GEMP-192
INFORMAL

Nuclear Materials & Propulsion Operation

COMPUTER PROGRAMS DESCRIBING COLLISION CASCADES IN BINARY MATERIALS
I. SQUARE PLANAR LATTICE

FLIGHT PROPULSION LABORATORY DEPARTMENT
GENERAL ELECTRIC

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COMPUTER PROGRAMS DESCRIBING COLLISION CASCADES IN BINARY MATERIALS I. SQUARE PLANAR LATTICE

D.G. Besco
J.R. Beeler, Jr.

February, 1963

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ABSTRACT

An IBM 7090 computer program calculates the results of the bombardment of a square planar lattice of binary material by a single atom of specified type, position, direction, and energy. The hard sphere model is used to compute the results of collisions. The collision radii are based on the Bohr screened coulomb potential. The computer records the entire history of the bombarding particle and all knock-ons, and prints a map of the defect configuration after the collision cascade, showing the location of all vacancies and interstitials.

I. INTRODUCTION

This program is the first member of a series of machine codes designed to describe the instantaneous point defect configurations created during ion bombardment of a binary solid and the absorption point distribution of these ions in the target material. This study is part of an analysis of experimental results on the injection of Kr and I atoms into BeO and their subsequent effusion at an elevated temperature.

Adopting the traditional philosophy of first solving a series of simple problems as preparation for the attempted solution of a difficult problem we have set out, initially, to describe the knock-on cascade in a binary system with a square planar lattice. The hard sphere collision model is assumed. The present report describes a machine code (IBM 7090) for this two-dimensional system. The hard sphere model will next be applied to the BeO Wurtzite structure and the body-centered cubic and face-centered cubic structure. Finally, we hope to use a more exact scattering model in the three-dimensional structures. The hard sphere calculations assume stationary target atoms prior to collision.

The intent of the two-dimensional hard sphere calculation was to describe: (1) The penetration distance and spatial trajectory of the bombarding atom; (2) The energy loss history of the bombarding atom. (This gives the primary knock-on spectrum); (3) Vacancy and interstitial clusters created in the knock-on cascade; (4) The fraction of the instantaneous defect configuration which is unstable and therefore anneals immediately.

II. PHYSICAL MODEL AND COMPUTATION METHODS

1. General Problem

The basic task of the program is to repeatedly solve the following problem and record the consequences of its solution.

Given: A moving particle (P_1) with mass M_1, energy E_1, position (x_1, y_1), and direction α in a two-dimensional square binary crystal with lattice constant c. (Figure 1).

Using the hard sphere model, the program must:

1) Identify the atom (P_2) with which P_1 will next collide.

2) Compute the hard sphere radius (r) implied by the screened coulomb potential, and from this the coordinates of the point of collision.

3) Determine the amount of energy transferred from P_1 to P_2 by the collision.

4) Calculate the basic scattering angles (θ, φ), and thereby the post-collision direction angles for the two particles (θ', φ').

The parameters of a single incident atom are input to the program, which then traces the history of all subsequent collisions, primary, secondary, etc., until the incident atom and all atoms which are dislodged from their lattice site at some point are finally absorbed or escape.

The output of the program consists of the collision history of the incident atom and all knock-ons, details of the resulting pattern of radiation damage, and statistics concerning the nature of the defects created.

The incident particle is assumed to be an iodine atom and the crystal beryllium oxide, but the analysis applies equally for other binary materials and bombarding atoms.

Hereafter, P_1 refers to the incident particle in a given collision, and P_2 refers to the target particle. Throughout, the subscripts 1 and 2 are used to denote quantities associated with the incident and target particles respectively.

2. Particle Tracing Method

The following indicates how an atom is selected for collision, given a set of initial conditions describing a moving particle.

A grid is imposed upon the lattice, consisting of horizontal and vertical lines joining the centers of atoms. The lattice position of an atom is defined to be the coordinates of its center in this grid. For example, spatial coordinates (c, 2c) are equivalent to lattice position (1, 2), where c is the lattice constant.

Consider a moving particle with free path originating at (x_1, y_1) and extending in direction α. (Figure 1). Let x_b be the x-coordinate of the next vertical grid line intersected by the path. Similarly, let y_b be the y-coordinate of the next horizontal grid line intersected by the path.

Compute

$$(1) \qquad r_x = \frac{|x_b - x_1|}{\cos\alpha} \qquad\qquad r_y = \frac{|y_b - y_1|}{\sin\alpha}$$

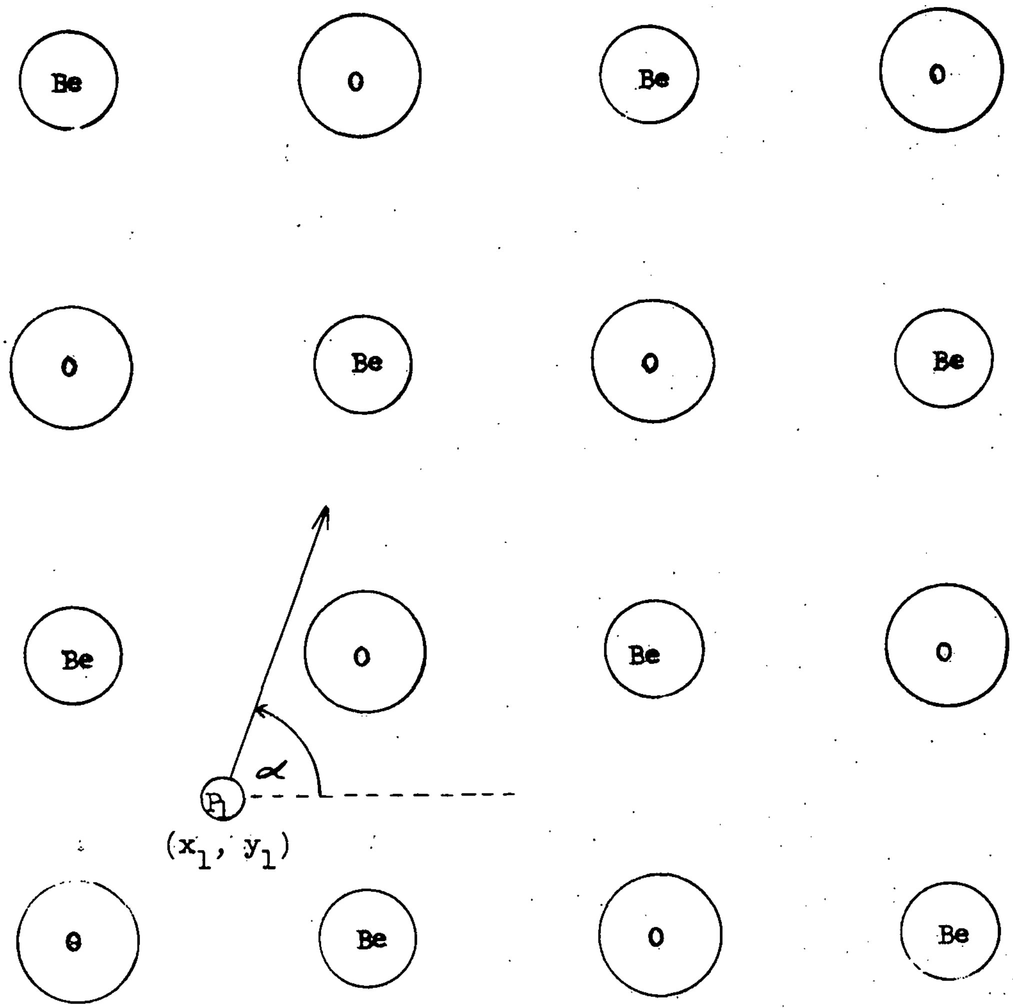

FIGURE 1

ENERGETIC ATOM (P_1) IN BeO SQUARE PLANAR LATTICE

Depending upon which of r_x, r_y is the smaller, the grid line next intersected by the path is identified.

Three lattice positions are then selected for testing:

a) the two positions adjoining the point of intersection of the path with the grid line. (S_1, S_2).

b) the corresponding interstitial position. (I).

See Figure 3.

The type of atom (beryllium oxygen, vacant) at each of the three positions is determined. For the non-vacant positions

(2) $$q = (x_3 - x_1) \cos \alpha + (y_3 - y_1) \sin \alpha$$

is computed, where (x_3, y_3) is the center of the atom being tested. This quantity is proportional to the projection along the free path of the line joining the centers.

The prospective target atom for which q has its smallest positive value is the one for which the results of a collision are to be computed.

If each of the three positions is vacant or has a negative q, the free path is traced unperturbed to its next intersection with a grid line and the process is repeated, using this intersection as a take-off point.

3. Collision Parameters

The following calculations are made after the atom has been selected for which the interaction is to be measured.

