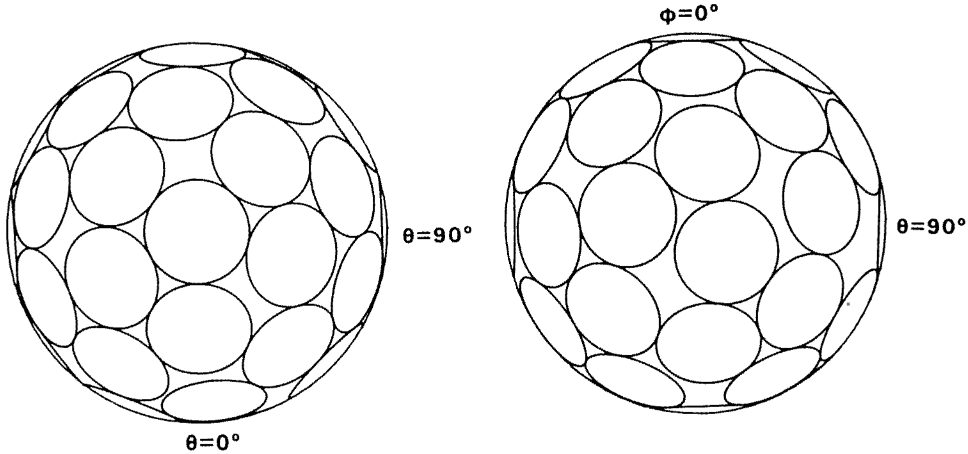

Fig. 7. Packing for $x = 43$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$.

$x = 44$

For $x = 44$, a highly symmetric structure is available of cubic symmetry. A rhombic dodecahedron can be considered as an interpenetrating cube and octahedron. If the octahedral vertices are truncated to give a truncated rhombic dodecahedron, a 32-vertex figure is formed with six square faces and twelve hexagonal faces; capping the latter produces a capped truncated rhombic dodecahedron, $l = 0.549275r$. Circles at the capping sites are free to rattle, and the packing can be improved to $l = 0.550610r$ by twisting about one of the fourfold axes, as shown by Karabinta and Székely [7]. A further improvement was found in this work, to $l = 0.550873r$. The structure is given in fig. 8. The structure has D_4 symmetry, but the four circles on the twofold axes are free to rattle and further improvements with a lowering of symmetry may be possible. The packing density of $p = 0.850977$ is only exceeded, for structures of lower x, for the octahedron, icosahedron and snub cube.

$x = 45$

In the literature, the best packing is the structure with fourfold symmetry found by Székely: $l = 0.538257r$. The structure in this work contains no symmetry elements and has a substantially larger edge length, $l = 0.539493r$ (fig. 9).

$x = 46$

The structure found contains a twofold axis, $l = 0.532147r$ (fig. 10).

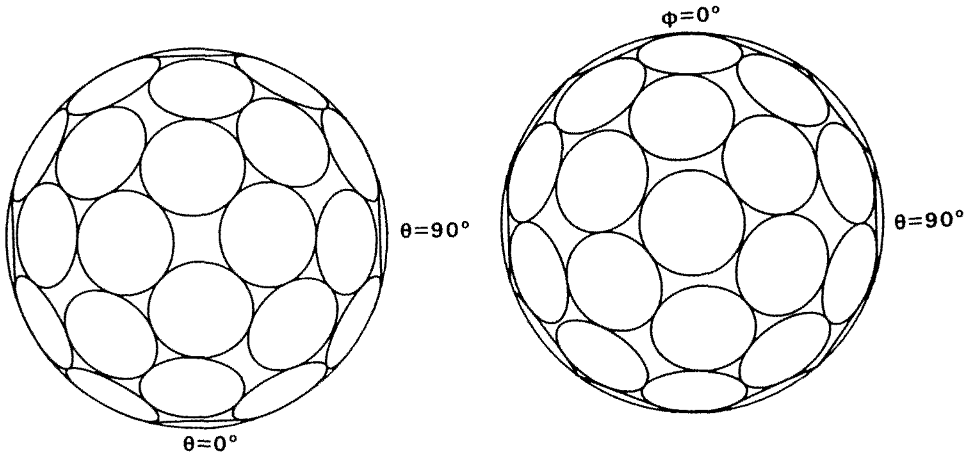

Fig. 8. Packing for $x = 44$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$. A fourfold axis passes through $\phi = 0$, 180° and twofold axes through $\phi = 90°$, $\theta = 0$, 90°, 180°, 270°.

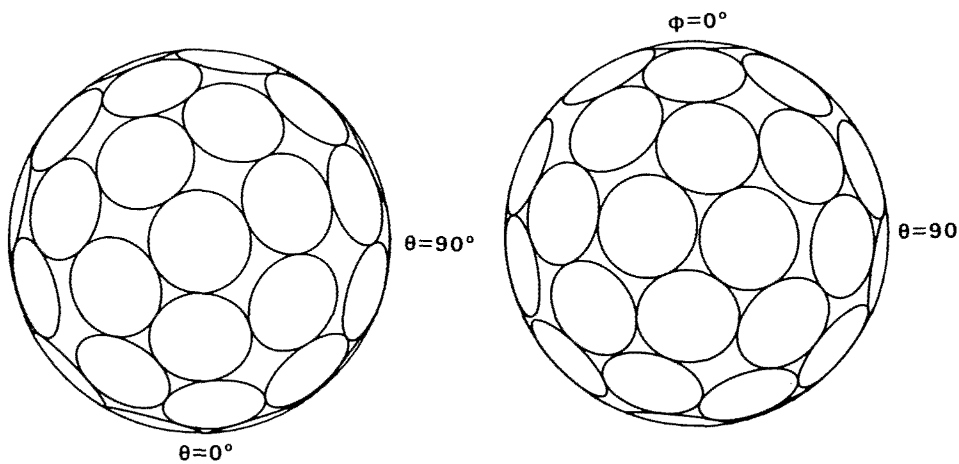

Fig. 9. Packing for $x = 45$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$.

