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A Vectorial Subdivision for Spatial Integration of Functions

With Cubic Symmetry*

by

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Abstract

A scheme is devised for subdividing the irreducible trihedral angle determined by the highest cubic symmetry into elemental tetrahedral (or trihedral) cones, each of which subtends a solid angle of $(4\pi/48)(1/489)$ steradians. The centroid of the solid figure formed by each cone and the surface cut by it on a sphere is located. The direction cosines of the 489 vectors through these centroids are tabulated to ten decimals. The IBM 7030 (STRETCH) was used for the calculations. Numerical spatial integrations employing the new subdivision are greatly simplified since separate weightings of the functions evaluated on each vector are not required. Applications to a wide range of cubic crystal problems in solid state physics are contemplated.

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1. Introduction

One encounters in physics a number of theoretical problems in which three-dimensional spacial integration of functions is required. Among these are problems in lattice dynamics and in the calculation of the energies of electrons in crystals, both kinds of which involve integrations over the reciprocal space defined by Brillouin zones. Such problems are often so complex that practical results can be obtained only with the aid of a digital computer.

This paper is concerned with a vectorial method for spacial integration whereby the appropriate functions of the problem are evaluated for a set of vector directions, appropriately weighted, and then summed over all the chosen vectors of the space. The accuracy of such calculations depends mainly on the density and distribution in space of the chosen vectors. The advantages and disadvantages of this vectorial method, when compared with a number of other commonly-used integration methods, will not be taken up as a topic in this paper.

More specifically, we are interested in spacial integration of functions which obey cubic symmetry. With these, integration is required only within a certain basic trihedral angle of the space; the value for the full 4π steradians of all space can then be obtained by merely multiplying by the appropriate integer. The irreducible trihedral angle for functions obeying the highest cubic

symmetry may be any of 48 equally suitable ones determined by the highest symmetry cubic group operations [3 , 4]. A typical choice is shown in Figs. 1a,b.

In some earlier works [1,5], as shown in Fig. 1a, a subdivision of the trihedral angle into 70 elemental cones was devised. While satisfactory for many problems this subdivision was found to be too crude for problems involving highly anisotropic cubic functions, even though the calculations for any particular cone centroid vector could be carried out almost exactly. Moreover the subdivision was such that the cones did not subtend equal areas on the surface of the sphere. To compensate for this in spacial integration required the assignment of a weighting factor to each vectorial function.

The motivation for the present work was to design an improvement over the earlier subdivision in the form of a much finer one which would lead to greater accuracy in spacial integrations. Furthermore, it was desired to design it so that all the cones surrounding the particular vectors would subtend the same size solid angle and thus avoid the necessity of introducing weighting factors.

In this paper we report a method of subdividing the basic trihedral angle into 489 equal elemental solid angle cones. We give to 10 decimal places the direction cosines, p_k , q_k , r_k , of the vectors which pierce the centroids of these cones. An outline of the subdivision is shown in Fig. 1b.

While the trihedral angle shown in Fig. 1b characterizes only cubic functions of highest cubic symmetry, the results of our subdivision are applicable to a wide range of cubic crystal problems, and indeed, to many problems which do not even invoke cubic symmetry. The reason for this is that one can use the basic set p_k, q_k, r_k to generate a corresponding set of 489 additional vectors which are uniformly distributed throughout any one of the other 47 basic trihedral angles. Thus, there is the possibility of generating 23,742 vectors uniformly distributed throughout the full 4π steradians.

In certain areas of mathematical physics one encounters the functions $(p^2q^2 + q^2r^2 + r^2p^2)$ and $(p^2q^2r^2)$ [2,6]. Using these as a basis a host of cubic invariant polynomials [2] can be generated. Although the integrals of these functions over all space can be obtained in closed form, tabulations of the functions for a well-ordered set of specific vectors apparently have not been prepared. Such tables can be calculated directly from our basic set of p_k, q_k, r_k .

In Secs. 2 and 3 we devise the particular method by which the surface of a sphere cut out by the basic trihedral angle can be further subdivided into 489 elemental surface areas. The labeling for these areas and for the bounding planes of each element is given in Table 1.

In Sec. 4 we calculate the coordinates of the centroids of the elemental solid figures formed by the bounding planes and the element of surface cut out by them on a sphere. From these centroid coordinates we calculate the final product, Table 2, the table of direction cosines of the vectors passing through the centroids. The calculations have been carried out with the aid of an IBM 7030 (STRETCH) computer.

2. Subdivision Design

In this section we discuss the first stage of the subdivision design, e.g., the method of dividing the area on a unit sphere cut out by the basic trihedral angle into j strips such that each strip contains $n_j \Delta\omega$ ($n_j = \text{integer}$). The strips are indicated in Fig. 1b. If we select N as the total number of $\Delta\omega$'s subtended by the trihedral angle, then $\sum_j n_j = N$. The choice $N = 489$ is the result of subdivision design compromises which we need not discuss further.

The subdivision is discussed in terms of Cartesian and polar coordinates and the crystallographic vectors. Let the $[100]$, $[010]$, and $[001]$ directions of Fig. 1a coincide with x, y, z of Fig. 1b. Standard polar coordinates ρ, θ, φ are then measured in the usual way with respect to x, y, z .

In our earlier work [5] we used $\theta = \text{constant}$, $\varphi = \text{constant}$ to define the sides of each elemental area as shown in Fig. 12. This does not lead, in any convenient way, to a set of equal areas. However, now we cut the sphere by a set of wedge planes all of which have a common intercept in the y axis. By appropriate adjustments of the angles between these planes, the strips cut out by them can be made to contain n_j equal $\Delta\omega$'s for all j .

We define 29 strips labeled j by the cuts of 30 planes labeled $i = 0, 1, 2, \dots, 29$. Plane $i = 0$ is the y - z plane; plane $i = 29$ is the y - $[101]$ plane. For any point $P(x, y, z)$ in the i th plane

we must have $x = a_1 z$ where

$$(2.01) \quad a_1 = \tan \theta_1^0.$$

The superscript 0 specifies a θ value measured from the z axis to a vector lying in the x - z plane.

