CHAPTER 4

THE DETERMINATION OF THE STRUCTURE

The structure of Nb_3As was calculated by using various computer programs as shown in Table 4.0.

Table 4.0 The crystallographic calculations were performed on a CDC 3100 computer using these programs.

Program	Calculation
FFCRL	Film factors.
LPARL	Correction for Lorentz-polarization effects and absorption for cylindrical or spherical crystals.
XSFRL	Interpolation of the X-ray scattering factors.
SFCRL	Calculation of structure factors, the temperature factor may be isotropic and or anisotropic and the anomalous dispersion correction terms may be included.
EXPRL	Expansion of reflection data for Fourier summations.
FORRL	Fourier summation.
LSQRL	Full matrix least-squares refinements.
DISTAN	Calculation of interatomic distances and angles.

These programs were obtained from the Institute of Chemistry, University of Uppsala, Sweden and were modified to be used with the CDC 3100 computer at Bangkok Data Center Co.,Ltd. by Professor R. Liminga of the University of Uppsala and the Crystallography Group, Faculty of Science, Chulalongkorn University.

4.1 Structure factor calculation

The collected observed intensity data as previously described constituted the material from which the crystal structure was derived.

The structure factor, $|F_{hkl}|$, is the most important quantity derived from these intensities. The relationship between the observed structure factor, $|F_o|$, and the intensity depends on the Lorentz-polarization factor,

$$|F_o|_{hkl} = \sqrt{\frac{KI_{hkl}}{Lp}} \quad \text{... (4.1.1)}$$

where L is the Lorentz-factor,

p is the polarization factor,

K is a constant for any given set of measurements.

The results of $|F_{relative}|$'s, $|F_{rel}|$, are defined by

$$|F_{rel}| = k'|F_o|$$

$$= \sqrt{\frac{I_{hkl}}{Lp}} \quad \text{... (4.1.2)}$$

In the course of this crystal structure analysis, structure factors were computed many times by using the program adapted from those used in the University of Uppsala, Sweden.

Some essential input of the computer program consists of raw intensity data from the five layers of the Weissenberg photographs, each reflection intensity being identified by its indices, h, k and l, and the cell parameters, and a list of atomic positions, which needed to be estimated first.

Before starting the computation of the structure factors, it was necessary to derive some constant functions for correcting the raw intensity data and we had to know the atomic positions in the unit cell of Nb_3As. These atomic positions could be obtained from Patterson functions and included in the F_o synthesis.

The input of the LPARL program were the observed intensities, the cell parameters and the absorption correction values of the crystal, A^*, and the output of this program was data corrected for the Lorentz-polarization factor.

The input data of the scattering factor values of both Nb and As at the appropriate $\frac{\sin\theta}{\lambda}$ values were the atomic scattering data at fixed interval as shown in Table 4.1.1. The input information is available in tabular form in the International Tables for X-ray Crystallography, Vol. III.

The anomalous dispersion is the effect when the wavelength of the incident beam lies near an absorption edge in the scattering element. This effect causes the scattering factor to be complex, it can be represented by

$$f_o^{anom.} = f_o + \Delta f' + i\,\Delta f'' \quad \ldots (4.1.3)$$

where f_o is the normal scattering factor,

$\Delta f'$ is a real correction term and

$\Delta f''$ is the imaginary component.

Table 4.1.1 The scattering factor of Nb and As atom, for MoK_α radiation, $\lambda_{K_\alpha} = 0.71068$ Å .

$\frac{\sin\theta}{\lambda}$	f_{Nb}	f_{As}
0.00	41.00	33.00
0.05	40.04	32.32
0.10	37.82	30.61
0.15	35.23	28.53
0.20	32.64	26.49
0.25	30.19	24.63
0.30	27.95	22.95
0.35	25.97	21.39
0.40	24.24	19.93
0.45	22.74	18.54
0.50	21.43	17.21
0.55	20.28	15.95
0.60	19.23	14.76
0.65	18.26	13.66
0.70	17.34	12.65
0.75	16.47	11.73
0.80	15.62	10.91
0.85	14.80	10.18
0.90	14.00	9.54
0.95	13.24	8.97
1.00	12.51	8.48
1.05	11.82	8.05
1.10	11.17	7.68
1.15	10.56	7.35
1.20	10.00	7.07

The correction terms $\Delta f'$ and $\Delta f''$ which arise from anomalous scattering are independent of $\sin\theta$.

For Nb atom, $\Delta f' = -2.19$ and $\Delta f'' = 0.86$.

For As atom, $\Delta f' = 0.12$ and $\Delta f'' = 2.17$.

For structure factor calculation, the space group $P4_2/n$ is classified as centrosymmetric.

The correction for thermal motion was applied to structure factor calculations. All of the atoms were assumed to be vibrating with the same amplitude about their rest positions, i.e. the vibration is isotropic. For the first structure factor calculation, we set the values of B's for Nb and As atoms as 0.25, where B is thermal parameter related to the magnitude of vibration.

The structure factor program usually puts out some summary information about the agreement between the observed and calculated data. The general agreement in magnitude is given by some sort of rescale factor.

The linear rescale factor is

$$LRS = \frac{\Sigma|F_c|}{\Sigma|F_o|} \qquad \ldots (4.1.4)$$

This rescale factors for individual levels were then used as the input scale factors for the corresponding levels in the next cycle of calculations. The over-all scale should be adjusted to bring $\Sigma|F_o|$ and $\Sigma|F_c|$ into agreement.

4.2 Determination of atomic positions

It is not possible to determine atomic positions directly from the intensities of X-ray diffraction. The interatomic vectors were determined from the Patterson synthesis.

Nb_3As is a tetragonal crystal, space group $P4_2/n$ whose co-ordinates of equivalent positions are :

$$\left.\begin{array}{l} x,\ y,\ z \\ \frac{1}{2}-x,\ \frac{1}{2}-y,\ z \\ \bar{y},\ \frac{1}{2}+x,\ \frac{1}{2}+z \\ \frac{1}{2}+y,\ \bar{x},\ \frac{1}{2}+z \\ \bar{x},\ \bar{y},\ \bar{z} \\ \frac{1}{2}+x,\ \frac{1}{2}+y,\ \bar{z} \\ y,\ \frac{1}{2}-x,\ \frac{1}{2}-z \\ \frac{1}{2}-y,\ x,\ \frac{1}{2}-z \end{array}\right\} \quad \text{for origin at } \bar{1}$$

and

$$\left.\begin{array}{l} x,\ y,\ z \\ \bar{x},\ \bar{y},\ z \\ \frac{1}{2}+x,\ \frac{1}{2}+y,\ \frac{1}{2}-z \\ \frac{1}{2}-x,\ \frac{1}{2}-y,\ \frac{1}{2}-z \\ \bar{y},\ x,\ \bar{z} \\ y,\ \bar{x},\ \bar{z} \\ \frac{1}{2}-y,\ \frac{1}{2}+x,\ \frac{1}{2}+z \\ \frac{1}{2}+y,\ \frac{1}{2}-x,\ \frac{1}{2}+z \end{array}\right\} \quad \text{for origin at } \bar{4}$$

The interatomic vectors of this space group, for the origin at $\bar{1}$, are shown in Table 4.2.1.

The Patterson function was calculated three dimentionally as projections about the c-axis.

The cell parameters of Nb_3As are a = 10.294, b = 10.294, c = 5.1958 Å, and there are 24 Nb atoms and 8 As atoms in each unit cell.

The Patterson function was projected along the c-axis at an interval of ca. 0.25 Å from W = 0.00 to 0.50. All of the significant peaks were found only on three sections at W = 0, 0.25 and 0.50 as shown in Fig.4.2.1. Therefore it was concluded that the niobium atoms must lie in the planes with the difference of $\frac{1}{4}c$ in height.

The peaks on the Harker line, as caused by the n-glide perpendicular to c, at $\frac{1}{2}\ \frac{1}{2}$ W where W(=2z) = 0 and 0.50 clearly indicate that the niobium atoms are at the heights of 0 (or 0.50) and 0.25 (or 0.75) respectively.

The first two sets of niobium atoms were found from the Harker plane UV0.5. The peak at 0.40, 0.02, 0.5, assumed to be corresponding to the vector $(x+y, -\frac{1}{2}-(x-y), \frac{1}{2})$, yields the values of x = -0.06 and y = 0.46. This information and that obtained from the Harker line led to the likely combination of certain co-ordinates of the "possible" set of atoms, which were then tested for their validity in generating the vectors which had to correspond to the actual Patterson peaks. An atom belonging to the first set of niobium atoms, Nb(1), was consequently assigned at -0.06, 0.46, 0.75. Another atom representing the second set of niobium atoms, Nb(2), was similarly deduced from the peak at 0.00, 0.18, 0.50 as the vector $-\frac{1}{2}+(x-y)$, $(x+y)$, $\frac{1}{2}$ which in turn gave its co-ordinates in real space at 0.34,-0.16, 0.75. The third and last set of niobium atoms,Nb(3), were expected to lie in the planes z = 0.00 and 0.50, and an atom of this set was located at x = 0.10, y = 0.26, z = 0.50 from the peak 0.34, 0.36, 0.50 found in the P(UV0.5) section corresponding to the vector $\frac{1}{2}+(x-y)$, $(x+y)$, $\frac{1}{2}$. These co-ordinates of the three crystallographically non-equivalent types of niobium atoms are tabulated in Table 4.2.2.

Table 4.2.1 Interatomic vectors derived from a general set of atoms in the space group $P4_2/n$ with the origin at $\bar{1}$.

Atomic position	x,y,z	$\frac{1}{2}-x,\frac{1}{2}-y,z$	$\bar{y},\frac{1}{2}+x,\frac{1}{2}+z$	$\frac{1}{2}+y,\bar{x},\frac{1}{2}+z$	$\bar{x},\bar{y},\bar{z}$	$\frac{1}{2}+x,\frac{1}{2}+y,\bar{z}$	$y,\frac{1}{2}-x,\frac{1}{2}-z$	$\frac{1}{2}-y,x,\frac{1}{2}-z$
x,y,z	$0,0,0$	$\frac{1}{2}-2x,\frac{1}{2}-2y,0$	$-(x+y), \frac{1}{2}+(x-y),\frac{1}{2}$	$\frac{1}{2}-(x-y), -(x+y),\frac{1}{2}$	$2\bar{x},2\bar{y},2\bar{z}$	$\frac{1}{2},\frac{1}{2},2\bar{z}$	$-(x-y), \frac{1}{2}-(x+y),\frac{1}{2}-2z$	$\frac{1}{2}-(x+y),x-y, \frac{1}{2}-2z$
$\frac{1}{2}-x,\frac{1}{2}-y,z$	$-\frac{1}{2}+2x,-\frac{1}{2}+2y, 0$	$0,0,0$	$-\frac{1}{2}+(x-y), x+y,\frac{1}{2}$	$x+y,-\frac{1}{2}-(x-y), \frac{1}{2}$	$-\frac{1}{2},-\frac{1}{2},2\bar{z}$	$2x,2y,2\bar{z}$	$-\frac{1}{2}+(x+y), -(x-y),\frac{1}{2}-2z$	$x-y,-\frac{1}{2}+(x+y), \frac{1}{2}-2z$
$\bar{y},\frac{1}{2}+x,\frac{1}{2}+z$	$x+y, -\frac{1}{2}-(x-y),-\frac{1}{2}$	$\frac{1}{2}-(x-y), -(x+y),-\frac{1}{2}$	$0,0,0$	$\frac{1}{2}+2y,-\frac{1}{2}-2x,0$	$-(x-y), -\frac{1}{2}-(x+y),-\frac{1}{2}-2z$	$\frac{1}{2}+(x+y), -(x-y),-\frac{1}{2}-2z$	$2y,2\bar{x},2\bar{z}$	$\frac{1}{2},-\frac{1}{2},2\bar{z}$
$\frac{1}{2}+y,\bar{x},\frac{1}{2}+z$	$-\frac{1}{2}+(x-y), x+y,-\frac{1}{2}$	$-(x+y), \frac{1}{2}+(x-y),-\frac{1}{2}$	$-\frac{1}{2}-2y,\frac{1}{2}+2x,0$	$0,0,0$	$-\frac{1}{2}-(x+y), x-y,-\frac{1}{2}-2z$	$x-y,\frac{1}{2}+(x+y), -\frac{1}{2}-2z$	$-\frac{1}{2},\frac{1}{2},2\bar{z}$	$2\bar{y},2x,2\bar{z}$
$\bar{x},\bar{y},\bar{z}$	$2x,2y,2z$	$\frac{1}{2},\frac{1}{2},2z$	$x-y,\frac{1}{2}+(x+y), \frac{1}{2}+2z$	$\frac{1}{2}+(x+y), -(x-y),\frac{1}{2}+2z$	$0,0,0$	$\frac{1}{2}+2x,\frac{1}{2}+2y,0$	$x+y,\frac{1}{2}-(x-y), \frac{1}{2}$	$\frac{1}{2}+(x-y),x+y, \frac{1}{2}$
$\frac{1}{2}+x,\frac{1}{2}+y,\bar{z}$	$-\frac{1}{2},-\frac{1}{2},2z$	$2\bar{x},2\bar{y},2z$	$-\frac{1}{2}-(x+y),x-y, \frac{1}{2}+2z$	$-(x-y), -\frac{1}{2}-(x+y),\frac{1}{2}+2z$	$-\frac{1}{2}-2x, -\frac{1}{2}-2y,0$	$0,0,0$	$-\frac{1}{2}-(x-y), -(x+y),\frac{1}{2}$	$-(x+y), -\frac{1}{2}+(x-y),\frac{1}{2}$
$y,\frac{1}{2}-x,\frac{1}{2}-z$	$x-y,-\frac{1}{2}+(x+y), -\frac{1}{2}+2z$	$\frac{1}{2}-(x+y),x-y, -\frac{1}{2}+2z$	$2\bar{y},2x,2z$	$\frac{1}{2},-\frac{1}{2},2z$	$-(x+y),-\frac{1}{2}-2y, -\frac{1}{2}$	$\frac{1}{2}+(x-y), -(x+y),-\frac{1}{2}$	$0,0,0$	$\frac{1}{2}-2y,-\frac{1}{2}+2x, 0$
$\frac{1}{2}-y,x,\frac{1}{2}-z$	$-\frac{1}{2}+(x+y), -(x-y),-\frac{1}{2}+2z$	$-(x-y), \frac{1}{2}-(x+y),-\frac{1}{2}+2z$	$-\frac{1}{2},\frac{1}{2},2z$	$2y,2\bar{x},2z$	$-\frac{1}{2}-(x-y), -(x+y),-\frac{1}{2}$	$x+y,\frac{1}{2}-(x-y), -\frac{1}{2}$	$-\frac{1}{2}+2y,\frac{1}{2}-2x,0$	$0,0,0$

Fig.4.2.1 Patterson sections for triniobium arsenide. (i) P(UV0), (ii) P(UV0.25), (iii) P(UV0.5), (iv) P(UV0.75).

(i)

TYPE OF SYNTHESIS = PATT

RMAX = 7.55 Z = .000 C = 132.3438542

	Y = 0.000	Y = 0.020	Y = 0.040	Y = 0.060	Y = 0.080	Y = 0.100	Y = 0.120	Y = 0.140	Y = 0.160	Y = 0.180	Y = 0.200	Y = 0.220	Y = 0.240
X= .0000	993	728	250	16	-26	-12	-5	-19	-18	7	31	39	29
X= .0201	720	519	160	-23	-57	-41	-25	-38	-43	-17	6	9	-3
X= .0401	253	166	15	-62	-84	-77	-52	-68	-64	-35	-19	-20	-27
X= .0601	15	-3	-41	-67	-90	-92	-33	-86	-75	-44	-34	-40	-41
X= .0801	-25	-32	-56	-74	-91	-89	-93	-89	-75	-41	-32	-40	-36
X= .1001	-12	-31	-67	-82	-95	-78	-70	-72	-57	-25	-18	-27	-25
X= .1201	-5	-31	-68	-82	-83	-81	-74	-65	-44	-9	3	-13	-26
X= .1401	-19	-36	-64	-72	-76	-84	-33	-63	-18	44	65	24	-22
X= .1601	-18	-25	-47	-44	-39	-50	-52	-30	32	123	148	70	-7
X= .1801	7	-1	-30	-24	-4	-2	4	9	52	145	165	76	-2
X= .2001	31	18	-23	-24	7	36	59	49	59	132	146	64	-1
X= .2201	39	30	-14	-26	1	47	86	73	67	125	131	52	-9
X= .2401	28	27	-11	-28	-16	20	37	43	29	71	73	12	-34
X= .2601	22	13	-16	-25	-13	17	37	45	2	2	3	-21	-34
X= .2801	49	17	-14	-14	10	66	112	104	34	-7	-13	-15	-9
X= .3001	71	30	-6	-13	7	53	105	99	36	-4	-18	-8	-5
X= .3201	50	27	-5	-23	-21	2	35	29	-7	-22	-17	-14	-17
X= .3401	11	13	-9	-31	-36	-29	-13	-15	-31	-31	-24	-25	-28
X= .3601	-7	2	-22	-41	-35	-31	-28	-30	-35	-23	-21	-35	-49
X= .3801	-3	-1	-29	-44	-23	-19	-22	-29	-31	-15	-3	-29	-57
X= .4001	11	[illegible]	-22	-33	-16	-7	-15	-28	-32	-13	-2	-32	-57
X= .4201	9	-7	-24	-28	-13	-17	-35	-46	-50	-35	-25	-50	-64
X= .4401	-6	-19	-35	-33	-16	-25	-47	-51	-47	-27	-10	-33	-52
X= .4601	2	-11	-31	-20	7	4	-19	-27	-15	20	49	20	-23
X= .4801	23	2	-20	6	49	55	25	-2	2	45	82	53	2
X= .5001	30	7	-12	30	98	114	70	22	5	23	56	48	15

	Y = 0.260	Y = 0.280	Y = 0.300	Y = 0.320	Y = 0.340	Y = 0.360	Y = 0.380	Y = 0.400	Y = 0.420	Y = 0.440	Y = 0.460	Y = 0.480	Y = 0.500
X= .0000	22	48	71	50	11	-7	-3	11	9	-6	2	23	30
X= .0201	4	49	80	51	3	-17	-6	28	36	2	-12	2	7
X= .0401	-22	16	45	19	-13	-22	-10	29	35	-12	-31	-14	-12
X= .0601	-34	2	31	-3	-37	-36	-28	-6	-3	-23	1	37	30
X= .0801	-13	50	92	40	-21	-24	-18	-18	-21	-2	72	124	98
X= .1001	9	91	140	78	1	-8	-0	-13	-28	0	98	145	114
X= .1201	-6	57	94	45	-12	-17	-9	-15	-34	-25	37	87	70
X= .1401	-31	-7	11	-7	-25	-19	-11	-5	-14	-24	3	32	22
X= .1601	-33	-29	-24	-31	-33	-22	-12	-4	-8	-20	-13	3	5
X= .1801	-21	-14	-10	-23	-35	-34	-26	-19	-24	-36	-32	-6	28
X= .2001	-18	-10	6	-3	-24	-31	-28	-23	-26	-35	-30	4	56
X= .2201	-35	-33	-11	-14	-34	-39	-36	-32	-26	-27	-24	2	48
X= .2401	-58	-62	-41	-37	-47	-35	-24	-29	-31	-33	-27	-0	15
X= .2601	-47	-54	-35	-26	-13	30	46	8	-28	-38	-22	19	26
X= .2801	-12	-13	2	6	29	88	97	32	-22	-36	-10	45	53
X= .3001	-2	20	50	45	39	71	68	12	-24	-26	13	85	94
X= .3201	-4	51	105	89	37	17	3	-27	-36	-23	27	106	114
X= .3401	-6	57	107	82	14	-25	-34	-39	-37	-29	3	63	67
X= .3601	-29	16	41	18	-18	-17	4	8	-1	-21	-27	0	13
X= .3801	-40	-7	-0	-15	-11	38	81	73	40	-6	-43	-30	-4
X= .4001	-33	-1	4	-11	-10	43	87	67	29	-12	-48	-36	-12
X= .4201	-39	-10	1	-19	-48	-23	10	-10	-31	-38	-50	-35	-17
X= .4401	-39	-19	-1	-18	-66	-65	-45	-66	-76	-64	-58	-35	-10
X= .4601	-30	-17	7	3	-45	-54	-38	-59	-74	-64	-40	24	73
X= .4801	-8	8	40	50	6	-18	-11	-27	-40	-30	31	178	273
X= .5001	26	53	94	114	67	13	-4	-12	-17	-10	73	273	396

(ii)