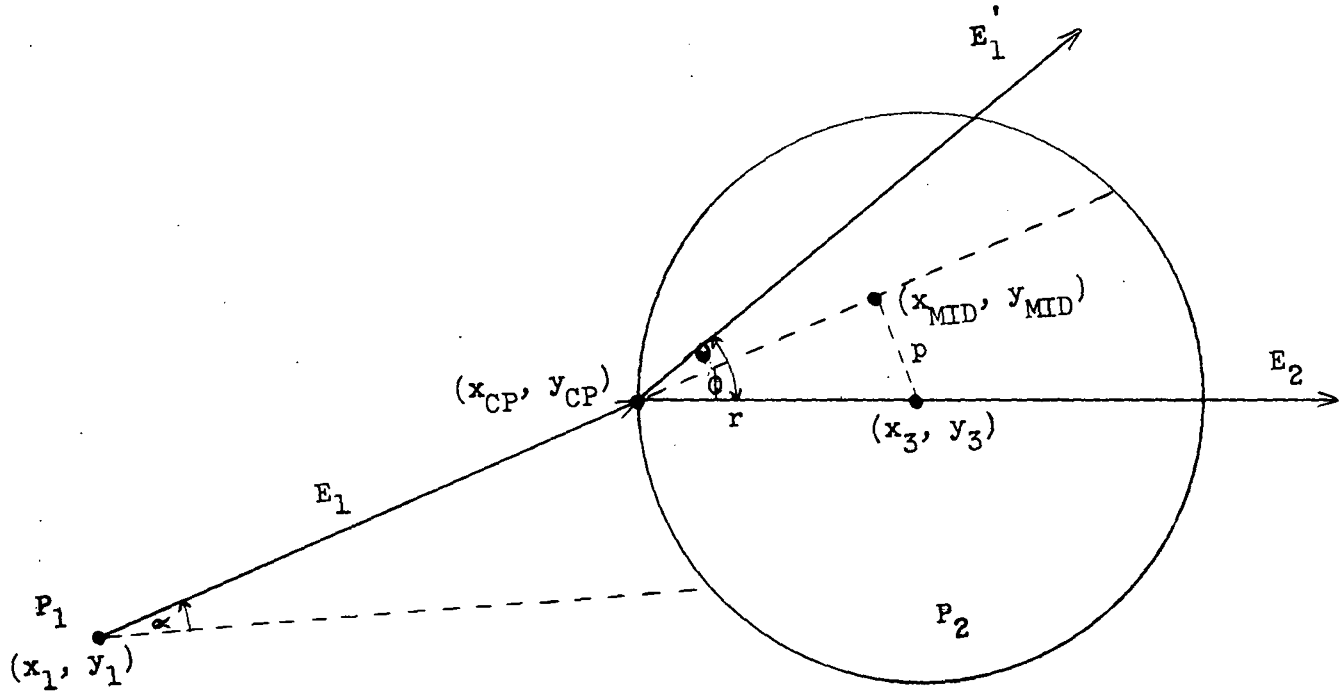

FIGURE 2

HARD SPHERE COLLISION

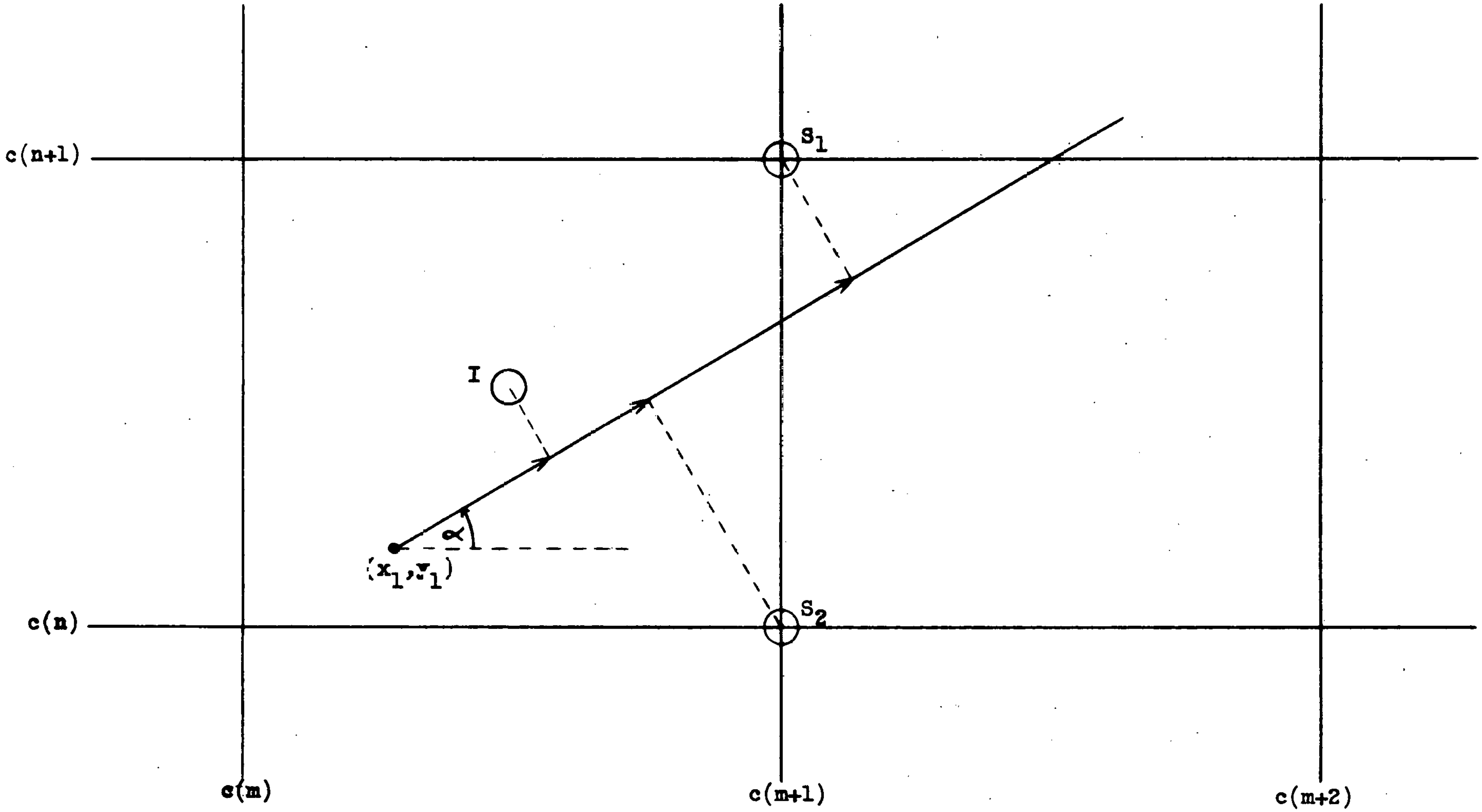

FIGURE 3
COLLISION TRACE
(See II. 2)

a) impact parameter

The impact parameter p is the normal distance from the unperturbed free path to the center of the target. [1]

(3) $$p = [\, x_3 \tan\alpha - y_3 + (y_1 - x_1 \tan\alpha)\,] \cos\alpha$$

b) distance of closest approach (collision radius)

The distance of closest approach of the two atoms is the separation distance at which the radial velocity component dr/dt vanishes in the center-of-mass coordinate system.

This occurs when the screened coulomb potential

(4) $$V(r) = \frac{M_2}{M_1 + M_2} \quad E \quad \left(1 - \frac{p^2}{r^2}\right)$$

But,

(5) $$V(r) = \frac{z_1 \; z_2 \quad e^{-r/a}}{r} \qquad [2]$$

So the proper value of r satisfies

(6) $$r = \frac{M_1 + M_2}{M_2} \quad \frac{z_1 \; z_2}{E} \quad e^{-r/a} \quad \left(1 - \frac{p^2}{r^2}\right)^{-1}$$

where m = mass, z = charge, and a is the Bohr screening radius [2]:

(7) $$a = \frac{\lambda\,(.529172 \times 10^{-8})}{(z_1^{2/3} + z_2^{2/3})^{1/2}} \quad \text{cm.}$$

A Newton-Raphson iteration is used to compute r.

For larger values of p, r will be only slightly greater than p, and the hard-sphere calculations will result in a small energy loss and small deflection, corresponding to the weakness of the two-body interaction for large impact parameters.

When $p > 1.0\text{Å}$, the following approximation is made in order to save the computer time normally required to iterate to a solution for r:

(8) $$r = p\,(1 + \epsilon)$$

where

(9) $$\epsilon = \frac{z_1 z_2 \left(\frac{M_1 + M_2}{M_2}\right) e^{-p/a}}{E_1 \; p}$$

c) point of collision

The coordinates of the point of collision are given by [3]:

(10) $$x_{cp} = x_3 - \sqrt{r^2 - p^2} \quad \cos \alpha - p \sin \alpha$$

(11) $$y_{cp} = y_1 + (x_3 - x_1) \tan \alpha$$

4. Hard Sphere Approximation [4]

The results of the collision are computed on the assumption of an elastic (hard-sphere) collision of a moving point with mass M_1 and a stationary circle with radius r and mass M_2.

The relationship between the three scattering angles:

θ = scattering angle of P_1 - laboratory coordinates

φ = scattering angle of P_2 - laboratory coordinates

Θ = scattering angle - center-of-mass coordinates

is given by the mnemonic drawing (Figure 7 in Evans) and the half-angle formula:

(12) $$\varphi = 1/2\ (\Pi - \Theta)$$

φ is the fundamental angle in the sense that one can find its trigonometric functions directly in terms of the impact parameter p and the collision radius r.

(13) $$\sin \varphi = \frac{|p|}{r}$$

(13') $$\cos \varphi = \sqrt{1 - \sin^2 \varphi}$$

If we let M_1 and M_2 be the masses, V_1 and V_2 the post-collision velocities, and V the pre-collision velocity of P_1, the equations for conservation of momentum are:

(14) $$M_1 V = M_1 V_1 \cos \theta + M_2 V_2 \cos \varphi$$

(15) $$0 = M_1 V_1 \sin \varphi - M_2 V_2 \sin \varphi$$

From (12),

(16) $$\sin \Theta = 2 \sin \varphi \cos \varphi$$

(17) $$\cos \Theta = \sin^2 \varphi - \cos^2 \varphi = 2 \sin^2 \varphi - 1$$

From the mnemonic triangle,

(18) $$\sin \theta = \frac{\sin \Theta}{\sqrt{\left(\frac{M_1}{M_2}\right)^2 + 2\left(\frac{M_1}{M_2}\right) \cos \Theta + 1}}$$

$$= \frac{2 \sin \varphi \cos \varphi}{\sqrt{\left(\frac{M_1}{M_2}\right)^2 + 2\left(\frac{M_1}{M_2}\right) (2 \sin^2 \varphi - 1) + 1}}$$

(19) $$\cos \theta = \frac{\frac{M_1}{M_2} + \cos \Theta}{\sqrt{\left(\frac{M_1}{M_2}\right)^2 + 2\left(\frac{M_1}{M_2}\right) \cos \Theta + 1}}$$

$$= \frac{\frac{M_1}{M_2} + 2 \sin^2 \varphi - 1}{\sqrt{\left(\frac{M_1}{M_2}\right)^2 + 2\left(\frac{M_1}{M_2}\right) (2 \sin^2 \varphi - 1) + 1}}$$

Since the absolute value of p was used, we have $\sin \varphi > 0$, $\cos \varphi > 0$.