The i th plane intersects any sphere in a circular section; thus, the θ_i and φ of any vector from the origin to a point on this section are related according to

$$(2.02) \quad \theta_i = \cot^{-1}(\cos \varphi / a_i).$$

The area cut out on a unit sphere within the trihedral angle between two such planes i and $i+1$ is given by

$$(2.03) \quad A_{i,i+1} = \int_{\varphi=0}^{\pi/4} d\varphi \int_{\theta_i}^{\theta_{i+1}} \sin \theta \, d\theta,$$

$$(2.04) \quad = \int_0^{\pi/4} \left\{ -\cos \left[\cot^{-1} \left(\frac{\cos \varphi}{a_{i+1}} \right) \right] + \cos \left[\cot^{-1} \left(\frac{\cos \varphi}{a_i} \right) \right] \right\} d\varphi,$$

$$(2.05) \quad = \left[\sin^{-1} \left(\frac{\sin \varphi}{\sqrt{1+a_i^2}} \right) - \sin^{-1} \left(\frac{\sin \varphi}{\sqrt{1+a_{i+1}^2}} \right) \right] \bigg|_0^{\pi/4}.$$

Since j labels the strip between i and $i+1$ (2.05) will be identified as the area of the j th strip.

If we put $\theta_1 = 0$, $\theta_{i+1} = \pi/4$, we observe that (2.05) gives the solid angle $(4\pi/48)$ of the basic trihedral angle. Otherwise, when i and $i+1$ correspond to our finally-selected wedge planes, (2.05) must give $n_j \Delta\omega$, where

$$(2.06) \quad \Delta\omega = (\pi/12)(1/489) = 0.00053 \ 53770 \ 71163 \ 90478 \ \dots$$

The process of solving for the θ_i^0 values which guarantee integral numbers of $\Delta\omega$'s in each strip is an inverse one. If we fix i , $i+1$ for a particular strip j , then the left side of (2.05), $n_j \Delta\omega$, is known exactly, while the right side contains two unknowns a_1 and a_{i+1} or $\cos\theta_1^0$ and $\cos\theta_{i+1}^0$. To avoid this problem we let $a_1 = 0 \sim \theta_1^0 = 0$ and solve for the single unknown θ_{i+1}^0 . In this case the left side of (2.05) is again known exactly; it takes the form

$$(2.07) \quad \Lambda_{0,i+1} = \sigma_j = \sum_{j=1}^{i+1} n_j \Delta\omega.$$

One finds then for the revised (2.05),

$$(2.08) \quad \sigma_j = \pi/4 - \sin^{-1}(\cos\theta_{i+1}^0/\sqrt{2}), \text{ or,}$$

$$\cos\theta_{i+1}^0 = \sqrt{2} \sin(\pi/4 - \sigma_j),$$

$$(2.09) \quad = \cos \sigma_j - \sin \sigma_j .$$

From the selected σ_j we were thus able to evaluate the θ_1^0 's to 14-place accuracy by simply using the existing STRETCH subroutines. Table 1 shows these results to 10 places.

3. Element Subdivision

The individual elements are labeled by k as in Table 1. The lower and upper edges are defined by (2.02). Let φ_{k-1} denote the left edge and φ_k the right edge. Thus, each element is defined by two wedge planes and two planes of constant φ .

The area $\Delta\omega$ of a single element is given by (2.05) with its limits 0 and $\pi/4$ being replaced by φ_{k-1} and φ_k , respectively. While the left side of such an equation is known exactly, the right side contains the two unknowns φ_{k-1} and φ_k . The area of a portion of a strip containing $s_j(k)\Delta\omega$ is found by simply replacing the upper limit $\pi/4$ of (2.05) by φ_k , while leaving the lower limit unchanged; here $1 \leq s_j(k) = \text{integer} \leq n_j$. For this equation the left side is again known exactly while the right side contains only the one unknown φ_k . This equation is thus the revised form of (2.05) which we shall use to solve for φ_k , i.e.,

$$(3.01) \quad s_j(k)\Delta\omega = \sin^{-1}(\cos\theta_1^0 \sin\varphi_k) - \sin^{-1}(\cos\theta_{i+1}^0 \sin\varphi_k) .$$

By use of an anti-trigonometric identity we can express (3.01) in the more convenient form

$$(3.02) \quad \sin[s_j(k)\Delta\omega] = \sin\varphi_k [\cos\theta_1^0 \sqrt{1 - \cos^2\theta_{i+1}^0 \sin^2\varphi_k} - \cos\theta_{i+1}^0 \sqrt{1 - \cos^2\theta_1^0 \sin^2\varphi_k}] .$$

We used a machine program involving Newton-Raphson interpolation to solve for the $\sin \varphi_k$ which satisfy (3.02). A check of the absolute accuracy of these $\sin \varphi_k$ is available in each strip: When $s_j(k) = n_j$, the φ_k must $= \pi/4$ so that $\sin \varphi_k = 1/\sqrt{2}$. This always checked to ± 2 in the 12th decimal place. Note, however that this represents a loss in accuracy of two significant figures since the initial $s_j(k)\Delta\omega$ and the $\cos \theta_1^0$'s were accurate to 14 decimals. Thus, even though the closure of the interpolation scheme was ± 3 in the 14th place, the errors came in the 12th place because (3.02) involves taking the difference of two numbers which are within a few parts in a thousand of each other.

4. Calculation of Centroids

The wedge planes and the planes of constant φ cutting out the elemental areas on a unit sphere define also solid angle cones. The solid angles are tetrahedral angles for elements $k = 3$ to 489 and trihedral angles for elements 1 and 2. (Note Fig. 1b.) We close these solid angles and form solid figures by any sphere of radius a . This is done merely for the convenience of defining a solid figure whose centroid vector we wish to identify.