TYPE OF SYNTHESIS = PATT

RHK(= 7.55 ***** Z = .251 ***** C = 132.3438542

	Y = 0. 0	Y = 0. 20	Y = 0. 40	Y = 0. 60	Y = 0. 80	Y = 0. 100	Y = 0. 120	Y = 0. 140	Y = 0. 160	Y = 0. 180	Y = 0. 200	Y = 0. 220	Y = 0. 240	Y = 0. 260	Y = 0. 280	Y = 0. 300	Y = 0. 320	Y = 0. 340	Y = 0. 360	Y = 0. 380	Y = 0. 400	Y = 0. 420	Y = 0. 440	Y = 0. 460	Y = 0. 480	Y = 0. 500
X= .0000	-13	-8	-9	-10	1	-12	-36	-38	-40	-40	-34	-35	-16	15	5	-16	-8	-11	-33	-39	-32	-26	-30	-49	-59	-57
X= .0231	-8	-7	-10	-1	19	5	-26	-32	-33	-32	-27	-26	-5	22	6	-9	5	-4	-27	-18	-10	-21	-28	-42	-57	-56
X= .0431	-9	-13	-15	-0	18	6	-19	-27	-28	-17	6	6	4	17	10	5	17	-8	-7	31	42	18	6	-13	-39	-44
X= .0691	-10	-14	-8	5	12	-1	-14	-12	-6	25	74	79	52	44	38	35	43	27	36	92	104	73	58	30	-11	-27
X= .0891	1	-3	10	16	12	-4	-11	-0	9	43	105	118	85	68	95	41	38	27	39	86	94	68	59	32	-7	-22
X= .1091	-12	-11	5	8	3	-8	-17	-11	-8	17	69	79	49	35	23	9	3	-5	7	41	42	25	21	3	-22	-24
X= .1231	-36	-30	-16	-11	-7	-7	-17	-19	-16	7	49	48	9	-11	-18	-24	-25	-29	-9	27	25	2	-6	-21	-36	-32
X= .1491	-39	-35	-27	-24	-11	-3	-13	-22	-16	13	48	41	-6	-34	-36	-39	-45	-50	-30	8	8	-17	-30	-44	-45	-25
X= .1601	-40	-41	-34	-26	1	24	7	-15	-14	0	13	8	-23	-39	-36	-40	-46	-52	-50	-30	-26	-39	-45	-50	-34	2
X= .1891	-40	-40	-26	-4	46	86	65	32	22	7	-13	-19	-30	-28	-24	-33	-35	-37	-43	-38	-33	-35	-29	-27	-22	4
X= .2001	-34	-36	-13	16	74	119	97	64	55	27	-5	-18	-25	-18	-17	-34	-37	-35	-38	-24	-11	-7	4	1	-12	-7
X= .2231	-35	-35	-21	5	54	87	63	37	32	11	-18	-16	-25	-22	-19	-31	-33	-34	-35	-8	21	26	32	30	15	16
X= .2491	-16	-27	-15	7	40	55	28	3	-4	-15	-18	-14	-24	-23	-14	-19	-28	-18	-18	8	40	40	35	30	18	26
X= .2691	15	6	20	32	44	46	14	-16	-21	-24	-20	-15	-24	-20	-9	-15	-12	-1	-1	19	48	37	10	-6	-17	-9
X= .2891	5	7	22	28	26	22	-6	-33	-33	-33	-29	-17	-23	-23	-13	-10	10	33	34	55	79	50	2	-20	-31	-31
X= .3091	-16	-19	-9	-6	-10	-11	-23	-34	-33	-33	-34	-17	-22	-29	-19	-8	24	56	62	86	106	53	7	-16	-28	-32
X= .3231	-8	-31	-36	-38	-36	-30	-37	-42	-36	-33	-35	-24	-31	-34	-21	-14	-0	18	26	51	71	35	-10	-31	-42	-42
X= .3401	-11	-42	-55	-51	-40	-22	-29	-49	-50	-45	-40	-34	-39	-28	2	8	-10	-21	-18	1	15	-2	-28	-40	-45	-40
X= .3601	-33	-51	-49	-37	-19	15	16	-23	-41	-33	-33	-35	-35	-13	31	41	7	-18	-18	-11	-7	-14	-23	-29	-35	-32
X= .3891	-39	-46	-28	-11	2	35	41	-8	-22	-20	-24	-22	-15	1	37	42	5	-17	-18	-16	-13	-10	-6	-10	-27	-30
X= .4001	-32	-	-5	18	23	46	49	11	-2	3	10	17	28	40	64	55	10	-12	-14	-17	-11	0	13	12	-11	-11
X= .4231	-26	-17	22	52	61	88	88	43	30	44	44	48	95	72	101	88	35	8	0	-9	-4	9	17	16	0	4
X= .4491	-30	-20	17	40	66	98	92	42	31	45	39	34	35	43	70	65	22	8	-6	-12	0	13	9	1	-6	-7
X= .4691	-43	-45	-20	2	17	48	29	-4	5	23	13	17	19	5	8	5	-17	-22	-19	-16	11	27	8	-8	-10	-12
X= .4891	-59	-55	-40	-27	-18	-9	-19	-22	7	17	3	20	32	1	-21	-25	-35	-30	-23	-19	11	27	4	-12	-14	-18
X= .5001	-57	-56	-44	-27	-22	-24	-32	-25	2	4	-7	16	26	-9	-31	-32	-42	-40	-32	-30	-11	4	-7	-12	-18	-25

TYPE OF SYNTHESIS = PATT

RMAX= 7.55

Z = .500

C = 132.3438542

(iii)

X	Y = 0. 0	Y = 0. 20	Y = 0. 40	Y = 0. 60	Y = 0. 80	Y = 0. 100	Y = 0. 120	Y = 0. 140	Y = 0. 160	Y = 0. 180	Y = 0. 200	Y = 0. 220	Y = 0. 240	Y = 0. 260	Y = 0. 280	Y = 0. 300	Y = 0. 320	Y = 0. 340	Y = 0. 360	Y = 0. 380	Y = 0. 400	Y = 0. 420	Y = 0. 440	Y = 0. 460	Y = 0. 480	Y = 0. 500
X= .0001	-43	-35	18	75	45	-18	-25	12	78	115	67	7	-4	-8	-12	-0	21	48	72	98	116	79	8	-16	8	26
X= .0201	-35	-37	1	50	29	-15	-19	-10	14	37	14	-14	-17	-17	-6	20	36	101	119	91	53	16	-19	-21	7	17
X= .0401	18	-19	-39	-22	-23	-26	-17	-24	-26	-13	-13	-2	-22	-25	-10	19	55	108	124	71	10	-21	-38	-33	-12	-11
X= .0601	75	12	-47	-53	-45	-26	-7	-22	-34	-2	-27	-32	-35	-41	-23	1	17	50	66	27	-17	-37	-52	-47	-30	-30
X= .0801	45	-6	-48	-37	-11	27	59	13	-22	-20	-25	-36	-48	-53	-28	-5	-8	-2	6	-9	-26	-37	-50	-42	-23	-23
X= .1001	-18	-45	-47	-4	44	99	127	68	1	-11	-14	-26	-41	-50	-26	-7	-14	-18	-16	-22	-28	-38	-51	-43	-23	-16
X= .1201	-25	-38	-32	7	51	[illegible]	144	91	13	-15	-23	-33	-46	-54	-38	-23	-20	-15	-16	-29	-35	-42	-53	-47	-25	2
X= .1401	12	6	-19	-16	10	65	113	103	37	-13	-34	-46	-49	-47	-39	-25	-13	-3	-6	-29	-42	-40	-38	-27	-7	26
X= .1601	78	79	5	-35	-26	22	38	116	63	5	-28	-44	-41	-32	-30	-21	-9	2	8	-13	-40	-38	-27	-11	6	32
X= .1801	115	114	25	-33	-43	-10	36	85	47	7	-20	-46	-51	-40	-38	-31	-15	13	43	29	-13	-28	-25	-14	6	29
X= .2001	67	61	-3	-33	-41	-26	15	34	22	23	8	-36	-53	-40	-37	-31	-8	45	104	92	32	-3	-16	-19	-2	12
X= .2201	7	-4	-36	-44	-41	-29	-5	7	25	59	43	-21	-47	-30	-20	-12	4	52	115	104	34	-7	-25	-32	-19	-13
X= .2401	-4	-16	-44	-53	-55	-44	-24	-13	17	54	30	-35	-61	-37	4	53	65	50	57	38	-17	-46	-51	-44	-20	-18
X= .2601	-3	-22	-48	-56	-59	-53	-34	-23	-7	12	-7	-43	-62	-34	64	170	182	87	18	-9	-39	-51	-48	-37	-11	1
X= .2801	-12	-29	-42	-38	-34	-34	-23	-15	-11	-4	-15	-41	-49	-24	75	221	218	98	14	-8	-17	-20	-31	-37	-21	-11
X= .3001	-0	-25	-37	-31	-25	-27	-23	-15	-10	-3	-13	-36	-44	-32	39	136	144	72	35	20	4	-7	-35	-49	-27	-17
X= .3201	21	-14	-32	-34	-29	-29	-21	-11	-11	-12	-21	-37	-38	-33	-3	59	86	89	131	74	23	-10	-42	-46	-16	-9
X= .3401	48	8	-13	-17	-9	-8	0	13	3	-11	-21	-34	-33	-28	-15	24	64	106	132	91	20	-24	-46	-43	-18	-17
X= .3601	72	35	3	-13	-4	-2	2	15	8	2	5	-11	-27	-30	-23	2	39	68	77	48	-9	-42	-50	-42	-29	-28
X= .3801	98	90	38	-21	-30	-19	-10	2	7	33	53	47	-5	-30	-28	-12	-3	-2	11	6	-29	-51	-52	-47	-33	-25
X= .4001	115	[illegible]	63	-17	-47	-26	-5	5	16	68	120	83	7	-42	-51	-33	-25	-35	-29	-23	-46	-50	-58	-52	-26	-7
X= .4201	79	116	61	-29	-30	-25	2	16	19	54	89	54	-14	-61	-76	-58	-41	-46	-43	-39	-56	-52	-50	-41	-1	34
X= .4401	9	30	-2	-44	-39	-12	27	56	44	31	24	-5	-32	-47	-64	-61	-48	-42	-31	-29	-47	-51	-40	-31	20	78
X= .4601	-16	-12	-29	-40	-23	5	59	105	92	57	7	-25	-28	-19	-34	-47	-45	-39	-26	-22	-39	-37	-21	0	81	156
X= .4801	8	-1	-25	-35	-23	-3	43	86	82	53	15	-21	-19	-5	-17	-30	-31	-35	-31	-26	-23	5	44	102	237	334
X= .5001	26	17	-11	-30	-23	-16	2	26	32	23	12	-13	-10	1	-11	-17	-9	-17	-28	-25	-7	34	78	156	334	449

Table 4.2.2 The determination of atomic positions from the Patterson map.

Atom	Patterson peak in vector space P(UVW)	Atomic co-ordinate in real space (xyz)
Nb(1)	0.40, 0.02, 0.5	-0.06, 0.46, 0.75
Nb(2)	0.00, 0.18, 0.5	0.34,-0.16, 0.75
Nb(3)	0.34, 0.36, 0.5	0.10, 0.26, 0.50

The positions of the remaining atoms can be obtained from the Fourier synthesis, that is the calculation of the electron density map. The phases assigned were obtained from the atomic co-ordinates shown in Table 4.2.2. New atomic parameters which were more accurate than before could then be assigned.

The electron density was calculated in two dimensions. The result was a map representing the projection of the electron density of the cell down the c axis onto the ab plane.

The Fourier map was calculated at four sections z = 0, 0.25, 0.50 and 0.75 as shown in Fig.4.2.2.

Peaks from the F_o synthesis, by drawing closed curves through points of constant electron density. The atomic positions can be obtained from the points of the highest value of the electron density. We can get the position of As atom thus

As is at 0.04, 0.27, 0

The fractional and absolute co-ordinates of all atoms in the unit cell of Nb_3As are tabulated in Table 4.2.3.

Fig.4.2.2 F_o synthesis, based on the three Nb atoms only,

(i) z=0, (ii) z=0.25, (iii) z=0.5

(i)

TYPE OF SYNTHESIS = FOBS

RMAX= 27.09

Z = .000

C = 36.8743589

	Y = 0. 0	Y = 0. 20	Y = 0. 40	Y = 0. 60	Y = 0. 80	Y = 0. 100	Y = 0. 120	Y = 0. 140	Y = 0. 160	Y = 0. 180	Y = 0. 200	Y = 0. 220	Y = 0. 240	Y = 0. 260	Y = 0. 280	Y = 0. 300	Y = 0. 320	Y = 0. 340	Y = 0. 360	Y = 0. 380	Y = 0. 400	Y = 0. 420	Y = 0. 440	Y = 0. 460	Y = 0. 480	Y = 0. 500
X= .0000	-80	-52	-32	-16	14	-16	-51	-38	-71	-94	-62	-64	-34	17	-19	-36	1	4	1	-1	-3	21	26	-4	-44	-68
X= .0201	-53	-73	-79	-40	38	32	-10	-17	-42	-62	-65	-47	121	351	322	105	-2	-15	-26	-18	3	39	66	48	2	-46
X= .0401	3	15	3	-8	59	91	52	21	12	25	-0	-27	208	600	607	228	-9	-13	3	18	19	-0	16	28	15	-10
X= .0601	10	36	13	-25	23	84	48	-11	-27	7	2	-65	91	429	427	105	-50	-47	-33	22	33	-28	-43	-15	12	5
X= .0801	-49	-61	-71	-54	-17	24	11	-49	-89	-45	16	-33	-12	140	103	-42	-38	-47	-62	26	44	-6	-4	-11	-26	-13
X= .1001	-66	-100	-109	-62	-0	31	18	-43	-74	-2	62	-4	-56	-8	-25	-44	38	28	-34	15	22	-12	15	-16	-82	-59
X= .1201	-43	-70	-116	-102	3	63	21	-55	-75	-21	-10	-73	-95	-78	-82	-52	15	1	-56	-17	13	-44	-43	-21	-58	-56
X= .1401	-57	-67	-86	-82	-10	40	-8	-28	-85	-63	-88	-110	-81	-61	-78	-74	-64	-88	-97	-26	30	-46	-103	-58	-24	5
X= .1601	-62	-65	-27	0	21	14	-50	-87	-39	-27	-81	-105	-65	-24	-36	-54	-51	-78	-99	-44	-1	-59	-125	-124	-78	-3
X= .1801	-67	-108	-66	-27	-5	-17	-89	-111	-57	-55	-105	-119	-104	-77	-70	-77	-50	-52	-82	-62	-64	-89	-73	-88	-114	-64
X= .2001	-91	-117	-67	-64	37	159	66	-81	-120	-124	-108	-91	-105	-101	-94	-103	-77	-50	-53	-49	-76	-95	-20	20	-43	-66
X= .2201	-53	-39	15	64	382	698	482	74	-77	-79	-44	-23	-45	-50	-51	-50	-24	-25	-7	90	119	10	-30	41	19	-68
X= .2401	-16	1	27	147	613	999	711	177	-8	-2	1	3	-19	-23	-13	2	23	-2	89	451	631	354	42	9	11	-47
X= .2601	-43	7	8	41	350	629	453	108	-2	24	2	-12	-23	-20	2	-0	-4	-11	123	705	998	616	149	29	7	-13
X= .2801	-59	18	41	-29	9	117	90	-7	-26	-24	-50	-52	-50	-46	-23	-44	-81	-79	71	478	637	387	64	16	-34	-58
X= .3001	-65	-44	20	-19	-94	-75	-46	-53	-50	-76	-103	-95	-102	-105	-90	-108	-125	-119	-80	65	150	38	-65	-67	-114	-90
X= .3201	-64	-115	-89	-73	-89	-63	-62	-83	-53	-49	-77	-70	-78	-105	-118	-165	-56	-56	-111	-90	-17	-3	-28	-66	-107	-67
X= .3401	-1	-78	-123	-125	-59	-1	-43	-100	-79	-51	-54	-36	-25	-65	-105	-82	-27	-39	-88	-53	18	22	0	-28	-65	-64
X= .3601	7	-24	-56	-101	-46	31	-24	-96	-87	-64	-74	-78	-61	-81	-109	-88	-69	-86	-79	-10	45	-10	-82	-80	-66	-58
X= .3801	-57	-60	-21	-42	-45	13	-17	-58	1	16	-54	-85	-78	-92	-69	-8	-20	-75	-54	21	64	3	-101	-117	-77	-44
X= .4001	-60	-85	-17	15	-13	21	13	-37	26	39	-47	-29	-8	-51	-0	63	-1	-73	-41	19	32	1	-60	-108	-100	-67
X= .4201	-12	-27	-11	-3	-7	44	26	-63	-47	-37	-44	100	141	-8	-31	-15	-45	-88	-48	11	24	-16	-54	-72	-61	-48
X= .4401	9	13	-14	-41	-27	33	22	-33	-47	-50	103	419	431	94	-65	1	7	-26	-12	48	83	23	-26	12	36	11
X= .4601	-7	15	28	17	1	19	17	1	-14	-11	225	605	601	210	-26	0	25	11	19	52	92	60	-9	3	16	2
X= .4801	-45	0	47	66	40	4	-19	-28	-16	-2	103	320	352	123	-46	-64	-62	-42	-18	-10	72	38	-40	-79	-73	-55
X= .5001	-68	-45	-5	25	21	-2	-0	0	4	3	-35	-20	17	-34	-65	-62	-93	-71	-37	-50	-16	13	-17	-31	-51	-80
X= .5201	-46	-44	3	17	1	17	45	29	7	11	-18	-53	-43	-26	1	-5	-64	-55	-19		1	38	44	71	33	-52
X= .5401	-9	-20	30	84	27	13	2	-34	-28	-6	-1	-1	-12	0	32	17	-32	-36	0	33	71	85	72	81	54	4
X= .5601	5	-34	-9	47	22	-5	-12	-40	-27	-10	-24	-23	-31	-22	5	-9	-27	-14	35	99	117	98	67	23	-1	10
X= .5801	-14	-21	-29	-26	-40	-21	16	4	-1	11	-27	-53	-21	-0	-32	-79	-82	-36	35	92	86	55	34	-15	-49	-46
X= .6001	-57	-24	-36	-32	-52	-25	-7	-27	-36	-17	-31	-43	8	24	-42	-97	-104	-63	-1	20	22	36	39	18	-25	-67
X= .6201	-54	-38	-44	-9	29	39	24	-36	-70	-53	-29	15	57	45	4	-31	-52	-24	4	-15	23	81	49	7	-12	-48
X= .6401	7	13	-18	29	88	89	100	68	-1	-23	-3	58	85	37	15	-2	-35	1	29	11	63	70	-23	-72	-52	-58
X= .6601	-5	17	-31	-10	39	44	96	121	49	3	3	18	18	-29	-45	-43	-65	-24	22	16	36	15	-63	-65	-36	-59
X= .6801	-65	-28	-61	-67	-32	-4	39	57	-7	-58	-49	-38	-24	-44	-91	-91	-69	-54	-36	-12	32	15	-54	-29	5	-66
X= .7001	-63	-25	-24	-48	-45	-18	1	-1	-47	-101	-81	-23	11	-13	-80	-80	-47	-78	-62	-16	32	-7	-86	-58	-14	-95

(ii)

