Spherical Designs in Four Dimensions (Extended Abstract)

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Abstract — **A preliminary report on our investigations into the existence of spherical t-designs on the unit sphere Ω_4 in 4-dimensional Euclidean space. Tables are given of the putatively best t-designs with up to 100 points. Some general constructions are proposed and explicit constructions are given for N-point strength t designs with $N = 4p$ and $t = \min\{p-1, 5\}$, $N = 6p$ and $t = \min\{p-1, 7\}$, and $N = 12p$ and $t = \min\{p-1, 11\}$, for all $p \geq 1$.**

I. Introduction

Spherical t-designs have received a great deal of attention in recent years. They were the subject of a conference at the University of Geneva in October 2002, organized by Pierre de la Harpe, and there was a special session on spherical codes and designs at the annual meeting of the American Mathematical Society in Baltimore in January 2003, organized by Béla Bajnok and N.J.A.S.

Beginning in the early 1990's, the first two authors carried out a systematic search for solutions to many versions of the problem of finding the "best" way to place N points on the unit sphere Ω_n in n-dimensional Euclidean space, concentrating on up to about 100 points in three, four and sometimes five dimensions. We originally considered just the packing problem, but the algorithm seemed to perform well on other problems, so we also tackled the covering, minimal energy and maximal volume problems, the spherical t-design problem and the problem of constructing optimal experimental designs. We also modified the algorithm to compute clusters of spheres with minimal second moment about their centroid, isometric embeddings and packings in Grassmannian spaces.

Some parts of this work have been described in [14], [15], [16], [17], [18], [28], and tables containing many of the results can be found on N.J.A.S.'s homepage [27]. The algorithm we used was a modification of the "pattern search" of Hooke and Jeeves [20]. It has been described in our earlier papers and we will say no more about it here.

Of course our computer program just produces numerical coordinates for the points $P_1, \ldots, P_N$, typically specified to 12 decimal places. If we want to prove theorems about the results (rather than just to use them), we must show (for example) that there *is* a spherical t-design in the neighborhood of the numerical points. We will say more about this "beautification" process later.

The purpose of the present paper is to give a preliminary report (in Section III) on the search for spherical designs in four dimensions. In Section IV we present some new constructions for four-dimensional designs that emerged from the beautification process. Full details will be published elsewhere.

II. Spherical t-designs

We give five equivalent definitions.

(D1) A set of N points $\{P_1, \ldots, P_N\}$ on the unit sphere $\Omega_n = S^{n-1} = \{x = (x_1, \ldots, x_n) \in \mathbb{R}^n : x \cdot x = 1\}$ forms a *spherical t-design* if the identity

$$\int_{\Omega_n} f(x) d\mu(x) = \frac{1}{N} \sum_{i=1}^{N} f(P_i) \tag{1}$$

holds for all polynomials f of degree $\leq t$, where μ is uniform measure on the sphere normalized to have total measure 1 ([10]; [12]; [9, §3.2]).

Of course a t-design is also a t'-design for all $t' \leq t$. The largest t for which the points form a t-design is called the *strength* of the design.

It is known that if N is large enough then a t-design in Ω_n always exists ([25]). The problem is to find the smallest value of N for a given strength and dimension, or equivalently to find the largest strength t that can be achieved with N points in Ω_n.

(D2) $P_1, \ldots, P_N$ is a spherical t-design if and only if

$$\sum_{i=1}^{N} f(P_i) = 0 \tag{2}$$

for all harmonic polynomials f of degrees from 1 to t. (f is harmonic if the Laplacian

$$\Delta f = \sum_{j=1}^{n} \frac{\partial^2 f}{\partial x_j^2}$$

vanishes.)

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(D3) $P_1, \dots, P_N$ is a spherical t-design if and only if

$$\sum_{i=1}^{N} f(P_i^T) = \sum_{i=1}^{N} f(P_i) \qquad (3)$$

for all polynomials f of degrees from 1 to t and all orthogonal transformations $T \in O(n, \mathbb{R})$.