Let $\vec{\rho}_k$ be the centroid vector of the solid figure defined by the k th tetrahedral (or trihedral) cone. The components of $\vec{\rho}_k$ are given by well-known formulas which we express in terms of the problem at hand as follows:

$$(4.01) \quad \bar{x}_k = V_k^{-1} \iiint (\rho \sin\theta \cos\varphi) (\rho^2 \sin\theta \, d\rho \, d\theta \, d\varphi) ,$$

$$= (a^4/4V_k) \int_{\varphi_{k-1}}^{\varphi_k} \cos\varphi \left\{ \int_{\theta_1(\varphi)}^{\theta_{1+1}(\varphi)} \sin^2\theta \, d\theta \right\} d\varphi ,$$

where $\theta_1(\varphi)$ is defined by (1b).

$$(4.02) \quad \bar{y}_k = (a^4/4V_k) \int_{\varphi_{k-1}}^{\varphi_k} \sin\varphi \left\{ \int_{\theta_1(\varphi)}^{\theta_{1+1}(\varphi)} \sin^2\theta \, d\theta \right\} d\varphi .$$

$$(4.03) \quad \bar{z}_k = (a^4/4V_k) \int_{\varphi_{k-1}}^{\varphi_k} \left\{ \int_{\theta_1(\varphi)}^{\theta_{1+1}(\varphi)} \sin\theta \cos\theta \, d\theta \right\} d\varphi .$$

The volume of the kth solid figure is

$$(4.04) \quad V_k = (a^3/3) \int_{\varphi_{k-1}}^{\varphi_k} \left\{ \int_{\theta_1(\varphi)}^{\theta_{i+1}(\varphi)} \sin \theta \, d\theta \right\} d\varphi ,$$

which integrates to $(a^3/3)$ times the same result expressed by (2.05) when its limits $\pi/4$ and 0 are replaced by φ_k and φ_{k-1} , respectively. Thus,

$$(4.05) \quad V_k = (a^3/3)\Delta\omega,$$

for all k. Equations (4.01), (4.02), and (4.03) also integrate directly to give, respectively,

$$(4.06) \quad \bar{x}_k = (3a/8\Delta\omega) \left[\sin\varphi \tan^{-1} \left(\frac{a_{i+1}}{\cos\varphi} \right) - \sin\varphi \tan^{-1} \left(\frac{a_1}{\cos\varphi} \right) - \frac{1}{\sqrt{1+a_{i+1}^2}} \tan^{-1} \left(\frac{a_{i+1} \tan\varphi}{\sqrt{1+a_{i+1}^2}} \right) + \frac{1}{\sqrt{1+a_1^2}} \tan^{-1} \left(\frac{a_1 \tan\varphi}{\sqrt{1+a_1^2}} \right) \right] \Big|_{\varphi_{k-1}}^{\varphi_k} ,$$

$$(4.07) \quad \bar{y}_k = (3a/8\Delta\omega) \left[-\cos\varphi \tan^{-1} \left(\frac{a_{i+1}}{\cos\varphi} \right) + \cos\varphi \tan^{-1} \left(\frac{a_1}{\cos\varphi} \right) \right] \Big|_{\varphi_{k-1}}^{\varphi_k} ,$$

$$(4.08) \quad \bar{z}_k = (3a/8\Delta\omega) \left[\frac{a_{i+1}}{\sqrt{1+a_{i+1}^2}} \tan^{-1} \left(\frac{a_{i+1} \tan\varphi}{\sqrt{1+a_{i+1}^2}} \right) - \frac{a_1}{\sqrt{1+a_1^2}} \tan^{-1} \left(\frac{a_1 \tan\varphi}{\sqrt{1+a_1^2}} \right) \right] \Big|_{\varphi_{k-1}}^{\varphi_k} .$$

The inverse tangents in (4.06), (4.07), and (4.08) can be evaluated by standard subroutines to an accuracy of 14 decimals. However, although the a_1 or the $\cos\theta_1^0$'s are accurate to 14 decimals, the $\sin\varphi_k$ and $\cos\varphi_k$ are only accurate to 12 decimals. Moreover, the differences involved in calculating these $\bar{x}$, $\bar{y}$, $\bar{z}$ cause a further loss in absolute accuracy of two or more decimals. Consequently, because of the nature of the problem, the absolute error of the final results becomes increased; it is $\wedge \pm 3$ in the 9th place to about ± 3 in the 10th place, depending on the particular vector.

The desired end product of this work is Table 2, a table of the direction cosines of the vectors passing through the centroids of the 489 elemental solid figures. They are defined as follows:

$$(4.09) \quad p_k = \bar{x}_k / \rho_k = \sin\bar{\theta}_k \cos\bar{\varphi}_k ,$$

$$(4.10) \quad q_k = \bar{y}_k / \rho_k = \sin\bar{\theta}_k \sin\bar{\varphi}_k ,$$

$$(4.11) \quad r_k = \bar{z}_k / \rho_k = \cos\bar{\theta}_k ,$$

$$(4.12) \quad \rho_k = (\bar{x}_k^2 + \bar{y}_k^2 + \bar{z}_k^2)^{1/2} .$$

These direction cosines have been calculated without any further loss in the absolute accuracy.

A limited number of Fortran decks containing the direction cosines of Table 2 have been prepared. These are available upon request to laboratories having computer facilities.

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Table and Figure Captions

Fig. 1. A symmetry-irreducible trihedral angle determined by highest cubic symmetry; 1(a), subdivision into 70 surface elements on a unit sphere; 1(b), subdivision into 29 strips containing 489 equal surface elements.

Table 1. Labeling for subdivision shown in Fig. 1b: i labels planes cutting out strips on unit sphere, j labels strips, n_j = integer = number of $\Delta\omega$'s in the j th strip. We show only six of 14 decimals of the $n_j\Delta\omega$'s and only 10 of 14 of the $\cos\theta_i^0$ values.

Table 2. The direction cosines p_k, q_k, r_k of the 489 vectors which pierce the centroids of their respective closed cones. An elemental cone is defined by wedge planes i and $i+1$ and planes of constant φ_{k-1} and φ_k , and is closed by its intersection with the unit sphere.