TYPE OF SYNTHESIS = FOBS

RMAX= 27.09

Z = .251

C = 36.8743589

X	Y = 0. 0	Y = 0. 20	Y = 0. 40	Y = 0. 60	Y = 0. 80	Y = 0. 100	Y = 0. 120	Y = 0. 140	Y = 0. 160	Y = 0. 180	Y = 0. 200	Y = 0. 220	Y = 0. 240	Y = 0. 260	Y = 0. 280	Y = 0. 300	Y = 0. 320	Y = 0. 340	Y = 0. 360	Y = 0. 380	Y = 0. 400	Y = 0. 420	Y = 0. 440	Y = 0. 460	Y = 0. 480	Y = 0. 500
X= .0000	-160	-105	64	127	-29	-117	-68	-78	-70	-22	-42	-76	-111	-131	-99	-70	-35	-8	-28	-52	-73	-63	-13	-12	-90	-164
X= .0201	-86	-115	-93	-77	-90	-14	42	-20	-28	15	-13	-58	-78	-101	-94	-34	10	2	-27	-75	-103	-59	-11	-37	-114	-105
X= .0401	-10	-41	-26	29	30	63	88	38	25	23	-15	-7	10	-58	-114	-32	56	41	19	-47	-116	-55	18	-21	-92	61
X= .0601	-12	-10	17	75	31	-20	3	6	-2	-33	-74	-23	42	1	-53	-23	28	58	79	10	-76	-21	72	29	-76	126
X= .0801	-61	-54	-55	-24	-26	-39	-17	-10	-13	-35	-78	-48	29	51	36	18	14	55	63	-7	-50	-27	28	29	-85	-26
X= .1001	-74	-103	-119	-81	-50	-20	7	8	-2	-24	-32	-6	32	48	39	31	33	44	25	-16	-20	-39	-23	61	-12	-117
X= .1201	-54	-76	-46	12	-6	-17	11	19	6	-8	10	30	33	41	17	9	46	51	26	12	7	-16	1	81	38	-78
X= .1401	-25	-28	20	41	62	23	26	35	28	12	2	0	18	28	-8	5	77	79	35	17	5	-11	4	33	-21	-76
X= .1601	-7	-2	38	57	52	46	56	80	65	23	-13	-22	9	-7	-50	12	84	67	28	4	-4	-13	-2	25	-25	-66
X= .1801	-37	8	51	24	10	34	51	77	83	55	13	0	46	16	-57	2	52	22	11	-8	-23	-35	-33	21	15	-19
X= .2001	-71	-32	-34	-27	15	29	9	2	11	4	-29	-16	60	34	-58	-28	10	-15	2	11	-32	-80	-75	-16	-15	-42
X= .2201	-98	-93	-117	-57	37	41	17	-12	-54	-53	-61	-47	7	-5	-44	-13	-2	-22	6	34	-5	-49	-21	-4	-60	-79
X= .2401	-131	-102	-60	1	54	53	47	30	-10	12	32	-5	-16	-16	7	59	43	10	25	39	36	33	46	14	-76	-113
X= .2601	-114	-80	12	45	30	35	42	27	10	44	60	7	-16	-16	-6	31	10	-12	26	41	52	57	2	-58	-97	-127
X= .2801	-78	-61	-4	-20	-50	-7	34	6	-23	-2	-14	-45	-6	6	-47	-62	-61	-56	-15	13	40	38	-57	-116	-88	-95
X= .3001	-41	-16	-17	-74	-79	-31	12	2	-15	11	-27	-59	33	60	-15	-29	3	11	3	8	30	15	-28	-33	-30	-70
X= .3201	-19	14	20	-34	-35	-22	-7	10	21	53	3	-57	15	46	1	13	54	84	78	50	34	12	24	51	9	-38
X= .3401	-64	-25	25	-1	-14	-4	6	28	66	84	12	-50	-8	9	-22	-13	22	65	79	53	45	54	57	38	-2	-8
X= .3601	-75	-21	35	6	-31	6	19	35	80	78	4	-9	28	18	1	2	12	28	34	24	23	62	81	20	-27	-26
X= .3801	-71	35	81	2	-16	6	12	24	51	47	8	15	41	36	33	12	-7	7	19	12	-16	-6	13	-45	-75	-55
X= .4001	-118	-15	59	-23	-40	-21	-18	22	43	33	28	35	48	37	-1	-30	-23	-1	10	8	-19	-49	-79	-118	-103	-75
X= .4201	-25	-87	29	27	-27	-50	-7	62	55	15	16	33	52	33	-47	-79	-35	-11	-8	-17	-39	-25	-23	-56	-55	-60
X= .4401	130	-75	30	74	-20	-77	11	29	59	28	-25	-55	2	44	-23	-75	-32	-1	6	2	-20	31	74	16	-10	-12
X= .4601	65	-92	-21	19	-53	-116	-49	17	40	52	-35	-116	-56	13	-6	-15	23	24	37	87	63	30	29	-27	-41	-12
X= .4801	-134	-115	-34	-11	-57	-102	-76	-29	2	10	-36	-96	-100	-75	-57	-12	16	-29	-20	42	-13	-90	-77	-94	-115	-86
X= .5001	-164	-51	-13	-14	-63	-72	-52	-29	-8	-33	-69	-100	-130	-111	-78	-43	-21	-70	-77	-67	-117	-30	127	65	-103	-160
X= .5201	-127	-74	-6	-16	-82	-84	-42	-12	12	-9	-50	-77	-102	-82	-56	-36	-2	-2	9	-13	7	380	705	508	71	-133
X= .5401	-89	-42	53	30	-66	-78	-20	5	3	14	20	-4	-31	-40	-60	-65	-33	14	59	15	66	528	944	786	177	-69
X= .5601	-102	-29	76	25	-75	-75	-40	-19	-20	-23	-20	-30	-43	-42	-65	-72	-56	-26	8	-54	-60	231	614	388	60	-78
X= .5801	-123	-67	-7	-65	-107	-67	-45	-9	12	-64	-103	-32	-112	-102	-67	-41	-10	8	21	-23	-88	-40	50	37	-52	-83
X= .6001	-103	-42	-23	-100	-102	-32	-8	38	53	-60	-106	-55	-78	-95	-76	-70	-16	36	37	24	-26	-87	-92	-61	-53	-74
X= .6201	-80	24	59	-30	-55	-40	-32	81	123	-23	-89	-20	-6	-19	-52	-83	-21	33	6	-5	-20	-75	-77	-39	-48	-94
X= .6401	-76	17	84	41	12	-3	69	364	482	214	8	-6	12	34	-12	-45	39	84	30	-5	-5	-17	-16	-4	-36	-72
X= .6601	-51	1	31	19	27	56	256	728	909	508	106	-9	1	35	-15	-51	42	92	41	11	28	35	26	28	-2	-34
X= .6801	23	18	-4	-31	-25	-16	172	602	744	364	-15	-121	-83	-27	-47	-92	-44	21	11	-13	-18	-24	19	62	11	-31
X= .7001	-21	-8	-16	-40	-49	-80	-33	156	191	7	-143	-179	-128	-51	-62	-125	-92	11	22	-36	-80	-109	-40	31	-27	-48

(iii)

TYPE OF SYNTHESIS = FOBS

RMAX= 27.09

Z = .500

C = 36.8743589

	Y = 0. 0	Y = 0. 20	Y = 0. 40	Y = 0. 60	Y = 0. 80	Y = 0. 100	Y = 0. 120	Y = 0. 140	Y = 0. 160	Y = 0. 180	Y = 0. 200	Y = 0. 220	Y = 0. 240	Y = 0. 260	Y = 0. 280	Y = 0. 300	Y = 0. 320	Y = 0. 340	Y = 0. 360	Y = 0. 380	Y = 0. 400	Y = 0. 420	Y = 0. 440	Y = 0. 460	Y = 0. 480	Y = 0. 500
X= .0001	-68	-46	-7	7	-13	-58	-54	7	-5	-65	-62	-56	-45	-15	-55	-94	-67	-60	-57	-49	-68	-46	11	3	-52	-80
X= .0201	-46	-1	17	11	-29	-83	-58	-24	-80	-115	-45	15	8	5	-36	-115	-109	-64	-65	-79	-130	-62	32	12	-75	-54
X= .0401	-6	45	32	-10	-11	-16	-20	-55	-122	-85	19	36	5	28	18	-65	-67	-27	-76	-115	-108	-75	11	3	-79	-31
X= .0601	24	62	18	-38	-1	15	-42	-101	-124	-69	-15	-31	36	145	65	-62	-28	0	-80	-100	-61	-56	-23	-4	-41	-19
X= .0801	22	38	1	-26	-7	-16	-46	-47	-64	-90	-91	8	343	604	378	37	-4	24	-9	4	2	-15	26	64	36	9
X= .1001	-3	3	18	32	41	16	12	33	-4	-65	-73	115	616	983	690	156	-18	21	46	63	33	24	82	94	33	-18
X= .1201	-5	-21	15	20	24	8	-17	-19	-43	-64	-48	88	442	697	477	65	-91	-47	-6	21	20	10	49	53	-6	-51
X= .1401	-2	-27	2	-34	-62	-37	-56	-92	-98	-84	-55	-7	96	169	73	-79	-112	-85	-75	-54	-41	-48	-11	21	-16	-41
X= .1601	5	-12	-12	-49	-48	26	1	-85	-75	-50	-50	-23	-0	-11	-76	-117	-56	-37	-84	-77	-77	-91	-26	11	-44	-74
X= .1801	1	-1	-10	-53	-41	37	14	-65	-48	-45	-78	-24	25	-4	-80	-123	-54	-25	-65	-22	-6	-48	10	26	-62	-92
X= .2001	-41	105	234	111	-39	-44	-51	-73	-51	-73	-108	-54	3	-1	-48	-111	-106	-82	-88	-7	62	16	5	-1	-67	-60
X= .2201	-24	325	620	433	105	-27	-80	-75	-32	-67	-97	-53	-11	3	-25	-93	-118	-103	-108	-68	1	-29	-63	-31	-51	-65
X= .2481	19	138	612	439	139	-13	-77	-59	-20	-73	-101	-50	-23	-20	-47	-105	-102	-61	-79	-93	-54	-8	98	242	126	-29
X= .2601	-31	123	211	97	-11	-56	-91	-78	-62	-101	-105	-46	-20	-23	-51	-103	-75	-23	-63	-83	-14	162	440	613	368	22
X= .2801	-64	-52	-30	-62	-30	-1	-68	-109	-104	-118	-93	-26	2	-11	-53	-98	-69	-34	-78	-34	-28	186	432	620	330	-21
X= .3001	-60	-67	-2	6	17	63	-7	-88	-82	-104	-110	-48	-2	3	-52	-108	-76	-51	-72	-51	-43	-39	109	234	108	-40
X= .3201	-92	-63	25	9	-48	-5	-21	-69	-26	-53	-122	-50	-5	25	-23	-79	-47	-47	-65	13	37	-39	-53	-10	-0	0
X= .3401	-73	-44	11	-25	-91	-77	-75	-85	-38	-55	-117	-77	-12	-1	-23	-51	-51	-75	-87	-1	26	-47	-49	-13	-12	4
X= .3601	-39	-17	23	-9	-48	-40	-52	-75	-85	-112	-80	72	169	96	-7	-55	-84	-98	-93	-58	-38	-62	-34	2	-26	-3
X= .3801	-52	-8	53	46	10	20	21	-7	-48	-90	63	474	697	449	91	-46	-63	-42	-19	-17	9	24	20	16	-20	-7
X= .4001	-19	30	92	82	22	32	61	43	19	-18	154	686	983	622	119	-72	-64	-3	34	13	17	43	33	19	3	-4
X= .4201	11	34	63	27	-16	2	4	-9	24	-3	35	375	605	347	10	-92	-89	-63	-46	-46	-16	-6	-25	0	38	23
X= .4401	-15	-41	-3	-21	-56	-61	-100	-80	1	-28	-64	63	146	41	-31	-16	-68	-123	-101	-42	15	-1	-38	17	62	25
X= .4601	-23	-79	4	13	-73	-109	-117	-78	-28	-69	-68	15	29	7	37	20	-85	-123	-57	-21	-16	-10	-11	32	45	-8
X= .4801	-53	-77	11	32	-60	-99	-80	-66	-65	-103	-117	-38	6	10	16	-44	-116	-81	-25	-58	-62	-28	11	17	-2	-49
X= .5001	-80	-53	2	10	-46	-67	-49	-58	-60	-65	-94	-56	-15	-46	-58	-62	-64	-5	6	-53	-58	-13	7	-7	-45	-68
X= .5201	-52	30	51	-2	-49	-25	-13	-53	-37	5	-14	-3	28	-9	-29	-26	-27	17	14	-37	-24	-21	-31	-16	-41	-44
X= .5401	-33	67	78	24	-14	19	8	-73	-65	-29	-58	-36	23	30	15	-25	-61	-31	-19	-44	-38	-33	-10	32	5	-4
X= .5601	-19	41	73	72	37	40	50	-23	-63	-53	-85	-82	-33	-10	-12	-49	-67	-9	30	-9	-53	-30	43	63	18	25
X= .5801	13	38	88	102	85	35	81	69	14	16	-7	-44	-8	15	-18	-46	-32	40	88	30	-50	-40	19	26	2	21
X= .6001	-16	2	73	118	84	21	24	52	36	33	31	24	87	110	27	-19	-5	45	89	37	-25	-20	-6	12	18	-2
X= .6201	-50	-32	34	99	91	21	-13	9	14	-12	-16	38	132	145	52	1	40	99	102	23	-8	17	-13	1	45	0
X= .6401	-38	-20	1	34	34	-1	2	25	19	-35	-82	-18	83	86	24	-2	57	124	72	-29	-26	5	-39	-33	30	1
X= .6601	-72	-66	-36	-15	-37	-64	-27	-3	-24	-52	-77	-43	19	16	-25	-50	-11	48	2	-69	-36	-0	-26	-28	8	5
X= .6801	-93	-64	-32	-28	-62	-104	-53	-35	-62	-66	-46	-8	40	34	-45	-102	-62	1	-23	-59	-18	10	-12	-7	11	3
X= .7001	-63	-5	18	-6	-78	-96	-31	-1	-40	-93	-80	5	88	83	-10	-81	-51	1	-3	-29	-30	-27	-25	-1	-18	-36

(iv)

TYPE OF SYNTHESIS = FOBS

RMAX= 27.09

Z = .750

C = 36.8743589

X	Y = 0. 0	Y = 0. 20	Y = 0. 40	Y = 0. 60	Y = 0. 80	Y = 0. 100	Y = 0. 120	Y = 0. 140	Y = 0. 160	Y = 0. 180	Y = 0. 200	Y = 0. 220	Y = 0. 240	Y = 0. 260	Y = 0. 280	Y = 0. 300	Y = 0. 320	Y = 0. 340	Y = 0. 360	Y = 0. 380	Y = 0. 400	Y = 0. 420	Y = 0. 440	Y = 0. 460	Y = 0. 480	Y = 0. 500
X= .0000	-104	-127	-87	-39	-122	-104	-61	-25	-31	23	-21	-88	-91	-84	-66	-40	-33	-34	-72	-95	-75	-82	-77	-70	-133	-160
X= .0201	-134	-103	-29	-31	-47	-37	-46	-52	-11	32	-17	-73	-25	5	-7	10	8	-14	-65	-120	-38	-43	-43	-55	-100	-123
X= .0401	-70	-57	0	16	22	36	40	23	21	28	-14	-26	44	38	-21	2	24	12	-13	-71	-82	-45	-24	-1	-26	-86
X= .0601	-79	-42	-20	-20	-24	-20	18	24	25	43	3	-26	26	30	13	17	12	48	68	-1	-54	-66	-24	16	-30	-100
X= .0801	-84	-41	-42	-63	-62	-57	-26	-7	29	73	2	-76	-43	-15	21	36	19	68	51	-26	-59	-61	-25	21	-45	-122
X= .1001	-75	-88	-82	-65	-60	-56	-17	11	28	30	-35	-59	-23	-45	-41	13	38	45	-7	-64	-55	-55	-18	39	-33	-102
X= .1201	-96	-122	-74	-4	-28	-65	-24	-3	-15	-30	-50	-1	55	8	-41	4	66	47	-16	-24	-15	-25	17	42	-44	-81
X= .1401	-74	-64	-14	65	57	-10	-16	-20	-18	8	-6	20	73	34	-30	-2	69	46	-22	-2	14	-8	22	23	-53	-78
X= .1601	-33	-11	13	45	64	41	45	49	55	90	65	32	43	6	-28	21	79	52	-19	-16	29	30	27	23	-11	-34
X= .1801	-30	7	23	14	22	37	62	65	77	110	78	16	6	-10	-15	51	112	90	7	-31	29	80	53	33	33	19
X= .2001	-40	6	3	23	39	11	2	-3	19	49	13	-21	-12	-24	-37	12	20	65	-6	-49	-34	1	-1	-16	-16	-24
X= .2201	-69	-11	-17	18	19	-43	-38	-24	-24	-14	-36	-32	-9	-19	-35	-24	15	29	13	-3	-54	-75	-32	-30	-70	-69
X= .2401	-88	2	42	35	-14	-42	12	35	8	-11	-26	-20	-0	-1	-12	-16	5	38	63	51	-17	-36	30	47	-21	-91
X= .2601	-92	-24	46	28	-40	-18	53	64	38	5	-16	-11	-1	-1	-21	-27	-12	5	31	6	-44	-11	37	44	7	-85
X= .2801	-88	-71	-29	-31	-76	-50	-3	13	29	15	-24	-35	-20	-9	-32	-36	-16	-26	-27	-41	-44	20	17	-16	-7	-66
X= .3001	-23	-17	-16	-0	2	-33	-48	-6	65	73	12	-38	-25	-12	-19	13	48	19	-2	2	12	39	22	3	9	-39
X= .3201	19	32	31	53	80	30	-30	7	69	113	52	-16	-11	6	17	78	109	78	68	61	37	23	14	23	8	-31
X= .3401	-32	-11	24	27	29	29	-14	-20	52	73	21	-28	6	43	32	64	89	54	47	42	41	66	45	12	-11	-34
X= .3601	-76	-53	24	24	-8	15	-1	-22	47	71	-3	-31	34	74	20	-6	8	-18	-21	-18	-11	57	64	-14	-63	-75
X= .3801	-82	-46	42	19	-26	-16	-24	-18	46	60	3	-44	8	58	2	-47	-29	-15	-3	-23	-65	-28	-3	-73	-121	-99
X= .4001	-103	-36	37	-18	-56	-56	-66	-10	44	34	11	-45	-45	-17	-54	-33	31	29	13	-15	-55	-59	-63	-81	-88	-76
X= .4201	-120	-46	21	-24	-62	-59	-26	60	68	20	35	18	-14	-39	-74	1	79	30	-6	-25	-57	-61	-62	-42	-41	-83
X= .4401	-96	-29	17	-23	-65	-64	-1	69	48	12	15	11	31	28	-26	2	50	26	24	17	-20	-24	-21	-21	-41	-78
X= .4601	-83	-26	-1	-23	-44	-82	-73	-14	11	22	-2	-23	39	47	-25	-13	29	20	22	40	36	22	18	-0	-57	-72
X= .4801	-122	-101	-57	-43	-42	-87	-121	-67	-15	8	8	-9	6	-22	-72	-17	32	-12	-53	-46	-36	-46	-32	-29	-103	-136
X= .5001	-160	-135	-71	-78	-82	-73	-35	-73	-34	-31	-39	-67	-84	-91	-90	-21	24	-31	-75	-80	-104	-123	-100	-87	-126	-164
X= .5201	-104	68	174	59	-53	-54	-49	-30	-3	11	-28	-85	-94	-73	-54	-8	19	2	18	25	-43	-67	-26	-38	-70	-90
X= .5401	63	504	703	389	35	-61	-38	-4	27	63	31	-36	-24	-5	-21	-17	-4	31	83	56	-25	-10	77	55	-5	-11
X= .5601	125	703	849	518	53	-90	-76	-17	25	20	-39	-84	-35	-2	-33	-47	-31	20	41	-30	-101	-68	21	29	-17	-14
X= .5801	-30	360	672	234	-40	-66	-76	-13	34	-23	-108	-112	-66	-37	-36	-50	-25	28	13	-54	-100	-107	-77	-67	-81	-64
X= .6001	-110	7	89	-60	-91	-27	-19	-5	28	-13	-80	-67	-54	-55	-57	-80	-17	57	[illegible]	-41	-31	-66	-76	-78	-83	-72
X= .6201	-67	-13	16	-54	-24	25	-3	-7	9	-12	-36	-34	-44	-63	-83	-33	173	260	71	-34	-9	-44	-41	-21	-41	-51
X= .6401	-78	8	60	7	21	37	4	26	39	11	21	31	12	-17	-43	155	602	732	[illegible]	82	36	-8	-18	6	-11	-28
X= .6601	-70	-2	15	-27	7	35	30	81	93	23	12	52	57	14	-43	188	760	908	484	125	53	12	-19	4	13	-7
X= .6801	-22	-2	-32	-56	-10	-15	-22	39	46	-41	-90	-59	-25	-33	-90	5	364	566	213	-28	-60	-65	-30	13	-9	-33
X= .7001	-43	-36	-63	-71	-40	-69	-84	-43	-48	-91	-125	-144	-116	-54	-83	-142	-17	105	9	-99	-105	-103	-21	20	-49	-78

Table 4.2.3 The atomic positions in the unit cell of Nb_3As.