(20) $$\therefore \quad 0 < \varphi < \pi/2$$

and $\sin \theta > 0$

(21) $\therefore \quad 0 < \theta < \pi$

θ' and φ', which are the post-collision directions of P_1 and P_2, are calculated by the following scheme, which merely determines the directions in which the deflections are to be applied.

(22) $$y_{MID} = y_1 + \left(\frac{R_1 + R_2}{2}\right) \sin \alpha$$

	$y_{MID} - y_3 > 0$	$y_{MID} - y_3 < 0$
$\cos \alpha > 0$	$\varphi' = \alpha - \varphi$ $\theta' = \alpha + \theta$	$\varphi' = \alpha + \varphi$ $\theta' = \alpha - \theta$
$\cos \alpha < 0$	$\varphi' = \alpha + \varphi$ $\theta' = \alpha - \theta$	$\varphi' = \alpha - \varphi$ $\theta' = \alpha + \theta$

By convention, $0 < \alpha < 2\pi$

Now, from equation (31) in Evans,

(23) $$\frac{E_1'}{E_1} = \left[1 - 2\,(1-\cos\Theta)\,\frac{M_1 M_2}{(M_1 + M_2)^2} \right]$$

$$= \left[1 - 4 \cos^2 \varphi \,\frac{M_1 M_2}{(M_1 + M_2)^2} \right]$$

where

(24) $$M_o \equiv \frac{M_1 M_2}{M_1 + M_2} \equiv \text{the reduced mass of the system}$$

So the percent energy transfer is given by:

$$(25) \qquad E_{TR} = \frac{E_2}{E_1} = \frac{4\, M_o^2 \cos^2 \varphi}{M_1\, M_2} = \frac{4\, M_1\, M_2 \cos^2 \varphi}{(M_1 + M_2)^2}$$

5. Types of Collisions

At this point, the post-collision energies for P_1 and P_2 are known. In determining the nature of the collision, the assumption is made that a sharp threshold energy (E_D) exists for the displacement of an atom from a lattice site. In the program E_D, referred to as the displacement energy, depends upon the type of P_2 and whether P_2 is an interstitial.

The assumption leads to the classification of each collision as one of four types [5]:

Type 1 - scattering - $E_1' > E_D \quad E_2 < E_D$

P_1 continues on at angle θ' with energy E_1'

P_2 remains in position, not having received enough energy to be dislodged.

Type 2 - displacement - $E_1' > E_D \quad E_2 > E_D$

P_1 continues on at angle θ' with energy E_1'

P_2 dislodged and becomes a free particle with angle φ' and energy $E_2 - E_D$.

Type 3 - replacement - $E_1' < E_D \qquad E_2 > E_D$

P_1 becomes bound and occupies the position in the lattice formerly occupied by P_2.

P_2 dislodged and becomes a free particle with angle φ' and energy $E_2 - E_D$.

Type 4 - interstitial absorption - $E_1' < E_D \qquad E_2 < E_D$

P_1 becomes bound and occupies an interstitial position. If P_2 is itself an interstitial, P_1 will share P_2's position. If not, it goes into one of the four positions adjacent to P_2, corresponding to the quadrant containing the point $(x_{CP} - x_3, y_{CP} - y_3)$.

P_2 remains in its original position.

6. Order of Calculations

At any given point in the calculations, tables exist which allow the computer rapid access to the following information.

I. The type, position, direction, and energy of every free particle moving in the crystal.

II. The occupancy (vacancy or type of atom) of every lattice site and interstice.

Tables I and II are up-dated each time the results of a collision are computed.

The number of new free particles after a collision may be either zero (type 4 collision), one (type 1 or 3), or two (type 2). In any event, Table I is up-dated by entering at the end of the table the new free particles, if any. If there are two, the one with greatest velocity is entered first. Information about the next particle to be traced is picked up from the beginning of the table and then erased from the table. The calculations are complete at such time as Table I contains no more entries.

If a type 2, 3, or 4 collision occurs, the appropriate change in the lattice configuration is recorded in Table II.

The result of this calculation scheme is that the collision cascade is approximated by a series of separate two-body interactions (hard sphere collisions) between moving knock-ons and stationary lattice atoms.

III. PROGRAM USAGE

1. Input

The program data is loaded by the decimal input routine DING, and must be punched accordingly. Input for a sample case is listed in the Appendix.

The following quantities are required as data:

a) Initial direction angle

α Symbol: ALPHA

The incident angle measured in degrees from the positive x - axis, i.e. from a line normal to the face of the crystal.

b) Lattice constant

c Symbol: CLAT

The separation between lattice planes (lines, in 2D) in centimeters.

c) Initial energy

E_o Symbol: EO

Initial energy in electron volts.

d) Displacement energies

E_{Di}, E_{Ds} Symbols: EDI, EDS

EDS (1) = Threshold energy for displacement of a B_E atom from a lattice site.

EDS (2) = Same for O.

EDS (3) = Same for I.

EDI (1), EDI (2), EDI (3) = Corresponding energies for displacement from an interstice. Units are electron volts.

e) Prefactor for screening radius calculation

λ Symbol: XLMDA

$1 \leq \lambda \leq 2$

See equation (7).

f) Initial coordinates

(x_o, y_o) Symbols: XO, YO

The initial position of the incident particle expressed in centimeters:

$x_o \geq 0$, $y_o > 0$.

The crystal occupies the first quadrant of the coordinate system. The y-axis corresponds to the surface which is being bombarded. Hence x_o is normally equal to zero. y_o must be large enough to insure that no collisions will occur at positions with negative y coordinates.

g) Output control

Symbol: KRTAB

KRTAB = 1 causes the results of every collision to be printed. When KRTAB = 2 or omitted, only the collisions involving the incident (iodine) atoms are printed.

h) Bombardment other than iodine - BeO

Calculations for materials other than BeO and/or bombarding ions other than iodine may be performed by loading the appropriate atomic numbers (nuclear charges) and mass numbers into the absolute decimal locations indicated:

ATOMIC NUMBER		MASS NUMBER	
PARTICLE	LOCATION	PARTICLE	LOCATION
Incident	9980	Incident	22476
Type 1	9978	Type 1	22802
Type 2	9979	Type 2	22475

Calculations for monatomic material may be made by setting the data for atom types 1 and 2 equal.

For the normal case of iodine - BeO no data need be loaded into the above locations.

i) Change cases

Any number of cases may be run successively. Each case constitutes one record, where an end of record is indicated by an equal sign (=) in column 1. For any given case, only those data items need be changed which differ from the preceding case.

2. Output (See sample in Appendix)

a) Input printout

x_o, y_o, α, E_o, lattice constant.

b) Collision history

The results of each collision involving the iodine atom are printed. If KRTAB = 1, results are printed for all collisions. The meanings of the column headings are as follows:

N O - sequential number of the collision

C - type of collision (see II.5)

P1 - incident particle type for this collision

1 - beryllium

2 - oxygen

3 - iodine

P2 - target particle type

K O X, K O Y - lattice position of target particle

E2 - E_2

THETA-P - θ'

P - p

R - r

CPX - x_{CP}

CPY - y_{CP}

INT - = 1 if target is an interstitial

= 0 otherwise.

c) Lattice map

The labeled coordinates in the map refer to the site at the lower left corner of the block below which the coordinates appear.

The numbers at the sites are to be interpreted as follows:

0 or 4 vacancy

1 or 5 beryllium

2 or 6 oxygen

3 or 7 iodine

Codes 4-7 differ from 0-3 in that they indicate that the interstitial position at the lower left of the site is filled, in addition to conveying the above information about site occupancy.

d) Interstitial table

A list of all atoms occupying interstitial positions, and the type of each.

Type 0 indicates the position was filled at one time but was subsequently displaced.

e) Interstitial and vacancy totals

The sputtering yield is the difference between the number of vacancies and the number of interstitials.

f) Final position of iodine atom

3. Error Returns

The "impossible" branches of tests in the program have been coded to call ERRORA and then dump core. Such a result indicates either a program malfunction or an error on omission in the data.

Input errors detectable by DING result in the usual error messages.

The message "particle table overflowed" indicates the program was required to keep track of more than 500 particles simultaneously. This does not happen at bombardment energies for which the hard sphere model is valid.

IV. PROGRAMMING INFORMATION

1. System and Set-up

The program is in the form of a relocatable deck. The deck and all necessary library subroutines are loaded via the FORTRAN-FAP monitor system with the usual control cards: (ISL③FORTRAN, $\not{S}$ ⑤ XEQ). The standard ECO set-up is used: input on tape A2, output on tape A3. (Also on line if sense switch 3 is down).

2. Subroutines (See Fig. 4)

The following summarizes the subroutines (other than library) which make up the program, and the general functions performed by each.