(D4) For $\alpha \in [-1, 1]$, let A_α be the number of ordered pairs (i, j) such that $P_i \cdot P_j = \alpha$. The numbers $\{A_\alpha\}$ are the *distance distribution* of the design. Then the Gegenbauer transform

$$\sum_\alpha A_\alpha Q_k(\alpha) \geq 0 \text{ for all } k, \qquad (4)$$

and $P_1, \dots, P_N$ is a spherical t-design if and only if equality holds in (4) for all $k = 1, \dots, t$. The $Q_k(x)$ are Gegenbauer or ultraspherical polynomials defined by the recurrence

$$Q_0 = 1, \quad Q_1 = nx,$$

$$\lambda_{k+1} Q_{k+1} = x Q_k - (1 - \lambda_{k-1}) Q_{k-1} \,,$$

where $\lambda_k = k/(n + 2k - 2)$.

The inequalities (4) are the basis for the linear programming bound for spherical designs.

(D5) $P_1, \dots, P_N$ forms a spherical t-design if and only if the polynomial identities

$$\frac{1}{N} \sum_{i=1}^{N} (P_i \cdot x)^{2s} = \left(\prod_{j=0}^{s-1} \frac{2j+1}{2j+n} \right) (x \cdot x)^s \,, \qquad (5)$$

and

$$\frac{1}{N} \sum_{i=1}^{N} (P_i \cdot x)^{2\overline{s}+1} = 0 \,,$$

hold, where s and $\overline{s}$ are defined by $\{2s, 2\overline{s}+1\} = \{t-1, t\}$ ([12]; [23, p. 114], [24]).

Spherical t-designs from groups. Let G be a finite subgroup of $O(n, \mathbb{R})$. Consider the ring R of polynomials in $x_1, \dots, x_n$ that are invariant under G, ignoring the trivial invariant $x_1^2 + \cdots + x_n^2$. If R_j is the linear subspace of R consisting of homogeneous invariants of degree j, then the dimensions $d_j = \dim R_j$ are given by the Molien series

$$\Phi_G(\lambda) = \frac{1}{|G|} \sum_{T \in G} \frac{1 - \lambda^2}{\det(I - \lambda T)} = \sum_{j=0}^{\infty} d_j \lambda^j \,. \qquad (6)$$

Let $\mathcal{P} = \{P_1, \dots, P_N\}$ be a union of m orbits under G (not necessarily all of the same size). There are $m(n-1)$ degrees of freedom in choosing $\mathcal{P}$.

Then $\mathcal{P}$ is a spherical t-design if and only if the average of f over $\mathcal{P}$ is equal to the average of f over Ω_n for all $f \in R_1 \cup R_2 \cup \cdots \cup R_t$ [11], [13], [19]. This imposes a total of $e_t = d_1 + \cdots + d_t$ conditions on $\mathcal{P}$. So if $m(n-1) \geq e_t$, we may hope that we can choose the orbits to form a t-design.

In particular, suppose that $d_1 = \cdots = d_t = 0$ for some t. Then there are no conditions to be satisfied, and so every orbit under G is a t-design. (This result seems to be due to Sobolev [29], cf. [9].)

Furthermore, if $d_{t+1} = 1$, and ψ is the unique (up to scalars) invariant of degree m, then the orbit of any real zero of ψ is at least a $(t+1)$-design.

III. Four dimensions

Table 1 gives our lower bounds for $\tau_4(N)$. The third column gives the order of the largest symmetry group we have found for a design with the specified strength. **Bold** entries indicate where $\tau_4(N)$ appears to exceed $\tau_4(k)$ for all $k < N$.

Notes on Table 1. (i) For each entry in the table we have a numerical approximation to the claimed design; that is, numerical coordinates for points such that the magnitude of the difference between the left and right sides of (5) is less than 10^{-8}. These designs will be placed on N.J.A.S.'s home page [27].

(ii) The entries with $N \leq 20$, 24, 48 and 120 were previously known to exist (Mimura [21], Bajnok [2], [3], Hardin and Sloane [14], Delsarte, Goethals and Seidel [10]); and the entries with $N = 21 - 23$ and 25, 26, 27, 31 were previously conjectured to exist [14].

(iii) In the present investigation the entries with $N = 21$, 26, 28, 32, 36, 39, 40, 42, 44, 52, 54, 60, 65, 66, 72, 78, 84, 90 have been beautified (and so shown to exist).