Atom	Fractional co-ordinate from Patt.map and F_o synthesis.	The equivalent positions	
		Fractional co-ordinate	Absolute co-ordinate
Nb(1)	-0.06, 0.46, 0.75	-0.06, 0.46, 0.75	9.676, 4.735, 3.897
		0.56, 0.04, 0.75	5.765, 0.412, 3.897
		0.54, 0.44, 0.25	5.559, 4.529, 1.299
		-0.04, 0.06, 0.25	9.882, 0.618, 1.299
		0.06, 0.54, 0.25	0.618, 5.559, 1.299
		0.44, -0.04, 0.25	4.529, 9.882, 1.299
		0.46, 0.56, 0.75	4.735, 5.765, 3.897
		0.04, -0.06, 0.75	0.412, 9.676, 3.897
Nb(2)	0.34, -0.16, 0.75	0.34, -0.16, 0.75	3.500, 8.647, 3.897
		0.16, 0.66, 0.75	1.647, 6.794, 3.897
		0.16, -0.16, 0.25	1.649, 8.647, 1.299
		0.34, 0.66, 0.25	3.500, 6.794, 1.299
		0.66, 0.16, 0.25	6.794, 1.647, 1.299
		-0.16, 0.34, 0.25	8.647, 3.500, 1.299
		-0.16, 0.16, 0.75	8.647, 1.647, 3.897
		0.66, 0.34, 0.75	6.794, 3.500, 3.897
Nb(3)	0.10 , 0.26 , 0.50	0.10, 0.26, 0.50	1.029, 2.676, 2.598
		0.40, 0.24, 0.50	4.118, 2.471, 2.598
		-0.26, 0.60, 0	7.618, 6.176, 0
		0.76, -0.10, 0	7.823, 9.265, 0
		-0.10, -0.26, 0.50	9.265, 7.618, 2.598
		0.60, 0.76, 0.50	6.176, 7.823, 2.598
		0.26, 0.40, 0	2.676, 4.118, 0
		0.24, 0.10, 0	2.471, 1.029, 0

Table 4.2.3

(continued)

Atom	Fractional co-ordinate from Patt.map and F_o synthesis.	The equivalent positions	
		Fractional co-ordinate	Absolute co-ordinate
As	0.04 , 0.27 , 0	0.04, 0.27, 0	0.412, 2.779, 0
		0.46 0.23, 0	4.735, 2.368, 0
		0.73, 0.54, 0.5	7.515, 5.559, 2.598
		0.77, -0.04, 0.5	7.926, 9.882, 2.598
		-0.04, 0.73, 0	9.882, 7.515, 0
		0.54, 0.77, 0	5.559, 7.926, 0
		0.27, 0.46, 0.5	2.779, 4.735, 2.598
		0.23, 0.04, 0.5	2.368, 0.412, 2.598

Fig.4.2.3 shows the positions of Nb atoms and As atoms in four neighbouring unit cells of Nb_3As in the three sections of z.

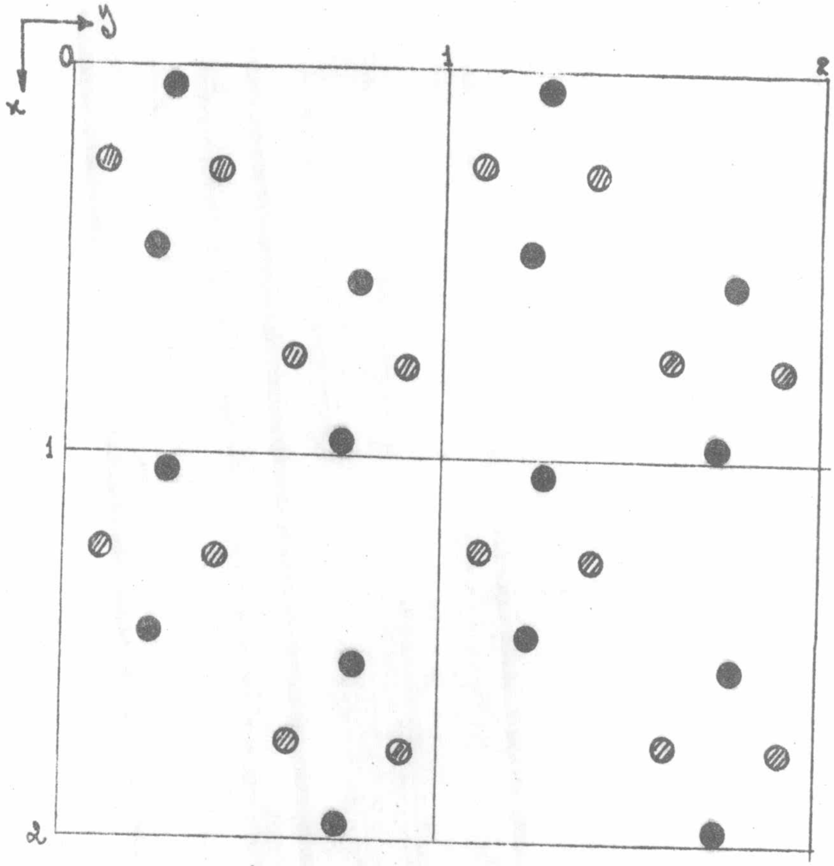


Fig.4.2.3.(i)

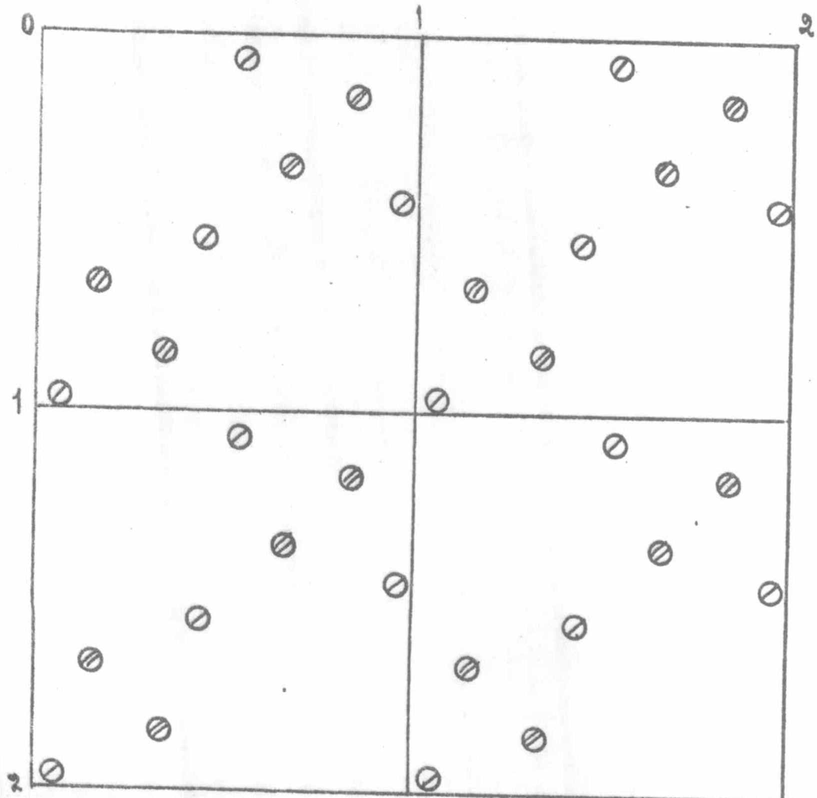


Fig.4.2.3.(ii)

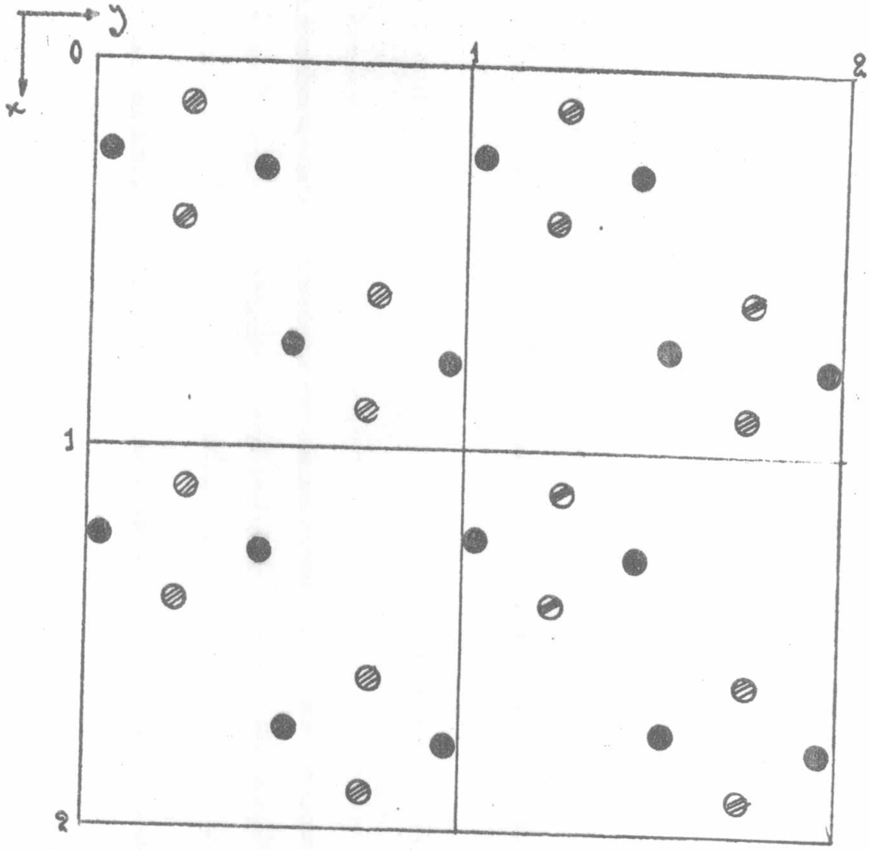
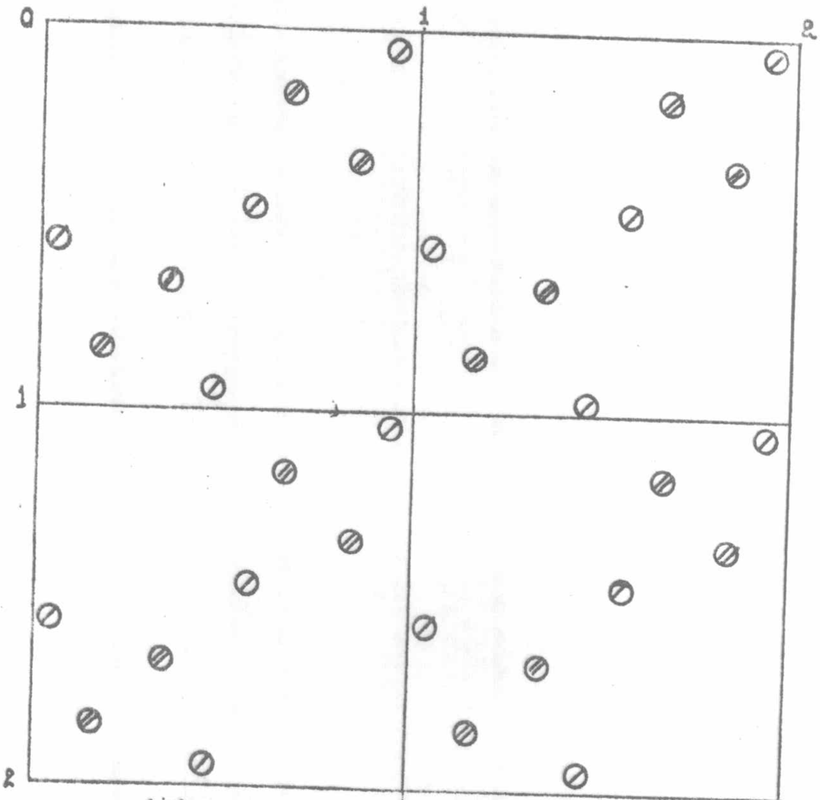


Fig.4.2.3.(iii)



(iv)

Fig.4.2.3. The atomic positions in four unit cells. (i) z=0, (ii) z =0.25, (iii) z=0.5, (iv) z=0.75 .

4.3 Refinement

4.3.1 Refinement by F_o synthesis

The accurate positional parameters of each atom can be determined from this F_o synthesis as given in section 4.2.

The Booth's method gives the accurate determination, provided the electron density is computed at equidistant points. The maximum in the xy section of an F_o synthesis for Nb(1) atom was determined as shown in Fig. 4.3.1 (i). As the peak near the line x = 0.56, y = 0.04 corresponded to Nb(1) was more conveniently observed than that at x = -0.06, y = 0.46. The peak was therefore chosen and subjected to the Booth method, and these are tabulated in Table 4.3.1.

Using the equation

$$X_m = \frac{(\rho_2/\rho_1) - 4}{(2\rho_2/\rho_1) - 4}$$

and

$$Y_m = \frac{(\rho_2/\rho_1) - 4}{(2\rho_2/\rho_1) - 4}$$

the data in Table 4.3.1 gives $X_m = 0.0255$ and $Y_m = 0.0262$ and the actual x and y co-ordinates of the Nb(1) atom are 0.5655 and 0.0462.

Following the same criterion, the Nb(2) atom appearing at x = 0.66, y = 0.16, z = 0.25 rather than that at x = 0.34, y = -0.16, z = 0.75 was chosen to undergo the Booth treatment. The chosen peaks of Nb(2), Nb(3) and As atomic co-ordinates were similarly determined from the xy section shown in Fig. 4.3.1 (ii), (iii) and (iv) respectively. The tables of function $\Delta\rho$ of the x and y co-ordinates were shown in Table 4.3.2, 4.3.3 and 4.3.4.

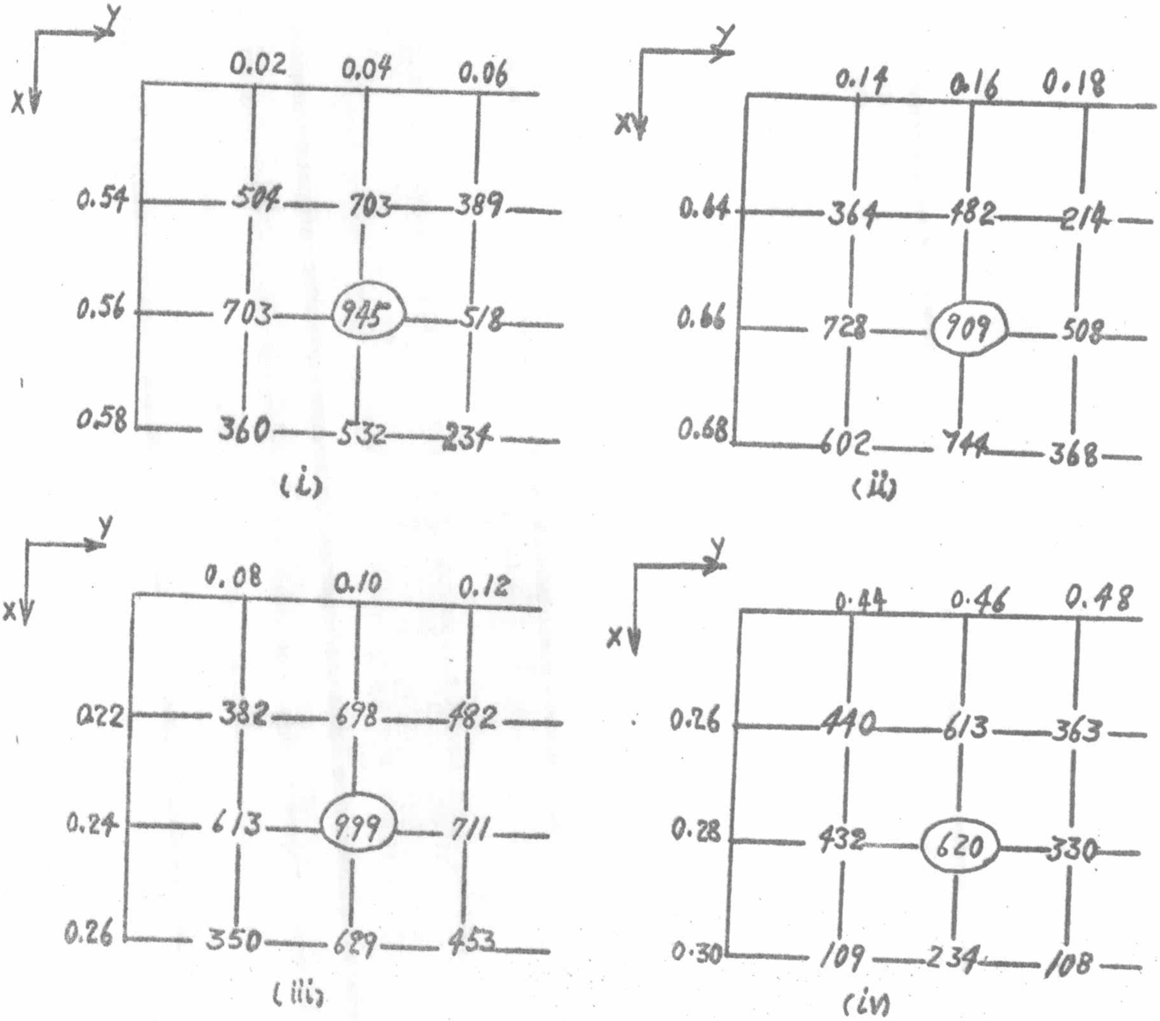


Fig.4.3.1 (i) Section through a Nb(1) atom in F_o synthesis at z = 0.75.

(ii) Section through a Nb(2) atom in F_o synthesis at z = 0.25.

(iii) Section through a Nb(3) atom in F_o synthesis at z = 0.

(iv) Section through a As atom in F_o synthesis at z = 0.5.

Table 4.3.1 The function $\Delta\rho$ of the x and y co-ordinates of Nb(1) atom.

x	0.54	0.56	0.58
Δx	0	0.02	0.04
$\Delta\rho$	0	242	171

y	0.02	0.04	0.06
Δy	0	0.02	0.04
$\Delta\rho$	0	242	185

Table 4.3.2 The function $\Delta\rho$ of the x and y co-ordinates of Nb(2) atom.

x	0.64	0.66	0.68
Δx	0	0.02	0.04
$\Delta\rho$	0	427	262

y	0.14	0.16	0.18
Δy	0	0.02	0.04
$\Delta\rho$	0	181	220

Table 4.3.3 The function $\Delta\rho$ of the x and y co-ordinates of Nb(3) atom.

x	0.22	0.24	0.26
Δx	0	0.02	0.04
$\Delta\rho$	0	301	69

y	0.08	0.10	0.12
Δy	0	0.02	0.04
$\Delta\rho$	0	386	98

Table 4.3.4 The function $\Delta\rho$ of the x and y co-ordinates of As atom.

x	0.26	0.28	0.30
Δx	0	0.02	0.04
$\Delta\rho$	0	7	379

y	0.44	0.46	0.48
Δy	0	0.02	0.04
$\Delta\rho$	0	188	102

And from the other peaks, the co-ordinate of these atoms were given. The average value of the positional co-ordinates were given in the Table 4.3.5.

Table 4.3.5 The co-ordinates of Nb atoms and As atom were obtained from F_o synthesis.

Atom	x	y	z
Nb(1)	0.5465	0.4386	0.2500
Nb(2)	0.6644	0.1455	0.2500
Nb(3)	0.2401	0.0998	0
As	0.0402	0.2699	0

By assuming the atoms were at exactly z = 0, and 0.25, it was inspected that the calculated values of the structure factors of a number of reflections were zero whereas the corresponding observed values were small. It was therefore concluded that the co-ordinates in z were approximately correct, however they needed be slightly shifted. The following set of atomic parameters with the newly adjusted values of z and the smaller values in the x-direction, were thus employed later on in the subsequent calculation which yielded a better agreement between the observed and calculated structure factors.

Table 4.3.6 The positional parameters of atoms in Nb_3As.

Atom	x	y	z	Biso
Nb(1)	0.0614	0.5465	0.2400	0.2500
Nb(2)	0.1644	0.6755	0.7400	0.2500
Nb(3)	0.0988	0.2599	0.5100	0.2500
As	0.0402	0.2699	0.0100	0.2500

4.3.2 Least-squares refinement

After the structure factor calculation, the R value that is $\frac{\sum_{hkl} |F_o| - |F_c|}{\sum_{hkl} |F_o|}$ was given. The output included the scale factors for each layers.

In the initial stage, refinement was restricted to the scale factors, isotropic temperature factors, and the positional parameters of the four atoms.

The weighting function was a measure of the relative of the observation. According to Cruickshank this was calculated, thus,

$$W = \frac{1}{(a + |F_o| + c|F_o|^2)}$$

where $a = 2\ F_{o\ min}$

and $c = 2/F_{o\ max}$

F_{min} and F_{max} are the minimum and maximum values of the observed structure factors.

The atomic positions and thermal par. eters were calculated for each atom to decrease R. Then the scale factor for each layer were introduced in the refinement. So the least shift of the parameters was given. The final R value being in the range of 0.1244, the parameters are shown in Table 4.3.7.

Table 4.3.7 The results from the last cycle of the least-square method for the isotropic temperature factor.

Atom	x	σ (x)	y	σ(y)	z	σ (z)	Biso
Nb(1)	0.0568	0.0005	0.5361	0.0005	0.239	0.001	0.5730
Nb(2)	0.1651	0.0005	0.5544	0.0005	0.730	0.001	0.6104
Nb(3)	0.1024	0.0005	0.2621	0.0005	0.516	0.001	0.6356
As	0.0419	0.0006	0.2714	0.0005	0.017	0.002	0.5166

From the last LSQRL program, the observed structure factors were compared with the calculated structure factors for observed reflections of Nb_3As crystal in 5 layers as shown in Table 4.3.8.

Table 4.3.8 The observed and calculated structure factors for the observed reflections of Nb_3As.