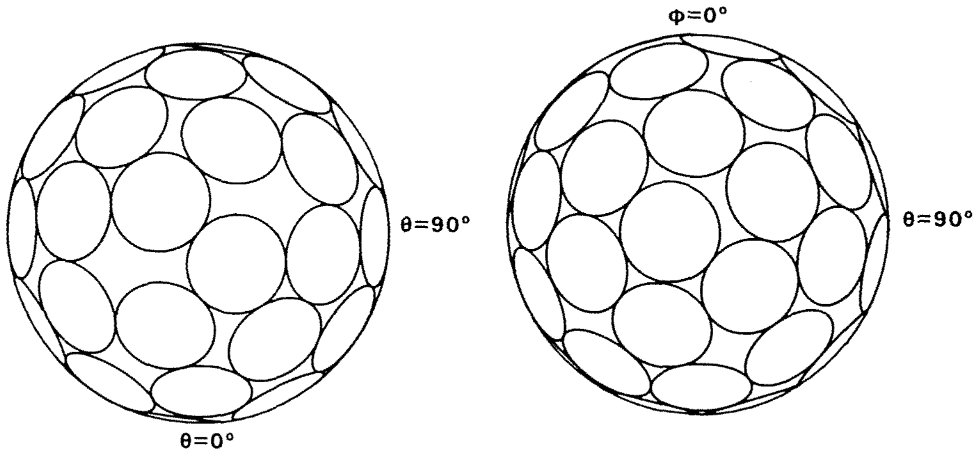

Fig. 10. Packing for $x = 46$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$. A C_2 axis passes through $\phi = 0, 180°$.

$x = 47$

The optimization procedure yielded a structure with a moderately high packing density, $l = 0.53076r$, $p = 0.84262$. Repeated attempts to select 92 edge lengths to solve for the 92 unknowns were, however, unsuccessful. It is commonly found that when the value of x is one less than a number producing a particularly favourable packing, as in this case where the packing for $x = 48$ is particularly good, then the structure approximates to the latter but with one circle missing, which tend to be very nonrigid structures for which the optimization procedures do not converge very well. Other examples of this behaviour are for $x = 5$, 11, 23, 31 and 42.

$x = 48$

The structure obtained from the optimization procedure had octahedral O symmetry, with the three fourfold axes, four threefold axes and six twofold axes of the regular octahedron, but without the mirror planes and centre of symmetry. The structure can be considered as a "snub cuboctahedron" and has the six square faces and eight equilateral triangular faces of the cuboctahedron, with an additional two equilateral triangles linking these squares and triangles along each of the 24 edges of the cuboctahedron. The snubbing of a non-regular polyhedron produces non-regular polygons at each vertex of the polyhedron, which in the case of the cuboctahedron are diamonds, or more correctly, pairs of isosceles triangles. The structure is given in fig. 11 and table 5, and has been described by Robinson [13]. There are 120 edge lengths of $0.530486r$ with five edges meeting at each vertex, and a further 12 edges of $0.645437r$. The packing density of $p = 0.859642$ is bettered only by the octahedron, icosahedron and snub cube for structures with fewer than 48 circles.

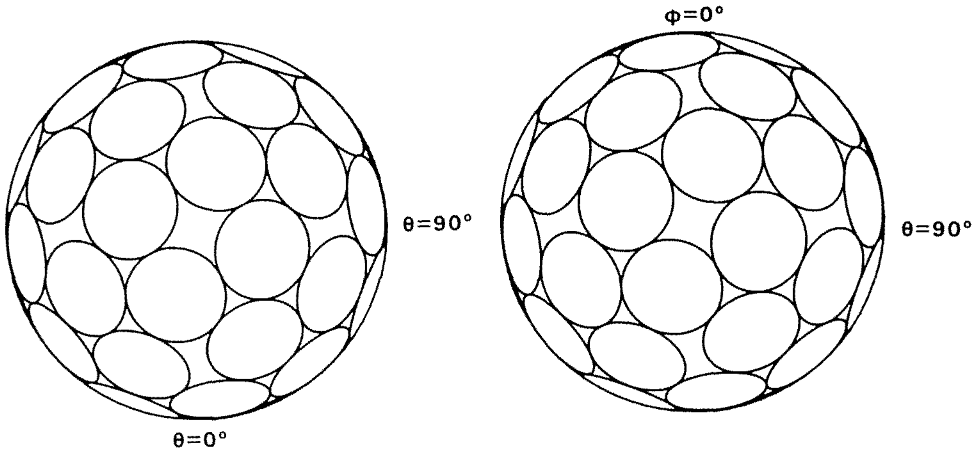

Fig. 11. Packing for $x = 48$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$. The structure has octahedral O symmetry, with fourfold axes passing through $\phi = 0$, 180°, and $\phi = 90°$, $\theta = 0$, 90°, 180°, 270°.

Table 5

Angular parameters (in degrees) for structure with $x = 48$

Vertex	ϕ	θ
1	22.031128	72.093037
2	42.941549	27.093037

$x = 49$

The structure obtained in this work contains no symmetry elements and is shown in fig. 12.