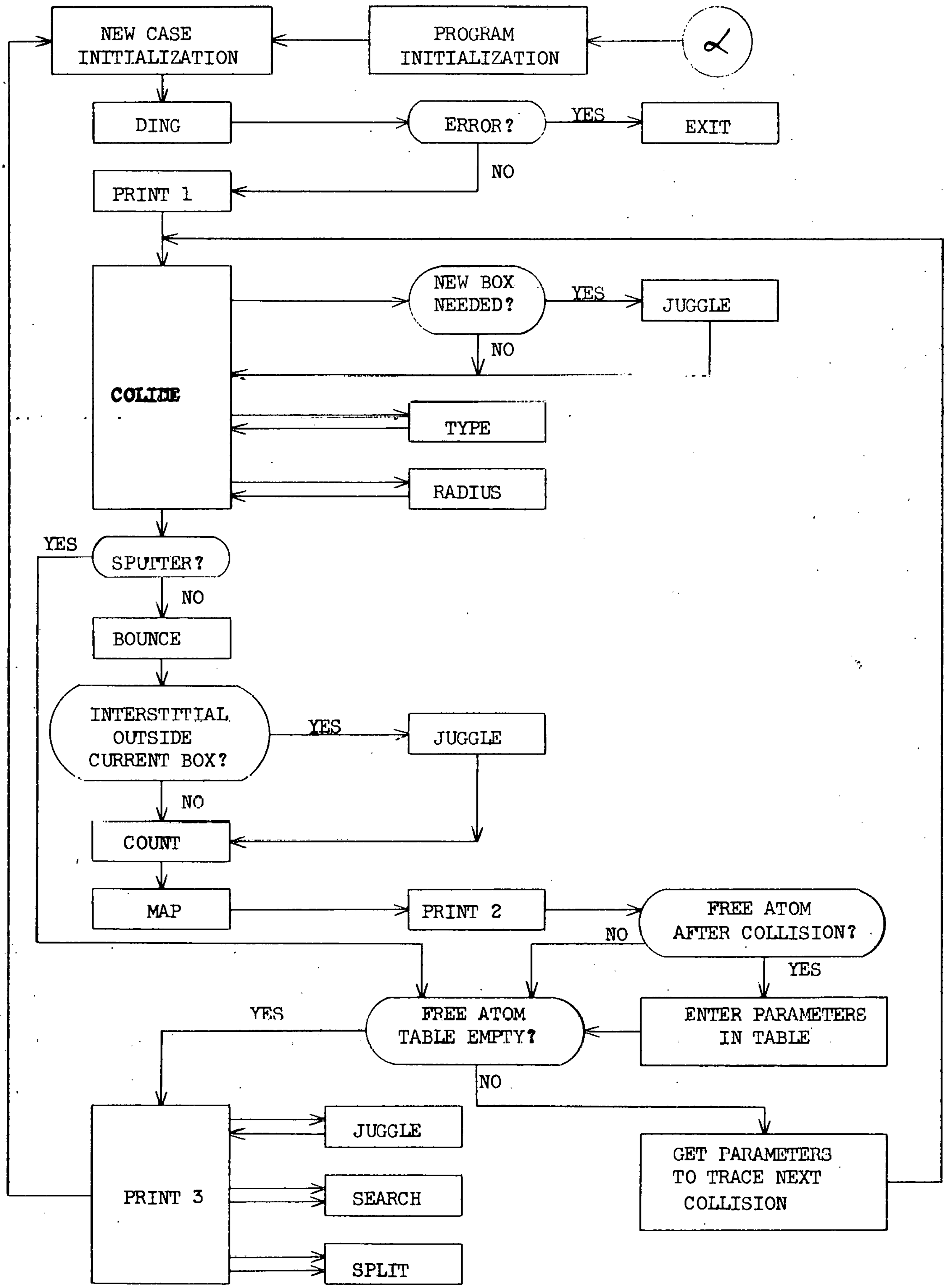

FIGURE 4

FLOW CHART

MAIN

The main program performs initialization and controls the overall flow of the program.

In addition, it makes the decision as to type of collision and up-dates the table of free particles.

BOUNCE

Computes the post-collision angles and energies.

COLIDE

Given the position, direction, and energy of a particle, determines the atom of collision and computes the point of collision and the impact parameter.

COUNT

Keeps a running tally of the number of vacancies in the lattice, and the number of interstitials of each type.

JUGGLE (Coded in FAP)

When a new block of the lattice map is required, looks it up in the table, brings it into the working area, and saves the previous block in the table. See IV.3 for description of lattice map.

MAP (Coded in FAP)

Up-dates the lattice map and/or the interstitial table after each collision.

PRINT 1

Input printout routine.

PRINT 2

Collision history printout routine.

PRINT 3

Prints out statistics, lattice map, and table of interstitials at end of case.

RADIUS

Computes the collision radius.

SEARCH (Coded in FAP)

Locates position in lattice map of block desired for printing.

SPLIT (Coded in FAP)

Unpacks information in interstitial table for printing.

TYPE (Coded in FAP)

Determines occupancy of the position being tested for collision.

3. Lattice Map

It is necessary for the program to know at any particular point in time exactly what positions are occupied by what type atoms. However, it was not known initially how much or precisely what parts of the crystal will be affected by a given bombardment.

In order to provide flexibility and to avoid unnecessarily consuming storage for mapping parts of the crystal unaffected by the bombardment, the following scheme was adopted for the lattice map:

The lattice is divided into blocks of dimensions 12 x 12 lattice spacings. Information about these blocks is stored in a table (referred to as Table II in II.6), table entries being made only for those blocks which are actually needed in the trace.

For the Nth block needed, the following table entries are made:

X-coordinate of lower left position of block stored in decrement of LXY(N).

Y-coordinate in address of LXY(N). Lattice map for the Nth block stored in A(N, 1), A(N, 2), . . . , A(N, 12).

The 36 bits of each machine word are considered to be 12 octal digits representing the types of atoms to be found in a horizontal row of 12 lattice positions.

The octal codes are as follows:

0 - vacancy

1 - beryllium atom

2 - oxygen atom

3 - iodine atom

4 - vacancy - interstitial

5 - beryllium - interstitial

6 - oxygen - interstitial

7 - iodine - interstitial

In codes 4 thru 7, the interstitial inferred to occupies the position at the immediate lower left of the indicated lattice site.

The types of atoms occupying the interstitial positions are kept in a separate table (ITYPE).

V. REFERENCES

1. J.R. Beeler, Monte Carlo Research Series: Fortran Monte Carlo Programs: Part I p. 21, DC 59-12-83, (1959).

2. G.J. Dienes, G.H. Vineyard, Radiation Effects in Solids, p. 10 (1957).

3. Beeler, p. 22.

4. R.D. Evans, The Atomic Nucleus, pp. 828-835, McGraw-Hill, (1955).

5. Dienes and Vineyard, p. 20.

VI. APPENDIX

1. Sample Input

2. Sample Output

Sample Input

Col. 1	2
	ALPHA, 30,
	CLAT, 2.5/-8,
	EO, 5000,
	EDI, 25, 50, 100,
	EDS, 25, 50, 100,
	KRTAB, 1,
	XO, 0,
	XLMDA, 1,
	YO, 250.4/-8
=	
8	

ION BOMBARDMENT -- TWO-DIMENSIONS

ENTRY POINT
X= 0. CM.
Y= 2.5040000-06 CM.

DIRECTION
ALPHA= 30.00 DEGREES

ENERGY
E= 5000.00 ELECTRON VOLTS

LATTICE CONSTANT
CLAT= 2.50000-08 CM.