H	K	L	F_o	F_c
0	4	0	98.01	95.43
0	6	0	80.39	73.86
0	10	0	261.73	256.28
0	14	0	139.03	114.49
0	16	0	117.96	100.60
1	5	0	459.21	415.60
1	7	0	214.60	223.29
1	9	0	121.48	138.90
1	13	0	87.47	69.60
1	15	0	174.79	169.82
2	4	0	143.75	160.71
2	8	0	138.26	149.41
2	10	0	111.82	98.91
2	12	0	161.74	128.16
2	14	0	92.71	95.13
3	1	0	41.02	45.57
3	3	0	528.12	480.08
3	7	0	202.76	228.06
3	9	0	60.96	52.17
3	11	0	72.18	68.42
3	15	0	136.90	32.05
3	17	0	97.76	75.53
4	0	0	98.01	95.43
4	2	0	435.74	408.16
4	6	0	111.66	117.48
4	8	0	165.90	167.63
4	10	0	99.03	101.74
4	12	0	280.27	272.15
4	16	0	79.30	46.00
5	1	0	139.75	135.22
5	3	0	129.99	134.83
5	5	0	210.35	203.22
5	13	0	135.37	121.02
5	15	0	136.37	112.66
6	0	0	80.39	73.86
6	2	0	166.73	173.75
6	4	0	83.78	195.13
6	6	0	122.38	223.48
6	8	0	174.40	168.88
6	10	0	110.71	101.78
7	1	0	194.05	193.11
7	3	0	193.07	196.60
7	5	0	184.01	169.95
7	7	0	109.71	91.48
7	9	0	96.34	65.20
7	11	0	107.58	78.67
8	2	0	117.58	100.89
9	1	0	173.90	167.60
9	7	0	114.84	105.32
9	11	0	171.82	161.46
10	0	0	261.73	256.28
10	2	0	63.83	69.25
10	8	0	167.66	105.13
11	1	0	236.34	230.87
11	3	0	111.24	103.14
11	5	0	153.70	104.91
11	7	0	71.42	57.51
11	11	0	101.75	66.47
12	6	0	181.93	188.98
12	10	0	99.52	117.25
12	12	0	65.22	71.00
13	11	0	75.48	49.53
14	0	0	128.48	114.49
14	6	0	140.90	138.36
15	3	0	153.86	141.63
16	0	0	117.96	100.60
16	2	0	119.69	115.68
16	8	0	77.65	83.53
0	3	1	62.94	53.49
0	4	1	190.57	162.13
0	10	1	171.31	156.40
0	11	1	64.68	81.81
0	13	1	90.49	105.51
1	3	1	126.63	109.01
1	4	1	354.90	341.85
1	5	1	112.59	104.61
1	6	1	216.54	223.44
1	7	1	175.87	171.76
1	9	1	84.42	91.43
1	10	1	62.09	67.88
1	14	1	122.04	134.31
2	3	1	257.41	268.33
2	4	1	185.46	174.80
2	5	1	69.54	67.73
2	6	1	37.84	57.57
2	7	1	105.33	104.94
2	9	1	132.66	136.79
2	10	1	134.53	128.55
2	12	1	52.47	62.36
2	13	1	48.77	64.45
2	15	1	52.76	66.31
3	0	1	62.94	53.49
3	1	1	70.18	66.03
3	2	1	336.55	316.10
3	3	1	94.64	93.34
3	5	1	79.55	77.75
3	6	1	115.67	108.73
3	7	1	129.79	132.20
3	8	1	201.84	216.98
3	9	1	94.31	103.20
3	10	1	53.78	58.78
3	12	1	69.41	83.90
3	16	1	51.72	94.89
4	0	1	190.57	162.13
4	1	1	300.12	235.38
4	2	1	192.77	186.92
4	3	1	[illegible]	51.23
4	4	1	[illegible]	44.45
4	6	1	171.52	185.96
4	9	1	165.85	152.95
4	10	1	59.50	74.47
4	12	1	58.48	73.40
5	1	1	308.81	170.78
5	4	1	137.37	119.46
5	5	1	87.03	86.12
5	6	1	56.89	72.30
5	7	1	232.40	226.34
5	11	1	66.99	81.19
5	13	1	76.20	71.36
6	1	1	173.14	154.99
6	4	1	123.54	118.60
6	6	1	146.77	135.79
6	7	1	72.45	58.69

Table 4.3.8

(continued)

H	K	L	F_o	F_c
5	9	1	178.38	159.67
7	1	1	93.28	90.11
7	2	1	205.96	167.00
7	3	1	233.47	217.82
7	4	1	77.02	80.97
7	5	1	98.21	98.89
7	8	1	79.33	90.32
7	9	1	190.61	168.57
7	10	1	66.80	66.18
7	14	1	108.03	99.23
8	1	1	42.25	54.05
8	2	1	100.69	100.06
8	3	1	184.05	165.43
8	4	1	249.57	226.83
8	5	1	92.96	109.78
8	7	1	226.85	183.87
8	8	1	116.94	130.10
8	10	1	129.23	128.20
8	11	1	144.18	119.06
8	13	1	63.58	75.40
8	14	1	62.95	77.43
9	1	1	119.14	117.53
9	4	1	264.78	186.41
9	8	1	55.36	61.88
9	9	1	143.61	123.47
10	0	1	171.31	156.40
10	1	1	51.15	45.93
10	2	1	87.44	94.64
10	3	1	74.14	76.51
10	6	1	206.14	197.25
10	9	1	82.18	83.03
10	12	1	59.51	66.88
11	0	1	64.68	81.81
11	1	1	79.43	83.78
11	2	1	97.06	107.50
11	4	1	130.44	129.49
11	5	1	108.18	110.54
11	6	1	48.10	64.61
11	7	1	127.85	124.08
11	10	1	76.04	25.18
11	11	1	105.80	108.24
12	6	1	56.21	77.00
13	0	1	90.49	105.51
13	2	1	135.04	138.16
13	9	1	74.37	88.37
13	10	1	76.22	100.89
14	4	1	83.60	41.82
14	8	1	75.36	94.85
15	4	1	91.67	89.77
15	8	1	51.83	30.96
0	3	2	130.88	105.15
0	4	2	178.65	180.13
0	5	2	34.79	33.87
0	6	2	353.31	327.05
0	7	2	60.36	66.09
0	8	2	194.25	201.51
0	10	2	160.28	143.75
1	3	2	45.52	52.51
1	7	2	74.82	93.24
1	9	2	148.32	148.97
1	11	2	107.32	106.07
1	13	2	166.68	177.04
2	2	2	317.98	405.83
2	5	2	78.14	15.50

H	K	L	F_o	F_c
2	6	2	131.77	136.26
2	8	2	78.35	80.80
2	10	2	124.03	137.26
2	12	2	59.05	69.25
2	14	2	144.34	167.20
3	0	2	119.68	105.15
3	1	2	257.18	245.14
3	3	2	204.16	183.86
3	5	2	116.05	114.47
3	9	2	97.30	100.89
4	0	2	191.05	180.13
4	2	2	63.83	70.84
4	4	2	163.77	158.80
4	5	2	82.20	78.84
4	6	2	243.71	227.73
4	10	2	151.60	161.03
4	16	2	166.90	169.78
5	0	2	44.80	33.87
5	3	2	218.40	209.04
5	5	2	411.74	375.53
5	6	2	39.62	43.98
5	13	2	66.58	67.93
6	0	2	353.31	327.05
6	1	2	41.64	55.88
6	2	2	47.57	41.54
6	14	2	84.58	96.32
7	0	2	65.49	66.09
7	1	2	225.29	218.99
7	3	2	85.24	93.14
7	7	2	166.33	165.61
7	11	2	56.86	81.96
7	13	2	136.52	158.62
8	0	2	226.61	201.51
8	2	2	150.70	148.72
8	18	2	71.94	67.00
9	1	2	59.68	65.62
9	3	2	118.47	109.35
9	5	2	70.68	71.52
9	7	2	92.13	98.03
10	0	2	175.65	143.75
10	2	2	139.72	124.04
10	4	2	94.24	95.40
10	8	2	127.50	128.22
10	10	2	164.85	141.31
10	16	2	67.86	28.71
11	5	2	101.81	96.79
11	7	2	67.43	72.32
11	13	2	130.11	133.13
12	2	2	[illegible]42	191.44
12	6	2	114.19	103.78
14	4	2	95.91	110.69
15	6	2	104.84	28.06
15	8	2	74.07	9.54
16	12	2	59.71	63.96
17	1	2	248.26	216.82
19	13	2	58.25	22.28
0	3	3	36.51	43.99
0	4	3	152.82	139.11
0	6	3	32.55	50.95
0	7	3	93.45	99.05
0	10	3	124.78	116.17
1	4	3	249.97	212.05
1	5	3	55.36	64.67
1	6	3	157.08	147.61

Table 4.3.8

(continued)

H	K	L	F_o	F_c
1	7	3	72.52	82.71
1	9	3	83.60	86.86
1	10	3	101.07	94.25
1	13	3	57.17	69.18
2	1	3	31.63	36.48
2	2	3	43.30	47.79
2	3	3	164.35	191.64
2	4	3	225.16	210.71
2	5	3	55.12	59.90
2	6	3	60.50	66.67
2	7	3	150.58	144.41
2	8	3	59.07	57.85
2	9	3	76.86	81.47
2	10	3	57.80	75.31
2	12	3	61.52	30.55
2	19	3	94.33	56.73
3	0	3	36.51	43.99
3	1	3	131.87	116.19
3	2	3	262.11	240.98
3	3	3	21.71	8.74
3	4	3	32.65	43.59
3	6	3	146.83	134.46
3	7	3	81.11	88.78
3	8	3	192.27	159.78
3	9	3	191.93	163.86
3	10	3	78.23	74.55
4	0	3	151.44	139.11
4	1	3	211.03	198.34
4	2	3	38.01	62.00
4	3	3	95.77	93.67
4	4	3	42.74	43.35
4	5	3	45.36	50.37
4	6	3	137.81	129.00
4	8	3	63.33	71.35
4	9	3	91.82	81.07
5	1	3	157.68	133.80
5	4	3	37.80	54.33
5	5	3	63.13	76.90
5	7	3	175.97	168.70
5	12	3	72.11	44.77
6	0	3	50.29	50.95
6	1	3	191.34	161.97
6	4	3	96.37	112.82
6	5	3	107.91	139.52
6	7	3	86.17	80.22
6	9	3	214.69	188.06
6	11	3	57.17	55.25
6	14	3	71.58	33.18
7	0	3	95.17	99.05
7	1	3	106.10	100.81
7	2	3	69.28	77.72
7	3	3	237.28	225.39
7	4	3	54.46	55.47
7	5	3	102.69	104.93
7	6	3	56.63	52.63
7	8	3	61.96	87.97
7	9	3	113.02	103.79
8	2	3	47.55	62.27
8	3	3	137.55	136.17
8	4	3	97.67	102.55
8	5	3	138.20	135.97
8	7	3	99.50	88.94
8	8	3	141.51	143.24
8	10	3	148.67	132.57
8	14	3	74.16	21.63
9	1	3	97.00	101.41
9	3	3	71.62	80.59
9	4	3	237.07	193.47
9	6	3	63.76	75.17
9	7	3	73.92	72.53
9	9	3	89.71	85.07
9	13	3	70.10	39.87
10	0	3	114.63	116.17
10	2	3	92.15	107.95
10	6	3	174.24	178.71
10	9	3	124.55	124.29
10	11	3	76.91	38.68
11	2	3	99.64	119.06
11	3	3	53.66	20.99
11	5	3	110.86	112.47
11	7	3	75.84	80.33
12	2	3	51.55	69.55
12	3	3	70.88	56.03
12	4	3	70.78	81.34
13	2	3	111.56	129.51
13	3	3	74.63	87.77
13	6	3	89.66	89.30
13	9	3	108.49	123.55
14	2	3	59.65	74.76
14	3	3	78.29	86.47
18	5	3	79.51	38.24
0	3	4	53.54	63.56
0	4	4	61.55	66.90
0	6	4	5[illegible].56	55.97
0	10	4	1[illegible].33	179.46
0	11	4	55.92	73.25
0	14	4	77.51	86.12
1	4	4	81.58	82.50
1	5	4	321.81	248.29
1	6	4	71.58	71.74
1	7	4	149.46	142.02
1	8	4	51.88	45.84
1	9	4	97.23	96.20
1	15	4	109.07	126.70
2	3	4	41.36	57.04
2	4	4	92.87	94.37
2	5	4	82.90	85.90
2	8	4	101.88	107.22
2	10	4	74.91	78.10
2	12	4	93.48	98.12
2	14	4	48.70	67.50
3	0	4	5	63.56
3	3	4	319.[illegible]	286.02
3	4	4	60.53	54.46
3	5	4	66.63	67.91
3	7	4	161.21	150.96
3	8	4	52.67	49.88
4	0	4	52.70	66.90
4	1	4	49.78	49.58
4	2	4	279.43	240.63
4	6	4	68.12	74.03
4	7	4	39.03	17.91
4	8	4	139.60	121.25
4	10	4	58.36	64.74
4	12	4	223.80	196.85
5	1	4	64.09	70.86
5	2	4	141.90	121.99
5	3	4	74.56	90.84

Table 4.3.8

(continued)

H	K	L	F_o	F_c
5	5	4	129.77	133.13
5	6	4	69.25	71.43
5	13	4	71.83	88.51
5	15	4	83.36	83.84
6	0	4	47.83	55.97
6	2	4	86.63	106.69
6	3	4	36.27	46.52
6	4	4	132.92	124.60
6	5	4	44.24	44.16
6	6	4	173.52	146.51
6	7	4	70.79	64.06
6	8	4	119.09	117.62
7	1	4	126.37	126.91
7	2	4	48.43	49.33
7	3	4	137.86	137.33
7	5	4	147.38	126.13
7	7	4	55.33	63.60
8	2	4	67.75	64.82
8	6	4	53.26	20.19
9	1	4	134.93	116.15
9	7	4	66.67	76.82
10	0	4	202.07	179.46
10	1	4	88.13	76.96
10	2	4	51.35	55.21
10	8	4	86.26	80.22
11	0	4	53.88	73.25
11	1	4	161.39	159.37
11	3	4	63.68	75.46
11	5	4	62.87	73.23
12	1	4	52.56	16.53
12	6	4	167.78	137.77
13	1	4	55.37	14.03
13	5	4	65.95	44.90
14	0	4	57.97	86.12
15	4	4	61.71	13.76
15	2	4	82.06	83.64

4.4 Determination of accurate lattice constants

The precise cell constants of Nb_3As can be obtained from the powder method by using the XDC 700 focusing camera.

The procedure for identifying a powder diffraction pattern involved measuring the positions of the diffraction lines in the photograph shown in Fig.3.6.3. In turn, the diffraction angles, the spacing d of these reflecting planes were calculated.

From the diffraction patterns, the six strongest reflections probably those of silicon were used to plot the graph of $\theta/(S-S_0)$ against $(S-S_0)$ shown in Fig.4.4.1, the values of $\theta/(S-S_0)$ and θ for each reflection were obtained. These lines were then confirmed as silicon. S_0 is the reference primary line read in mm. and S is the reading in mm. of each diffraction lines. The values of $\theta/(S-S_0)$ of silicon corresponding to $(S-S_0)$ and the values of reflecting angles θ were obtained in Table 4.4.1.

The Miller indices of the diffraction lines were obtained by the trial-and-error method. These angles θ and the d-spacings have to be related to the unit cell parameters and Miller indices assigned to the individual reflections. For the tetragonal system, the value of $\sin^2\theta_{hkl}$ can be expressed, thus

$$\sin^2\theta_{hkl} \quad = \quad A(h^2 + k^2) + Cl^2 \qquad \ldots (4.4.1)$$

where a and c are values of rough cell constants,

$$A = \frac{\lambda^2}{4a^2}$$

$$C = \frac{\lambda^2}{4c^2}$$

All possible values of $\sin^2\theta_{hkl}$ based on the values of A, C and indices hkl are calculated and compared with the observed values of $\sin^2\theta_{hkl}$. If the agreement is better than 0.0005, the indexing is probably correct.

Table **4.4.1** **The standard silicon lines** for CuK_{α_1} **radiation.**

hkl	θ^o	$(S-S_o)_{cal}$ (mm)	$(S-S_o)_o$ (mm)	$\theta/(S-S_o)_{cal}$	$\theta/(S-S_o)_o$
111	14.2214	49.725	49.68	0.28600	0.28626
220	23.6517	82.698	82.62	0.28600	0.28627
311	28.0616	98.117	98.06	0.28600	0.28617
400	34.5655	120.858	120.69	0.28600	0.28640
331	38.1887	133.527	133.42	0.28600	0.286[illegible]3
422	44.0158	153.901	153.73	0.28600	0.28632

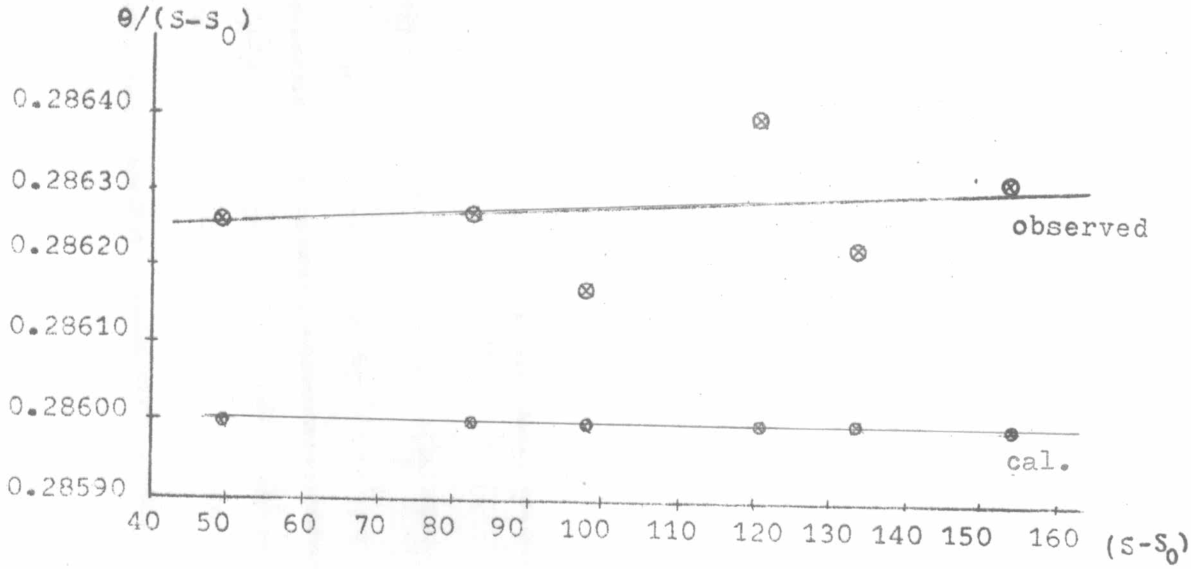


Fig.4.4.1 The graph of the observed values and those obtained from the calculation of $\theta/(S-S_0)$ against $(S-S_0)$ of silicon.

The data leading to the d-spacing as obtained from the powder pattern were shown in Table 4.4.2.

Table 4.4.2 The powder data obtained from powder pattern of Nb_3As where S_o = 26.05 mm., λ = 1.54051 Å .