(iv) Many entries still have not yet been beautified, for example those with $N = 22, 23, \dots, 30, \dots$ points, and especially the putative 8-design with $N = 96$ points. (The biggest group we have found for such a design has order only 6, with 16 orbits, which leaves too many unknown parameters for our present beautification methods to handle.)

(v) For definitions of orthoplex, diplo-simplex, etc., see [8].

(vi) This is only a preliminary version of the table. It is possible that some entries — especially the group orders — may change in the final version.

The data in Table 1 can be summarized as follows. It appears that spherical designs in four dimensions with strength t and N points exist if and only if:

t	N
2	≥ 5
3	$8, \geq 10$
4	≥ 20
5	$24, 28, 30, \geq 32$
6	$42, 48, \geq 50$
7	$48, 54, 56, 60, 62, 64, 66, \geq 68$
8	≥ 96
$\cdots$	$\cdots$

For $t = 2$ this is known to be true from the work of Mimura [21], and for $t = 3$ from Bajnok [2], [3] and Boyvalenkov, Danev and Nikova [4]. For $t \geq 4$ these are only conjectures.

Examples. Our beautification technique begins by computing the distance distribution of the points, their apparent automorphism group and its orbits on the points.

For small numbers of points this is often enough to reveal the structure immediately.

7 points, strength 2. The group has order 14 and acts transitively on the points. By a suitable change of coordinates we can make the generators for the group look like

$$\begin{bmatrix} \cos\theta_1 & \sin\theta_1 & 0 & 0 \\ -\sin\theta_1 & \cos\theta_1 & 0 & 0 \\ 0 & 0 & \cos\theta_2 & \sin\theta_2 \\ 0 & 0 & -\sin\theta_2 & \cos\theta_2 \end{bmatrix} \tag{7}$$

and $\operatorname{diag}\{1,-1,1,-1\}$, where $\theta_1 = 2\pi/7$, $\theta_2 = 4\pi/7$. This transformation also beautifies the points, which become

$$\frac{1}{\sqrt{2}}(\cos j\theta, \sin j\theta, \cos 2j\theta, \sin 2j\theta)$$

($j = 0,\ldots,6$). We may specify this design more simply as $\{(\omega^j, \omega^{2j}),\ j = 0,\ldots,6\}$, where $\omega = e^{2\pi i/7}$, which is how it is listed in Table 1. Once we have these simple coordinates it is straightforward to use a symbolic algebra package such as Maple [6] to verify that the strength is as claimed.

Of course this design has been known for a long time, but we have described the process in detail to illustrate the beautification technique.

The designs for $N = 9$ and 13 are of the same type.

20 points, strength 4. This was already beautified in [14]. The points consist of the orbit of a single point (a,b,c,d) under a certain group of order 20. The equations that a,b,c,d must satisfy are given in [14]. At that time we found that a,b,c,d were roots of integral polynomials of degree 72. We have now found that these polynomials can be factored, and so a simpler description is possible. It turns out that $c = -0.4594335\ldots$ is a root of the following polynomial of degree 20 over $\mathbf{Q}[\sqrt{3}]$:

$$\begin{aligned}
&1019215872\,x^{20} - 2548039680\,x^{18} \\
&+849346560\,x^{18}\sqrt{3} + 3609722880\,x^{16} \\
&-1804861440\,x^{16}\sqrt{3} - 3185049600\,x^{14} \\
&+1769472000\,x^{14}\sqrt{3} + 1761177600\,x^{12} \\
&-1006387200\,x^{12}\sqrt{3} - 608587776\,x^{10} \\
&+350631936\,x^{10}\sqrt{3} + 128240640\,x^{8} \\
&-74108160\,x^{8}\sqrt{3} - 15465600\,x^{6} \\
&+8950080\,x^{6}\sqrt{3} + 930300\,x^{4} \\
&-538800\,x^{4}\sqrt{3} - 20100\,x^{2} \\
&+11650\,x^{2}\sqrt{3} - 63 + 36\sqrt{3}\,,
\end{aligned}$$

and a, b and d are roots of similar polynomials of the same degree.

A different 20-point 4-design will be given in Section V.

