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The closest packing of equal circles on a sphere

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The closest packing of x circles on the surface of a sphere is examined with the use of techniques that have been developed to determine the stereochemical arrangement of atoms packed around a central atom. The technique is based on the concept that the centres of the circles repel one another, and minimizing the total 'repulsion energy' leads to an approximate structure from which exact solutions can be determined.

A number of improved packings have been discovered for values of x in the range 20–40. Many different types of structure are found that are of lower symmetries than those previously described.

The packing density p, defined as the fraction of the spherical surface that is enclosed by the circles, is found to increase as the number of circles increases, in contrast to the conclusion from previous studies. However, this increase in p is very slight and the values remain substantially below that for an infinite number of circles, or a close-packed plane.

1. INTRODUCTION

The determination of the closest packing of circles on a plane is a trivial problem, but the closest packing of circles on curved surfaces is more difficult to determine (Coxeter 1962). The optimal packing of circles, or spheres, onto the surface of a sphere is basic to studies as diverse as the shape of the enzymes and the arrangement of dimples on golf balls. This problem is usually known as the Tammes problem and originated from a study of the pattern of orifices in spherical pollen grains (Tammes 1930). Our interest stems from the arrangement of ligand atoms around a central atom in coordination complexes, [M(ligand)$_x$] (Kepert 1982), the packing of atoms into clusters, M_x (Fuller & Kepert 1983; Clare & Kepert 1984), and the concentric arrangement of ligand atoms about clusters of metal atoms, [M_y(ligand)$_x$] (Clare *et al.* 1985). The chemical interest in this packing problem has been summarized by others (Melnyk *et al.* 1977; Mackay *et al.* 1977; Benfield & Johnson 1980).

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.

There is general agreement concerning the closest packing for low values of x. Indeed, for $x = 2$–12 and for $x = 24$ there are geometric proofs that these packings are the optimum solutions. In other cases rigorous proofs are not available and improved packings are discovered from time to time. The best packings in the literature are summarized in table 1 for values of x from 3 to 40. (In some instances the numerical values quoted in table 1 are more precise or slightly revised compared with the values quoted in the cited reference). Few results are available for $x > 40$. A number of points should be made concerning the data in table 1.

(1) Most of these best packings have a fairly high degree of symmetry. However, the symmetry is lower than for the well known geodesic domes based on smaller

Table 1. The best packing of circles on a sphere available from the literature (x = 3–40)

x	symmetry	Föppl notation	$l(r)$	p	reference
3	D_{3h}	3	1.732051	0.750000	Melnyk *et al.* (1977)
4	T_d	13	1.632993	0.845299	Melnyk *et al.* (1977)
5	C_{4v} or lower (see text)	—	1.414214	0.732233	Melnyk *et al.* (1977)
6	O_h	141	1.414214	0.878680	Melnyk *et al.* (1977)
7	C_{3v}	$11\bar{3}$	1.256870	0.777483	Melnyk *et al.* (1977)
8	D_{4d}	$4\bar{4}$	1.215563	0.823582	Melnyk *et al.* (1977)
9	D_{3h}	$3\bar{3}\bar{3}$	1.154701	0.825765	Melnyk *et al.* (1977)
10	C_{2v}	$2(\bar{4})\bar{2}\bar{2}$	1.091426	0.810140	Melnyk *et al.* (1977)
11	C_{5v}	$15\bar{5}$	1.051462	0.821421	Melnyk *et al.* (1977)
12	I_h	$15\bar{5}1$	1.051462	0.896095	Melnyk *et al.* (1977)
13	C_{4v}	$14\bar{4}\bar{4}$	0.956414	0.791393	Melnyk *et al.* (1977)
14	D_{2d}	$1(4)\bar{2}\bar{2}(\bar{4})1$	0.933863	0.809946	Melnyk *et al.* (1977)
15	C_3	$3\bar{3}\tilde{3}\tilde{3}\bar{3}$	0.902656	0.807314	Melnyk *et al.* (1977)
16	D_{4d}	$4\bar{4}\bar{4}\bar{4}$	0.880574	0.817143	Melnyk *et al.* (1977)
17	D_{5h}	$15\bar{5}\bar{5}1$	0.861440	0.828873	Melnyk *et al.* (1977)
18	D_{4d}	$14\bar{4}\bar{4}\bar{4}1$	0.838137	0.828409	Goldberg (1965)
19	C_{3v} or C_s (see text)	—	0.804392	0.802240	van der Waerden (1952)
20	D_{3h}	$13\bar{3}(\bar{6})\bar{3}\bar{3}1$	0.804392	0.844463	van der Waerden (1952)
21	D_3	$3\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}$	0.774344	0.818921	Karabinta & Székely (1974)
22	D_2	$14\tilde{4}\tilde{4}\tilde{4}\tilde{4}1$	0.765659	0.837992	Goldberg (1969)
23	E (see text)	—	0.744206	0.825799	—
24	O	$\bar{4}\bar{4}\bar{4}\tilde{4}\bar{4}\bar{4}$	0.744206	0.861703	Robinson (1961)
25	C_4	$14\tilde{4}\tilde{4}\tilde{4}\tilde{4}\tilde{4}$	0.708108	0.809688	Székely (1974)
26	C_5	$15\bar{5}\bar{5}\bar{5}\bar{5}$	0.700842	0.824300	Goldberg (1967*a*)
27	D_{5h}	$15\bar{5}\bar{5}\bar{5}\bar{5}1$	0.695141	0.841673	Székely (1974)
28	C_3	$13\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}$	0.668291	0.804699	Székely (1974)
29	C_4	$14\tilde{4}\tilde{4}\tilde{4}\tilde{4}\tilde{4}\tilde{4}$	0.654483	0.798359	Székely (1974)
30	D_5	$5\bar{5}\bar{5}\tilde{5}\bar{5}\bar{5}$	0.653791	0.824093	Goldberg (1967*a*)
31	C_5	$15\bar{5}\bar{5}\tilde{5}\bar{5}\bar{5}$	0.646346	0.831731	Strohmajer (1963)
32	D_5	$15\bar{5}\bar{5}\tilde{5}\bar{5}\bar{5}1$	0.641736	0.846017	Goldberg (1967*a*)
33	D_3	$3\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}$	0.622751	0.820265	Goldberg (1967*c*)
34	C_{3v}	$16\bar{6}\bar{6}\bar{6}\bar{6}\bar{3}$	0.607876	0.804239	Székely (1974)
35	C_{2v}	$16\bar{6}\bar{6}\bar{6}\bar{6}\bar{2}\bar{2}$	0.599036	0.803414	Székely (1974)
36	C_3	$3\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}$	0.596162	0.818270	Karabinta & Székely (1974)
37	C_3	$13\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}$	0.589220	0.821075	Székely (1974)
38	D_{6d}	$16\bar{6}\bar{6}\bar{6}\bar{6}\bar{6}1$	0.588926	0.842404	Székely (1974)
39	C_3	$3\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}$	0.574333	0.821327	Karabinta & Székely (1974)
40	C_3	$16\tilde{6}\tilde{6}\tilde{6}\tilde{6}\tilde{6}\bar{3}$	0.567309	0.821469	Székely (1974)