S (mm.)	$S-S_o$ (mm.)	θ (degree)	$\theta/(S-S_o)$	$d = \lambda/2\sin\theta$ d-spacings identified as those of lines, (Å)		
				Unidentifiable	Nb_7As_4	Nb_3As
61.29	35.24	10.0875	0.28625		4.398	
62.88	36.83	10.5428	0.28626			4.210
78.45	52.40	15.0000	0.28626		2.976	
79.54	53.49	15.3121	0.28626		2.917	
81.56	55.51	15.8903	0.28626		2.813	
82.71	55.66	16.2195	0.28626			2.758
83.02	56.97	16.3082	0.28626		2.743	
83.24	57.19	16.3712	0.28626		2.733	
85.97	59.92	17.1527	0.28626		2.612	
87.19	61.14	17.5019	0.28626		2.561	
88.66	62.61	17.9227	0.28626			2.503
88.93	62.88	18.0003	0.28626		2.483	
89.36	63.31	18.1234	0.28627		2.476	
90.13	64.08	18.3439	0.28627			2.447
90.67	64.62	18.4984	0.28627			2.428
92.68	66.63	19.0738	0.28627		2.357	

Table 4.4.2

(continued)

S (mm.)	$S-S_o$ (mm.)	θ (degree)	$\theta/(S-S_o)$	d = λ/2sin θ d-spacings identified as those of lines, (Å)		
				Unidentifiable	Nb_7As_4	Nb_3As
93.59	67.54	19.3343	0.28627			2.327
93.90	67.85	19.4231	0.28627		2.316	
94.29	68.24	19.5347	0.28627			2.304
94.51	68.46	19.5977	0.28627		2.297	
94.80	68.75	19.6807	0.28627		2.287	
95.29	69.24	19.8210	0.28627		2.272	
95.95	69.90	20.0099	0.28627			2.251
97.11	71.06	20.3420	0.28627		2.216	
97.59	71.54	20.4794	0.28627		2.202	
98.95	72.90	20.8687	0.28627			2.162
99.46	73.41	21.0147	0.28627		2.143	
100.65	74.60	21.3554	0.28627			2.115
101.02	74.97	21.4613	0.28627			2.105
101.62	75.57	21.6331	0.28627		2.089	
102.94	76.89	22.0109	0.28627		2.055	
103.33	77.28	22.1226	0.28627		2.045	
103.91	77.86	22.2889	0.28627			2.031
104.38	78.33	22.4235	0.28627			2.019
105.99	79.94	22.8844	0.28627		1.981	

Table 4.4.2

(continued)

S (mm.)	$S-S_o$ (mm.)	θ (degree)	$\theta/(S-S_o)$	$d = \lambda/2\sin\theta$ d-spacings identified as those of lines, (Å)		
				Unidentifiable	Nb_7As_4	Nb_3As
107.52	81.47	23.3224	0.28627		1.946	
108.07	82.02	23.4399	0.28627		1.933	
108.99	82.94	23.7432	0.28627			1.913
110.50	84.45	24.1747	0.28626			1.881
111.88	85.83	24.5688	0.28625		1.853	
113.12	87.07	24.9229	0.28625			1.828
114.39	88.34	25.2860	0.28624		1.803	
114.94	88.89	25.4429	0.28623			1.793
115.25	89.20	25.5313	0.28623		1.787	
116.00	89.95	25.7455	0.28622			1.773
116.63	90.58	25.9258	0.28622		1.762	
117.08	91.03	26.0546	0.28622		1.754	
118.84	92.79	26.5570	0.28621			1.723
119.10	93.05	26.6310	0.28620			1.718
124.44	98.39	28.1563	0.28617		1.632	
125.98	99.93	28.5990	0.28619			1.609
127.51	101.46	29.0379	0.28620		1.587	
128.40	102.35	29.2936	0.28621		1.574	
132.16	106.11	30.3740	0.28625		1.523	

Table 4.4.2

(continued)

S (mm.)	$S-S_o$ (mm.)	θ (degree)	$\theta/(S-S_o)$	$d = \lambda/2\sin\theta$ d-spacings identified as those of lines, (Å)		
				Unidentifiable	Nb_7As_4	Nb_3As
132.63	106.58	30.5091	0.28626		1.517	
134.38	108.33	31.0116	0.28627		1.495	
135.01	108.96	31.1931	0.28628		1.487	
135.58	109.53	31.3568	0.28628		1.480	
137.26	111.21	31.8394	0.28630			1.460
137.69	111.64	31.9631	0.28631			1.455
139.36	113.31	32.4429	0.28632		1.436	
140.26	114.21	32.7018	0.28633		1.426	
140.60	114.55	32.7997	0.28634		1.422	
141.04	114.99	32.9262	0.28634		1.417	
141.99	115.94	33.1994	0.28635		1.407	
142.69	116.64	33.4005	0.28636		1.399	
143.05	117.00	33.5041	0.28636		1.395	
143.58	117.53	33.6565	0.28637		1.390	
144.01	117.96	33.7802	0.28637		1.385	
144.83	118.78	34.0156	0.28638		1.377	
145.53	119.48	34.2173	0.28639		1.370	
146.11	120.06	34.3840	0.28639			1.364
147.30	121.25	34.7248	0.28639			1.352

Table 4.4.2

(continued)

S (mm.)	$S-S_o$ (mm.)	θ (degree)	$\theta/(S-S_o)$	$d = \lambda/2\sin\theta$ d-spacings identified as those of lines , (Å)		
				Unidentifiable	Nb_7As_4	Nb_3As
147.95	121.90	34.9085	0.28637		1.346	
149.20	123.15	35.2640	0.28635		1.334	
150.30	124.25	35.5778	0.28634		1.324	
151.25	125.20	35.8500	0.28634			1.315
151.74	125.69	35.9888	0.28633		1.311	
152.16	126.11	36.1085	0.28633		1.307	
153.06	127.01	36.3642	0.28631			1.299
156.46	130.41	37.3325	0.28627			1.270
159.96	133.91	38.3291	0.28623			1.242
160.61	134.56	38.5158	0.28624			1.237
161.60	135.55	38.8012	0.28625		1.229	
163.70	137.65	39.4023	0.28625			1.213
169.30	143.25	41.0089	0.28628		1.174	
170.21	144.16	41.2694	0.28628		1.166	
170.48	144.43	41.3474	0.28628		1.134	
172.50	146.45	41.9316	0.28632		1.153	
173.70	147.65	42.2766	0.28633			1.145
175.50	149.45	42.7875	0.28630	1.134		
176.00	149.95	42.9307	0.28630		1.131	

Table 4.4.2

(continued)

S (mm.)	$S-S_o$ (mm.)	θ (degree)	$\theta/(S-S_o)$	$d = \lambda/2\sin\theta$ d-spacings identified as those of lines, (Å)		
				Unidentifiable	Nb_7As_4	Nb_3As
177.01	150.96	43.2274	0.28635		1.125	
177.70	151.65	43.4189	0.28631			1.121
180.37	154.32	44.1849	0.28632	1.105		
181.10	155.05	44.3947	0.28632			1.101
182.72	156.67	44.8593	0.28633			1.092

The unit cell dimensions were refined by the least-squares method using CELSP program. This program was written by J. Tegenfeldt and N-O Ersson, Institute of Chemistry, University of Uppsala, Sweden, and modified for the NEAC 2200 computer by the Crystallography Group, Department of Physics, Chulalongkorn University, under the supervision of R-Liminga, Institute of Chemistry, University of Uppsala, Sweden. For this program, the maximum number of input reflections is 50.

From the diffraction lines of the photograph in Fig.3.6.3, it was found that there were more than two compounds other than the standard silicon in the sample. In the refinement, the data of the Nb_3As compound was chosen to be refined. Ten diffraction lines were used to be refined first, the cell parameters obtained were :

$$a = 10.294 \pm 0.001 \text{ Å} \quad , \quad c = 5.1965 \pm 0.0004 \text{ Å}$$

The other diffraction lines of Nb_3As were refined further and the results of refinement are shown in Table 4.4.3.

The final cell parameters obtained were :

$$a = 10.294 \pm 0.001 \text{ Å} \quad , \quad c = 5.1958 \pm 0.0007 \text{ Å}$$

and $v = 550.58 \text{ Å}^3$

Table 4.4.3 The comparison of the $\sin^2\theta_{obs}$ and $\sin^2\theta_{cal}$ (a = 10.294 Å , c = 5.1958 Å) from powder diffraction data of Nb_3As

hkl	$\sin^2\theta_o \times 10^5$	$\sin^2\theta_c \times 10^5$	d (Å)
311	7802	7797	2.758
321	9470	9477	2.503
112	9905	9911	2.447
411	11709	11717	2.251
222	13261	13270	2.115
312	14385	14390	2.031
510	14550	14559	2.019
402	17758	17750	1.828
332	18868	18870	1.773
422	19989	19990	1.723
611	22913	22916	1.609
532	27830	27829	1.460
004	35155	35163	1.299
722	38462	38468	1.242

4.5 Interatomic distances and angles

The distance between two atoms in fractional co-ordinates (x_1,y_1,z_1) and (x_2,y_2,z_2), which are at the points A and B in Fig.4.5.1, is given by the law of cosines in three dimensions,

$$l = \sqrt{(\Delta xa)^2 + (\Delta yb)^2 + (\Delta zc)^2 + 2ab\,\Delta x\,\Delta y\cos\gamma + 2ac\,\Delta x\,\Delta z\cos\beta + 2bc\,\Delta y\,\Delta z\cos\alpha} \quad \ldots (4.5.1)$$

where $a, b, c, \alpha, \beta, \gamma$ are the unit cell parameters,

Δx is $(x_2 - x_1)$, Δy is $(y_2 - y_1)$ and Δz is $(z_2 - z_1)$

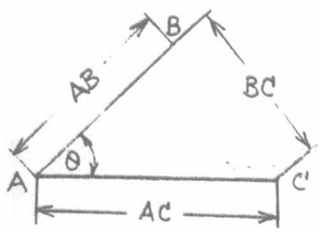


Fig. 4.5.1 A set of three atoms showing the interatomic distances AB, BC, AC and the bond angles θ.

In Fig.4.5.1., the angle θ subtended by bonds AB and AC can be calculated by the law of cosines,

$$\theta = \cos^{-1}\left[\frac{(AB)^2 + (AC)^2 - (BC)^2}{2(AB)(AC)}\right] \quad \ldots (4.5.2)$$

For Nb_3As, all of the positional parameters were obtained from the last refinement so the interatomic distances and interatomic angles could be solved by using the DISTAN program as shown in Table 4.5.1

Table 4.5.1 The interatomic distances (≤4Å) and angles of Nb_3As.

*** DISTANCES ***

ATOM1	TO ATOM2	X,Y,Z OF ATOM1			X,Y,Z OF ATOM2			DISTANCE	S.D.
NB1	NB1	-0.0568	.4639	-0.2388	.0568	.5361	.2388	2.8411	.0125
NB1	NB1	-0.0568	.4639	.7612	.0568	.5361	.2388	3.0474	.0127
NB2	NB1	.1651	.6544	-0.2698	.0568	.5361	.2388	3.1155	.0088
NB2	NB1	.1651	.6544	.7302	.0568	.5361	.2388	3.0411	.0087
NB2	NB1	.3456	.6651	.2302	.0568	.5361	.2388	3.2567	.0058
NB2	NB1	.1544	.8349	.2302	.0568	.5361	.2388	3.2371	.0054
NB2	NB1	-0.1651	.3456	.2698	.0568	.5361	.2388	3.0139	.0051
NB3	NB1	.1024	.2621	.5161	.0568	.5361	.2388	3.2017	.0080
NB3	NB1	-0.2621	.6024	.0161	.0568	.5361	.2388	3.5465	.0063
NB3	NB1	-0.1024	.7379	.4839	.0568	.5361	.2388	2.9366	.0069
NB3	NB1	.2621	.3976	-0.0161	.0568	.5361	.2388	2.8727	.0077
AS	NB1	.0419	.2714	.0167	.0568	.5361	.2388	2.9624	.0083
AS	NB1	-0.2714	.5419	.5167	.0568	.5361	.2388	3.6744	.0071
AS	NB1	-0.0419	.7286	-0.0167	.0568	.5361	.2388	2.5925	.0083
AS	NB1	.2714	.4581	.4833	.0568	.5361	.2388	2.6725	.0083

ATOM1	TO ATOM2	X,Y,Z OF ATOM1			X,Y,Z OF ATOM2			DISTANCE	S.D.
NB1	NB2	.0568	.5361	.2388	.1651	.6544	.7302	3.0411	.0087
NB1	NB2	.0568	.5361	1.2388	.1651	.6544	.7302	3.1156	.0088
NB1	NB2	.4639	.5568	.7388	.1651	.6544	.7302	3.2371	.0055
NB1	NB2	.0361	.9432	.7388	.1651	.6544	.7302	3.2567	.0056
NB1	NB2	-0.0568	.4639	.7612	.1651	.6544	.7302	3.0139	.0051
NB2	NB2	.3349	.8456	.7302	.1651	.6544	.7302	2.6329	.0084
NB2	NB2	.3456	.6651	.2302	.1651	.6544	.7302	3.1961	.0035
NB2	NB2	.3456	.6651	1.2302	.1651	.6544	.7302	3.1961	.0035
NB2	NB2	.1544	.8349	.2302	.1651	.6544	.7302	3.1961	.0035
NB2	NB2	.1544	.8349	1.2302	.1651	.6544	.7302	3.1961	.0035
NB3	NB2	-0.1024	.7379	.4839	.1651	.6544	.7302	3.1554	.0047
NB3	NB2	.2621	.3976	.9839	.1651	.6544	.7302	3.1180	.0068
AS	NB2	-0.0419	.7286	.9833	.1651	.6544	.7302	2.6177	.0062
AS	NB2	.2714	.4581	.4833	.1651	.6544	.7302	2.6322	.0078

ATOM1	TO ATOM2	X,Y,Z OF ATOM1			X,Y,Z OF ATOM2			DISTANCE	S.D.
NB1	NB3	.0568	.5361	.2388	.1024	.2621	.5161	3.2017	.0080
NB1	NB3	.0361	-0.0568	.7388	.1024	.2621	.5161	3.5465	.0061
NB1	NB3	-0.0568	.4639	.7612	.1024	.2621	.5161	2.9366	.0069
NB1	NB3	-0.0361	.0568	.2613	.1024	.2621	.5161	2.8727	.0071
NB2	NB3	-0.1651	.3456	.2698	.1024	.2621	.5161	3.1554	.0047
NB2	NB3	-0.1544	.1651	.7698	.1024	.2621	.5161	3.1180	.0082
NB3	NB3	.3976	.2379	.5161	.1024	.2621	.5161	3.0493	.0069
NB3	NB3	.2621	.3976	-0.0161	.1024	.2621	.5161	3.5066	.0113
NB3	NB3	.2621	.3976	.9839	.1024	.2621	.5161	3.2490	.0108
NB3	NB3	.2379	.1024	-0.0161	.1024	.2621	.5161	3.5066	.0113
NB3	NB3	.2379	.1024	.9839	.1024	.2621	.5161	3.2490	.0107
AS	NB3	.0419	.2714	.0167	.1024	.2621	.5161	2.6704	.0110
AS	NB3	.0419	.2714	1.0167	.1024	.2621	.5161	[illegible]	.0110
AS	NB3	.2714	.4581	.4833	.1024	.2621	.5161	2.6696	.0069
AS	NB3	.2286	.0419	.4833	.1024	.2621	.5161	2.6179	.0063

ATOM1	TO ATOM2	X,Y,Z OF ATOM1			X,Y,Z OF ATOM2			DISTANCE	S.D.
NB1	AS	.0568	.5361	.2388	.0419	.2714	.0167	2.9624	.0083
NB1	AS	.0361	-0.0568	-0.2612	.0419	.2714	.0167	3.6744	.0068
NB1	AS	-0.0568	.4639	-0.2388	.0419	.2714	.0167	2.5925	.0083
NB1	AS	-0.0361	.0568	.2613	.0419	.2714	.0167	2.6725	.0074
NB2	AS	-0.1651	.3456	.2698	.0419	.2714	.0167	2.6177	.0062
NB2	AS	-0.1544	.1651	-0.2302	.0419	.2714	.0167	2.6322	.0086
NB3	AS	.1024	.2621	-0.4839	.0419	.2714	.0167	2.6759	.0110
NB3	AS	.1024	.2621	.5161	.0419	.2714	.0167	2.6704	.0110
NB3	AS	.2621	.3976	-0.0161	.0419	.2714	.0167	2.6179	.0073
NB3	AS	.2379	.1024	-0.0161	.0419	.2714	.0167	2.6696	.0069
AS	AS	.2714	.4581	.4833	.0419	.2714	.0167	3.8927	.0117
AS	AS	.2286	.0419	.4833	.0419	.2714	.0167	3.8927	.0115

Table 4.5.1

(continued)