21 points, strength 4. The group of this design is the same as the group of the above 7-point design. The 21 points fall into two orbits, with representatives (u,v,w,x) and $(y,0,z,0)$ (say), whose approximate values are

$$(0.01210\ldots, -0.83898\ldots, -0.04657\ldots, -0.54202\ldots)$$

and

$$(0.30292\ldots, 0, -0.95301\ldots, 0)\,.$$

After a considerable amount of simplification we find that the following equations must be satisfied for this to be a 4-design:

$$\begin{aligned}
u^2+v^2+w^2+x^2 = y^2+z^2 &= 1\,, \\
u^2+v^2 &= \frac{1}{4}(3-2y^2)\,, \\
(u^2+v^2)^2 &= \frac{1}{2}(1-y^4)\,, \\
(u^2+v^2)(w^2+x^2) &= \frac{1}{4}(1-2y^2z^2)\,, \\
(w^2+x^2)^2 &= \frac{1}{2}(1-z^4)\,, \\
2w(u^2-v^2)+4uvx &= -y^2z\,, \\
6wx(ux+vw)-2uw^3-2vx^3 &= -yz^3\,.
\end{aligned}$$

These imply

$$\begin{aligned}
12y^4-12y^2+1 &= 0\,, \\
u^2+v^2 &= \frac{1}{2}+\frac{1}{2\sqrt{6}}\,,
\end{aligned}$$

and finally that u is a root of the irreducible polynomial

$$\begin{aligned}
&3700643019850472505033743306588160000000\,u^{56} \\
&-25904501138953307535236203146117120000000\,u^{54} \\
&+84999144362190540349993791573196800000000\,u^{52} \\
&-173910947750577153192288884663255040000000\,u^{50} \\
&+248993876622795373683247148873809920000000\,u^{48} \\
&-265381298465540615880932583863746560000000\,u^{46} \\
&+218698123408994140417405690073579520000000\,u^{44} \\
&-142881480631246174121831584280544679034888\,u^{42} \\
&+75284982077502453833675720618229293383680\,u^{40} \\
&-32374809500551735712198447668228427612160\,u^{38} \\
&+11454997471679407431575166084758215065600\,u^{36} \\
&-3352159649429319897729550611614552555520\,u^{34} \\
&+813574916637025869466185176594063032320\,u^{32} \\
&-163862407167379920445022461706234757120\,u^{30} \\
&+27348994563778297262612218663151861760\,u^{28} \\
&-3769083413703449793932677741459537920\,u^{26} \\
&+426384216532181799588302388713226240\,u^{24} \\
&-39253745700791543310477080238489600\,u^{22} \\
&+2905467386561335010342830426030080\,u^{20} \\
&-170031342417598620867220922695680\,u^{18} \\
&+7685045911891937295873217658880\,u^{16} \\
&-259360492235099623193428623360\,u^{14} \\
&+6208592090672404227568435200\,u^{12} \\
&-96802309887404637487104000\,u^{10} \\
&+834705885375722041920000\,u^{8} \\
&-2644802466521769792000\,u^{6} \\
&+1397410700711592000\,u^{4} \\
&-24494390617200\,u^{2} \\
&+1383468025\,.
\end{aligned}$$

IV. A NEW CONSTRUCTION

The most interesting example that we beautified was the 6-design in Ω_4 with 42 points. This turned out to consist of six heptagons, each in a different plane, with a group of order 42 acting transitively on the 42 points. Or, to put it another way: the computer-produced design was suggesting to us that we should choose six planes in $\mathbb{R}^4$, i.e. six points in the Grassmann manifold $G(4,2)$, and draw a heptagon in each plane.

This was an appealing idea, in view of the recent work on finding packings and designs in Grassmann manifolds (cf. [1], [5], [7], [26])! It immediately suggested a general construction.

Informally stated, we take a "nice" set of M planes in $\mathbb{R}^4$, draw a regular p-gon in each plane for a given value of p, obtaining a set of $N = Mp$ points that will form a spherical t-design for some t (possibly 0).

The following are two more precise versions.