COLLISION HISTORY

TYPES OF COLLISIONS

1-SCATTERING
2-KNOCKOUT
3-REPLACEMENT
4-INTERSTITIAL FORMED
5-MULTIPLE INTERSTITIAL FORMED

NO	C	P1	P2	KOX	KOY	E1	E1-P	E2	THETA-P	P	R	CPX	CPY	INT
1	1	3	2	1	100	5000.000	4999.964	0.036	5.24539-01	1.59641-08	1.59643-08	1.69583-08	2.51379-06	0
2	2	3	1	1	101	4999.964	4832.384	142.580	4.79239-01	5.67471-09	6.11669-09	2.58660-08	2.51894-06	0
3	2	3	2	2	101	4832.384	4586.534	195.850	5.54733-01	5.75535-09	6.17439-09	4.53622-08	2.52908-06	0
4	1	1	1	2	102	142.580	142.579	0.001	1.71550+00	2.82877-08	2.82878-08	2.20079-08	2.54592-06	0
5	1	3	1	2	102	4586.534	4586.480	0.055	5.53829-01	1.53435-08	1.53439-08	5.79900-08	2.53690-06	0
6	1	2	1	3	101	195.850	195.601	0.248	5.53545+00	1.65038-08	1.65152-08	6.36448-08	2.51301-06	0
7	2	1	2	1	102	142.579	63.736	28.842	2.93197+00	3.54908-09	5.61169-09	2.21148-08	2.54519-06	0
8	1	3	1	3	101	4586.480	4586.477	0.002	5.54020-01	1.90680-08	1.90681-08	6.49471-08	2.54120-06	0
9	3	2	2	3	100	195.601	21.166	124.435	6.77105+00	1.81647-09	5.52192-09	7.24117-08	2.50488-06	0
10	1	2	1	2	102	28.842	28.825	0.018	1.04935+00	2.14427-08	2.14499-08	3.13242-08	2.56055-06	0
11	2	3	2	3	102	4586.477	3236.784	1299.693	4.42882-01	2.19239-09	4.46101-09	7.28495-08	2.54609-06	0
12	1	2	1	4	100	124.435	124.422	0.013	5.19271+00	2.20834-08	2.20846-08	8.03845-08	2.48985-06	0
13	1	2	1	1	103	28.825	26.890	1.934	8.54433-01	1.26815-08	1.31701-08	3.42259-08	2.56560-06	0
14	1	3	1	4	102	3236.784	3212.425	24.359	4.65348-01	8.10384-09	8.23362-09	9.52115-08	2.55670-06	0
15	1	2	1	4	102	1299.693	1299.680	0.014	1.07022+00	2.19033-08	2.19035-08	8.07739-08	2.56049-06	0
16	1	2	2	4	99	124.422	118.372	6.051	4.97036+00	1.05329-08	1.07988-08	8.95586-08	2.47224-06	0
17	4	2	2	2	103	26.890	10.758	16.132	1.74043+00	5.72523-09	9.05146-09	4.10785-08	2.57347-06	0
18	1	3	2	4	103	3212.425	3212.258	0.167	4.62827-01	1.42071-08	1.42081-08	1.06228-07	2.56223-06	0
19	1	2	1	3	103	1299.680	1296.726	2.953	1.03447+00	1.20275-08	1.20423-08	8.52648-08	2.56870-06	0
20	2	2	1	4	98	118.372	54.837	38.534	4.42153+00	4.42078-09	6.84096-09	9.43936-08	2.45392-06	0
21	1	3	2	5	102	3212.258	3212.256	0.002	4.63103-01	1.93243-08	1.93243-08	1.16350-07	2.56728-06	0
22	1	2	2	4	103	1296.726	1284.580	12.147	1.13140+00	9.44863-09	9.49320-09	9.14086-08	2.57904-06	0
23	1	2	2	3	98	54.837	54.744	0.094	4.46286+00	1.74549-08	1.74698-08	9.19287-08	2.44569-06	0
24	4	1	2	5	98	38.534	38.078	0.457	5.52742+00	1.43258-08	1.44188-08	1.15451-07	2.43920-06	0
25	2	3	1	5	103	3212.256	2725.911	461.345	3.95638-01	3.04242-09	4.99657-09	1.22813-07	2.57051-06	0
26	2	2	1	4	104	1284.580	283.728	975.852	5.44428-01	1.14157-09	2.90340-09	9.98975-08	2.59710-06	0
27	1	2	2	4	97	54.744	53.350	1.394	4.30260+00	1.29296-08	1.30974-08	8.79869-08	2.43022-06	0
28	2	3	2	6	103	2725.911	2589.143	86.768	4.70658-01	6.33217-09	6.78614-09	1.45308-07	2.57990-06	0
29	1	1	2	5	104	461.345	458.273	3.072	1.00879+00	1.09420-08	1.09818-08	1.34430-07	2.59437-06	0
30	1	2	2	5	104	283.728	277.497	6.231	6.93165-01	1.05192-08	1.06366-08	1.18203-07	2.60818-06	0
31	2	1	2	4	105	975.852	187.748	738.103	-3.16387-01	8.82381-10	2.50891-09	1.00799-07	2.62262-06	0
32	1	2	1	3	97	53.350	46.608	6.742	4.57078+00	9.83275-09	1.05852-08	8.55803-08	2.42468-06	0

33	1	3	1	6	104	2589.143	2589.106	0.038	4.69658-01	1.57845-08	1.57850-08	1.57048-07	2.58588-06	0
34	1	2	1	6	102	86.768	86.605	0.163	5.50834+00	1.72861-08	1.73037-08	1.61949-07	2.56252-06	0
35	1	1	1	6	104	458.273	452.291	5.981	1.12329+00	1.01760-08	1.02431-08	1.40766-07	2.60443-06	0
36	1	2	1	5	105	277.497	259.549	17.948	5.01823-01	8.59410-09	8.91252-09	1.28675-07	2.61688-06	0
37	1	1	1	5	105	187.748	181.022	6.727	5.77637+00	9.79012-09	9.97035-09	1.20160-07	2.61628-06	0
38	2	2	1	4	106	738.103	709.471	3.632	2.04288+00	7.96098-09	8.13401-09	9.29848-08	2.64588-06	0
39	1	2	1	4	96	46.608	46.482	0.126	4.53179+00	1.77583-08	1.77844-08	8.25554-08	2.40346-06	0
40	1	3	1	7	103	2589.106	2589.099	0.007	4.70087-01	1.78230-08	1.78231-08	1.66881-07	2.59087-06	0
41	1	2	1	7	103	86.605	86.498	0.108	5.48189+00	1.80511-08	1.80633-08	1.61897-07	2.56257-06	0
42	3	1	2	6	105	452.291	47.999	354.293	-1.28254+00	5.74939-10	3.31490-09	1.49106-07	2.62181-06	0
43	2	2	1	6	105	259.549	100.547	134.003	1.07954+00	3.13933-09	5.42172-09	1.44615-07	2.62563-06	0
44	1	1	2	5	104	181.022	179.234	1.788	5.90920+00	1.18870-08	1.19512-08	1.29688-07	2.61099-06	0
45	1	2	2	3	106	709.471	708.793	0.678	2.01197+00	1.41455-08	1.41523-08	8.77972-08	2.65604-06	0
46	4	1	2	5	107	3.632	2.711	0.921	1.25395+00	1.26537-08	1.48640-08	1.11869-07	2.65697-06	0
47	4	2	2	4	97	46.482	27.728	18.753	5.22004+00	6.81110-09	8.81854-09	8.27064-08	2.40429-06	0
48	2	3	2	7	104	2589.099	2200.318	338.781	3.54817-01	4.46520-09	5.70321-09	1.73859-07	2.59441-06	0
49	3	2	2	7	102	86.498	0.903	35.595	4.01343+00	6.67869-10	6.53789-09	1.69995-07	2.55421-06	0
50	2	2	1	6	106	354.293	306.569	22.723	1.02065+00	6.74504-09	7.29955-09	1.55742-07	2.64549-06	0
51	1	2	2	7	106	100.547	100.208	0.339	1.13761+00	1.52939-08	1.53198-08	1.61095-07	2.65643-06	0
52	1	1	1	6	104	134.003	133.998	0.005	6.17354+00	2.48328-08	2.48333-08	1.52717-07	2.62468-06	0
53	2	1	1	6	104	179.234	59.690	94.544	6.86484+00	2.81285-09	4.87422-09	1.47322-07	2.60407-06	0
54	1	2	2	4	107	708.793	708.759	0.035	2.01899+00	1.91290-08	1.91295-08	8.27599-08	2.66671-06	0
55	2	3	1	8	104	2200.318	1922.021	253.297	4.23563-01	3.84176-09	5.57809-09	1.94873-07	2.60220-06	0
56	2	2	1	7	105	338.781	236.618	77.163	9.53313-01	4.99987-09	6.09565-09	1.79202-07	2.62058-06	0
57	1	2	1	7	101	35.595	35.535	0.060	5.61504+00	1.91370-08	1.91559-08	1.86606-07	2.54010-06	0
58	1	2	2	7	106	306.569	305.856	0.713	1.06889+00	1.40601-08	1.40765-08	1.62660-07	2.65677-06	0
59	4	1	2	6	107	22.723	22.698	0.026	2.52080+00	1.96655-08	1.96775-08	1.38398-07	2.65911-06	0
60	1	2	2	6	107	100.208	100.134	0.073	1.11052+00	1.78652-08	1.78718-08	1.66012-07	2.66706-06	0
61	1	1	2	8	105	133.998	94.150	39.848	5.37850+00	5.48802-09	6.66833-09	1.95634-07	2.61996-06	0
62	1	1	2	8	105	59.690	57.458	2.232	8.42008-01	1.14556-08	1.16954-08	1.91738-07	2.63328-06	0
63	1	1	1	7	103	94.544	75.347	19.197	4.82659+00	7.15373-09	8.01342-09	1.67039-07	2.57409-06	0
64	2	2	1	3	107	708.759	420.417	263.342	1.53625+00	3.40128-09	4.55098-09	7.93756-08	2.67375-06	0
65	1	3	2	8	105	1922.021	1922.018	0.003	4.23093-01	1.86803-08	1.86803-08	2.07641-07	2.60795-06	0
66	1	1	2	9	104	253.297	247.863	5.434	5.68191+00	9.84839-09	9.96505-09	2.19723-07	2.59155-06	0
67	1	2	2	8	105	236.618	236.038	0.580	1.00285+00	1.44008-08	1.44185-08	1.87845-07	2.63276-06	0
68	1	1	2	7	106	77.163	77.068	0.094	2.37787+00	1.72316-08	1.72430-08	1.62948-07	2.63767-06	0
69	1	2	1	8	102	35.535	35.203	0.332	5.54251+00	1.59586-08	1.60401-08	1.88845-07	2.53847-06	0
70	1	2	2	6	107	305.856	305.834	0.023	1.06028+00	1.98676-08	1.98683-08	1.67335-07	2.66529-06	0
71	2	2	1	7	107	100.134	45.538	29.596	1.66300+00	4.52646-09	7.08309-09	1.68525-07	2.67213-06	0
72	1	1	1	9	105	94.150	94.147	0.003	5.37323+00	2.62030-08	2.62033-08	2.04313-07	2.60892-06	0
73	2	1	1	8	106	57.458	27.373	5.085	3.30028-02	4.97310-09	7.20510-09	2.00238-07	2.64280-06	0
74	1	1	1	6	102	75.347	75.291	0.056	4.85375+00	1.96726-08	1.96798-08	1.69484-07	2.55277-06	0
75	2	2	2	3	108	420.417	309.064	61.353	9.95653-01	5.27967-09	6.15777-09	8.01671-08	2.69665-06	0
76	1	1	2	2	107	263.342	236.345	26.997	2.42431+00	6.87296-09	7.29039-09	5.42273-08	2.68094-06	0
77	1	3	2	9	104	1922.018	1921.874	0.144	4.26116-01	1.43798-08	1.43812-08	2.18914-07	2.61303-06	0
78	1	1	1	9	103	247.863	243.232	4.631	5.81903+00	1.06596-08	1.07606-08	2.29817-07	2.58462-06	0
79	1	2	2	7	106	236.038	236.018	0.020	9.93704-01	2.01043-08	2.01051-08	1.91849-07	2.63903-06	0
80	1	1	2	6	107	77.068	77.006	0.062	2.41569+00	1.80083-08	1.80162-08	1.37930-07	2.66162-06	0
81	4	2	2	8	102	35.203	3.211	31.992	6.80649+00	2.41662-09	8.00126-09	1.96001-07	2.53193-06	0
82	1	2	2	7	108	305.834	298.560	7.273	9.05450-01	1.02716-08	1.03960-08	1.83179-07	2.69358-06	0
83	4	2	2	7	108	45.538	36.854	8.685	2.11493+00	9.01395-09	1.00199-08	1.66427-07	2.69481-06	0
84	4	1	2	8	108	29.596	29.592	0.005	4.00429-01	2.28551-08	2.28571-08	1.83987-07	2.67898-06	0
85	1	1	2	9	104	94.147	90.996	3.152	5.12717+00	1.08587-08	1.10615-08	2.15133-07	2.59500-06	0
86	1	1	1	9	105	27.373	27.281	0.092	9.10713-02	1.86062-08	1.86376-08	2.23305-07	2.64356-06	0
87	4	1	1	9	107	5.085	5.082	0.003	1.62862+00	2.58113-08	2.58193-08	1.99224-07	2.67351-06	0
88	4	1	2	7	103	75.291	42.528	32.763	3.83732+00	5.07080-09	6.97955-09	1.69304-07	2.55403-06	0
89	1	2	1	4	108	309.064	308.441	0.623	1.02933+00	1.48201-08	1.48363-08	8.71868-08	2.70748-06	0
90	1	2	1	2	108	61.353	60.147	1.206	2.46118+00	1.35989-08	1.37463-08	5.90820-08	2.71032-06	0
91	1	1	1	2	108	236.345	233.453	2.892	2.53515+00	1.15851-08	1.16566-08	4.33563-08	2.69042-06	0
92	1	3	1	9	105	1921.874	1903.575	18.299	4.00928-01	8.38412-09	8.55510-09	2.26916-07	2.61666-06	0
93	1	1	1	10	104	243.232	243.219	0.013	5.81177+00	2.27861-08	2.27867-08	2.39652-07	2.57970-06	0
94	1	2	2	8	107	236.018	234.481	1.537	9.12918-01	1.27935-08	1.28354-08	2.10157-07	2.66715-06	0
95	3	1	1	6	107	77.006	0.335	51.671	3.92046+00	3.69228-10	5.59578-09	1.41431-07	2.65852-06	1
96	1	2	1	8	108	298.560	285.832	12.728	1.06064+00	9.27156-09	9.49374-09	1.91445-07	2.70412-06	0
97	3	1	1	9	103	90.996	2.974	63.022	3.73815+00	9.70433-10	5.36821-09	3.21984-07	2.57944-06	0
98	4	1	2	9	106	27.281	15.353	11.927	-9.28703-01	6.25882-09	8.63304-09	2.19648-07	2.64323-06	0