Table I

i	j	k	n_j	$n_j \Delta \omega$	$\cos \theta_1^0$	$\theta_{i+1}^0 - \theta_i^0$ (degrees)
0	1	1-2	2	0.001071	1.00000 00000	2.6524
1	2	3-5	3	0.001606	0.99892 86728	1.5436
2	3	6-10	5	0.002677	0.99731 95350	1.7453
3	4	11-16	6	0.003212	0.99463 19235	1.5794
4	5	17-23	7	0.003748	0.99139 73834	1.5075
5	6	24-31	8	0.004283	0.98761 08262	1.4681
6	7	32-40	9	0.004818	0.98326 63508	1.4457
7	8	41-51	11	0.005889	0.97835 72598	1.5686
8	9	52-63	12	0.006424	0.97232 64245	1.5373
9	10	64-75	12	0.006424	0.96570 88787	1.4052
10	11	76-89	14	0.007495	0.95905 14739	1.5138
11	12	90-104	15	0.008031	0.95123 44909	1.5058
12	13	105-120	16	0.008566	0.94279 98623	1.5023
13	14	121-137	17	0.009101	0.93373 59209	1.5023
14	15	138-155	18	0.009637	0.92403 04273	1.5055
15	16	156-174	19	0.010172	0.91367 06112	1.5121
16	17	175-194	20	0.010708	0.90264 32177	1.5142
17	18	195-215	21	0.011243	0.89093 45556	1.5253
18	19	216-236	21	0.011243	0.87853 05501	1.4667
19	20	236-258	22	0.011778	0.86601 54966	1.4827
20	21	259-281	23	0.012314	0.85278 71062	1.4992
21	22	282-305	24	0.012849	0.83883 09626	1.5162
22	23	306-330	25	0.013384	0.82413 24605	1.5338
23	24	331-355	25	0.013384	0.80867 68743	1.4929
24	25	356-380	25	0.013384	0.79307 64215	1.4568
25	26	381-406	26	0.013920	0.77733 38968	1.4811
26	27	407-433	27	0.014455	0.76081 39930	1.5175
27	28	434-461	28	0.014991	0.74350 27247	1.5176
28	29	462-489	28	0.014991	0.72538 62547	1.5010
29					0.70710 67812

TABLE 2.