Construction 1. Fix integers M and p, and let $\theta = 2\pi/p$. Let Π_i $(i = 1,\ldots,M)$ be a plane in $\mathbb{R}^4$ spanned by a pair of orthogonal vectors u_i, v_i, and let $\phi_1,\ldots,\phi_M \in [0,2\pi)$ be phase angles. Then the design consists of the $N = Mp$ points

$$\{\cos(j\theta+\phi_i)u_i + \sin(j\theta+\phi_i)v_i : 0 \le j < p,\ 1 \le i \le M\}\,. \tag{8}$$

Construction 2. Fix integers M and p, and let $\theta = 2\pi/p$. For $i = 1,\ldots,M$ let $\Pi_i = \langle u_i, v_i\rangle$, $\Pi_i' = \langle w_i, x_i\rangle$ be a pair of perpendicular planes in $\mathbb{R}^4$, where $\{u_i, v_i, w_i, x_i\}$ is a coordinate frame, let $\phi_1,\ldots,\phi_M \in [0,2\pi)$ be phase angles, and let $k_1,\ldots,k_M$ be integers. Then the design consists of the $N = Mp$ points

$$\begin{aligned}\{&\cos(j\theta+\phi_i)u_i + \sin(j\theta+\phi_i)v_i \\ &+ \cos(jk_i\theta+\phi_i)w_i + \sin(jk_i\theta+\phi_i)x_i : \\ &0 \le j < p,\ 1 \le i \le M\}\,.\end{aligned} \tag{9}$$

The first construction generalizes the 42-point design and the second construction generalizes the 7-, 9- and 13-point designs (and others).

We are far from completing our investigations of these constructions. At present three concrete examples have emerged, applications of Construction 1 with all phase angles ϕ_i set to 0. (There are also simpler applications of Construction 1 using a pair of planes to obtain 3-designs, which we will not describe here.)

Theorem 1 *Let $\Pi_1,\ldots,\Pi_4$ be the planes with generator matrices*

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & s & s & s \end{bmatrix},\ \begin{bmatrix} 0 & 1 & 0 & 0 \\ s & 0 & s & -s \end{bmatrix},$$

$$\begin{bmatrix} 0 & 0 & 1 & 0 \\ s & -s & 0 & s \end{bmatrix},\ \begin{bmatrix} 0 & 0 & 0 & 1 \\ s & s & -s & 0 \end{bmatrix},$$

where $s = 1/\sqrt{3}$. Then (8) (with all $\phi_i = 0$) forms a $4p$-point spherical t-design with $t = \min\{p-1, 5\}$.

Theorem 1 yields the following t-designs:

p	2	3	4	5	6	7	8	9	10	11	12	$\cdots$
N	8	12	16	20	24	28	32	36	40	44	48	$\cdots$
t	3	2	3	4	5	5	5	5	5	5	5	$\cdots$
group	384	18	96	15	1152	21	192	27	240	33	288	$\cdots$

Notes. (i) $p = 2$ gives the orthoplex, which has higher strength than was guaranteed by the theorem. (ii) $p = 5$ gives a simpler construction for a 20-point 4-design than the one in [14]. (iii) $p = 6$ gives the 24-cell. (iv) The designs are antipodal if and only if p is even, and this is reflected in the fact that the designs with p odd have much smaller groups.

Theorem 2 *Let $\Pi_1,\ldots,\Pi_6$ be the planes with generator matrices*

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix},\ \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix},$$

$$\begin{bmatrix} s & 0 & -h & h \\ 0 & s & -h & -h \end{bmatrix},\ \begin{bmatrix} -h & h & s & 0 \\ -h & -h & 0 & s \end{bmatrix},$$

$$\begin{bmatrix} -s & 0 & -h & -h \\ 0 & -s & h & -h \end{bmatrix},\ \begin{bmatrix} -h & -h & -s & 0 \\ h & -h & 0 & -s \end{bmatrix},$$

where now $s = 1/\sqrt{2}$, $h = 1/2$. Then (8) (with all $\phi_i = 0$) forms a $6p$-point t-design with $t = \min\{p-1, 7\}$.

Theorem 2 yields the following t-designs:

p	2	3	4	5	6	7	8	9	10	11	12	$\cdots$
N	12	18	24	30	36	42	48	54	60	66	72	$\cdots$
t	1	2	3	4	5	6	7	7	7	7	7	$\cdots$
group	24	36*	128*	30	144*	42	2304	54	120	66	192*	$\cdots$

Notes. (i) The starred group orders were obtained using a slightly different set of six planes. (ii) $p = 6$ is the 42-point design that the computer found. (iii) $p = 8$ gives the 48-point design formed from two copies of the 24-cell. Its group is the Clifford group $\mathcal{C}(2)$ from [22].