99	1	2	1	3	109	308.441	308.390	0.050	1.01976+00	1.94736-08	1.94754-08	9.15545-08	2.71474-06	0
100	4	2	2	3	109	60.147	29.876	30.271	3.24987+00	5.69824-09	8.08516-09	5.08737-08	2.71696-06	0
101	2	1	2	1	108	233.453	84.505	98.948	1.15475+00	2.59204-09	4.67278-09	2.96720-08	2.69991-06	0
102	2	3	2	10	105	1903.575	1214.936	638.639	4.69388-01	1.33249-09	5.12519-09	2.44923-07	2.62430-06	0
103	3	1	2	10	103	243.219	22.551	170.668	3.21690+00	5.13473-10	4.11941-09	2.46125-07	2.57640-06	0
104	2	2	1	9	107	234.481	196.214	13.267	1.21809+00	6.94685-09	7.65789-09	2.17533-07	2.67670-06	0
105	1	1	2	6	107	51.671	51.597	0.074	2.40015+00	1.76773-08	1.76910-08	1.37909-07	2.66209-06	0
106	2	2	2	8	109	285.832	76.807	159.025	3.47919-02	2.73217-09	5.27062-09	2.00183-07	2.71973-06	0
107	1	1	1	10	103	63.022	62.987	0.034	5.28556+00	2.06819-08	2.06876-08	2.32619-07	2.56378-06	0
108	3	2	2	4	109	308.390	42.073	216.317	2.21223+00	1.82428-09	4.93900-09	9.60427-08	2.72204-06	0
109	1	1	1	1	109	84.505	83.802	0.703	1.06343+00	1.44119-08	1.44722-08	3.76491-08	2.71797-06	0
110	1	3	1	10	106	1214.936	1214.935	0.001	4.69190-01	2.06282-08	2.06283-08	2.59303-07	2.63159-06	0
111	2	2	1	11	105	638.639	370.765	242.874	6.27854-01	3.43700-09	4.65620-09	2.71416-07	2.62797-06	0
112	1	2	1	11	103	170.668	153.550	17.118	5.69809+00	8.48878-09	8.99219-09	2.69327-07	2.56802-06	0
113	3	2	2	9	108	196.214	7.275	138.939	-1.58941-01	1.04183-09	5.41059-09	2.24144-07	2.69466-06	0
114	4	1	2	10	107	13.267	5.359	7.908	4.76311+00	5.54210-09	9.32496-09	2.41459-07	2.67126-06	0
115	3	1	1	5	107	51.597	0.847	25.750	3.84246+00	8.06199-10	6.29198-09	1.29058-07	2.67019-06	0
116	1	2	2	9	108	76.807	76.792	0.015	4.87301-02	2.05839-08	2.05859-08	2.23997-07	2.72056-06	0
117	1	2	2	9	110	159.025	159.024	0.001	1.60770+00	2.58545-08	2.58545-08	1.99163-07	2.74905-06	0
118	1	1	1	10	102	62.987	46.534	16.454	4.74910+00	7.13012-09	8.29544-09	2.41710-07	2.54970-06	0
119	1	2	1	5	109	216.317	215.740	0.577	6.80175-01	1.49586-08	1.49803-08	1.15404-07	2.73650-06	0
120	1	1	2	2	109	83.802	68.621	15.181	1.66040+00	7.37847-09	8.23173-09	4.17778-08	2.72540-06	0
121	1	3	2	11	106	1214.935	1203.314	11.621	4.35265-01	9.32417-09	9.44128-09	2.77894-07	2.64101-06	0
122	1	2	2	11	106	370.765	370.502	0.263	6.01234-01	1.57214-08	1.57270-08	2.83896-07	2.63703-06	0
123	1	1	2	11	104	242.874	242.842	0.032	5.60607+00	1.92427-08	1.92441-08	2.87107-07	2.61496-06	0
124	1	2	2	11	102	153.550	150.895	2.655	5.82998+00	1.18920-08	1.19962-08	2.80253-07	2.56079-06	0
125	1	2	1	10	108	138.939	138.936	0.003	1.41546+00	2.46849-08	2.46852-08	2.25607-07	2.70378-06	0
126	4	1	2	5	108	25.750	25.579	0.171	2.38058+00	1.61221-08	1.61806-08	1.13565-07	2.68855-06	0
127	2	2	1	9	109	76.792	31.075	20.718	-5.23210-01	4.38444-09	7.36892-09	2.19298-07	2.72033-06	0
128	3	2	1	8	110	159.024	16.041	117.983	1.96489+00	8.71572-10	5.58158-09	1.99332-07	2.74446-06	0
129	1	1	1	9	101	46.534	46.385	0.149	4.80572+00	1.76052-08	1.76335-08	2.42557-07	2.52664-06	0
130	2	2	2	5	110	215.740	110.264	55.476	-9.41268-02	4.45794-09	6.23568-09	1.24414-07	2.74379-06	0
131	1	1	1	2	110	68.621	63.524	5.098	1.93644+00	1.03909-08	1.07998-08	3.99142-08	2.74614-06	0
132	2	3	1	12	106	1203.314	926.541	251.773	4.65342-01	1.17217-09	5.58387-09	2.94555-07	2.64876-06	0
133	1	2	2	12	105	370.502	370.465	0.037	6.11230-01	1.90305-08	1.90314-08	2.89078-07	2.64059-06	0
134	1	1	2	12	105	242.842	242.648	0.194	5.56841+00	1.59043-08	1.59112-08	2.89670-07	2.61290-06	0
135	1	2	2	12	103	150.895	150.886	0.009	5.82220+00	2.14263-08	2.14269-08	2.90469-07	2.55581-06	0
136	1	2	2	10	109	138.936	138.923	0.013	1.42514+00	2.08173-08	2.08183-08	2.29402-07	2.72802-06	0
137	4	2	2	10	109	31.075	31.045	0.030	5.72886+00	1.93840-08	1.93934-08	2.39792-07	2.70851-06	0
138	4	1	2	10	110	20.718	20.518	0.200	8.17194-01	1.58359-08	1.59193-08	2.38709-07	2.73622-06	0
139	3	1	2	8	111	117.983	39.951	28.032	2.04655-02	2.99017-09	5.62733-09	2.02399-07	2.76991-06	0
140	4	1	2	10	102	46.385	34.150	12.235	4.06574+00	7.25771-09	8.59046-09	2.42346-07	2.52890-06	0
141	1	2	1	6	110	110.264	95.763	14.501	5.91543+00	8.58543-09	9.27246-09	1.45706-07	2.74178-06	0
142	3	2	1	5	111	55.476	9.558	20.919	9.24316-01	2.34970-09	7.36183-09	1.26684-07	2.76783-06	0
143	1	1	2	1	110	63.524	62.302	1.222	1.75061+00	1.25476-08	1.26806-08	3.73731-08	2.75278-06	0
144	1	3	2	12	107	926.541	926.540	0.000	4.65093-01	2.10059-08	2.10059-08	3.09404-07	2.65622-06	0
145	2	1	2	13	106	251.773	200.768	1.005	8.59302-01	5.54772-09	6.28082-09	3.20898-07	2.65476-06	0
146	2	2	1	13	107	370.465	338.462	7.003	3.89880-01	7.56883-09	7.95062-09	3.27350-07	2.66740-06	0
147	2	1	1	12	104	242.648	100.904	116.744	6.43836+00	2.97029-09	4.60608-09	2.99288-07	2.60455-06	0
148	3	2	1	12	102	150.886	15.847	110.039	6.20349+00	9.63389-10	5.66814-09	2.95426-07	2.55335-06	0
149	2	2	1	10	110	138.923	103.714	10.209	1.80639+00	6.63636-09	7.79400-09	2.30341-07	2.73442-06	1
150	4	2	2	9	112	28.032	28.032	0.000	2.01171+00	3.32711-08	3.32711-08	1.94911-07	2.78580-06	0
151	1	2	2	6	109	95.763	95.076	0.687	6.00022+00	1.41159-08	1.41668-08	1.53955-07	2.73860-06	0
152	4	1	2	5	112	20.919	9.854	11.064	2.97532+00	5.71721-09	8.75870-09	1.20952-07	2.79223-06	0
153	1	1	2	2	111	62.302	62.154	0.148	1.81561+00	1.63981-08	1.64193-08	3.40153-08	2.77125-06	0
154	2	3	2	14	107	926.540	588.249	288.291	5.29488-01	1.41935-09	5.84554-09	3.44295-07	2.67373-06	0
155	1	1	1	14	108	200.768	180.467	20.301	5.35694-01	7.50109-09	7.91175-09	3.54038-07	2.69320-06	0
156	4	2	1	14	106	1.005	0.942	0.064	5.23471+00	1.89304-08	1.96172-08	3.32305-07	2.64153-06	0
157	1	2	1	14	108	338.462	338.446	0.017	3.84602-01	2.15406-08	2.15411-08	3.58041-07	2.68002-06	0
158	4	1	2	13	108	7.003	3.589	3.414	2.97374+00	7.38977-09	1.07676-08	3.20255-07	2.69033-06	0
159	1	1	2	13	104	100.904	91.070	9.834	5.82381-01	8.46989-09	8.95670-09	3.20813-07	2.60792-06	0
160	2	1	2	12	103	116.744	54.269	12.475	6.05227+00	3.86385-09	5.96678-09	3.03115-07	2.58009-06	0
161	1	1	2	13	102	110.039	109.678	0.361	5.57497+00	1.47646-08	1.47910-08	3.15568-07	2.53861-06	0
162	1	2	1	10	110	103.714	103.706	0.009	1.81331+00	2.27531-08	2.27541-08	2.27927-07	2.74448-06	0
163	4	1	2	10	110	10.209	10.064	0.144	5.65555-01	1.64229-08	1.65505-08	2.41625-07	2.73927-06	0
164	1	2	2	7	110	95.076	94.940	0.136	5.96232+00	1.68192-08	1.68313-08	1.69692-07	2.73403-06	0