k	p _k	q _k	r _k
1	.03085 40704	.00770 95979	.99949 41663
2	.03084 01385	.02312 45349	.99925 67947
3	.06073 37520	.01010 40339	.99810 28604
4	.06070 57918	.03031 07268	.99769 53777
5	.06064 98618	.05051 33023	.99688 01335
6	.08919 57071	.00888 44273	.99597 44940
7	.08916 54072	.02665 27244	.99566 01641
8	.08901 38291	.06218 32048	.99408 74143
9	.08901 38291	.04441 93519	.99503 12846
10	.08889 24718	.07994 31905	.99282 78878
11	.11772 08682	.00974 31145	.99299 89269
12	.11767 45538	.02922 89952	.99262 19649
13	.11758 18838	.04871 38328	.99186 76641
14	.11744 27761	.06819 69384	.99073 52683
15	.11725 71064	.08767 76321	.98922 36369
16	.11702 47078	.10715 52473	.98733 12366
17	.14430 19881	.01020 20503	.98948 11036
18	.14424 05963	.03060 59101	.98906 92234
19	.14411 77463	.05010 90486	.98824 94859
20	.14393 33051	.07141 09898	.98700 74337
21	.14368 70720	.09181 12648	.98535 51223
22	.14337 87771	.11220 94145	.98328 61097
23	.14300 80793	.13260 49929	.98079 79431
24	.16986 62267	.01046 72119	.98541 15397
25	.16979 06666	.03160 14588	.98497 97348
26	.16963 94564	.05223 51762	.98411 55848
27	.16941 24150	.07326 80148	.98281 80054
28	.16910 92692	.09419 96307	.98108 53605
29	.16872 96519	.11512 96880	.97891 54506
30	.16855 78606	.13605 78606	.97630 54967
31	.16773 90455	.15698 38344	.97325 21196
32	.19481 50088	.01062 38921	.98078 24658
33	.19472 60835	.03187 15410	.98033 97152
34	.19454 81206	.05311 87852	.97945 36352
35	.19428 08945	.07436 53577	.97812 30636
36	.19392 40650	.09561 09960	.97634 62472
37	.19347 71745	.11665 54336	.97412 08284
38	.19293 96446	.13809 84519	.97144 38281
39	.19231 07721	.15933 97819	.96831 16238
40	.19158 97233	.18057 92061	.96471 99222
41	.22055 43543	.00979 02908	.97532 55492
42	.22046 89460	.02937 07759	.97495 16918
43	.22029 80373	.04895 09727	.97420 03193
44	.22004 14431	.06853 06903	.97308 07193
45	.21969 88846	.08810 97411	.97158 07088
46	.21926 99871	.10768 79407	.96970 30371
47	.21875 42783	.12726 51096	.96744 51703
48	.21815 11846	.14684 10742	.96480 45188
49	.21746 00280	.16641 56676	.96177 80211
50	.21668 00214	.18598 87309	.95836 21238
51	.21581 02634	.20556 01142	.95455 27590
52	.24686 50916	.00998 66837	.96899 83967
53	.24676 58527	.02995 99736	.96861 19006
54	.24656 72617	.04993 30315	.96783 84565
55	.24626 90912	.06990 57044	.96667 71577
56	.24587 09986	.08987 78413	.96512 66371
57	.24537 25235	.10984 92944	.96318 50587
58	.24477 30851	.12981 99198	.96085 01055
59	.24407 19782	.14978 95786	.95811 89653
60	.24326 83686	.16975 81374	.95498 83118
61	.24236 12877	.18972 54697	.95145 42829
62	.24134 96257	.20969 14564	.94751 24544
63	.24023 21241	.22965 39868	.94315 78099
64	.27160 47477	.27160 47477	.27160 47477
65	.27147 44548	.27147 44548	.27147 44548
66	.27121 36883	.27082 20853	.27082 20853
67	.27082 20853	.27029 90980	.27029 90980
68	.27029 90980	.26964 39899	.26964 39899
69	.26964 39899	.26885 58297	.26885 58297
70	.26885 58297	.26793 34847	.26793 34847
71	.26793 34847	.26687 56116	.26687 56116
72	.26687 56116	.26568 06455	.26568 06455
73	.26568 06455	.26434 67880	.26434 67880
74	.26434 67880	.26287 19912	.26287 19912
75	.26287 19912	.25116 95037	.25116 95037
76	.25116 95037	.24933 35226	.24933 35226
77	.24933 35226	.24749 69178	.24749 69178
78	.24749 69178	.24567 88804	.24567 88804
79	.24567 88804	.24385 77966	.24385 77966
80	.24385 77966	.24197 80077	.24197 80077
81	.24197 80077	.24013 67162	.24013 67162
82	.24013 67162	.23829 46930	.23829 46930
83	.23829 46930	.23645 20641	.23645 20641
84	.23645 20641	.23460 89597	.23460 89597
85	.23460 89597	.23276 55133	.23276 55133
86	.23276 55133	.23092 20664	.23092 20664
87	.23092 20664	.22908 86064	.22908 86064
88	.22908 86064	.22724 51606	.22724 51606
89	.22724 51606	.22540 17148	.22540 17148
90	.22540 17148	.22356 82690	.22356 82690
91	.22356 82690	.22172 48232	.22172 48232
92	.22172 48232	.21988 13774	.21988 13774
93	.21988 13774	.21804 79276	.21804 79276
94	.21804 79276	.21620 44818	.21620 44818
95	.21620 44818	.21436 10360	.21436 10360
96	.21436 10360	.21252 75862	.21252 75862
97	.21252 75862	.21068 41404	.21068 41404
98	.21068 41404	.20884 69306	.20884 69306
99	.20884 69306	.20700 34848	.20700 34848
100	.20700 34848	.20516 00390	.20516 00390
101	.20516 00390	.20332 65932	.20332 65932
102	.20332 65932	.20148 31474	.20148 31474
103	.20148 31474	.19964 97016	.19964 97016
104	.19964 97016	.19780 62558	.19780 62558
105	.19780 62558	.19596 28100	.19596 28100
106	.19596 28100	.19412 93642	.19412 93642
107	.19412 93642	.19228 59184	.19228 59184
108	.19228 59184	.19044 24726	.19044 24726
109	.19044 24726	.18860 90268	.18860 90268
110	.18860 90268	.18676 55810	.18676 55810
111	.18676 55810	.18492 21352	.18492 21352
112	.18492 21352	.18308 86894	.18308 86894
113	.18308 86894	.18124 52436	.18124 52436
114	.18124 52436	.17940 17978	.17940 17978
115	.17940 17978	.17756 83520	.17756 83520
116	.17756 83520	.17572 49062	.17572 49062
117	.17572 49062	.17388 14604	.17388 14604
118	.17388 14604	.17204 80146	.17204 80146
119	.17204 80146	.17020 45688	.17020 45688
120	.17020 45688	.16836 11230	.16836 11230
121	.16836 11230	.16652 76772	.16652 76772
122	.16652 76772	.16468 42314	.16468 42314
123	.16468 42314	.16284 78256	.16284 78256
124	.16284 78256	.16100 43798	.16100 43798
125	.16100 43798	.15916 93340	.15916 93340
126	.15916 93340	.15732 58882	.15732 58882
127	.15732 58882	.15548 24424	.15548 24424
128	.15548 24424	.15364 89966	.15364 89966
129	.15364 89966	.15180 55508	.15180 55508
130	.15180 55508	.14996 21050	.14996 21050
131	.14996 21050	.14812 86592	.14812 86592
132	.14812 86592	.14628 52134	.14628 52134
133	.14628 52134	.14444 17676	.14444 17676
134	.14444 17676	.14260 83218	.14260 83218
135	.14260 83218	.14076 48760	.14076 48760
136	.14076 48760	.13892 14302	.13892 14302
137	.13892 14302	.13708 79844	.13708 79844
138	.13708 79844	.13524 45386	.13524 45386
139	.13524 45386	.13340 10928	.13340 10928
140	.13340 10928	.13156 76470	.13156 76470
141	.13156 76470	.12972 42012	.12972 42012
142	.12972 42012	.12788 78354	.12788 78354
143	.12788 78354	.12604 43896	.12604 43896
144	.12604 43896	.12420 94438	.12420 94438
145	.12420 94438	.12236 60080	.12236 60080
146	.12236 60080	.12052 25622	.12052 25622
147	.12052 25622	.11868 91164	.11868 91164
148	.11868 91164	.11684 56706	.11684 56706
149	.11684 56706	.11500 22248	.11500 22248
150	.11500 22248	.11316 87790	.11316 87790
151	.11316 87790	.11132 53332	.11132 53332
152	.11132 53332	.10948 18874	.10948 18874
153	.10948 18874	.10764 84376	.10764 84376
154	.10764 84376	.10580 49918	.10580 49918
155	.10580 49918	.10396 15460	.10396 15460
156	.10396 15460	.10212 80002	.10212 80002
157	.10212 80002	.10028 45544	.10028 45544
158	.10028 45544	.9844 11086	.9844 11086
159	.9844 11086	.9680 76628	.9680 76628
160	.9680 76628	.9516 42170	.9516 42170
161	.9516 42170	.9352 78312	.9352 78312
162	.9352 78312	.9188 43854	.9188 43854
163	.9188 43854	.9024 94396	.9024 94396
164	.9024 94396	.8860 60038	.8860 60038
165	.8860 60038	.8696 25580	.8696 25580
166	.8696 25580	.8532 91122	.8532 91122
167	.8532 91122	.8368 56664	.8368 56664
168	.8368 56664	.8204 22206	.8204 22206
169	.8204 22206	.8040 87748	.8040 87748
170	.8040 87748	.7876 53290	.7876 53290
171	.7876 53290	.7712 18832	.7712 18832
172	.7712 18832	.7548 84374	.7548 84374
173	.7548 84374	.7384 49916	.7384 49916
174	.7384 49916	.7220 15458	.7220 15458
175	.7220 15458	.7056 81000	.7056 81000
176	.7056 81000	.6892 46542	.6892 46542
177	.6892 46542	.6728 12084	.6728 12084
178	.6728 12084	.6564 77626	.6564 77626
179	.6564 77626	.6400 43168	.6400 43168
180	.6400 43168	.6236 87710	.6236 87710
181	.6236 87710	.6072 53252	.6072 53252
182	.6072 53252	.5908 18794	.5908 18794
183	.5908 18794	.5744 84336	.5744 84336
184	.5744 84336	.5580 49878	.5580 49878
185	.5580 49878	.5416 15420	.5416 15420
186	.5416 15420	.5252 80962	.5252 80962
187	.5252 80962	.5088 46504	.5088 46504
188	.5088 46504	.4924 12046	.4924 12046
189	.4924 12046	.4760 77588	.4760 77588
190	.4760 77588	.4596 43130	.4596 43130
191	.4596 43130	.4432 87672	.4432 87672
192	.4432 87672	.4268 53214	.4268 53214
193	.4268 53214	.4104 18756	.4104 18756
194	.4104 18756	.3940 84298	.3940 84298
195	.3940 84298	.3776 49840	.3776 49840
196	.3776 49840	.3612 15382	.3612 15382
197	.3612 15382	.3448 80924	.3448 80924
198	.3448 80924	.3284 46466	.3284 46466
199	.3284 46466	.3120 12008	.3120 12008
200	.3120 12008	.2956 77550	.2956 77550