We remind the reader that there is a canonical way to specify a plane Π in $\mathbb{R}^4$ by a pair of points $(l,r) \in \Omega_3 \times \Omega_3$ (see [7], Theorem 1). A set of M planes is described by a "binocular spherical code" $\{(l_i, r_i) \in \Omega_3 \times \Omega_3 : i = 1,\ldots,M\}$. The sets of planes used in Theorems 1 and 2 correspond to the binocular spherical codes $\{$point $\times$ tetrahedron$\}$ and $\{$point $\times$ octahedron$\}$. The third theorem is a natural continuation:

Theorem 3 *By using the $M = 12$ planes described by $\{$point $\times$ icosahedron$\}$ we obtain from (8) a $12p$-point spherical t-design with $t = \min\{p-1, 11\}$.*

Theorem 3 yields the following t-designs:

p	6	7	8	9	10	11	12	13	14	15	$\cdots$
N	72	84	96	108	120	132	144	156	168	180	$\cdots$
t	5	6	7	8	9	10	11	11	11	11	$\cdots$
group	24	28	32	36	40	44	48	52	56	60	$\cdots$

Theorems 1–3 are established by computing the distance distribution of the design and working out its Gegenbauer transform (cf. (4)). This is simplified by the fact that the planes in the three theorems form isoclinic sets (cf. [7]). Details are postponed to the full version of this paper.

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Table 1: Conjectured values of $\tau_4(N)$, the largest t for which an N-point configuration on the sphere in 4 dimensions forms a spherical t-design.

N	$\tau_4(N)$	Group	Remarks
1	**0**	∞	single point
2	**1**	∞	two antipodal points
3	1	∞	equilateral triangle
4	1	48	tetrahedron
5	**2**	120	regular simplex
6	2	72	join of 2 triangles
7	2	14	$\{(\omega^j, \omega^{2j})\}$
8	**3**	384	orthoplex
9	2	72	$\{(\omega^j, \omega^k)\}$
10	3	240	diplo-simplex
11	3	22	
12	3	288	join of 2 hexagons
13	3	52	$\{(\omega^j, \omega^{5j})\}$
14	3	392	
15	3	60	
16	3	512	join of 2 octagons
17	3	68	
18	3	648	
19	3	48	
20	**4**	20	Theorem 1; [14]
21	4	14	
22	4	6	
23	4	6	
24	**5**	1152	24-cell
25	4	20	
26	4	52	
27	4	18	
28	5	28	Theorem 1
29	4	8	
30	5	40	
31	4	12	
32	5	192	Theorem 1
33	5	6	
34	5	12	
35	5	10	
36	5	144	Theorem 1
37	5	12	
38	5	48	
39	5	26	
40	5	240	Theorem 1
41	5	12	
42	**6**	42	Theorem 2
43	5	12	
44	5	96	Theorem 1
45	5	30	
46	5	96	
47	5	12	
48	**7**	2304	two 24-cells
49	5	4	
50	6	100	
51	6	4	
52	6	52	
53	6	6	
54	7	54	Theorem 2
55	6	20	
56	7	16	
57	6	9	
58	6	116	
59	6	12	
60	7	240	Theorem 2
61	6	8	
62	7	8	
63	6	18	
64	7	256	
65	6	52	
66	7	66	Theorem 2
67	6	12	
68	7	136	
69	7	3	
70	7	40	
71	7	6	
72	7	576	Theorem 2
73	7	6	
74	7	16	
75	7	6	
76	7	38	
77	7	22	
78	7	52	
79	7	8	
80	7	256	
81	7	36	
82	7	164	
83	7	12	
84	7	144	
85	7	34	
86	7	24	
87	7	18	
88	7	128	
89	7	12	
90	7	180	
91	7	52	
92	7	48	
93	7	36	
94	7	96	
95	7	38	
96	**8**	6	
97	8	1	
98	8	4	
99	8	11	
100	8	20	
...	...		
120	**11**	14400	600-cell [10]