polyhedra in which the regular faces are divided into smaller polygons and then projected onto the spherical surface with retention of the high symmetry of the original regular polyhedron. Most of the best packings in table 1 have axial symmetry and are described by using a modified Föppl notation in which the number of corners in the succession of planar polygons perpendicular to the principle axis of rotation are listed; 'a' signifies that the polygon is eclipsed relative to the polygon above it, '$\bar{a}$' signifies a staggered arrangement and '$\tilde{a}$' signifies an intermediate arrangement. Parentheses, (a), specify that the polygon is irregular.

(2) The closeness of packing is given in two forms in table 1. The shortest edge length of the polyhedron is given by l, which is also the diameter of the circles. The fraction of the surface of the sphere that is enclosed by the circles is defined as the packing density p. Relatively high values for the packing density are observed for the tetrahedron ($x = 4$), octahedron ($x = 6$), icosahedron ($x = 12$) and snub cube ($x = 24$). For higher values of x the packing density appears relatively constant at $p \approx 0.82$ and does not appear to be approaching the value expected for an infinite number of circles, $p = \pi/(2\sqrt{3}) = 0.906900$, corresponding to a close-packed plane. Indeed the trend from $x = 20$ to $x = 40$ is a *decrease* in p.

(3) For $x = 5$ an infinite range of equally good packings is possible. In each polyhedron there is a pair of vertices at opposite poles of the sphere at $\phi = 0$ and $\phi = 180°$ with the other three vertices forming a triangle on the equatorial great circle at $\phi = 90°$ so that there are six polar–equatorial edge lengths equal to $2^{\frac{1}{2}}r$. Any arrangement is possible on the equatorial plane provided no edge of this triangle is less than $2^{\frac{1}{2}}r$. A C_{4v} square pyramid (Föppl 14) is formed if the triangle is right-angled with edge lengths of $2^{\frac{1}{2}}r$, $2^{\frac{1}{2}}r$ and $2r$. A D_{3h} trigonal bipyramid (Föppl 131) is formed if the triangle is equilateral with edges of $3^{\frac{1}{2}}r$. An isosceles triangular arrangement corresponds to an intermediate $(12\bar{2})$ structure of C_{2v} symmetry whereas a scalene triangular arrangement forms a structure containing only the identity operation E.

A related type of non-rigid structure is observed if only some of the circles pack to form a rigid structure that includes holes that are larger than necessary to accommodate the remaining circles allowing them to 'rattle'. In these cases the maximum symmetry structure is given in table 1 where the circles are in the centres of their 'holes'. A number of similar examples will be described later.

(4) The square pyramid limit for $x = 5$ can be obtained by removal of one vertex from an octahedron with no change in edge length. A similar situation occurs for other dense-packed structures. For example, the capped pentagonal antiprismatic structure ($x = 11$) is obtained by removal of one vertex from an icosahedron and the structure for $x = 23$ in table 1 is obtained by removal of one vertex from a snub cube. Other examples will be described later.

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 about a central atom, or about a cluster of atoms, is best modelled by $n \approx 6$. As n gets 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 inflexible circles on the surface of a sphere. Within the range $x = 20$ to 40, it is usually sufficient to perform the energy minimization procedure for each value of x by using values of n up to 5000–10000. This generates an approximate polyhedron whose shortest edge lengths vary by only about 1 % and which also establishes the symmetry of the structure. Each of these edge lengths is a function of four angular coordinates:

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

If each of these 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 elements of symmetry). 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, particularly if the structure is close to one of higher symmetry, 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 the corresponding equations can be deleted from the set of equations to be solved and the circles reinserted later.

Examples of structures in which these techniques remain inadequate are described later under the individual structure.

Minimization techniques were variants of Fletcher–Powell–Davidon (Daniels 1978). Equations were solved by Newton–Raphson methods with the approximate structure as the starting point.

3. Results

For values of x from 20 to 40 a number of packing arrangements have been discovered that are an improvement on the best in the literature and these are described in turn. The symmetry and Föppl notation do not completely define the structure and a full listing of angular coordinates is required; in this work the angular coordinates are defined relative to the 'north pole' at $\phi = 0$ and the 'longitude' is given by θ.

(a) $x = 19, 20$

The structure obtained for $x = 20$ is the same as that obtained previously (van der Waerden 1952) although our precision is a little better. More recent solutions appear incorrect (Goldberg 1967*b*) or are inferior because a different set of simultaneous equations was chosen (Mackay *et al.* 1977). In the best structure,

$13\bar{3}(\bar{6})\bar{3}\bar{3}1$, the two polar circles are free to rattle. The polyhedral edge lengths to these polar vertices are $0.807\,656\,r$, compared with $0.804\,392\,r$ for the short edges.

The best structure found for $x = 19$ is obtained by removal of one vertex from the $x = 20$ structure. Four different structures can be obtained, depending upon which vertex is removed, and may be described as

$$C_{3v}\,3\bar{3}(\bar{6})\bar{3}\bar{3}1, \quad C_s\,1(2)\bar{3}(\bar{6})\bar{3}\bar{3}1, \quad C_s\,13(\bar{2})(\bar{6})\bar{3}\bar{3}1 \quad \text{and} \quad C_s\,13\bar{3}(\bar{5})\bar{3}\bar{3}1.$$

(*b*) $x = 23, 24$

The best packing for $x = 24$ is the snub cube and it has generally been assumed that removal of one vertex leads to the best arrangement for $x = 23$. An equally good arrangement is obtained if two adjacent vertices of a square face of a snub cube are replaced by one vertex at an intermediate position to form an 'edge-coalesced snub cube' (figure 1). The circle on this edge-coalesced site can rattle in the hole created by the rigid framework formed by the other 22 circles. However there is not a continuous series of structures between the snub cube with a missing vertex and an edge-coalesced snub cube. The optimum position for the edge-coalesced vertex is $0.770\,710\,r$ from three of the surrounding vertices, compared with the other edge lengths for the snub cube of $0.744\,206\,r$.