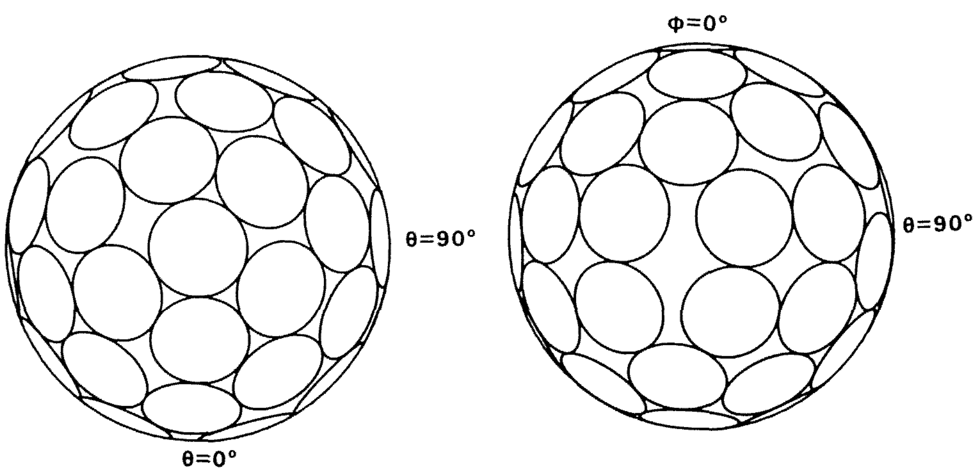

Fig. 12. Packing for $x = 49$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$.

$x = 52$

The best packed structure described in the literature has fivefold symmetry with $l = 0.501723r$ [9]. Our method produced a better structure with threefold symmetry, $l = 0.503577r$ (fig. 13).

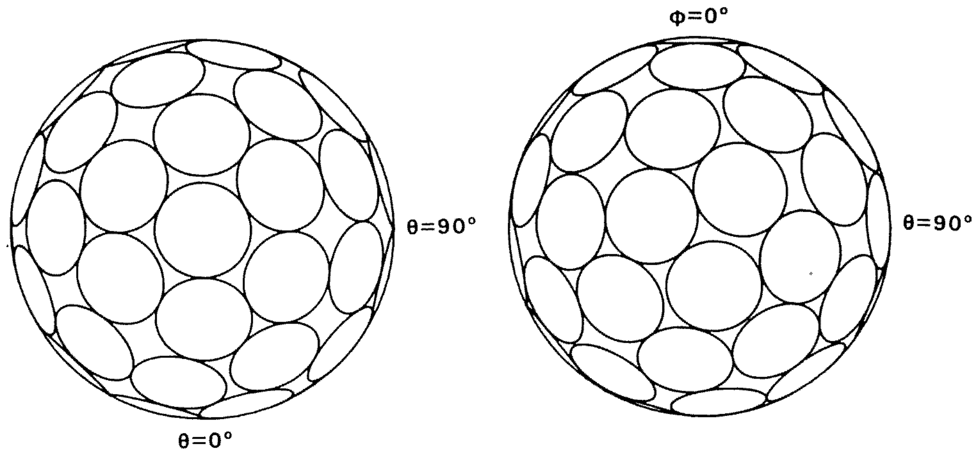

Fig. 13. Packing for $x = 52$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$. A C_3 axis passes through $\phi = 0, 180°$.

$x = 53$

The previous best structure has fourfold symmetry and $l = 0.490867r$ [9]. In this work, a structure with no symmetry was obtained with $l = 0.495986r$ (fig. 14).

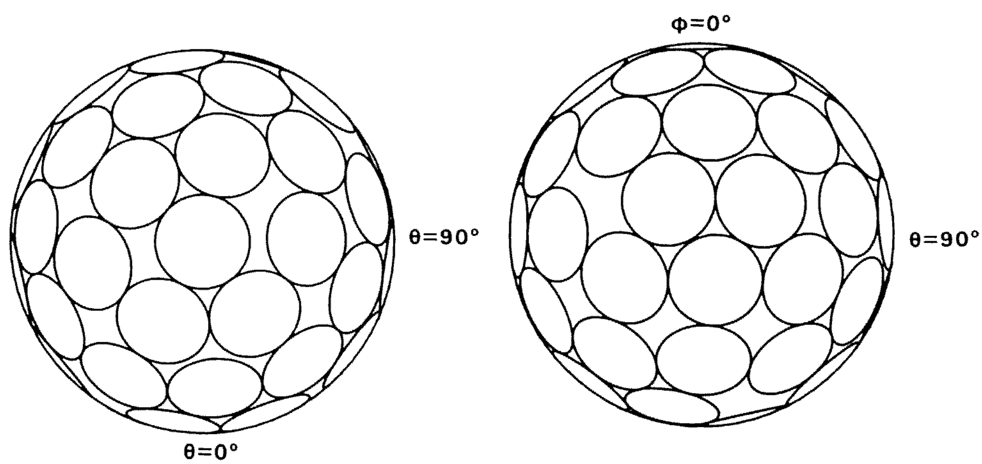

Fig. 14. Packing for $x = 53$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$.

$x = 54$

The structure obtained in this work contains a twofold axis (fig. 15). The edge length of $0.495259r$ is an improvement on $0.488512r$ for a structure of fourfold symmetry described in the literature [9].

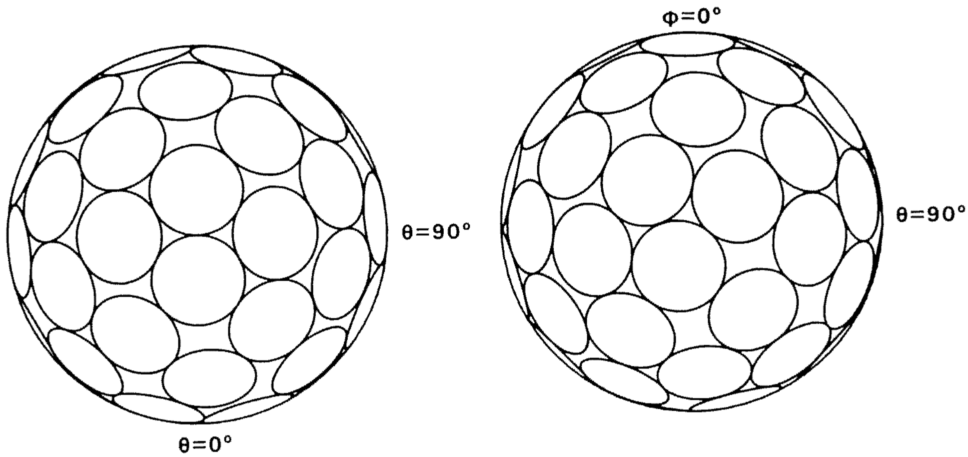

Fig. 15. Packing for $x = 54$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$. A C_2 axis passes through $\phi = 0, 180°$.