* ANGLES *

ATOM1	ATOM2	ATOM3	ANGLE	SD	DIST12	DIST23	DIST13	XYZ OF ATOM1			XYZ OF ATOM2			XYZ OF ATOM3		
NB1	NB1	NB1	123.82	.20	2.841	3.047	5.195	-0.057	.464	-0.239	.057	.536	.239	-0.057	.464	.761
NB1	NB1	NB2	60.58	.23	2.841	3.116	3.014	-0.057	.464	-0.239	.057	.536	.239	.165	.654	-0.270
NB1	NB1	NB2	171.39	.83	2.841	3.041	5.865	-0.057	.464	-0.239	.057	.536	.239	.165	.654	.730
NB1	NB1	NB2	118.05	.31	2.841	3.257	5.232	-0.057	.464	-0.239	.057	.536	.239	.346	.665	.230
NB1	NB1	NB2	111.35	.33	2.841	3.237	5.225	-0.057	.464	-0.239	.057	.536	.239	.154	.835	.230
NB1	NB1	NB2	64.22	.18	2.841	3.014	3.115	-0.057	.464	-0.239	.057	.536	.239	-0.165	.346	.270
NB1	NB1	NB3	102.30	.28	2.841	3.202	4.731	-0.057	.464	-0.239	.057	.536	.239	.102	.262	.516
NB1	NB1	NB3	54.03	.12	2.841	3.546	2.873	-0.057	.464	-0.239	.057	.536	.239	-0.262	.602	.016
NB1	NB1	NB3	109.52	.19	2.841	2.937	4.719	-0.057	.464	-0.239	.057	.536	.239	-0.102	.736	.404
NB1	NB1	NB3	76.73	.26	2.841	2.873	3.546	-0.057	.464	-0.239	.057	.536	.239	.271	.458	.403
NB1	NB1	AS	53.01	.23	2.841	2.962	2.592	-0.057	.464	-0.239	.057	.536	.239	.262	.398	-0.016
NB1	NB1	AS	88.24	.14	2.841	3.674	4.575	-0.057	.464	-0.239	.057	.536	.239	.042	.271	.017
NB1	NB1	AS	65.89	.26	2.841	2.592	2.962	-0.057	.464	-0.239	.057	.536	.239	-0.271	.542	.517
NB1	NB1	AS	132.60	.35	2.841	2.672	5.049	-0.057	.464	-0.239	.057	.536	.239	-0.042	.729	-0.017
NB1	NB1	NB2	171.37	.78	3.047	3.116	6.144	-0.057	.464	.761	.057	.536	.239	.165	.654	-0.270
NB1	NB1	NB2	59.34	.22	3.047	3.041	3.014	-0.057	.464	.761	.057	.536	.239	.165	.654	.730
NB1	NB1	NB2	117.49	.29	3.047	3.257	5.390	-0.057	.464	.761	.057	.536	.239	.346	.665	.230
NB1	NB1	NB2	111.27	.31	3.047	3.237	5.189	-0.057	.464	.761	.057	.536	.239	.154	.835	.230
NB1	NB1	NB2	60.22	.17	3.047	3.014	3.041	-0.057	.464	.761	.057	.536	.239	-0.165	.346	.270
NB1	NB1	NB3	55.99	.20	3.047	3.202	2.937	-0.057	.464	.761	.057	.536	.239	.102	.262	.516
NB1	NB1	NB3	89.00	.11	3.047	3.546	4.635	-0.057	.464	.761	.057	.536	.239	-0.262	.602	.016
NB1	NB1	NB3	64.66	.21	3.047	2.937	3.202	-0.057	.464	.761	.057	.536	.239	-0.102	.736	.404
NB1	NB1	NB3	124.89	.31	3.047	2.873	5.249	-0.057	.464	.761	.057	.536	.239	.271	.458	.403
NB1	NB1	AS	95.93	.20	3.047	2.962	4.464	-0.057	.464	.761	.057	.536	.239	.262	.398	-0.016
NB1	NB1	AS	45.65	.13	3.047	3.674	2.672	-0.057	.464	.761	.057	.536	.239	.042	.271	.017
NB1	NB1	AS	119.47	.24	3.047	2.592	4.677	-0.057	.464	.761	.057	.536	.239	-0.271	.542	.517
NB1	NB1	AS	79.65	.29	3.047	2.672	3.674	-0.057	.464	.761	.057	.536	.239	-0.042	.729	-0.017
NB2	NB1	NB2	115.10	.18	3.116	3.041	5.195	.165	.654	-0.270	.057	.536	.239	.165	.654	.730
NB2	NB1	NB2	60.10	.10	3.116	3.257	3.195	.165	.654	-0.270	.057	.536	.239	.346	.665	.230
NB2	NB1	NB2	60.37	.10	3.116	3.237	3.195	.165	.654	-0.270	.057	.536	.239	.154	.835	.230
NB2	NB1	NB2	124.80	.23	3.116	3.014	5.432	.165	.654	-0.270	.057	.536	.239	-0.165	.346	.270
NB2	NB1	NB3	132.35	.20	3.116	3.202	5.779	.165	.654	-0.270	.057	.536	.239	.102	.262	.516
NB2	NB1	NB3	88.81	.18	3.116	3.546	4.672	.165	.654	-0.270	.057	.536	.239	-0.262	.602	.016
NB2	NB1	NB3	106.93	.23	3.116	2.937	4.863	.165	.654	-0.270	.057	.536	.239	-0.102	.736	.404
NB2	NB1	NB3	62.60	.17	3.116	2.873	3.118	.165	.654	-0.270	.057	.536	.239	.271	.458	.403
NB2	NB1	AS	92.73	.20	3.116	2.962	4.400	.165	.654	-0.270	.057	.536	.239	.262	.398	-0.016
NB2	NB1	AS	130.93	.18	3.116	3.674	6.183	.165	.654	-0.270	.057	.536	.239	.042	.271	.017
NB2	NB1	AS	53.64	.19	3.116	2.592	2.619	.165	.654	-0.270	.057	.536	.239	-0.271	.542	.517
NB2	NB1	AS	102.99	.20	3.116	2.672	4.538	.165	.654	-0.270	.057	.536	.239	-0.042	.729	-0.017
NB2	NB1	NB2	60.80	.10	3.041	3.257	3.195	.165	.654	.730	.057	.536	.239	.346	.665	.230
NB2	NB1	NB2	61.11	.16	3.041	3.237	3.195	.165	.654	.730	.057	.536	.239	.154	.835	.230
NB2	NB1	NB2	119.57	.23	3.041	3.014	5.232	.165	.654	.730	.057	.536	.239	-0.165	.346	.270
NB2	NB1	NB3	85.48	.22	3.041	3.202	4.238	.165	.654	.730	.057	.536	.239	.102	.262	.516
NB2	NB1	NB3	122.41	.18	3.041	3.546	5.779	.165	.654	.730	.057	.536	.239	-0.262	.602	.016
NB2	NB1	NB3	63.69	.18	3.041	2.937	3.155	.165	.654	.730	.057	.536	.239	-0.102	.736	.404
NB2	NB1	NB3	108.43	.17	3.041	2.873	4.798	.165	.654	.730	.057	.536	.239	.271	.458	.403
NB2	NB1	AS	135.59	.26	3.041	2.962	5.559	.165	.654	.730	.057	.536	.239	.262	.398	-0.016
NB2	NB1	AS	90.03	.20	3.041	3.674	4.771	.165	.654	.730	.057	.536	.239	.042	.271	.017
NB2	NB1	AS	105.50	.27	3.041	2.592	4.492	.165	.654	.730	.057	.536	.239	-0.271	.542	.517
NB2	NB1	AS	54.40	.18	3.041	2.672	2.632	.165	.654	.730	.057	.536	.239	-0.042	.729	-0.017
NB2	NB1	NB2	47.84	.15	3.257	3.237	2.633	.346	.665	.230	.057	.536	.239	.154	.835	.230
NB2	NB1	NB2	163.27	.54	3.257	3.014	6.204	.346	.665	.230	.057	.536	.239	-0.165	.346	.270
NB2	NB1	NB3	103.38	.12	3.257	3.202	5.068	.346	.665	.230	.057	.536	.239	.102	.262	.516
NB2	NB1	NB3	139.64	.32	3.257	3.546	5.385	.346	.665	.230	.057	.536	.239	-0.262	.602	.016
NB2	NB1	NB3	103.10	.21	3.257	2.937	4.854	.346	.665	.230	.057	.536	.239	-0.102	.736	.404
NB2	NB1	NB3	61.59	.13	3.257	2.873	3.155	.346	.665	.230	.057	.536	.239	.271	.458	.403
NB2	NB1	AS	114.63	.15	3.257	2.962	5.237	.346	.665	.230	.057	.536	.239	.262	.398	-0.016
NB2	NB1	AS	146.93	.38	3.257	3.674	6.646	.346	.665	.230	.057	.536	.239	.042	.271	.017
NB2	NB1	AS	92.24	.19	3.257	2.592	4.241	.346	.665	.230	.057	.536	.239	-0.271	.542	.517
NB2	NB1	AS	51.25	.15	3.257	2.672	2.613	.346	.665	.230	.057	.536	.239	-0.042	.729	-0.017
NB2	NB1	NB2	146.68	.25	3.237	3.014	6.013	.154	.835	.230	.057	.536	.239	-0.165	.346	.270
NB2	NB1	NB3	142.92	.22	3.237	3.202	6.103	.154	.835	.230	.057	.536	.239	.102	.262	.516
NB2	NB1	NB3	95.73	.16	3.237	3.546	5.035	.154	.835	.230	.057	.536	.239	-0.262	.602	.016
NB2	NB1	NB3	60.44	.17	3.237	2.937	3.118	.154	.835	.230	.057	.536	.239	-0.102	.736	.404
NB2	NB1	NB3	103.69	.16	3.237	2.873	4.810	.154	.835	.230	.057	.536	.239	.271	.458	.403
NB2	NB1	AS	152.22	.29	3.237	2.962	6.019	.154	.835	.230	.057	.536	.239	.262	.398	-0.016
NB2	NB1	AS	105.96	.17	3.237	3.674	5.525	.154	.835	.230	.057	.536	.239	.042	.271	.017
NB2	NB1	AS	52.27	.18	3.237	2.592	2.632	.154	.835	.230	.057	.536	.239	-0.271	.542	.517
NB2	NB1	AS	92.02	.16	3.237	2.672	4.273	.154	.835	.230	.057	.536	.239	-0.042	.729	-0.017
NB2	NB1	NB3	60.93	.14	3.014	3.202	3.155	-0.165	.346	.270	.057	.536	.239	.102	.262	.516
NB2	NB1	NB3	56.05	.10	3.014	3.546	3.115	-0.165	.346	.270	.057	.536	.239	-0.262	.602	.016
NB2	NB1	NB3	96.83	.13	3.014	2.937	4.233	-0.165	.346	.270	.057	.536	.239	-0.102	.736	.404
NB2	NB1	NB3	105.93	.22	3.014	2.873	4.672	-0.165	.346	.270	.057	.536	.239	.271	.458	.403
NB2	NB1	AS	51.94	.15	3.014	2.962	2.618	-0.165	.346	.270	.057	.536	.239	.262	.398	-0.016
NB2	NB1	AS	45.02	.11	3.014	3.674	2.632	-0.165	.346	.270	.057	.536	.239	.042	.271	.017
NB2	NB1	AS	103.17	.14	3.014	2.592	4.400	-0.165	.346	.270	.057	.536	.239	-0.271	.542	.517
NB2	NB1	AS	113.93	.24	3.014	2.672	4.771	-0.165	.346	.270	.057	.536	.239	-0.042	.729	-0.017
NB3	NB1	NB3	116.88	.10	3.202	3.546	5.753	.102	.262	.516	.057	.536	.239	-0.262	.602	.016
NB3	NB1	NB3	120.66	.23	3.202	2.937	5.365	.102	.262	.516	.057	.536	.239	-0.102	.736	.404
NB3	NB1	NB3	76.26	.20	3.202	2.873	3.507	.102	.262	.516	.057	.536	.239	.271	.458	.403
NB3	NB1	AS	51.16	.21	3.202	2.962	2.67[illegible]	.102	.262	.516	.057	.536	.239	.262	.398	-0.016
NB3	NB1	AS	88.42	.14	3.202	3.674	4.807	.102	.262	.516	.057	.536	.239	.042	.271	.017
NB3	NB1	AS	164.00	.14	3.202	2.592	5.739	.102	.262	.516	.057	.536	.239	-0.271	.542	.517
NB3	NB1	AS	53.14	.14	3.202	2.672	2.678	.102	.262	.516	.057	.536	.239	-0.042	.729	-0.017
NB3	NB1	NB3	59.26	.17	3.546	2.937	3.249	-0.262	.602	.016	.057	.536	.239	-0.102	.736	.404
NB3	NB1	NB3	128.77	.25	3.546	2.873	5.795	-0.262	.602	.016	.057	.536	.239	.271	.458	.403
NB3	NB1	AS	90.13	.14	3.546	2.962	4.625	-0.262	.602	.016	.057	.536	.239	.262	.398	-0.016
NB3	NB1	AS	43.46	.17	3.546	3.674	2.676	-0.262	.602	.016	.057	.536	.239	.042	.271	.017
NB3	NB1	AS	47.41	.10	3.546	2.592	2.618	-0.262	.602	.016	.057	.536	.239	-0.271	.542	.517
NB3	NB1	AS	168.00	.81	3.546	2.672	6.185	-0.262	.602	.016	.057	.536	.239	-0.042	.729	-0.017

Table 4.5.1

(continued)

ATOM1	ATOM2	ATOM3	ANGLE	SD	DIST12	DIST23	DIST13	XYZ OF ATOM1			XYZ OF ATOM2			XYZ OF ATOM3		
NB3	NB1	NB3	164.04	.34	2.937	2.873	5.753	-0.102	.738	.484	.057	.536	.239	.262	.398	-0.016
NB3	NB1	AS	142.26	.13	2.937	2.962	5.562	-0.102	.738	.484	.057	.536	.239	.042	.271	.017
NB3	NB1	AS	45.97	.09	2.937	3.674	2.670	-0.102	.738	.484	.057	.536	.239	-0.271	.542	.517
NB3	NB1	AS	57.49	.23	2.937	2.592	2.675	-0.102	.738	.484	.057	.536	.239	-0.042	.729	-0.017
NB3	NB1	AS	117.87	.29	2.937	2.672	4.837	-0.102	.738	.484	.057	.536	.239	.271	.456	.483
NB3	NB1	AS	53.29	.14	2.873	2.962	2.615	.262	.398	-0.016	.057	.536	.239	.042	.271	.017
NB3	NB1	AS	149.37	.21	2.873	3.674	5.327	.262	.398	-0.016	.057	.536	.239	-0.271	.542	.517
NB3	NB1	AS	115.57	.30	2.873	2.592	4.625	.262	.398	-0.016	.057	.536	.239	-0.042	.729	-0.017
NB3	NB1	AS	57.44	.23	2.873	2.672	2.670	.262	.398	-0.016	.057	.536	.239	.271	.456	.483
AS	NB1	AS	96.94	.09	2.962	3.674	4.991	.042	.271	.017	.057	.536	.239	-0.271	.542	.517
AS	NB1	AS	118.91	.25	2.962	2.592	4.703	.042	.271	.017	.057	.536	.239	-0.042	.729	-0.017
AS	NB1	AS	87.23	.21	2.962	2.672	3.843	.042	.271	.017	.057	.536	.239	.271	.456	.483
AS	NB1	AS	80.12	.22	3.674	2.592	4.117	-0.271	.542	.517	.057	.536	.239	-0.042	.729	-0.017
AS	NB1	AS	125.33	.28	3.674	2.672	5.657	-0.271	.542	.517	.057	.536	.239	.271	.456	.483
AS	NB1	AS	142.85	.29	2.592	2.672	4.991	-0.042	.729	-0.017	.057	.536	.239	.271	.456	.483
NB1	NB2	NB1	115.10	.18	3.041	3.116	5.135	.057	.536	.239	.165	.654	.730	.057	.536	1.239
NB1	NB2	NB1	103.62	.21	3.041	3.237	4.935	.057	.536	.239	.165	.654	.730	.464	.557	.739
NB1	NB2	NB1	103.16	.20	3.041	3.257	4.935	.057	.536	.239	.165	.654	.730	.036	.943	.739
NB1	NB2	NB1	60.43	.23	3.041	3.014	3.047	.057	.536	.239	.165	.654	.730	-0.057	.464	.761
NB1	NB2	NB2	122.89	.14	3.041	2.633	4.987	.057	.536	.239	.165	.654	.730	.335	.846	.730
NB1	NB2	NB2	62.89	.13	3.041	3.196	3.257	.057	.536	.239	.165	.654	.730	.346	.665	.230
NB1	NB2	NB2	155.43	.16	3.041	3.196	6.094	.057	.536	.239	.165	.654	.730	.346	.665	1.230
NB1	NB2	NB2	62.47	.14	3.041	3.196	3.237	.057	.536	.239	.165	.654	.730	.154	.835	.230
NB1	NB2	NB2	154.54	.19	3.041	3.196	6.084	.057	.536	.239	.165	.654	.730	.154	.835	1.230
NB1	NB2	NB3	56.54	.16	3.041	3.155	2.937	.057	.536	.239	.165	.654	.730	-0.102	.738	.484
NB1	NB2	NB3	97.63	.22	3.041	3.118	4.635	.057	.536	.239	.165	.654	.730	.262	.398	.984
NB1	NB2	AS	143.91	.17	3.041	2.618	4.464	.057	.536	.239	.165	.654	.730	-0.042	.729	.983
NB1	NB2	AS	95.64	.23	3.041	2.632	2.672	.057	.536	.239	.165	.654	.730	.271	.456	.483
NB1	NB2	NB1	101.35	.21	3.116	3.237	4.936	.057	.536	1.239	.165	.654	.730	.464	.557	.739
NB1	NB2	NB1	101.51	.20	3.116	3.257	4.935	.057	.536	1.239	.165	.654	.730	.036	.943	.739
NB1	NB2	NB1	55.20	.22	3.116	3.014	2.841	.057	.536	1.239	.165	.654	.730	-0.057	.464	.761
NB1	NB2	NB2	122.00	.13	3.116	2.633	5.033	.057	.536	1.239	.165	.654	.730	.335	.846	.730
NB1	NB2	NB2	155.61	.15	3.116	3.196	6.169	.057	.536	1.239	.165	.654	.730	.346	.665	.230
NB1	NB2	NB2	62.11	.13	3.116	3.196	3.257	.057	.536	1.239	.165	.654	.730	.346	.665	1.230
NB1	NB2	NB2	154.74	.19	3.116	3.196	6.153	.057	.536	1.239	.165	.654	.730	.154	.835	.230
NB1	NB2	NB2	61.69	.13	3.116	3.196	3.237	.057	.536	1.239	.165	.654	.730	.154	.835	1.230
NB1	NB2	NB3	97.95	.13	3.116	3.155	4.731	.057	.536	1.239	.165	.654	.730	-0.102	.738	.484
NB1	NB2	NB3	54.86	.13	3.116	3.118	2.873	.057	.536	1.239	.165	.654	.730	.262	.398	.984
NB1	NB2	AS	52.93	.20	3.116	2.618	2.592	.057	.536	1.239	.165	.654	.730	-0.042	.729	.983
NB1	NB2	AS	105.18	.26	3.116	2.632	4.575	.057	.536	1.239	.165	.654	.730	.271	.456	.483
NB1	NB2	NB1	132.13	.22	3.237	3.257	5.935	.464	.557	.739	.165	.654	.730	.036	.943	.739
NB1	NB2	NB1	121.10	.25	3.237	3.014	5.446	.464	.557	.739	.165	.654	.730	-0.057	.464	.761
NB1	NB2	NB2	66.47	.08	3.237	2.633	3.257	.464	.557	.739	.165	.654	.730	.335	.846	.730
NB1	NB2	NB2	57.93	.18	3.237	3.196	3.116	.464	.557	.739	.165	.654	.730	.346	.665	.230
NB1	NB2	NB2	56.42	.18	3.237	3.196	3.041	.464	.557	.739	.165	.654	.730	.346	.665	1.230
NB1	NB2	NB2	102.96	.17	3.237	3.196	5.033	.464	.557	.739	.165	.654	.730	.154	.835	.230
NB1	NB2	NB2	101.66	.17	3.237	3.196	4.987	.464	.557	.739	.165	.654	.730	.154	.835	1.230
NB1	NB2	NB3	156.84	.47	3.237	3.155	6.262	.464	.557	.739	.165	.654	.730	-0.102	.738	.484
NB1	NB2	NB3	55.01	.17	3.237	3.118	2.937	.464	.557	.739	.165	.654	.730	.262	.398	.984
NB1	NB2	AS	149.02	.43	3.237	2.618	5.645	.464	.557	.739	.165	.654	.730	-0.042	.729	.983
NB1	NB2	AS	51.16	.21	3.237	2.632	2.592	.464	.557	.739	.165	.654	.730	.271	.456	.483
NB1	NB2	NB1	106.51	.17	3.257	3.014	5.027	.036	.943	.739	.165	.654	.730	-0.057	.464	.761
NB1	NB2	NB2	65.69	.22	3.257	2.633	3.237	.036	.943	.739	.165	.654	.730	.335	.846	.730
NB1	NB2	NB2	102.52	.18	3.257	3.196	5.033	.036	.943	.739	.165	.654	.730	.346	.665	.230
NB1	NB2	NB2	101.23	.18	3.257	3.196	4.987	.036	.943	.739	.165	.654	.730	.346	.665	1.230
NB1	NB2	NB2	57.73	.21	3.257	3.196	3.116	.036	.943	.739	.165	.654	.730	.154	.835	.230
NB1	NB2	NB2	56.23	.21	3.257	3.196	3.041	.036	.943	.739	.165	.654	.730	.154	.835	1.230
NB1	NB2	NB3	53.26	.15	3.257	3.155	2.873	.036	.943	.739	.165	.654	.730	-0.102	.738	.484
NB1	NB2	NB3	154.01	.32	3.257	3.118	6.212	.036	.943	.739	.165	.654	.730	.262	.398	.984
NB1	NB2	AS	52.77	.19	3.257	2.618	2.672	.036	.943	.739	.165	.654	.730	-0.042	.729	.983
NB1	NB2	AS	151.31	.35	3.257	2.632	5.707	.036	.943	.739	.165	.654	.730	.271	.456	.483
NB1	NB2	NB2	171.69	.26	3.014	2.633	5.632	-0.057	.464	.761	.165	.654	.730	.335	.846	.730
NB1	NB2	NB2	120.42	.26	3.014	3.196	5.391	-0.057	.464	.761	.165	.654	.730	.346	.665	.230
NB1	NB2	NB2	114.80	.24	3.014	3.196	5.232	-0.057	.464	.761	.165	.654	.730	.346	.665	1.230
NB1	NB2	NB2	113.31	.19	3.014	3.196	5.183	-0.057	.464	.761	.165	.654	.730	.154	.835	.230
NB1	NB2	NB2	107.99	.19	3.014	3.196	5.025	-0.057	.464	.761	.165	.654	.730	.154	.835	1.230
NB1	NB2	NB3	62.48	.14	3.014	3.155	3.202	-0.057	.464	.761	.165	.654	.730	-0.102	.738	.484
NB1	NB2	NB3	70.65	.20	3.014	3.118	3.546	-0.057	.464	.761	.165	.654	.730	.262	.398	.984
NB1	NB2	AS	63.01	.16	3.014	2.618	2.962	-0.057	.464	.761	.165	.654	.730	-0.042	.729	.983
NB1	NB2	AS	80.89	.23	3.014	2.632	3.674	-0.057	.464	.761	.165	.654	.730	.271	.456	.483
NB2	NB2	NB2	65.68	.06	2.633	3.196	3.196	.335	.846	.730	.165	.654	.730	.346	.665	.230
NB2	NB2	NB2	65.68	.06	2.633	3.196	3.196	.335	.846	.730	.165	.654	.730	.346	.665	1.230
NB2	NB2	NB2	65.68	.05	2.633	3.196	3.196	.335	.846	.730	.165	.654	.730	.154	.835	.230
NB2	NB2	NB2	65.68	.05	2.633	3.196	3.196	.335	.846	.730	.165	.654	.730	.154	.835	1.230
NB2	NB2	NB3	112.08	.26	2.633	3.155	4.810	.335	.846	.730	.165	.654	.730	-0.102	.738	.484
NB2	NB2	NB3	114.90	.16	2.633	3.118	4.854	.335	.846	.730	.165	.654	.730	.262	.398	.984
NB2	NB2	AS	108.82	.27	2.633	2.618	4.270	.335	.846	.730	.165	.654	.730	-0.042	.729	.983
NB2	NB2	AS	107.32	.17	2.633	2.632	4.241	.335	.846	.730	.165	.654	.730	.271	.456	.483
NB2	NB2	NB2	100.75	.18	3.196	3.196	5.195	.346	.665	.230	.165	.654	.730	.346	.665	1.230
NB2	NB2	NB2	48.65	.12	3.196	3.196	2.633	.346	.665	.230	.165	.654	.730	.154	.835	.230
NB2	NB2	NB2	131.35	.12	3.196	3.196	5.825	.346	.665	.230	.165	.654	.730	.154	.835	1.230
NB2	NB2	NB3	99.69	.19	3.196	3.155	4.854	.346	.665	.230	.165	.654	.730	-0.102	.738	.484
NB2	NB2	NB3	100.74	.17	3.196	3.118	4.863	.346	.665	.230	.165	.654	.730	.262	.398	.984
NB2	NB2	AS	150.65	.32	3.196	2.618	5.625	.346	.665	.230	.165	.654	.730	-0.042	.729	.983
NB2	NB2	AS	52.29	.18	3.196	2.632	2.618	.346	.665	.230	.165	.654	.730	.271	.456	.483
NB2	NB2	NB2	131.35	.12	3.196	3.196	5.825	.346	.665	1.230	.165	.654	.730	.154	.835	.230
NB2	NB2	NB2	48.65	.12	3.196	3.196	2.633	.346	.665	1.230	.165	.654	.730	.154	.835	1.230
NB2	NB2	NB3	145.56	.25	3.196	3.155	6.072	.346	.665	1.230	.165	.654	.730	-0.102	.738	.484
NB2	NB2	NB3	59.35	.15	3.196	3.118	3.155	.346	.665	1.230	.165	.654	.730	.262	.398	.984
NB2	NB2	AS	93.15	.23	3.196	2.618	4.241	.346	.665	1.230	.165	.654	.730	-0.042	.729	.983
NB2	NB2	AS	100.41	.22	3.196	2.632	4.492	.346	.665	1.230	.165	.654	.730	.271	.456	.483
NB2	NB2	NB2	108.75	.17	3.196	3.196	5.135	.154	.835	.230	.165	.654	.730	.154	.835	1.230
NB2	NB2	NB3	58.80	.21	3.196	3.155	3.119	.154	.835	.230	.165	.654	.730	-0.102	.738	.484
NB2	NB2	NB3	147.94	.23	3.196	3.118	6.063	.154	.835	.230	.165	.654	.730	.262	.398	.984
NB2	NB2	AS	102.17	.29	3.196	2.618	4.539	.154	.835	.230	.165	.654	.730	-0.042	.729	.983
NB2	NB2	AS	93.70	.21	3.196	2.632	4.270	.154	.835	.230	.165	.654	.730	.271	.456	.483
NB2	NB2	NB3	98.13	.24	3.196	3.155	4.799	.154	.835	1.230	.165	.654	.730	-0.102	.738	.484
NB2	NB2	NB3	99.23	.17	3.196	3.118	4.813	.154	.835	1.230	.165	.654	.730	.262	.398	.984
NB2	NB2	AS	52.70	.23	3.196	2.618	2.632	.154	.835	1.230	.165	.654	.730	-0.042	.729	.983