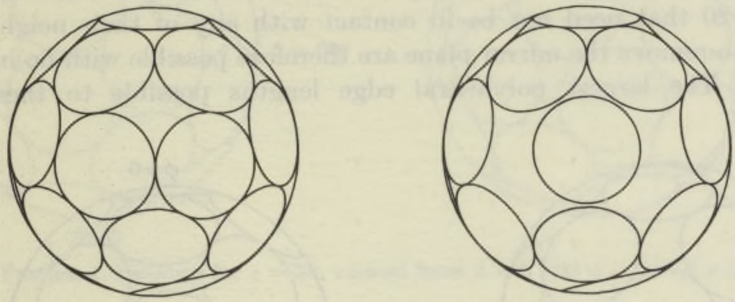

FIGURE 1. Snub cube and edge-coalesced snub cube (viewed down the edge-coalesced site).

(*c*) $x = 25$

The structure obtained by the energy minimization method is a $1(4)\bar{2}\bar{\bar{2}}\tilde{2}\tilde{\bar{2}}\tilde{2}\bar{2}\tilde{2}\tilde{\bar{2}}\bar{\bar{2}}\tilde{2}$ stack with C_2 symmetry (figure 2 and table 2). This structure is a slight improvement on the related $14\tilde{4}\tilde{4}\tilde{4}\tilde{4}$ stack (Székely 1974) or the $5\bar{5}\bar{5}\bar{5}\bar{5}$ stack

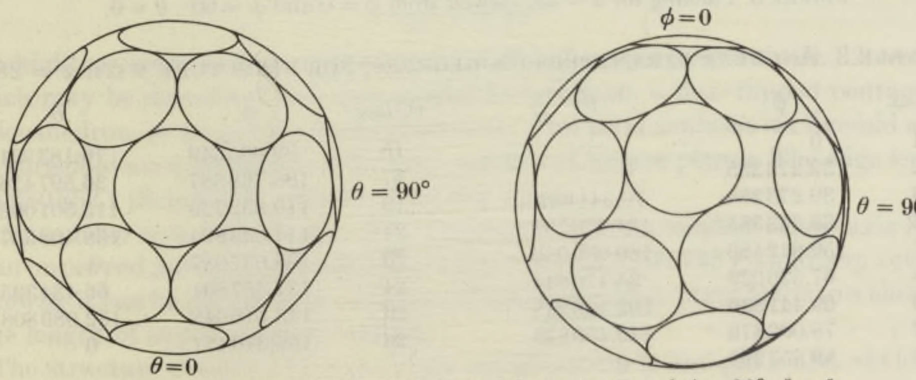

FIGURE 2. Packing for $x = 25$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$.

TABLE 2. ANGULAR PARAMETERS (IN DEGREES) FOR STRUCTURE WITH $x = 25$

vertex	ϕ	θ	vertex	ϕ	θ
1	0	—	14	91.786094	97.707933
2	41.596463	32.333930	16	109.352325	21.871512
4	41.596463	147.666070	18	119.831905	157.293309
6	50.797250	90.000000	20	120.965815	66.341288
8	73.745972	0	22	148.402264	112.783008
10	79.791658	54.892163	24	150.948596	22.050075
12	82.436495	138.339740			

(Jucovič 1959; Mackay *et al.* 1977). Circle 10 (and the symmetry-related 11) need not be in contact with any of the six surrounding circles and the largest circle that can be placed at this site corresponds to a polyhedral edge length of $0.726747\,r$ compared with $0.710156\,r$ for the shortest edges.

(*d*) $x = 28$

The best packing found contains no symmetry axis but does contain a mirror plane through $\theta = 0$, $\theta = 180°$. Six vertices, 1, 2, 7, 14, 23 and 28 are distributed very unevenly on this great circle (figure 3 and table 3). There are three circles, 14, 19 and 20 that need not be in contact with any of their neighbours and distortions to remove the mirror plane are therefore possible with no impairment of packing. The largest polyhedral edge lengths possible to these sites is

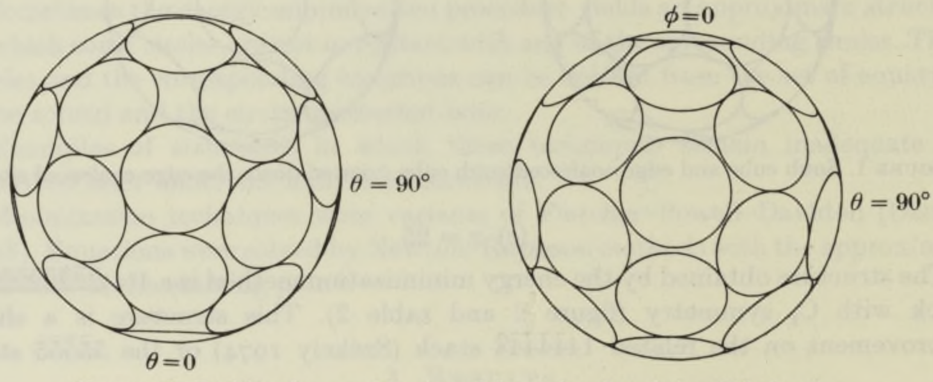

FIGURE 3. Packing for $x = 28$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$.

TABLE 3. ANGULAR PARAMETERS (IN DEGREES) FOR STRUCTURE WITH $x = 28$

vertex	ϕ	θ	vertex	ϕ	θ
1	0	—	15	99.065549	76.183921
2	39.273385	0	17	106.768587	36.597426
3	39.273385	70.341687	19	110.832729	115.501093
5	39.273385	134.470789	21	114.045824	158.408357
7	59.612189	180.000000	23	130.037087	0
8	67.520029	35.170844	24	137.457801	66.434395
10	69.441836	102.406238	26	148.616048	132.089808
12	78.000878	142.450843	28	169.310471	0
14	88.857263	0			

$l_{14} = 0.688769\ r$ and $l_{19} = l_{20} = 0.678122\ r$, compared with $l = 0.672110\ r$ for the remaining 25 vertices. This structure is a substantial improvement on previous structures with threefold (Székely 1984) or fourfold (Goldberg 1969) symmetry.