$x = 55$

The previous best result was for a structure of fivefold symmetry, $l = 0.480723r$ [9]. We have obtained a better structure that contains no symmetry, $l = 0.488077r$. A value of $l = 0.488285r$ has recently been claimed, but no details are available [10].

$x = 56$

The previous best structure has sixfold symmetry and $l = 0.480307r$ [9]. A structure with D_2 symmetry was found in this work, $l = 0.486351r$ (fig. 16 and table 6). The four symmetry-related circles 5, 6, 7 and 8 rattle.

$x = 57$

The structure obtained in this work is closely related to one containing a twofold axis with $l = 0.479818r$; this structure contains two pairs of rattlers, and the structure can be slightly improved to $l = 0.479905r$ by collapsing around one of them (fig. 17). This structure remains fairly flexible and further improvements may be possible.

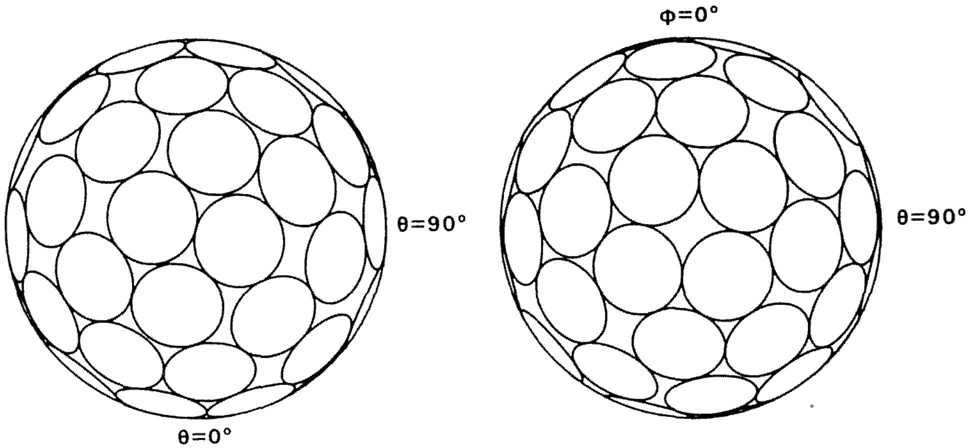

Fig. 16. Packing for $x = 56$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$. Twofold axes pass through $\phi = 0$, 180°; $\phi = 90°$, $\theta = 0$, 180°; $\phi = 90°$, $\theta = 90°$, 270°.

Table 6

Angular parameters (in degrees) for structure with $x = 56$

Vertex	ϕ	θ
1	14.074023	74.660274
5	25.157948	166.088130
9	37.565526	155.080655
13	39.006288	41.398104
17	50.513237	78.467558
21	51.204848	5.002105
25	52.795527	149.108034
29	65.499953	119.636314
33	67.023832	44.884125
37	75.203575	168.291463
41	76.054584	91.917397
45	77.183320	17.224854
49	84.521122	141.246264
53	86.809745	65.564717

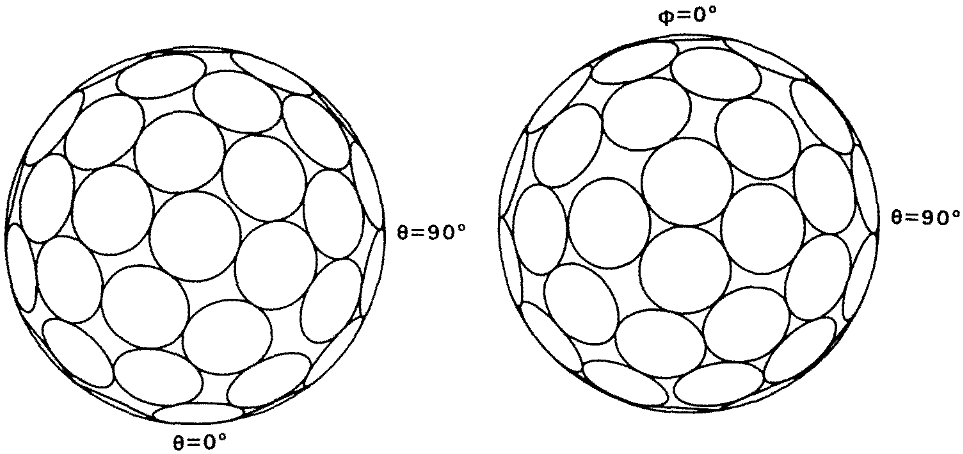

Fig. 17. Packing for $x = 57$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$.

$x = 59$

The most close-packed structure previously found for $x = 59$ was the same as for $x = 60$ but with one circle missing. The structure obtained from our method has an edge length of $0.473591r$, which is an improvement on the $x = 60$ structure (fig. 18).