165	1	1	1	1	111	62.154	49.505	12.649	1.34759+00	7.83693-09	8.78121-09	3.35634-08	2.77306-06	0
166	1	3	1	14	108	588.249	588.248	0.001	5.29089-01	1.97954-08	1.97954-08	3.59945-07	2.68288-06	0
167	1	2	1	14	108	288.291	288.287	0.004	2.17137-01	2.43984-08	2.43985-08	3.55231-07	2.67617-06	0
168	2	1	2	15	108	180.467	121.131	9.336	1.38140+00	4.84919-09	6.04620-09	3.69419-07	2.70233-06	0
169	1	2	1	15	107	338.446	333.238	5.208	4.77709-01	1.10124-08	1.11055-08	3.69538-07	2.68467-06	0
170	1	1	1	13	105	91.070	88.710	2.360	4.20693-01	1.19634-08	1.21215-08	3.29950-07	2.61394-06	0
171	1	1	2	13	104	54.269	54.267	0.002	6.04397+00	2.43910-08	2.43915-08	3.19264-07	2.57629-06	0
172	4	2	2	12	103	12.475	11.252	1.222	3.84481+00	1.30502-08	1.37407-08	2.91114-07	2.56048-06	0
173	2	1	1	13	101	109.678	52.285	32.394	6.38367+00	4.19927-09	6.08200-09	3.24390-07	2.53105-06	0
174	3	2	2	9	110	103.706	5.908	47.797	4.83528-01	1.51439-09	6.34468-09	2.27950-07	2.74438-06	0
175	2	2	1	7	109	94.940	68.389	1.551	6.36297+00	6.89277-09	8.25883-09	1.72857-07	2.73298-06	0
176	4	1	2	2	112	49.505	49.045	0.460	1.21874+00	1.43151-08	1.43878-08	3.86401-08	2.79542-06	0
177	1	3	1	15	107	588.248	588.128	0.120	5.32827-01	1.44050-08	1.44111-08	3.67367-07	2.68722-06	0
178	2	2	1	15	107	288.287	207.827	55.460	6.17382-01	5.40032-09	6.46776-09	3.70361-07	2.67951-06	0
179	1	1	2	14	109	121.131	121.128	0.004	1.37408+00	2.33408-08	2.33412-08	3.72898-07	2.72047-06	0
180	4	2	1	16	108	9.336	6.285	3.050	5.45503+00	9.61972-09	1.19735-08	3.89718-07	2.69386-06	0
181	2	2	2	16	108	333.238	251.728	31.510	9.95049-01	5.74423-09	6.60911-09	3.81956-07	2.69110-06	1
182	1	1	1	14	104	88.710	88.679	0.031	4.39377-01	2.09084-08	2.09121-08	3.41105-07	2.61893-06	0
183	3	1	1	13	103	54.267	0.015	29.252	4.48991+00	1.03408-10	6.17784-09	3.18974-07	2.57636-06	0
184	4	1	2	14	102	52.285	44.588	7.697	6.33118-01	8.58988-09	9.37084-09	3.45412-07	2.53317-06	0
185	4	1	2	14	101	32.394	6.035	26.358	6.68989+00	2.50793-09	7.32906-09	3.26804-07	2.50710-06	0
186	1	2	1	9	111	47.797	44.298	3.499	2.25797+00	1.16226-08	1.21137-08	2.16297-07	2.76657-06	0
187	1	2	2	8	110	68.389	67.936	0.453	-1.66929-03	1.48067-08	1.48559-08	1.99975-07	2.73514-06	0
188	4	1	2	8	109	1.551	0.488	1.063	6.46051+00	6.48825-09	1.28228-08	1.78395-07	2.71237-06	0
189	2	3	1	16	108	588.128	529.855	33.273	5.99542-01	5.57131-09	7.26428-09	3.93155-07	2.70243-06	0
190	1	2	2	16	109	207.827	207.805	0.022	6.07147-01	1.99370-08	1.99380-08	4.11375-07	2.70863-06	0
191	1	1	2	16	107	55.460	55.375	0.085	5.46002+00	1.74200-08	1.74345-08	3.87352-07	2.66300-06	0
192	3	1	1	15	109	121.120	6.056	09.272	2.70467+00	1.17669-09	4.94606-09	3.72907-07	2.72062-06	0
193	2	2	2	16	109	251.728	88.253	113.475	5.79232-02	3.32337-09	5.61279-09	4.00325-07	2.71940-06	0
194	4	2	2	16	108	31.510	6.113	25.397	6.82212+00	3.67906-09	8.35273-09	3.95713-07	2.68217-06	0
195	3	1	2	14	105	88.679	14.335	24.345	-1.55261+00	1.71335-09	5.70079-09	3.45808-07	2.62114-06	0
196	4	1	2	14	103	29.252	14.319	14.933	4.91885+00	5.51622-09	8.25908-09	3.42788-07	2.57098-06	0
197	1	2	1	8	111	44.298	28.968	15.331	1.81219+00	7.25307-09	9.17828-09	2.09175-07	2.77525-06	0
198	1	2	2	9	110	67.936	67.507	0.429	6.20199+00	1.48977-08	1.49449-08	2.23788-07	2.73510-06	0
199	1	3	2	17	108	529.855	529.853	0.001	6.00056-01	1.99763-08	1.99763-08	4.13689-07	2.71647-06	0
200	4	1	2	17	108	33.273	26.255	7.019	5.29170+00	8.36642-09	9.52756-09	4.17905-07	2.69364-06	0
201	1	2	2	17	108	207.805	207.365	0.441	6.53216-01	1.48571-08	1.48729-08	4.15961-07	2.71181-06	0
202	3	1	1	16	106	55.375	0.278	30.097	3.96012+00	4.35757-10	6.15147-09	3.95509-07	2.65420-06	0
203	1	1	2	15	110	89.272	85.593	3.678	8.60315-01	1.05789-08	1.08237-08	3.83617-07	2.74345-06	0
204	1	2	2	17	108	88.253	88.240	0.013	7.01591-02	2.07925-08	2.07941-08	4.23542-07	2.72074-06	0
205	1	2	2	17	110	113.475	113.474	0.001	1.63085+00	2.64053-08	2.64054-08	3.98642-07	2.74842-06	0
206	4	2	1	15	106	24.345	24.150	0.195	8.11748-01	1.69427-08	1.70167-08	3.62352-07	2.63638-06	0
207	5	2	2	9	112	28.968	13.275	15.693	2.63936+00	6.15646-09	9.09431-09	2.08122-07	2.77953-06	1
208	3	2	1	10	110	67.507	19.618	22.890	5.60484+00	3.49996-09	7.29393-09	2.30838-07	2.73453-06	1
209	2	3	1	17	109	529.853	403.696	101.158	5.85080-01	6.56314-10	6.42193-09	4.20098-07	2.72085-06	0
210	1	2	2	18	109	207.365	199.888	7.477	8.44259-01	1.02131-08	1.04023-08	4.42224-07	2.73191-06	0
211	4	1	2	17	106	30.097	29.995	0.102	5.45325+00	1.70824-08	1.71139-08	4.12570-07	2.63824-06	0
212	1	1	1	16	110	85.593	73.157	12.436	1.25138+00	8.14734-09	8.81268-09	3.91633-07	2.75277-06	0
213	1	2	1	18	108	88.240	88.230	0.010	7.80869-02	2.25466-08	2.25479-08	4.48172-07	2.72247-06	0
214	3	2	1	16	110	113.474	14.717	73.757	2.10700+00	1.45048-09	6.14815-09	3.98911-07	2.74395-06	0
215	5	1	2	10	110	22.890	22.751	0.139	5.23356-01	1.65061-08	1.65608-08	2.42052-07	2.73953-06	0
216	1	3	2	18	109	403.696	403.237	0.459	5.96851-01	1.30548-08	1.30739-08	4.42200-07	2.73549-06	0
217	1	1	2	18	109	101.158	100.988	0.169	7.56979-01	1.61519-08	1.61666-08	4.39039-07	2.73680-06	0
218	2	2	1	18	110	199.888	150.642	24.246	4.68421-01	6.20480-09	7.24890-09	4.52148-07	2.74308-06	0
219	1	1	1	15	111	73.157	73.144	0.013	1.23811+00	2.27730-08	2.27750-08	3.96526-07	2.76756-06	0
220	3	2	2	18	109	88.230	11.128	27.102	-1.12964+00	2.37601-09	6.69029-09	4.43950-07	2.72214-06	0
221	4	1	2	17	111	73.757	35.279	38.478	2.31518-01	4.42919-09	6.72372-09	4.03463-07	2.76924-06	0
222	2	3	2	19	110	403.237	352.314	0.923	7.06190-01	6.43544-09	7.83582-09	4.67685-07	2.75281-06	0
223	2	1	1	19	111	100.988	28.344	47.645	-2.55480-01	3.01202-09	5.68546-09	4.73563-07	2.76950-06	0
224	1	2	1	20	110	150.642	150.196	0.446	5.09253-01	1.54264-08	1.54513-08	4.92254-07	2.76337-06	0
225	4	1	2	18	111	24.246	16.136	8.109	2.72648+00	7.40892-09	9.28233-09	4.44581-07	2.76746-06	0
226	3	1	2	16	111	73.144	7.156	15.989	3.75124+00	8.54162-10	5.88276-09	3.97292-07	2.76978-06	0
227	4	2	1	19	110	27.102	21.748	5.354	7.77281-01	1.06746-08	1.20430-08	4.65400-07	2.73227-06	0
228	2	3	2	20	111	352.314	259.700	42.613	8.24984-01	4.08733-09	7.19770-09	4.92840-07	2.77427-06	0
229	4	2	1	20	110	0.923	0.917	0.006	5.97918+00	2.33369-08	2.34261-08	4.81463-07	2.74752-06	0
230	1	1	1	20	110	28.344	26.309	2.034	6.29893+00	1.21853-08	1.26476-08	4.99801-07	2.76265-06	0