(*e*) $x = 29, 30$

The best structure obtained for $x = 30$ is described by $3\bar{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\bar{3}$ (figure 4 and table 4). In addition to the obvious threefold axis there are three twofold axis through $\phi = 90$, $\theta = 0$, 60 and 120°, the symmetry being D_3. This packing is a substantial improvement on the structure with fivefold symmetry proposed previously (Schutte & Van der Waerden 1951; Goldberg 1967*a*; Székely 1974).

The best packings found for $x = 29$ are the same as that found for $x = 30$ but with one circle removed. This may be done in five different ways, none of which contain any symmetry elements. These packings are substantial improvements on the fourfold spiral found previously (Székely 1974).

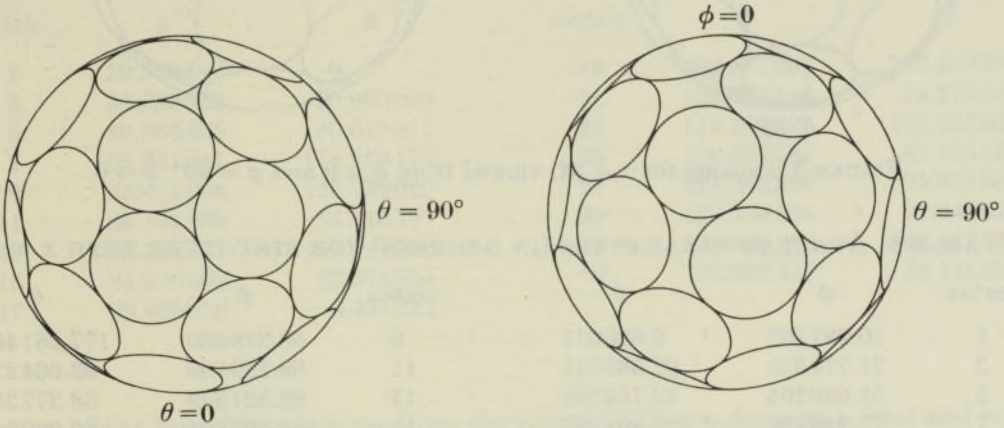

FIGURE 4. Packing for $x = 30$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$.

TABLE 4. ANGULAR PARAMETERS (IN DEGREES) FOR STRUCTURE WITH $x = 30$

vertex	ϕ	θ	vertex	ϕ	θ
1	22.433924	85.417486	10	72.361610	112.041504
4	45.761559	25.417486	13	82.796649	37.867631
7	60.081628	71.130768			

(*f*) $x = 32$

A highly symmetrical arrangement is possible for a polyhedron with 32 vertices which may be described as a face-capped icosahedron, a face-capped pentagonal dodecahedron, or a rhombic triacontahedron. This solid contains six fivefold axes, ten threefold axes, fifteen twofold axes and fifteen mirror planes. The edge length is $0.640852\ r$ (Schutte & van der Waerden 1951).

It has been noted previously that retention of only a single fivefold axis leads to an improved packing with a shortest edge length of $0.641736\ r$ (Goldberg 1967*a*). Likewise it can be shown that retention of only one mirror plane leads to a shortest edge length of approximately $0.6419\ r$.

The structure obtained by our energy minimization technique is also obviously related to the face-capped icosahedron but retains only three of the twofold axes, through $\phi = 0$; $\phi = 90$, $\theta = 0$; $\phi = 90$, $\theta = 90°$ (figure 5 and table 5). The high symmetry is destroyed by rotating 1, 2, 3, 4, anticlockwise about the twofold axis through $\theta = 0$ by 2.6° (figure 5), by rotating 15, 18, 10, 23 anticlockwise about the twofold axis through $\theta = 0$ by 4.4° (figure 5), and by rotating 11, 21, 13, 19 clockwise about the twofold axis through $\theta = 90$ by 7.0°. There are 17 symmetry-independent edge lengths of 0.642 294 r.

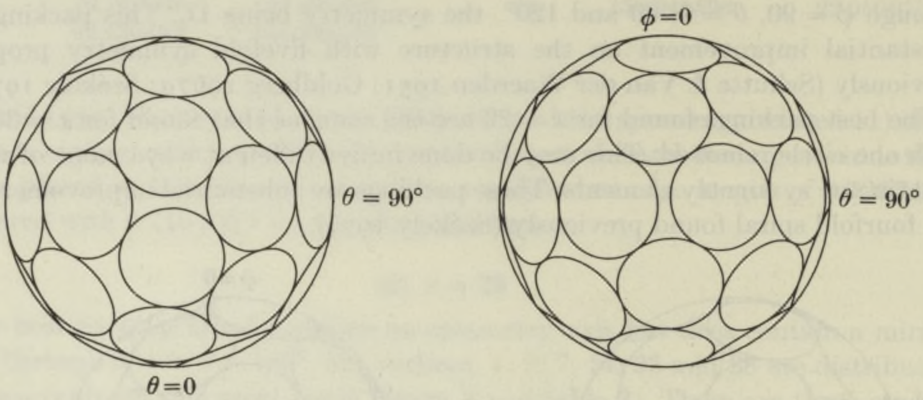

FIGURE 5. Packing for $x = 32$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$.

TABLE 5. ANGULAR PARAMETERS (IN DEGREES) FOR STRUCTURE WITH $x = 32$

vertex	ϕ	θ	vertex	ϕ	θ
1	20.987 303	2.588 011	9	58.328 680	177.281 463
3	31.774 535	92.588 011	11	69.239 100	92.664 275
5	51.669 294	42.762 798	13	86.321 349	58.377 355
7	57.749 352	132.801 297	15	88.426 891	20.929 047

(g) $x = 33$

The structure with D_3 symmetry (Goldberg 1967c) is confirmed although a significantly improved value for the edge length is found in this work, 0.622 751 r compared with 0.622 33 r.

(h) $x = 34$

The structure obtained contains only a single twofold axis and is represented by $2\bar{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\bar{2}$ (figure 6 and table 6). Circles 19 and 20 are not in contact with any of the neighbouring circles and hence equally good packings are possible with loss of the twofold axis. The polyhedral edge lengths to these vertices are 0.627 321 r, compared with 0.614 714 r for the shortest edges.