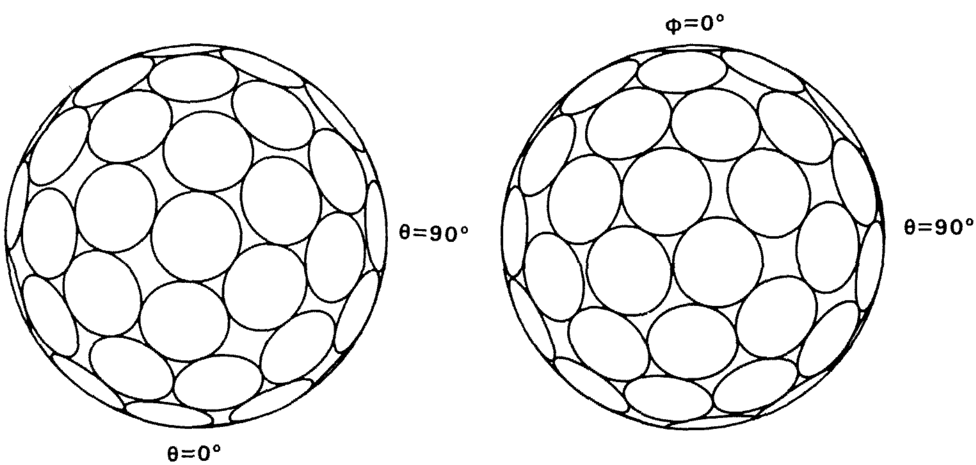

Fig. 18. Packing for $x = 59$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$.

$x = 60$

Chemical interest in the structure of 60-atom clusters originates from the observation of the C_{60} molecule in the gas phase, detected as an intense peak in the mass spectrum of graphite vaporized by a laser pulse [14–16].

There are a number of highly symmetrical polyhedra with 60 vertices, in which all vertices are identical. In addition to the trivial cases of the prism and antiprism formed from two 30-sided polygons, there are the truncated dodecahedron, the truncated icosahedron, the rhombicosidodecahedron, and the snub dodecahedron (which is the same as the snub icosahedron).

The truncated dodecahedron is composed of twelve decagonal and twenty triangular faces. The structure has the full I_h symmetry of the dodecahedron and icosahedron. The structure is not very close-packed, with only three edges meeting at each vertex, $l = 0.336763r$.

The truncated icosahedron has twenty hexagonal and twelve pentagonal faces, and again full I_h symmetry. There are again only three edges meeting at each vertex, but these are substantially longer at $l = 0.403548r$ than for the truncated dodecahedron. This is the structure that has been proposed for the C_{60} molecule, or Buckminsterfullerene.

The rhombicosidodecahedron has twelve pentagonal faces, thirty square faces and twenty triangular faces, and retains I_h symmetry. There are now four edges meeting at each vertex and the edge lengths are substantially longer than for the above two polyhedra, $l = 0.447838r$. The rhombicosidodecahedron contains pentagonal cupola units consisting of a pentagon surrounded by five squares and five triangles, and one or more of the pentagonal cupolas can be rotated by 36° to give a C_{5v} gyrate rhombicosidodecahedron, a D_{5d} para-gyrate rhombicosidodecahedron, a C_{2v} meta-bigyrate rhombicosidodecahedron, or a C_{3v} trigyrate rhombicosidodecahedron, in which the vertices are no longer identical but the edge lengths remain unchanged.

The snub dodecahedron has twelve pentagonal faces and eighty triangular faces. The six fivefold axes, ten threefold axes and fifteen twofold axes of the dodecahedron and icosahedron are retained, but the fifteen mirror planes are lost and the symmetry reduced to I. The edge length is longer than for the above structures, $l = 0.463859r$.

The snub dodecahedron is a member of the series of structures which have five edges meeting at each vertex, all of which are identical [13]. The smaller members of this series, the icosahedron for $x = 12$, the snub cube for $x = 24$ and the "snub cuboctahedron" for $x = 48$, are the best packings that are known for these values of x. It has been shown, however, for $x = 60$ the structure can be improved to $l = 0.467068r$ if the symmetry is lowered to C_3 [9].

Our calculations yield a structure of D_{3d} symmetry with a further improvement in packing, $l = 0.469826r$, $p = 0.839510$ (fig. 19 and table 7).

The remaining case of the series of structures with five edges meeting at each vertex is for $x = 120$ [13], but our optimized structure is again an improvement.

$x = 61$ to 80

The results obtained from the optimization of the repulsion energies are indicated in table 8. Only the value of the shortest edge length is given, and all

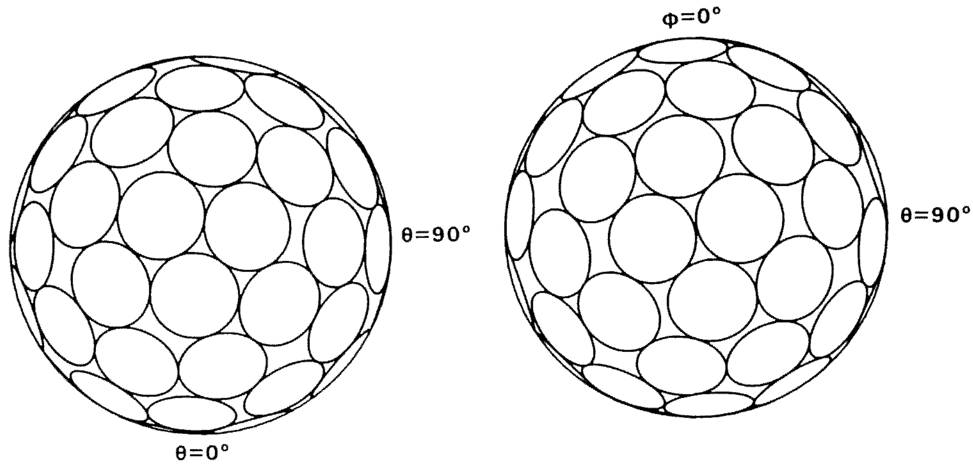

Fig. 19. Packing for $x = 60$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$. A threefold axis passes through $\phi = 0$, 180° and twofold axes through $\phi = 90°$, $\theta = 0$, 60°, 120°, 180°, 240°, 300°.