TABLE 2.

k	p_k	q_k	r_k	k	p_k	q_k	r_k
135	.35364 83310	.29616 45992	.88725 38465	206	.45338 81792	.23132 25797	.86077 23411
136	.35120 83166	.31658 53880	.88115 06173	207	.45105 28410	.25143 58943	.85634 76663
137	.34858 71405	.33700 54130	.87459 38240	208	.44850 93244	.27154 88179	.85152 84055
				209	.44575 41011	.29166 13317	.84630 78334
				210	.44278 32564	.31177 34205	.84067 84892
138	.39452 37167	.01019 48516	.91882 92017	211	.43959 24582	.33188 50718	.83463 21164
139	.39435 92378	.03058 45268	.91844 72648	212	.43617 69208	.35199 62770	.82815 95950
140	.39403 00779	.05097 41181	.91768 29174	213	.43253 13631	.37210 70308	.82125 08615
141	.39353 58315	.07136 35702	.91653 52095	214	.42864 99608	.39221 73322	.81389 48184
142	.39287 58870	.09175 28287	.91500 27081	215	.42452 62910	.41232 71841	.80607 92278
143	.39204 94228	.11214 18401	.91308 34889				
144	.39105 54024	.13253 05528	.91077 51231				
145	.38989 25669	.15291 89168	.90807 46617	216	.48894 99197	.01045 90707	.87224 91524
146	.38855 94269	.17330 68842	.90497 86161	217	.48873 56034	.03137 71951	.87186 75253
147	.38705 42528	.19369 44099	.90148 29344	218	.48830 66915	.05229 52688	.87110 37710
148	.38537 50620	.21408 14516	.89758 29731	219	.48766 26236	.07321 32584	.86995 68865
149	.38351 96056	.23446 79701	.89327 34649	220	.48680 25547	.09413 11311	.86842 53583
150	.38148 53516	.25485 39299	.88854 86798	221	.48572 53490	.11504 88546	.86650 71531
151	.37926 94661	.27523 92992	.88340 13812	222	.48442 95725	.13596 63979	.86419 97037
152	.37686 87913	.29562 40507	.87782 47745	223	.48291 34834	.15688 37311	.86149 98912
153	.37427 98202	.31600 81617	.87181 04484	224	.48117 50191	.17780 08255	.85840 40234
154	.37149 86675	.33639 16142	.86534 93063	225	.47921 17826	.19871 76544	.85490 78086
155	.36852 10360	.35677 43959	.85843 12881	226	.47702 10240	.21963 41927	.85100 63243
				227	.47459 96207	.24055 04176	.84669 39805
				228	.47194 40531	.26146 63083	.84196 44769
156	.41855 12610	.01016 09759	.90813 63315	229	.46905 03768	.28238 18469	.83681 07531
157	.41837 79773	.03048 29035	.90776 13457	230	.46591 41902	.30329 70182	.83122 49311
158	.41803 11980	.05080 47585	.90701 09117	231	.46253 05976	.32421 18098	.82519 82481
159	.41751 04978	.07112 64928	.90588 41020	232	.45889 41652	.34512 62128	.81872 09796
160	.41681 52355	.09144 80592	.90437 95176	233	.45499 88715	.36604 02218	.81178 23495
161	.41594 45496	.11176 94116	.90249 52799	234	.45083 80491	.38695 38350	.80437 04265
162	.41489 73532	.13209 05051	.90022 90180	235	.44640 43167	.40786 70550	.79647 20029
163	.41367 23265	.15241 12962	.89757 78535	236	.44168 95006	.42877 98884	.78807 24537
164	.41226 79087	.17273 17436	.89453 83817				
165	.41068 22864	.19305 18081	.89110 66485				
166	.40891 33826	.21337 14529	.88727 81236	237	.51123 39620	.01034 60231	.85937 93085
167	.40695 88406	.23369 06439	.88304 76686	238	.51101 47256	.03103 80543	.85901 14024
168	.40481 60083	.25400 93505	.87840 94998	239	.51057 59732	.05173 00408	.85827 51182
169	.40248 19178	.27432 75449	.87335 71457	240	.50991 71434	.07242 19533	.85716 95092
170	.39995 32625	.29464 52033	.86788 33977	241	.50903 73898	.09311 37626	.85569 31477
171	.39722 63716	.31496 23058	.86198 02525	242	.50793 55751	.11380 54404	.85384 41153
172	.39429 71792	.33527 88370	.85565 88467	243	.50661 02637	.13449 69594	.85161 99908
173	.39116 11900	.35559 47857	.84884 93811	244	.50505 97120	.15518 82929	.84901 78332
174	.38781 34385	.37591 01460	.84160 10332	245	.50328 18565	.17587 94158	.84603 41624
				246	.50127 42997	.19657 03043	.84266 49345
				247	.49903 42926	.21726 09361	.83890 55134
175	.44238 29338	.01011 46408	.89676 92200	248	.49655 87148	.23795 12909	.83475 06370
176	.44220 14976	.03034 39011	.89640 22998	249	.49384 40516	.25864 13502	.83019 43776
177	.44183 84050	.05057 30983	.89566 80108	250	.49088 63663	.27933 10979	.82523 00971
178	.44129 32139	.07080 21903	.89456 54527	251	.48768 12693	.30002 05202	.81985 03931
179	.44056 52580	.09103 11362	.89309 32682	252	.48422 38813	.32070 96059	.81404 70388
180	.43965 36422	.11125 98957	.89124 96342	253	.48050 87923	.34139 83466	.80781 09120
181	.43855 72372	.13148 84296	.88903 22506	254	.47653 00120	.36208 67370	.80113 19133
182	.43727 46720	.15171 67002	.88643 83251	255	.47228 09147	.38277 47551	.79399 88723
183	.43580 43251	.17194 46713	.88346 45551	256	.46775 41734	.40346 24623	.78639 94372
184	.43414 43138	.19217 23088	.88010 71063	257	.46294 16844	.42414 98039	.77831 99475
185	.43229 24809	.21239 95806	.87636 15859	258	.45783 44786	.44483 68090	.76974 52849
186	.43024 63804	.23262 64569	.87222 30126				
187	.42800 32597	.25285 29108	.86768 57814				
188	.42556 00394	.27307 89181	.86274 36221	259	.53341 95587	.01023 20717	.84578 89093
189	.42291 32900	.29330 44579	.85738 95521	260	.53319 58465	.03069 62020	.84543 47594
190	.42005 92054	.31352 95127	.85161 58222	261	.53274 81427	.05116 02929	.84472 60152
191	.41699 35712	.33375 40687	.84541 38532	262	.53207 58868	.07162 43183	.84366 17851
192	.41371 17300	.35397 81163	.83877 41637	263	.53117 82335	.09208 82525	.84224 07245
193	.41020 85394	.37420 16498	.83168 62867	264	.53005 40474	.11255 20706	.84046 10272
194	.40647 83250	.39442 46683	.82413 86730	265	.52870 18954	.13301 57483	.83832 04140
				266	.52712 00378	.15347 92620	.83581 61173
				267	.52530 64160	.17394 25894	.83294 48631
				268	.52325 86392	.19440 57093	.82970 28485
195	.46602 58234	.01005 78944	.88471 39485	269	.52097 39673	.21486 86021	.82608 57154
196	.46583 68706	.03017 36648	.88435 60143	270	.51844 92918	.23533 12494	.82208 85201
197	.46545 87378	.05028 93799	.88363 97126	271	.51568 11129	.25579 36349	.81770 56965
198	.46489 09692	.07040 50031	.88256 41746	272	.51266 55136	.27625 57439	.81293 10150
199	.46413 28779	.09052 04984	.88112 80900	273	.50939 81287	.29671 75640	.80775 75340
200	.46318 35408	.11063 58308	.87932 96995	274	.50587 41102	.31717 90849	.80217 75444
201	.46204 17939	.13075 09659	.87716 67832	275	.50208 80870	.33764 02989	.79618 25051
202	.46070 62241	.15086 58706	.87463 66469	276	.49803 41177	.35810 12007	.78976 29693
203	.45917 51602	.17098 05134	.87173 61047	277	.49370 56370	.37856 17880	.78290 84983
204	.45744 86622	.19109 48643	.86846 14580	278	.48909 53930	.39902 20616	.77560 75624
205	.45551 85082	.21120 88951	.86480 84709				