231	4	1	2	20	112	47.645	30.748	16.897	4.28218-01	6.31776-09	8.05487-09	4.79850-07	2.79357-06	0
232	2	2	1	21	111	150.196	100.806	24.390	9.43828-01	5.80975-09	7.24417-09	5.18389-07	2.77796-06	0
233	4	2	1	17	112	15.989	12.697	3.292	7.49165-01	1.15090-08	1.30598-08	4.07375-07	2.78922-06	0
234	1	3	1	20	112	259.700	259.277	0.423	8.14430-01	1.29032-08	1.29471-08	4.96255-07	2.77796-06	1
235	4	2	2	22	112	42.613	42.608	0.005	9.09701-02	2.23168-08	2.23183-08	5.27028-07	2.77777-06	0
236	4	1	2	21	111	26.309	25.395	0.914	2.66560-01	1.30413-08	1.32944-08	5.22213-07	2.76300-06	0
237	1	2	2	21	112	100.806	78.769	22.037	4.57309-01	7.57573-09	8.57016-09	5.28784-07	2.79231-06	0
238	4	1	2	22	111	24.390	20.358	4.032	5.29429+00	1.02252-08	1.12876-08	5.41455-07	2.76762-06	0
239	1	3	1	20	112	259.277	258.630	0.647	8.01388-01	1.24006-08	1.24654-08	5.08148-07	2.79057-06	0
240	1	2	2	22	112	78.769	63.248	15.521	9.17244-01	8.16457-09	9.11142-09	5.30266-07	2.79304-06	1
241	2	3	2	21	112	258.630	208.315	0.315	9.22965-01	5.54197-09	7.84871-09	5.17152-07	2.79986-06	0
242	1	2	1	22	112	63.248	59.318	3.930	1.10478+00	1.14354-08	1.18416-08	5.39052-07	2.80451-06	0
243	1	3	1	21	113	208.315	201.173	7.142	8.77216-01	8.91138-09	9.62332-09	5.29914-07	2.81673-06	0
244	5	2	2	22	112	0.315	0.025	0.291	1.30421+00	1.27158-08	4.53809-08	4.93722-07	2.79946-06	1
245	1	2	1	21	113	59.318	59.303	0.015	1.09288+00	2.17593-08	2.17623-08	5.44277-07	2.81490-06	0
246	1	3	2	22	113	201.173	195.429	5.744	9.34917-01	1.01559-08	1.05515-08	5.40361-07	2.82929-06	0
247	3	2	2	22	113	59.303	0.226	9.077	2.60195+00	4.36829-10	7.08201-09	5.46361-07	2.81892-06	0
248	2	3	1	22	114	195.429	163.796	6.633	8.68972-01	4.54310-09	7.94141-09	5.49787-07	2.84206-06	0
249	4	2	2	23	114	9.077	5.241	3.836	1.73887+00	8.60165-09	1.13202-08	5.63839-07	2.84811-06	0
250	1	3	2	23	114	163.796	163.146	0.650	8.90920-01	1.26535-08	1.27187-08	5.52007-07	2.84469-06	1
251	4	1	2	23	115	6.633	0.549	6.085	-1.28786+00	6.71010-10	9.77127-09	5.50409-07	2.86524-06	0
252	1	3	2	23	114	163.146	163.021	0.125	9.00579-01	1.45406-08	1.45549-08	5.63286-07	2.85864-06	0
253	2	3	1	23	115	163.021	129.539	8.482	8.49569-01	3.01440-09	7.87810-09	5.60341-07	2.85492-06	1
254	2	3	1	23	115	129.539	100.802	3.737	8.10470-01	2.24801-09	8.04861-09	5.71585-07	2.86771-06	0
255	4	1	2	23	115	8.482	8.239	0.243	1.06584+00	1.54468-08	1.56927-08	5.64097-07	2.86811-06	0
256	1	3	2	24	115	100.802	100.751	0.051	8.18335-01	1.55669-08	1.55771-08	5.88332-07	2.88532-06	0
257	4	1	2	24	116	3.737	3.732	0.005	1.18276+00	2.26384-08	2.26557-08	5.79124-07	2.88380-06	0
258	1	3	1	24	116	100.751	78.052	22.699	7.82666-01	2.09724-09	8.31279-09	5.83533-07	2.88019-06	1
259	1	3	1	24	116	78.052	60.766	17.286	7.43225-01	2.43108-09	8.61929-09	5.95851-07	2.89244-06	0
260	1	3	2	25	116	60.766	60.592	0.173	7.61837-01	1.41614-08	1.42137-08	6.14521-07	2.90960-06	0
261	1	3	1	25	117	60.592	48.734	11.859	7.05953-01	3.90765-09	9.04567-09	6.21794-07	2.91654-06	0
262	4	3	2	26	118	48.734	47.479	1.255	7.60874-01	1.18617-08	1.22760-08	6.39898-07	2.93198-06	0

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(    0,  96)
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TABLE OF INTERSTITIALS

TYPE 1 - BERYLLIUM
TYPE 2 - OXYGEN
TYPE 3 - IODINE
TYPE 4 - MULTIPLE

POSITION		TYPE
2	103	2
2	112	1
3	109	2
4	97	2
5	98	1
5	107	1
5	108	1
5	112	1
6	107	1
7	103	1
7	108	2
8	102	2
8	108	1
8	109	1
9	106	1
9	107	1
9	112	4
10	102	1
10	107	1
10	109	2
10	110	4
12	103	2
13	108	1
14	101	1
14	102	1
14	103	1
14	106	2
15	106	2
16	108	2
17	106	1
17	108	1
17	111	1
17	112	2
18	111	1
19	110	2
20	110	2
20	112	1
21	111	1
22	111	1
22	112	4
23	114	2
23	115	1
24	116	1
26	118	3

27 BERYLLIUM INTERSTITIALS

19 OXYGEN INTERSTITIALS

48 VACANCIES

FINAL POSITION OF IODINE ATOM - (26, 118)

FLIGHT PROPULSION LABORATORY DEPARTMENT

GENERAL ELECTRIC