(i) $x = 35$

The structure attained by using $n > 5000$ in the repulsive law did not contain any symmetry elements, thus requiring 68 simultaneous equations to be selected and solved to determine the structure. There were 71 edge lengths in the range 0.606 r to 0.613 r, the next shortest being significantly longer at 0.629 r. The

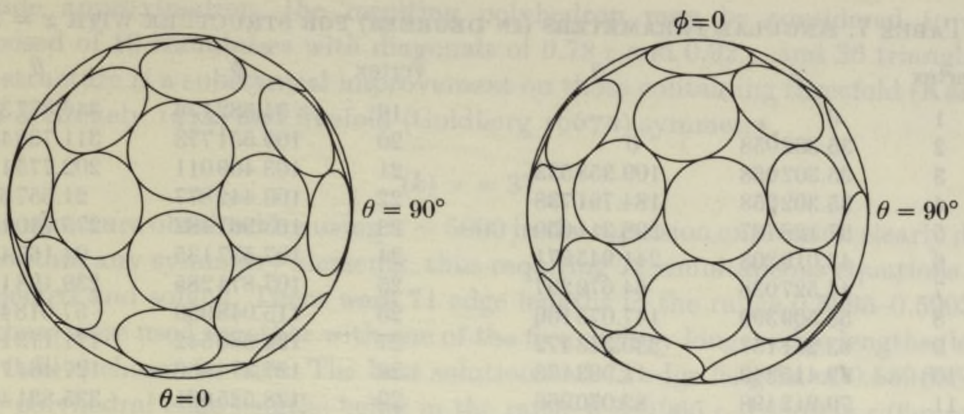

FIGURE 6. Packing for $x = 34$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$.

TABLE 6. ANGULAR PARAMETERS (IN DEGREES) FOR STRUCTURE WITH $x = 34$

vertex	ϕ	θ	vertex	ϕ	θ
1	19.589448	0	19	92.677967	110.240600
3	30.583029	90.000000	21	100.646448	74.278345
5	49.085255	40.018311	23	117.256228	138.543904
7	55.281041	174.866179	25	120.639784	42.255124
9	58.444004	123.739029	27	124.642876	179.691886
11	66.133535	84.010797	29	129.706124	97.843025
13	83.562377	151.047153	31	152.868196	144.115896
15	84.840503	42.014754	33	155.692388	54.115896
17	89.406810	6.451312			

selection of the best 68 equations from the possible 71 was done on a trial and error basis, the best solution having 68 edge lengths of $0.606437\,r$, the next shortest being $0.609801\,r$, $0.610378\,r$, $0.616873\,r$ and $0.633634\,r$ (figure 7 and table 7). This structure contains no elements of symmetry and packing is a substantial improvement on those with twofold (Székely 1974) or fivefold (Goldberg 1967*a*) symmetry.

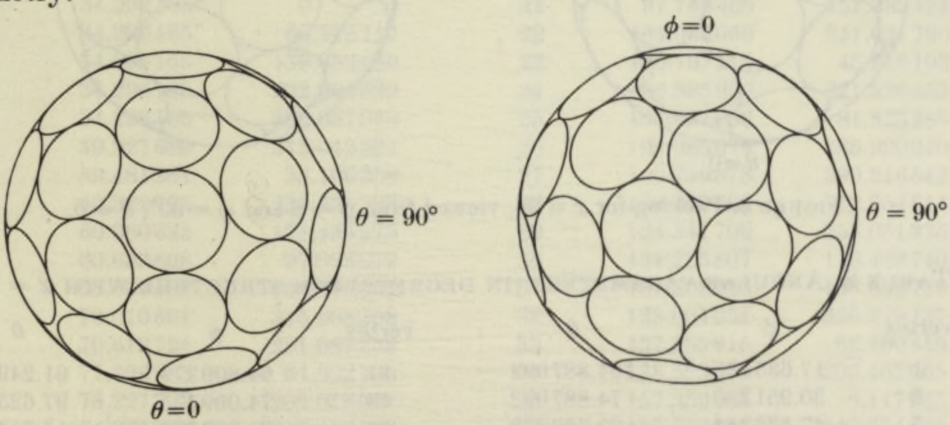

FIGURE 7. Packing for $x = 35$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$.

TABLE 7. ANGULAR PARAMETERS (IN DEGREES) FOR STRUCTURE WITH $x = 35$

vertex	ϕ	θ	vertex	ϕ	θ
1	0	—	19	94.682176	346.877358
2	35.302058	0	20	100.551773	311.730418
3	35.302058	109.358533	21	103.409011	202.775110
4	35.302058	184.791738	22	103.442877	21.557670
5	37.126727	298.311650	23	103.967482	275.740169
6	42.019208	241.945871	24	107.537135	94.167426
7	44.527038	54.679267	25	107.874285	239.198152
8	58.509399	147.075136	26	115.048958	57.018407
9	63.211151	330.343472	27	124.086542	171.173110
10	69.415843	11.993173	28	127.374486	127.484777
11	70.912198	83.070966	29	128.525661	335.831403
12	71.291236	217.641478	30	137.154424	215.161499
13	71.936130	290.789107	31	138.710950	23.429981
14	75.457241	180.993175	32	138.828096	268.990246
15	75.825657	254.207512	33	145.248122	81.961019
16	79.290929	47.506746	34	158.552249	157.688529
17	81.196597	117.955874	35	165.977477	326.446026
18	94.258820	150.851084			

(*j*) $x = 36$

The best structure found contains three twofold axes through $\phi = 0$; $\phi = 90$, $\theta = 0$; $\phi = 90$, $\theta = 90°$ (figure 8 and table 8). This structure is interesting in that the polyhedral edge lengths fall into two distinct groups. There are 23 independent edge lengths in the range 0.604–0.623 r (average 0.606 r), the remaining four independent edge lengths being in the range 0.767–0.791 r (average 0.781 r). To

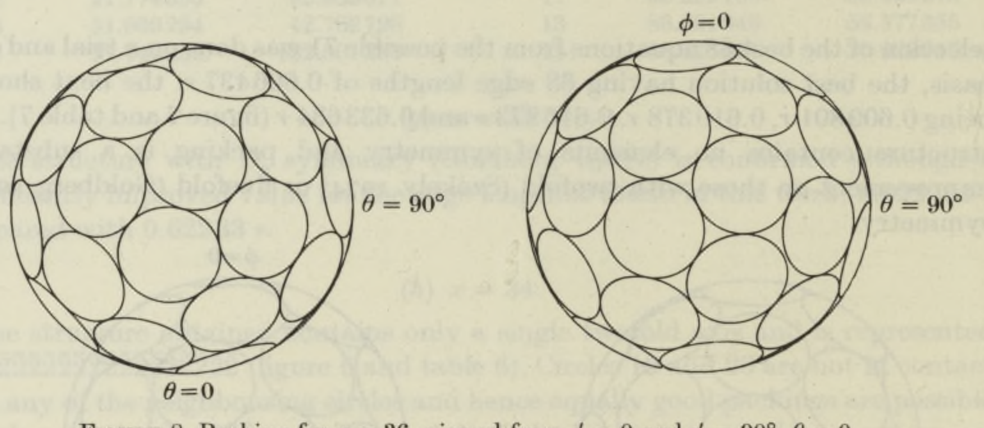

FIGURE 8. Packing for $x = 36$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$.