TABLE 2.

k	p _k	q _k	r _k
279	.48419 53747	.41948 20254	.76784 74259
280	.47348 96530	.46040 10568	.75961 40122
281			.75089 17467
282	.55548 73439	.01011 72035	.83146 34405
283	.55525 96027	.03035 15990	.83112 30679
284	.55448 38419	.05058 59595	.82941 91138
285	.55411 95035	.07082 02620	.82805 34306
286	.55320 57457	.09105 44839	.82634 31583
287	.55206 14382	.11128 86030	.82428 61558
288	.55068 51547	.13152 25976	.82187 98239
289	.54907 51641	.15175 64471	.81912 10888
290	.54722 94186	.17199 01314	.81600 63814
291	.54514 55410	.19222 36318	.81259 16136
292	.54282 08080	.21245 69306	.80869 21497
293	.54025 21314	.23269 00117	.80448 27739
294	.53743 60365	.25292 28601	.79989 76519
295	.53436 86365	.27315 54628	.79493 02870
296	.53104 56031	.29338 78085	.78957 34698
297	.52746 21330	.31361 98877	.78381 92195
298	.52361 29086	.33385 16933	.77765 87166
299	.51949 20535	.35408 32701	.77108 22259
300	.51509 30806	.37431 44657	.76407 90062
301	.51040 88220	.39454 54302	.75663 72067
302	.50543 14105	.41477 61164	.74874 37463
303	.49956 12618	.43500 65303	.74038 41723
304	.49456 12618	.45523 66810	.73154 24956
305	.48864 82451	.47546 65810	
306	.57741 68552	.01000 14437	.81638 82327
307	.57718 53212	.03000 43209	.81540 80665
308	.57672 26096	.05000 71671	.81442 67224
309	.57602 75333	.07000 99619	.81311 64240
310	.57509 96475	.09001 26853	.81147 55801
311	.57393 72899	.11001 53174	.80950 21835
312	.57253 95839	.13001 78391	.80719 37983
313	.57090 46347	.15002 32320	.80454 75447
314	.56903 04080	.17002 24783	.80156 00803
315	.56691 45472	.19002 45613	.79822 75780
316	.56455 43531	.21002 64653	.79454 57005
317	.56194 71664	.23002 81755	.79050 95702
318	.55908 83464	.25002 96789	.78611 37345
319	.55620 51879	.27003 09635	.78135 21259
320	.55366 24229	.29003 20190	.77621 80162
321	.55066 74208	.31003 28368	.77070 39635
322	.54746 33422	.33003 34101	.76480 17513
323	.54442 26083	.35003 37342	.75850 23187
324	.54167 37972	.37003 38064	.75179 56796
325	.53862 90295	.39003 36262	.74467 08290
326	.53527 97477	.41003 31958	.73711 56353
327	.53157 97477	.43003 25196	.72911 67135
328	.52781 64974	.45003 16053	.72065 92784
329	.52392 86534	.47003 04631	.71172 69714
330	.52000 52678	.49002 91068	
331	.51616 74116	.01027 49870	.80085 70481
332	.51247 42667	.03082 49515	.80051 88910
333	.50800 76575	.05137 48875	.79964 21485
334	.50323 11559	.07124 47766	.79882 59609
335	.49858 89983	.09247 46000	.79746 90320
336	.49422 88308	.11302 43398	.79576 96205
337	.48963 86634	.13357 39784	.79372 55288
338	.48542 86634	.15412 34991	.79133 40881
339	.48157 86634	.17467 28859	.78859 21413
340	.47726 85283	.19522 21234	.78549 60205
341	.47348 85283	.21577 11977	.78204 15221
342	.46968 85283	.23632 00958	.77822 38765
343	.46588 85283	.25686 88060	.77403 77132
344	.46208 85283	.27741 73180	.76947 70200
345	.45828 85283	.29796 56230	.76453 50963
346	.45448 85283	.31851 37140	.75920 44985
347	.45068 85283	.33906 15859	.75347 69780
348	.44688 85283	.35960 92353	.74734 34082
349	.44308 85283	.38015 66611	.74079 37013
350	.43928 85283	.40070 38644	.73381 67110
351	.43548 85283	.42125 08490	.72640 01199
352	.43168 85283		
353	.42788 85283		
354	.42408 85283		
355	.42028 85283		
356	.41648 85283		
357	.41268 85283		
358	.40888 85283		
359	.40508 85283		
360	.40128 85283		
361	.39748 85283		
362	.39368 85283		
363	.38988 85283		
364	.38608 85283		
365	.38228 85283		
366	.37848 85283		
367	.37468 85283		
368	.37088 85283		
369	.36708 85283		
370	.36328 85283		
371	.35948 85283		
372	.35568 85283		
373	.35188 85283		
374	.34808 85283		
375	.34428 85283		
376	.34048 85283		
377	.33668 85283		
378	.33288 85283		
379	.32908 85283		
380	.32528 85283		
381	.32148 85283		
382	.31768 85283		
383	.31388 85283		
384	.31008 85283		
385	.30628 85283		
386	.30248 85283		
387	.29868 85283		
388	.29488 85283		
389	.29108 85283		
390	.28728 85283		
391	.28348 85283		
392	.27968 85283		
393	.27588 85283		
394	.27208 85283		
395	.26828 85283		
396	.26448 85283		
397	.26068 85283		
398	.25688 85283		
399	.25308 85283		
400	.24928 85283		
401	.24548 85283		
402	.24168 85283		
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404	.23408 85283		
405	.23028 85283		
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407	.22268 85283		
408	.21888 85283		
409	.21508 85283		
410	.21128 85283		
411	.20748 85283		
412	.20368 85283		
413	.19988 85283		
414	.19608 85283		
415	.19228 85283		
416	.18848 85283		
417	.18468 85283		
418	.18088 85283		
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423	.16188 85283		
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433	.12388 85283		
434	.12008 85283		
435	.11628 85283		
436	.11248 85283		
437	.10868 85283		
438	.10488 85283		
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442	.08968 85283		
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444	.08208 85283		
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454	.04408 85283		
455	.04028 85283		
456	.03648 85283		
457	.03268 85283		
458	.02888 85283		
459	.02508 85283		
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TABLE 2.