Table 7

Angular parameters (in degrees) for structure with $x = 60$

Vertex	ϕ	θ
1	15.738927	110.945871
7	32.007533	51.665997
13	41.835673	8.495532
19	46.148978	89.430596
25	58.743683	58.747333
31	64.136761	28.320394
37	66.874697	115.221523
43	73.248271	87.068228
49	83.917516	47.828096
55	87.364685	13.648270

values are capable of improvement (the analytic solution for the edge length is usually about $0.0001r$ longer than the minimum edge length obtained in the optimization). The edge lengths in table 8 are all longer than the best values in the literature, which are for structures of high symmetry [2, 17, 18]. With the exception of the structure for $x = 72$, all structures obtained in this work appear to be of low symmetry. Analytic solutions were obtained only for $x = 61$, 65, 72 and 74.

Table 8

Best packings obtained from energy optimization

x	$l(r)$	p
61	0.46356	0.83058
62	0.46045	0.83278
63	0.45722	0.83417
64	0.45289	0.83124
65	0.45073	0.83610
66	0.44892	0.84205
67	0.44420	0.83671
68	0.43996	0.83287
69	0.43828	0.83857
70	0.43509	0.83824
71	0.43244	0.83977
72	0.43156	0.84810
73	0.42437	0.83112
74	0.42169	0.83178
75	0.41962	0.83467
76	0.41670	0.83393
77	0.41556	0.84025
78	0.41312	0.84107
79	0.40869	0.83348
80	0.40748	0.83899

The packing density for the structure with 72 circles is greater than for any of the structures above $x = 48$. The structure has D_{3d} symmetry, and the details given in fig. 20 and table 9. Figure 21(b) shows the relationship to the snub dodecahedron, the reduction in symmetry from I to D_{3d} leading to an increase in edge length from $0.430148r$ to $0.431609r$.

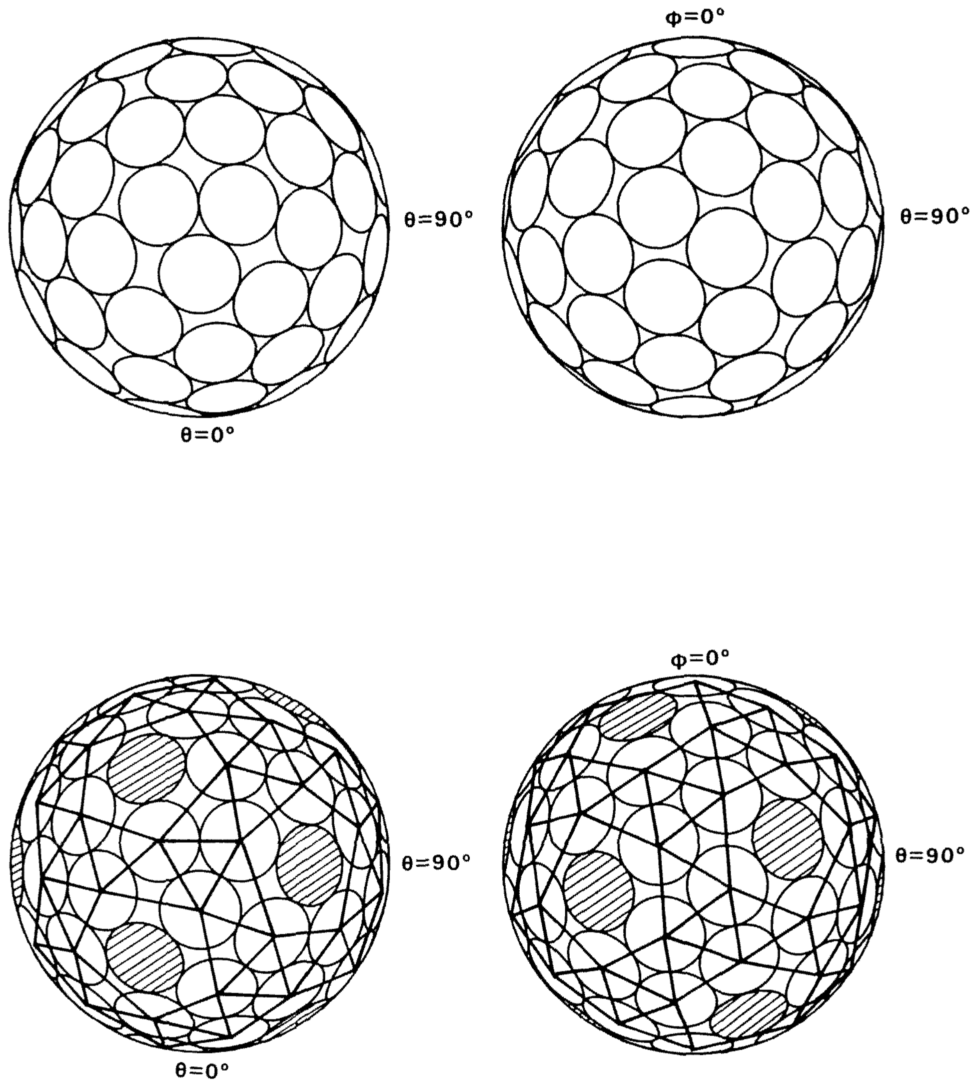

Fig. 20. Packing for x = 72, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$. A threefold axis passes through $\phi = 0$, 180° and twofold axes through $\phi = 90°$, θ = 0, 60°, 120°, 180°, 240°, 300°. The lower figures show the relation to the dodecacapped snub dodecahedron; the capping circles are hatched.

Table 9

Angular parameters (in degrees) for structure with $x = 72$

Vertex	ϕ	θ
1	14.429573	0.507154
7	33.239759	45.345849
13	36.312734	89.498418
19	43.089457	7.589568
25	54.403137	64.896854
31	57.086044	34.797258
37	59.377690	103.071935
43	67.973011	9.377054
49	74.489949	81.409992
55	78.179031	56.023866
61	81.757485	30.962961
67	83.613316	109.275820

4. Discussion

The best packings of x circles on a sphere that are currently known are summarized in table 8 (values obtained from the optimization of the repulsion energy) and table 10 (exact solutions). The packing density p as a function of x is shown in fig. 21. It must be remembered that these results should be considered only as lower limits and further improvements will be found from time to time. The results are sufficiently reliable, however, to allow the following conclusions:

(1) The large fluctuations in the value of the packing density as a function of x that are evident at low values of x have substantially diminished and have settled down to values within the range $p = 0.83$ and 0.85.