TABLE 8. ANGULAR PARAMETERS (IN DEGREES) FOR STRUCTURE WITH $x = 36$

vertex	ϕ	θ	vertex	ϕ	θ
1	17.635265	164.887092	11	64.809279	61.249285
3	30.951386	74.887092	13	74.099135	97.625810
5	47.536244	23.798073	15	81.992722	15.715907
7	48.078801	125.209554	17	82.661332	132.526303
9	62.741541	164.583628			

a crude approximation, the resulting polyhedron may be considered to be composed of 16 rhombuses with diagonals of 0.78 r and 0.92 r, and 36 triangles. This structure is a substantial improvement on those containing threefold (Karabinta & Székely 1974) and fivefold (Goldberg 1967*a*) symmetry.

(k) $x = 37$

The structure obtained by using $n \sim 5000$ in the repulsion expression clearly did not contain any symmetry elements, thus requiring 72 simultaneous equations to be selected and solved. There were 71 edge lengths in the range 0.5895–0.5903 r and these were used together with one of the five slightly longer edge lengths (less than 0.60 r) chosen in turn. The best solution had 72 edge lengths of 0.589685 r, other polyhedral edge lengths being in the range 0.589965 r–0.850934 r (figure 9 and table 9). This packing is only a marginal improvement on that found for a

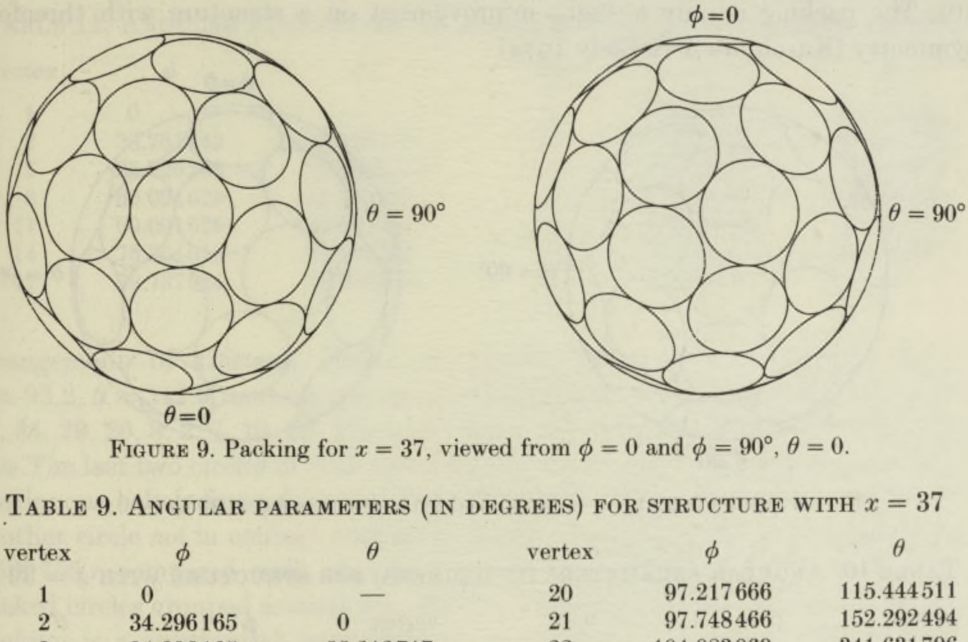

FIGURE 9. Packing for $x = 37$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$.

TABLE 9. ANGULAR PARAMETERS (IN DEGREES) FOR STRUCTURE WITH $x = 37$

vertex	ϕ	θ	vertex	ϕ	θ
1	0	—	20	97.217666	115.444511
2	34.296165	0	21	97.748466	152.292494
3	34.296165	66.212717	22	104.083069	341.631796
4	34.296165	139.882030	23	106.197115	45.976193
5	34.296165	202.984539	24	106.985959	221.926553
6	34.296165	266.087048	25	107.287086	81.823389
7	49.927689	313.043524	26	108.085674	185.920940
8	59.481201	33.106358	27	109.789878	290.215542
9	60.332795	234.535793	28	123.297065	12.954614
10	60.360882	171.485975	29	124.341709	255.051335
11	60.683608	97.098979	30	131.225807	110.459740
12	68.339599	134.306661	31	131.808246	156.832739
13	70.010691	345.608398	32	133.064654	320.279737
14	70.613724	281.087238	33	137.689815	62.460815
15	77.393205	64.802706	34	138.523530	205.402065
16	78.227738	203.018321	35	157.359904	6.117965
17	84.221885	313.452102	36	158.312854	263.334598
18	89.044129	14.781730	37	164.075624	131.654969
19	90.140422	252.328872			

structure containing a threefold axis, 0.589220 r (Székely 1974). Our structure is markedly irregular. In particular it may be noted that vertex 32 is linked by polyhedral edges to *seven* neighbouring vertices at distances ranging from 0.590 to 0.851 r.

(l) $x = 39$

The approximate structure obtained by the energy minimization method clearly had a twofold axis, requiring 38 simultaneous equations to obtain a solution. Even by using $n > 20000$ in the repulsion expression there was no clear division into 'short' and 'longer' polyhedral edges, there being 35 independent edge lengths in the range 0.5750–0.5753 r, another seven in the range 0.5753–0.5786 r with all others being greater than 0.6 r. All combinations involving the 35 short edge lengths and three of the next seven were solved, the best solution corresponding to 38 independent edge lengths of 0.575098 r with four others in the range 0.575485–0.578028 r, all the rest remaining greater than 0.6 r (figure 10 and table 10). The packing is only a slight improvement on a structure with threefold symmetry (Karabinta & Székely 1974).