k	p _k	q _k	r _k
425	.61030 67414	.37700 97469	.69669 88819
426	.60466 45522	.39738 73297	.69026 37826
427	.59866 81460	.41776 47523	.68342 45113
428	.59230 67888	.43814 20194	.67616 87946
429	.58556 86106	.45851 91380	.66848 30606
430	.57844 04671	.47889 61171	.66035 22810
431	.57090 77752	.49927 29687	.65175 97832
432	.56295 43189	.51964 97071	.64268 70286
433	.55456 20172	.54002 63501	.63311 33471
434	.67861 10131	.01002 78125	.73442 93947
435	.67833 78226	.03008 34312	.73413 40379
436	.67779 11128	.05013 90313	.73354 29674
437	.67697 02236	.07019 46007	.73265 54677
438	.67587 41604	.09025 01271	.73147 04600
439	.67450 15872	.11030 55989	.72998 64956
440	.67285 08189	.13036 10046	.72820 17468
441	.67091 98103	.15041 63330	.72611 39958
442	.66870 61433	.17047 15737	.72372 06205
443	.66620 70112	.19052 67166	.72101 85770
444	.66341 92002	.21058 17524	.71800 43804
445	.66033 90675	.23063 66724	.71467 40804
446	.65696 25160	.25069 14688	.71102 32345
447	.65328 49654	.27074 61347	.70704 68758
448	.64930 13178	.29080 06640	.70273 94770
449	.64500 59197	.31085 50519	.69809 49078
450	.64039 25165	.33090 92946	.69310 63869
451	.63545 42017	.35096 33897	.68776 64260
452	.63018 33571	.37101 73359	.68206 67658
453	.62457 15849	.39107 11336	.67599 83017
454	.61860 96282	.41112 47846	.66955 09984
455	.61228 72794	.43117 82926	.66271 37900
456	.60559 32732	.45123 16630	.65547 44647
457	.59851 51613	.47128 49032	.64781 95287
458	.59103 91660	.49133 80228	.63973 40476
459	.58315 00061	.51139 10338	.63120 14583
460	.57483 06913	.53144 39509	.62220 33457
461	.56606 22759	.55149 67915	.61271 91761
462	.69778 98676	.01021 92960	.71622 96186
463	.69749 81440	.03065 78824	.71593 04668
464	.69691 43317	.05109 64517	.71333 17879
465	.69603 76986	.07153 49929	.71443 28289
466	.69486 71403	.09197 34947	.71323 24541
467	.69340 11737	.11241 19465	.71172 91385
468	.69163 79271	.13285 03378	.70992 09572
469	.68957 51281	.15328 86585	.70780 55735
470	.68721 00884	.17372 68990	.70538 02230
471	.68453 96858	.19416 50504	.70264 16952
472	.68156 03427	.21460 31041	.69958 63113
473	.67826 80009	.23504 10524	.69620 98984
474	.67465 80919	.25547 88886	.69250 77592
475	.67072 55034	.27591 66064	.68847 46367
476	.66646 45391	.29635 42008	.68410 46745
477	.66186 88741	.31679 16677	.67939 13693
478	.65693 15018	.33722 90043	.67432 75173
479	.65164 46735	.35766 62087	.66890 51522
480	.64599 98287	.37810 32808	.66311 54729
481	.63998 75136	.39854 02215	.65694 87607
482	.63359 72876	.41897 70336	.65039 42823
483	.62681 76129	.43941 37214	.64344 01772
484	.61963 57267	.45985 02914	.63607 33258
485	.61203 74902	.48028 67516	.62827 91950
486	.60400 72109	.50072 31128	.62004 16547
487	.59552 74308	.52115 93879	.61134 27611
488	.58657 86740	.54159 55927	.60216 24973
489	.57713 91429	.56203 17462	.59247 84604