(2) In contrast to previous work, there is now a slight upward trend in the packing density as the number of circles increases. The slope of p/x of 0.0001 to 0.0002 indicates that packings as dense as that of an icosahedron may not be reached until there are many hundreds of circles on the sphere. A preliminary calculation for $x = 200$ using our techniques has indicated $l \sim 0.2583r$ corresponding to $p \sim 0.838$, which is not a particularly high value.

(3) Particularly favourable close-packed arrangements are found for the tetrahedron ($x = 4$), octahedron ($x = 6$), icosahedron ($x = 12$), snub cube ($x = 24$) and snub cuboctahedron ($x = 48$). However, high symmetry is not a condition for good close packing since there are a number of structures that have been described with tetrahedral, octahedral and icosahedral symmetry, for example, for $x = 30, 36, 54, 60, 72$ and 78 [2,3,17,18] that are not as close-packed as the lower symmetry structures found in this work.

Table 10

The best packings of circles on a sphere

x	Symmetry	Föppl notation	$l(r)$	p	Ref.
3	D_{3h}	3	1.732051	0.750000	[1]
4	T_d	13	1.632993	0.845299	[1]
5	C_{4v}	14	1.414214	0.732233	[1]
6	O_h	141	1.414214	0.878680	[1]
7	C_{3v}	$13\bar{3}$	1.256870	0.777483	[1]
8	D_{4d}	$4\bar{4}$	1.215563	0.823582	[1]
9	D_{3h}	$3\bar{3}^2$	1.154701	0.825765	[1]
10	C_{2v}	$2(\bar{4})\bar{2}^2$	1.091426	0.810140	[1]
11	C_{5v}	$15\bar{5}$	1.051462	0.821421	[1]
12	I_h	$15\bar{5}1$	1.051462	0.896095	[1]
13	C_{4v}	$14\bar{4}^2$	0.956414	0.791393	[1]
14	D_{2d}	$1(4)\bar{2}^2(\bar{4})1$	0.933863	0.809946	[1]
15	C_3	$3\,\bar{3}\,\tilde{3}^2\bar{3}$	0.902656	0.807314	[1]
16	D_{4d}	$4\bar{4}^3$	0.880574	0.817143	[1]
17	C_{2v}	$1(4)\bar{2}^2(\bar{4})\bar{2}^2$	0.862445	0.830912	[18]
18	C_2	$2\,\bar{2}\,\tilde{2}^7$	0.838217	0.828575	[18]
19	C_S	–	0.808558	0.810961	[6] [This work]
20	D_{3h}	$13\bar{3}(\bar{6})\bar{3}^2 1$	0.804392	0.844463	[19]
21	C_1	–	0.775239	0.820896	[This work]
22	pseudo-S_4	$\frac{2}{2}\bar{2}\,\tilde{2}^9\,\frac{2}{2}$	0.761175	0.827806	[This work]
23	C_1	–	0.744496	0.826468	[20]
			0.744517	0.826516	[10]
24	O	$\bar{4}\,4^2\tilde{4}\,\bar{4}^2$	0.744206	0.861703	[21]
25	C_3	$13\,\tilde{3}^7$	0.710776	0.816014	[6] [This work]
26	C_1	–	0.700983	0.824643	[This work]
27	C_{2v}	$1(4)\bar{2}^2(\bar{4})\bar{2}(\bar{4})(4)\bar{2}^2$	0.695141	0.841674	[18]
28	C_s	–	0.672110	0.814206	[1]
29	C_1	–	0.661981	0.817306	[This work]
	–	–	0.662797	0.819383	[10]
30	D_3	$3\,\bar{3}\,\tilde{3}^7\bar{3}$	0.660981	0.842861	[1]
31	C_5	$15\bar{5}^2\tilde{5}\,\bar{5}^2$	0.646346	0.831731	[19]
32	D_3	$13\,\bar{3}\,\tilde{3}^7\bar{3}1$	0.642469	0.848006	[18]
33	C_3	$3\bar{3}\,\tilde{3}^8\bar{3}$	0.622258	0.818933	[12] [This work]
34	C_2	$2\bar{2}\,\tilde{2}^{14}\bar{2}$	0.614714	0.822896	[1]
35	C_1	–	0.606437	0.823883	[1]
36	D_2	$2\bar{2}\,\tilde{2}^{15}\bar{2}$	0.604483	0.841834	[1]
37	C_1	–	0.589685	0.822400	[1]
38	D_{6d}	$16\bar{6}^5 1$	0.588926	0.842404	[9]
39	C_2	$1(4)\bar{2}^2\tilde{2}^{14}\bar{2}$	0.575098	0.823563	[1]
40	C_3	$13\bar{3}(\bar{6})\bar{3}^2(\bar{6})\bar{3}\,\tilde{3}^3\bar{3}$	0.570680	0.831473	[1]