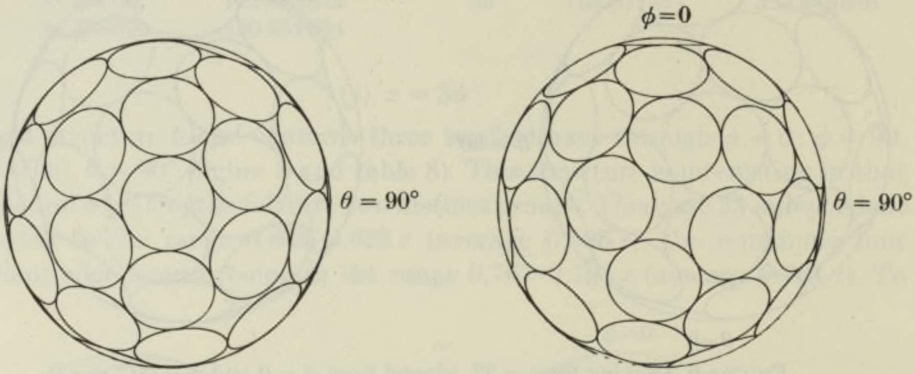

FIGURE 10. Packing for $x = 39$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$.

TABLE 10. ANGULAR PARAMETERS (IN DEGREES) FOR STRUCTURE WITH $x = 39$

vertex	ϕ	θ	vertex	ϕ	θ
1	0	—	20	96.848574	94.507455
2	33.422520	0	22	98.012009	60.813316
4	33.422520	116.954617	24	98.265401	128.202103
6	38.073158	58.477309	26	101.186298	27.050632
8	58.720466	148.477309	28	119.624919	177.079839
10	66.623850	5.248956	30	127.111802	78.928732
12	68.404117	76.615269	32	131.256452	122.166315
14	68.545303	112.625830	34	133.828960	35.354514
16	70.700521	40.953433	36	152.299351	166.307976
18	90.063846	160.719254	38	160.505357	76.307976

(m) $x = 40$

The structure obtained contains a threefold axis and can be represented by an unusual type of stacking sequence, $13\bar{3}(\bar{6})\bar{3}\bar{3}(\bar{6})\bar{3}\bar{3}\bar{3}\bar{3}\bar{3}$ (figure 11 and table 11). A remarkable feature of this structure that is evident from figure 12 is the spiral

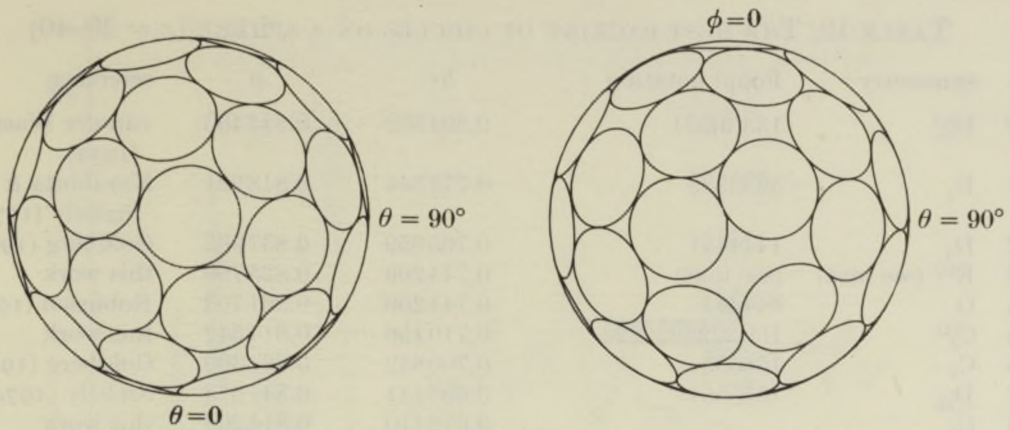

FIGURE 11. Packing for $x = 40$, viewed from $\phi = 0$ and $\phi = 90°$, $\theta = 0$.

TABLE 11. ANGULAR PARAMETERS (IN DEGREES) FOR STRUCTURE WITH $x = 40$

vertex	ϕ	θ	vertex	ϕ	θ
1	0	—	20	93.207555	43.753830
2	33.761143	13.324335	23	93.207555	102.894840
5	35.726298	73.324335	26	109.522371	73.324335
8	60.091629	42.001323	29	120.818211	24.299286
11	60.091629	104.647347	32	128.566808	104.751272
14	76.364015	73.324335	35	140.967520	60.000000
17	79.737824	13.324335	38	160.762641	0

arrangement of thirteen circles in contact commencing at circle 25 at $\phi \approx 93.2$, $\theta \approx 342.9°$ and continuing anticlockwise in the sequence 25, 17, 13, 16, 28, 34, 29, 20, 8, 2, 7, 10, 22. There are three such spirals related by the threefold axis. The last two circles of each spiral also belong to the adjacent spiral so that a continuous belt is formed around the middle of the structure. At $\phi = 0$ there is another circle *not* in contact with these spirals, the polyhedral edge length being $0.580755\,r$ compared with the short edges of $0.570680\,r$. Another six close-packed circles grouped around $\phi = 180°$ also do not form part of the spirals. This packing is a substantial improvement on alternative packings with threefold (Székely 1974), fourfold (Karabinta & Székely 1974) and fivefold (Goldberg 1969) symmetry.

4. DISCUSSION

The best packings of x circles on a sphere that are now known are summarized in table 12, for $x = 20$–40. A great variety in structural types is present, for example the corresponding polyhedra may have pentagonal, square or triangular faces, or square and triangular. Circles may be in contact with five, four or three other circles, and in those cases where a circle may rattle in its hole formed by the surrounding circles, may be in contact with two, one or zero other circles.