. . . continued

Table 10 (continued)

x	Symmetry	Föppl notation	$l(r)$	p	Ref.
41	C_2	$12\,\tilde{2}^{18}\,\bar{2}$	0.563219	0.829653	[This work]
	–	–	0.563488	0.830463	[10]
42	D_5	$15\,\bar{5}\,\tilde{5}^{5}\,\bar{5}1$	0.559765	0.839281	[9]
43	C_1	–	0.552622	0.837933	[This work]
44	D_4	$4\,\bar{4}\,\tilde{4}^{8}\bar{4}$	0.550873	0.850977	[This work]
45	C_1	–	0.539493	0.834044	[This work]
46	C_2	$2\,\bar{2}\,\tilde{2}^{21}$	0.532147	0.829086	[This work]
47	C_1	–	0.53076	0.84262	[This work]
48	O	$4\,\bar{4}\,\tilde{4}^{9}\bar{4}$	0.530486	0.859642	[13]
49	C_1	–	0.515905	0.829139	[This work]
50	D_6	$16\,\bar{6}^{2}\tilde{6}^{3}\,\bar{6}^{2}1$	0.513472	0.837961	[9]
51	C_5	$15\,\tilde{5}^{7}\bar{5}^{2}$	0.505892	0.829249	[9]
52	C_3	$13\,\bar{3}\,\tilde{3}^{15}$	0.503577	0.837660	[This work]
53	C_1	–	0.495986	0.827811	[This work]
54	C_2	$2\,\bar{2}\,\tilde{2}^{25}$	0.495259	0.840920	[This work]
55	C_1	–	0.488077	0.831449	[This work]
	–	–	0.488285	0.832169	[10]
56	D_2	$2\,\bar{2}\,\tilde{2}^{25}\bar{2}$	0.486351	0.840494	[This work]
57	C_1	–	0.479904	0.832638	[This work]
58	D_7	$17\,\bar{7}^{2}\tilde{7}^{3}\,\bar{7}^{2}1$	0.476143	0.833817	[9]
59	C_1	–	0.473591	0.838994	[This work]
60	D_{3d}	$3\,\tilde{3}^{19}$	0.469826	0.839510	[This work]
61	C_1	–	0.463620	0.830787	[This work]
65	C_1	–	0.450806	0.836366	[This work]
72	D_{3d}	$3\,\tilde{3}^{23}$	0.431609	0.848284	[This work]
74	C_1	–	0.421747	0.832005	[This work]

(4) In some cases, the closest packed structures are superficially related to structures of higher symmetry. Examples include the D_2 structure for $x = 32$ which is related to the rhombic triacontahedron (or an icosahedron with all faces capped), the D_{4d} structure for $x = 44$ which is related to a truncated rhombic dodecahedron, and the D_{3d} structure for $x = 72$ which is based on a dodecacapped snub dodecahedron. In the latter case, the structure for $x = 72$ based on dodecahedral symmetry has shorter edge lengths than one based on octahedral symmetry [2], but when the packing of both are improved by a lowering of symmetry, the order is reversed and the distorted capped snub dodecahedron now has the longer edges, again demonstrating that the high symmetry structures are not a reliable guide for the most favourably packed structures. It is probable that many of the high symmetry structures that have been

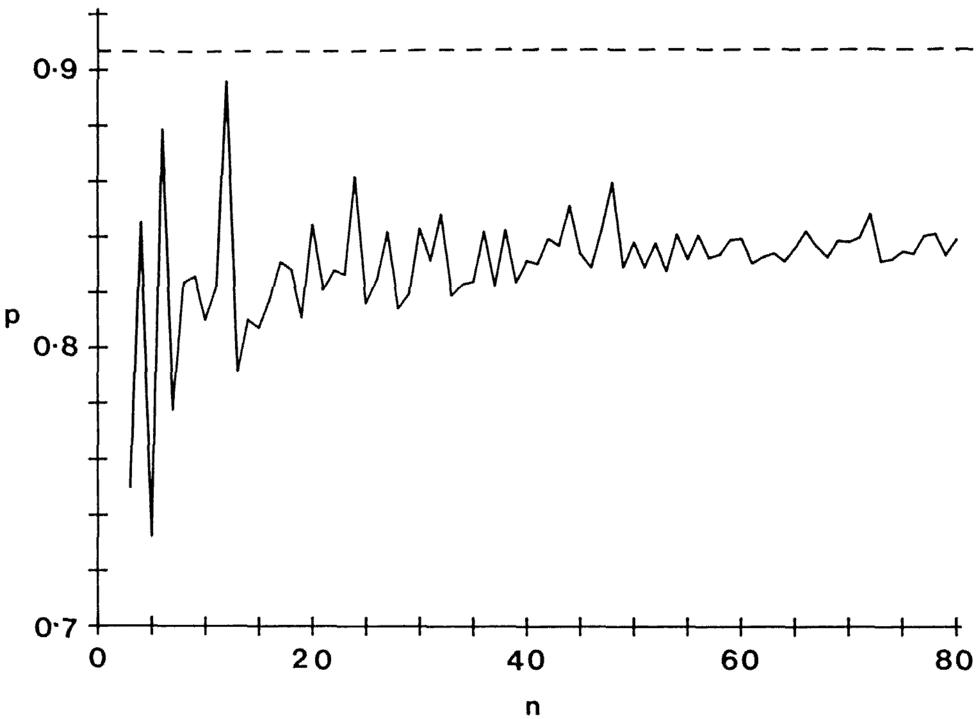

Fig. 21. Packing density p as a function of the number of circles x, for the best closest packings of circles on the surface of a sphere. The broken line indicates the value for an infinite number of circles, p = 0.906900.

described [2,3,17,18] for x = 120, 132, 180, 270, 360, 480, 750 and 1080 (p = 0.846 to 0.861) are capable of improvement.

(5) There is no obvious correlation between the type of structure observed and the number of circles. For example, structures are known with no rotational symmetry as well as with twofold, threefold, fourfold, fivefold, sixfold and even sevenfold symmetry, but their occurrence is not a simple function of x. One feature of possible significance is the rarity of structures containing a mirror plane for $x > 20$, and these can exist as pairs of optical isomers. Likewise, there is no apparent pattern for other structural features, such as the coordination number or degree of connectivity between a circle and its neighbours, or the number and type of faces of the polyhedron.

It is clearly not possible at this stage to predict the most close-packed structure for a given value of x.

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