Eleven new improved packings have been discovered in this work, some of which are substantial improvements on the previous best in the literature particularly for $x = 28$, 29, 30, 34, 35, 36 and 40. This improvement in packing has been

TABLE 12. THE BEST PACKING OF CIRCLES ON A SPHERE (x = 20–40)

x	symmetry	Foppl notation	$l(r)$	p	reference
20	$D_{3h}^{(1)}$	$13\bar{3}(\bar{6})\bar{3}\bar{3}1$	0.804392	0.844463	van der Waerden (1952)
21	D_3	$3\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}$	0.774344	0.818921	Karabinta & Székely (1974)
22	D_2	$14\tilde{4}\tilde{4}\tilde{4}\tilde{4}1$	0.765659	0.837992	Goldberg (1969)
23	$E^{(1)}$ (see text)	(see text)	0.744206	0.825799	this work
24	O	$4\bar{4}\bar{4}\tilde{4}\bar{4}\bar{4}$	0.744206	0.861703	Robinson (1961)
25	$C_2^{(1)}$	$1(4)\bar{2}\bar{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}$	0.710156	0.814542	this work
26	C_5	$15\bar{5}\bar{5}\bar{5}\bar{5}$	0.700842	0.824300	Goldberg (1967*a*)
27	D_{5h}	$15\bar{5}\bar{5}\bar{5}51$	0.695141	0.841673	Székely (1974)
28	C_s	—	0.672110	0.814206	this work
29	E	—	0.660981	0.814766	this work
30	D_3	$3\bar{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\bar{3}$	0.660981	0.842861	this work
31	C_5	$15\bar{5}\bar{5}\tilde{5}\bar{5}\bar{5}$	0.646346	0.831731	Strohmajer (1963)
32	D_2	$2\bar{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\bar{2}$	0.642294	0.847530	this work
33	D_3	$3\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}\tilde{3}$	0.622751	0.820265	this work
34	$C_2^{(1)}$	$2\bar{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\bar{2}$	0.614714	0.822896	this work
35	E	—	0.606437	0.823883	this work
36	D_2	$2\bar{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\bar{2}$	0.604483	0.841834	this work
37	E	—	0.589685	0.822400	this work
38	D_{6d}	$16\bar{6}\bar{6}\bar{6}\bar{6}\bar{6}1$	0.588926	0.842404	Székely (1974)
39	C_2	$1(4)\bar{2}\bar{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\tilde{2}\bar{2}$	0.575098	0.823563	this work
40	$C_3^{(1)}$	$13\bar{3}(\bar{6})\bar{3}\bar{3}(\bar{6})\bar{3}\tilde{3}\tilde{3}\tilde{3}\bar{3}$	0.570680	0.831473	this work

(1) Or lower symmetry if one or more circles are allowed to 'rattle' in their holes, see text.

achieved by not imposing any symmetry upon the structures, the symmetry of the new structures being low. In general, the symmetries of the structures for x = 20–40 are lower than those found for $x < 20$. This observation has implications for the structures found for molecules of the type $[M_y(\text{ligand})_x]$, many of which are very complex and difficult to understand. It is particularly noteworthy that the structures discovered for x = 29, 35 and 37 contain no symmetry elements. On the other hand, our method confirms the highly symmetric snub cube for x = 24, the D_{6d} structure for x = 38, and the C_5 and D_{5h} structures for x = 26 and 27 respectively. The structure obtained for x = 32 is only of D_2 symmetry but is close to a highly symmetric structure of icosahedral I_h symmetry. Only the structures for x = 27, 28 and 38 contain a mirror plane; each of the other structures may therefore occur as its optical antipode. In sharp contrast, all structures for $x < 20$ contain a mirror plane, except that for x = 15.

There is no discernable periodicity in symmetry properties or other structural features, apparent as x increases.

The packing density p (fig. 12) now shows a very slight upward trend with increasing values of x, in contrast to the trend observed for results from the earlier literature. However, the slope is not pronounced; even by using linear extrapolation the packing density does not equal that for a close-packed plane until many hundreds of circles are packed into the sphere.

It should be remembered that the best results that are described here should only be considered as lower limits and it may be possible to find further improvements in packing in the future.

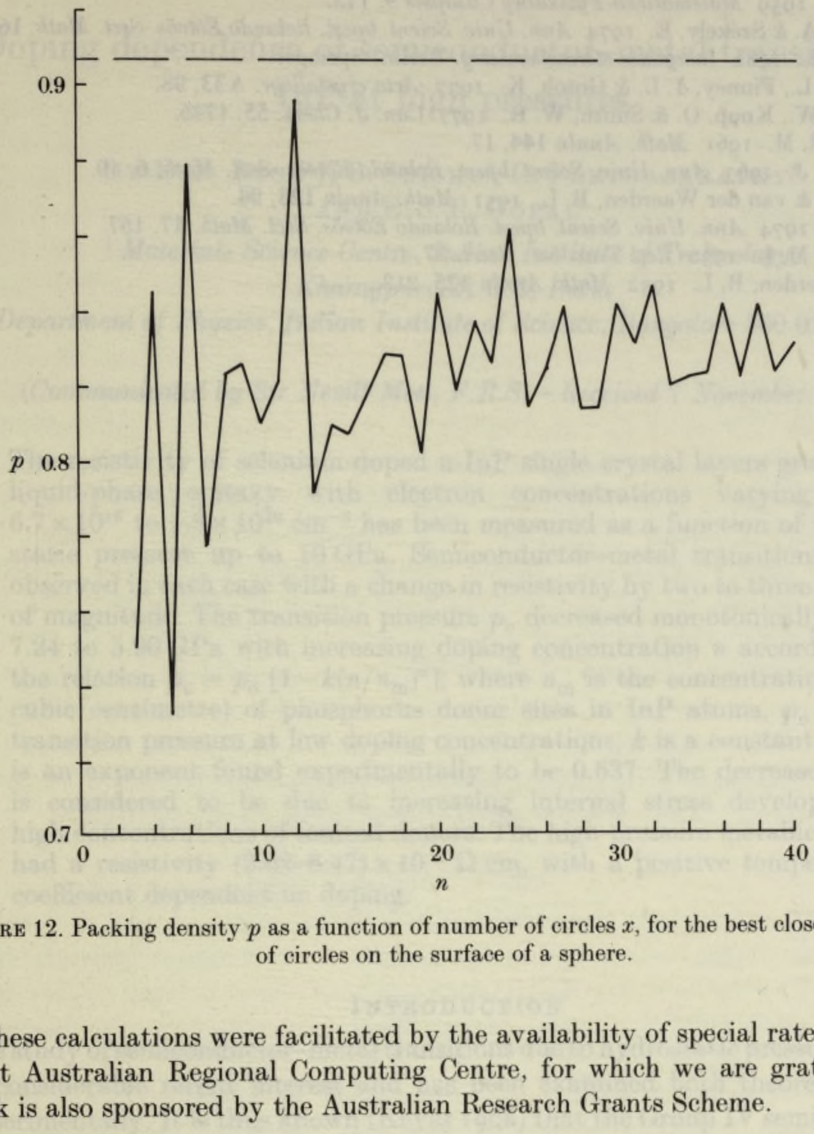

FIGURE 12. Packing density p as a function of number of circles x, for the best closest packings of circles on the surface of a sphere.

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