Table 4.5.1

(continued)

ATOM1	ATOM2	ATOM3	ANGLE	SD	DIST12	DIST23	DIST13	XYZ OF ATOM1			XYZ OF ATOM2			XYZ OF ATOM3		
N33	N33	AS	99.75	.25	3.249	2.618	4.504	.262	.398	.984	.102	.262	.515	.229	.042	.483
N33	N33	N33	100.48	.10	3.507	3.249	5.195	.238	.102	-0.016	.102	.262	.515	.238	.102	.984
N33	N33	AS	48.94	.22	3.507	2.670	2.679	.238	.102	-0.016	.102	.262	.515	.042	.271	.017
N33	N33	AS	151.14	.24	3.507	2.676	5.991	.236	.102	-0.016	.102	.262	.515	.042	.271	1.017
N33	N33	AS	92.56	.24	3.507	2.670	4.501	.238	.102	-0.016	.102	.262	.515	.271	.458	.483
N33	N33	AS	49.11	.20	3.507	2.618	2.673	.236	.102	-0.016	.102	.262	.515	.229	.042	.483
N33	N33	AS	147.70	.26	3.249	2.670	5.688	.230	.102	.994	.102	.262	.515	.042	.271	.017
N33	N33	AS	52.48	.24	3.249	2.676	2.670	.239	.102	.984	.102	.262	.515	.042	.271	1.017
N33	NB3	AS	98.64	.24	3.249	2.670	4.504	.230	.102	.994	.102	.262	.515	.271	.458	.483
N33	NB3	AS	52.95	.20	3.249	2.618	2.676	.236	.102	.984	.102	.262	.515	.229	.042	.483
AS	N33	AS	152.75	.05	2.676	2.676	5.195	.042	.271	.017	.102	.262	.515	.042	.271	1.017
AS	N33	AS	93.60	.26	2.670	2.670	3.893	.042	.271	.017	.102	.262	.515	.271	.458	.483
AS	N33	AS	94.79	.27	2.670	2.618	3.893	.042	.271	.017	.102	.262	.515	.229	.042	.483
AS	NB3	AS	100.75	.27	2.676	2.670	4.117	.042	.271	1.017	.102	.262	.515	.271	.458	.483
AS	N33	AS	102.10	.28	2.676	2.618	4.117	.042	.271	1.017	.102	.262	.516	.229	.042	.483
AS	N33	AS	109.07	.05	2.670	2.618	4.307	.271	.458	.483	.102	.262	.515	.229	.042	.483
NB1	AS	N31	177.98	.11	2.962	3.674	6.036	.057	.536	.239	.042	.271	.017	.036	-0.057	-0.261
NB1	AS	N31	61.09	.25	2.962	2.592	2.841	.057	.536	.239	.042	.271	.017	-0.057	.464	-0.239
NB1	AS	N31	126.20	.31	2.962	2.672	5.027	.057	.536	.239	.042	.271	.017	-0.036	.057	.261
NB1	AS	N32	65.04	.19	2.962	2.618	3.014	.057	.536	.239	.042	.271	.017	-0.165	.346	.270
NB1	AS	N32	127.73	.17	2.962	2.632	5.025	.057	.536	.239	.042	.271	.017	-0.154	.165	-0.230
NB1	AS	NB3	113.55	.28	2.962	2.676	4.713	.057	.536	.239	.042	.271	.017	.102	.262	-0.484
NB1	AS	N33	69.05	.25	2.962	2.670	3.202	.057	.536	.239	.042	.271	.017	.102	.262	.516
NB1	AS	N33	61.60	.16	2.962	2.618	2.873	.057	.536	.239	.042	.271	.017	.262	.398	-0.016
NB1	AS	N33	125.82	.18	2.962	2.670	5.015	.057	.536	.239	.042	.271	.017	.238	.102	-0.016
NB1	AS	AS	43.29	.14	2.962	3.893	2.672	.057	.536	.239	.042	.271	.017	.271	.458	.483
NB1	AS	AS	106.86	.31	2.962	3.893	5.537	.057	.536	.239	.042	.271	.017	.229	.042	.483
NB1	AS	N31	119.55	.27	3.674	2.592	5.446	.036	-0.057	-0.251	.042	.271	.017	-0.057	.464	-0.239
NB1	AS	N31	54.67	.25	3.674	2.672	3.047	.036	-0.057	-0.261	.042	.271	.017	-0.036	.057	.261
NB1	AS	N32	116.39	.19	3.674	2.618	5.390	.036	-0.057	-0.261	.042	.271	.017	-0.165	.346	.270
NB1	AS	N32	54.09	.17	3.674	2.632	3.014	.036	-0.057	-0.251	.042	.271	.017	-0.154	.165	-0.230
NB1	AS	N33	65.73	.21	3.674	2.676	3.546	.036	-0.057	-0.251	.042	.271	.017	.102	.262	-0.484
NB1	AS	N33	110.65	.24	3.674	2.670	5.249	.036	-0.057	-0.251	.042	.271	.017	.102	.262	.516
NB1	AS	N33	116.42	.21	3.674	2.618	5.377	.036	-0.057	-0.261	.042	.271	.017	.262	.398	-0.016
NB1	AS	N33	52.27	.18	3.674	2.670	2.937	.036	-0.057	-0.251	.042	.271	.017	.238	.102	-0.016
NB1	AS	AS	135.12	.19	3.674	3.893	6.995	.036	-0.057	-0.251	.042	.271	.017	.271	.458	.483
NB1	AS	AS	72.24	.15	3.674	3.893	4.464	.036	-0.057	-0.261	.042	.271	.017	.229	.042	.483
NB1	AS	N31	139.27	.21	2.592	2.672	4.935	-0.057	.464	-0.239	.042	.271	.017	-0.036	.057	.261
NB1	AS	N32	73.45	.20	2.592	2.618	3.115	-0.057	.464	-0.239	.042	.271	.017	-0.165	.346	.270
NB1	AS	N32	70.57	.20	2.592	2.632	3.237	-0.057	.464	-0.239	.042	.271	.017	-0.154	.165	-0.230
NB1	AS	N33	67.73	.26	2.592	2.676	2.937	-0.057	.464	-0.239	.042	.271	.017	.102	.262	-0.484
N31	AS	N33	128.04	.33	2.592	2.670	4.731	-0.057	.464	-0.239	.042	.271	.017	.102	.262	.516
NB1	AS	N33	65.79	.22	2.592	2.618	3.545	-0.057	.464	-0.239	.042	.271	.017	.262	.398	-0.016
N31	AS	N33	139.62	.36	2.592	2.670	4.939	-0.057	.464	-0.239	.042	.271	.017	.238	.102	-0.016
N31	AS	AS	100.35	.23	2.592	3.893	5.049	-0.057	.464	-0.239	.042	.271	.017	.271	.458	.483
N31	AS	AS	167.48	.49	2.592	3.893	5.443	-0.057	.464	-0.239	.042	.271	.017	.229	.042	.483
N31	AS	N32	75.99	.24	2.672	2.618	3.257	-0.036	.057	.251	.042	.271	.017	-0.165	.346	.270
N31	AS	N32	69.96	.21	2.672	2.632	3.041	-0.036	.057	.251	.042	.271	.017	-0.154	.165	-0.230
N31	AS	NB3	120.16	.30	2.672	2.676	4.605	-0.036	.057	.251	.042	.271	.017	.102	.262	-0.484
N31	AS	NB3	65.05	.26	2.672	2.670	2.873	-0.036	.057	.251	.042	.271	.017	.102	.262	.516
N31	AS	N33	134.53	.29	2.672	2.618	4.879	-0.036	.057	.251	.042	.271	.017	.262	.398	-0.016
N31	AS	N33	73.64	.23	2.672	2.670	3.202	-0.036	.057	.251	.042	.271	.017	.238	.102	-0.016
N31	AS	AS	107.11	.36	2.672	3.893	5.331	-0.036	.057	.251	.042	.271	.017	.271	.458	.483
N31	AS	AS	49.48	.24	2.672	3.893	2.962	-0.036	.057	.251	.042	.271	.017	.229	.042	.483
N32	AS	NB2	75.06	.15	2.618	2.632	3.195	-0.165	.346	.270	.042	.271	.017	-0.154	.165	-0.230
N32	AS	NB3	133.48	.33	2.618	2.676	4.855	-0.165	.346	.270	.042	.271	.017	.102	.262	-0.484
N32	AS	NB3	73.26	.25	2.618	2.670	3.155	-0.165	.346	.270	.042	.271	.017	.102	.262	.516
N32	AS	NB3	126.34	.32	2.618	2.618	4.672	-0.165	.346	.270	.042	.271	.017	.262	.398	-0.016
N32	AS	NB3	146.86	.42	2.618	2.670	5.069	-0.165	.346	.270	.042	.271	.017	.238	.102	-0.016
N32	AS	AS	92.12	.33	2.618	3.893	4.771	-0.165	.346	.279	.042	.271	.017	.271	.458	.483
N32	AS	AS	165.42	.38	2.618	3.893	5.237	-0.165	.346	.270	.042	.271	.017	.229	.042	.483
N32	AS	NB3	71.94	.26	2.632	2.676	3.113	-0.154	.165	-0.230	.042	.271	.017	.102	.262	-0.484
NB2	AS	NB3	129.61	.28	2.632	2.670	4.795	-0.154	.165	-0.230	.042	.271	.017	.102	.262	.516
NB2	AS	NB3	147.00	.42	2.632	2.618	5.035	-0.154	.165	-0.230	.042	.271	.017	.262	.398	-0.016
N32	AS	NB3	106.14	.28	2.632	2.670	4.235	-0.154	.165	-0.230	.042	.271	.017	.238	.102	-0.016
N32	AS	AS	167.12	.34	2.632	3.893	6.455	-0.154	.165	-0.230	.042	.271	.017	.271	.458	.483
N32	AS	AS	115.48	.24	2.632	3.893	5.559	-0.154	.165	-0.230	.042	.271	.017	.229	.042	.483
N33	AS	N33	152.75	.05	2.676	2.670	5.195	.102	.262	-0.484	.042	.271	.017	.102	.262	.516
N33	AS	N33	75.71	.25	2.676	2.618	3.249	.102	.262	-0.494	.042	.271	.017	.262	.398	-0.016
N33	AS	NB3	74.96	.26	2.676	2.670	3.249	.102	.262	-0.494	.042	.271	.017	.238	.102	-0.016
N33	AS	AS	118.81	.19	2.676	3.893	5.689	.102	.262	-0.484	.042	.271	.017	.271	.458	.483
N33	AS	AS	117.96	.21	2.676	3.893	5.604	.102	.262	-0.484	.042	.271	.017	.229	.042	.483
N33	AS	NB3	88.06	.25	2.670	2.618	3.507	.102	.262	.516	.042	.271	.017	.262	.398	-0.016
N33	AS	NB3	82.39	.26	2.670	2.670	3.507	.102	.262	.516	.042	.271	.017	.238	.102	-0.016
N33	AS	AS	43.19	.21	2.670	3.893	2.670	.102	.262	.515	.042	.271	.017	.271	.458	.483
N33	AS	AS	42.98	.21	2.670	3.893	2.618	.102	.262	.516	.042	.271	.017	.229	.042	.483
NB3	AS	NB3	70.43	.04	2.618	2.670	3.049	.262	.398	-0.016	.042	.271	.017	.238	.102	-0.016
N33	AS	AS	43.13	.16	2.618	3.893	2.670	.262	.398	-0.016	.042	.271	.017	.271	.458	.483
N33	AS	AS	65.08	.17	2.618	3.893	4.501	.262	.398	-0.016	.042	.271	.017	.229	.042	.483
N33	AS	AS	54.42	.18	2.670	3.893	4.501	.238	.102	-0.016	.042	.271	.017	.271	.458	.483
NB3	AS	AS	43.21	.16	2.670	3.893	2.670	.238	.102	-0.016	.042	.271	.017	.229	.042	.483
AS	AS	AS	67.17	.22	3.893	3.893	4.307	.271	.458	.483	.042	.271	.017	.229	.042	.483

Table 4.5.1

(continued)

ATOM1	ATOM2	ATOM3	ANGLE	SD	DIST12	DIST23	DIST13	XYZ OF ATOM1			XYZ OF ATOM2			XYZ OF ATOM3		
N32	N32	AS	148.97	.27	3.196	2.632	5.618	.154	.635	1.239	.165	.654	.730	.271	.456	.483
N33	N32	N33	132.99	.14	3.155	3.118	5.753	-0.102	.736	.484	.165	.654	.730	.262	.390	.984
N33	N32	AS	54.14	.21	3.155	2.618	2.670	-0.102	.736	.484	.165	.654	.730	-0.042	.729	.983
N33	N32	AS	111.99	.29	3.155	2.632	4.807	-0.102	.736	.484	.165	.654	.730	.271	.456	.483
N33	N32	AS	107.20	.28	3.118	2.618	4.025	.262	.398	.984	.165	.654	.730	-0.042	.729	.983
N33	N32	AS	54.68	.23	3.118	2.632	2.675	.262	.398	.984	.165	.654	.730	.271	.456	.483
AS	N32	AS	143.84	.38	2.618	2.632	4.991	-0.042	.729	.983	.165	.654	.730	.271	.456	.483
N31	N33	N31	159.03	.16	3.202	3.546	6.035	.057	.536	.239	.102	.262	.515	.036	-0.057	.739
N31	N33	N31	59.34	.23	3.202	2.937	3.047	.057	.536	.239	.102	.262	.515	-0.057	.464	.761
N31	N33	N31	111.58	.18	3.202	2.873	5.327	.057	.536	.239	.102	.262	.515	-0.036	.057	.261
N31	N33	N32	56.60	.13	3.202	3.155	3.014	.057	.536	.239	.102	.262	.515	-0.165	.346	.270
N31	N33	N32	110.37	.12	3.202	3.118	5.189	.057	.536	.239	.102	.262	.515	-0.154	.165	.770
N31	N33	N33	102.60	.19	3.202	3.049	4.879	.057	.536	.239	.102	.262	.515	.398	.238	.516
N31	N33	N33	50.46	.16	3.202	3.507	2.873	.057	.536	.239	.102	.262	.515	.262	.398	-0.016
N31	N33	N33	91.88	.18	3.202	3.249	4.635	.057	.536	.239	.102	.262	.515	.262	.398	.984
N31	N33	N33	96.68	.26	3.202	3.507	5.015	.057	.536	.239	.102	.262	.515	.238	.102	-0.016
N31	N33	N33	147.72	.26	3.202	3.249	5.195	.057	.536	.239	.102	.262	.515	.238	.102	.984
N31	N33	AS	59.78	.21	3.202	2.670	2.962	.057	.536	.239	.102	.262	.515	.042	.271	.017
N31	N33	AS	111.82	.24	3.202	2.676	4.877	.057	.536	.239	.102	.262	.515	.042	.271	1.017
N31	N33	AS	53.22	.19	3.202	2.670	2.672	.057	.536	.239	.102	.262	.516	.271	.456	.483
N31	N33	AS	143.72	.30	3.202	2.618	5.533	.057	.536	.239	.102	.262	.515	.229	.042	.483
N31	N33	N31	113.95	.15	3.546	2.937	5.445	.036	-0.057	.739	.102	.262	.516	-0.057	.464	.761
N31	N33	N31	51.23	.23	3.546	2.873	2.841	.036	-0.057	.739	.102	.262	.515	-0.036	.057	.261
N31	N33	N32	102.50	.15	3.546	3.155	5.232	.036	-0.057	.739	.102	.262	.516	-0.165	.346	.270
N31	N33	N32	53.30	.13	3.546	3.118	3.014	.036	-0.057	.739	.102	.262	.515	-0.154	.165	.770
N31	N33	N33	96.68	.23	3.546	3.049	4.939	.036	-0.057	.739	.102	.262	.515	.398	.238	.516
N31	N33	N33	135.70	.24	3.546	3.507	6.533	.036	-0.057	.739	.102	.262	.516	.262	.398	-0.016
N31	N33	N33	104.53	.26	3.546	3.249	5.377	.036	-0.057	.739	.102	.262	.515	.262	.398	.984
N31	N33	N33	84.26	.17	3.546	3.507	4.731	.036	-0.057	.739	.102	.262	.515	.238	.102	-0.016
N31	N33	N33	50.98	.17	3.546	3.249	2.937	.036	-0.057	.739	.102	.262	.516	.238	.102	.984
N31	N33	AS	107.73	.23	3.546	2.670	5.043	.036	-0.057	.739	.102	.262	.516	.042	.271	.017
N31	N33	AS	70.82	.21	3.546	2.676	3.674	.036	-0.057	.739	.102	.262	.515	.042	.271	1.017
N31	N33	AS	147.75	.25	3.546	2.670	5.977	.036	-0.057	.739	.102	.262	.515	.271	.456	.483
N31	N33	AS	46.80	.21	3.546	2.618	2.592	.036	-0.057	.739	.102	.262	.515	.229	.042	.483
N31	N33	N31	116.35	.15	2.937	2.873	4.935	-0.057	.464	.751	.102	.262	.515	-0.036	.057	.261
N31	N33	N32	59.76	.16	2.937	3.155	3.041	-0.057	.464	.751	.102	.262	.515	-0.165	.346	.270
N31	N33	N32	64.56	.12	2.937	3.118	3.237	-0.057	.464	.751	.102	.262	.516	-0.154	.165	.770
N31	N33	N33	127.86	.24	2.937	3.049	5.377	-0.057	.464	.751	.102	.262	.515	.398	.238	.516
N31	N33	N33	108.79	.25	2.937	3.507	5.243	-0.057	.464	.751	.102	.262	.516	.262	.398	-0.016
N31	N33	N33	69.76	.23	2.937	3.249	3.546	-0.057	.464	.751	.102	.262	.515	.262	.398	.984
N31	N33	N33	153.60	.36	2.937	3.507	6.274	-0.057	.464	.751	.102	.262	.516	.238	.102	-0.016
N31	N33	N33	105.85	.32	2.937	3.249	4.933	-0.057	.464	.751	.102	.262	.516	.238	.102	.984
N31	N33	AS	105.43	.22	2.937	2.670	4.464	-0.057	.464	.751	.102	.262	.516	.042	.271	.017
N31	N33	AS	54.76	.20	2.937	2.676	2.592	-0.057	.464	.751	.102	.262	.516	.042	.271	1.017
N31	N33	AS	81.75	.20	2.937	2.670	3.674	-0.057	.464	.761	.102	.262	.516	.271	.456	.483
N31	N33	AS	156.58	.36	2.937	2.618	5.433	-0.057	.464	.761	.102	.262	.516	.229	.042	.483
N31	N33	N32	65.20	.17	2.873	3.155	3.257	-0.036	.057	.251	.102	.262	.516	-0.165	.346	.270
N31	N33	N32	62.52	.18	2.873	3.118	3.115	-0.036	.057	.251	.102	.262	.516	-0.154	.165	.770
N31	N33	N33	115.74	.26	2.873	3.049	5.015	-0.036	.057	.251	.102	.262	.516	.398	.238	.516
N31	N33	N33	99.31	.29	2.873	3.507	4.879	-0.036	.057	.261	.102	.262	.516	.262	.398	-0.016
N31	N33	N33	155.76	.30	2.873	3.249	5.985	-0.036	.057	.251	.102	.262	.516	.262	.398	.984
N31	N33	N33	59.26	.23	2.873	3.507	3.202	-0.036	.057	.261	.102	.262	.516	.238	.102	-0.016
N31	N33	N33	100.69	.22	2.873	3.249	4.713	-0.036	.057	.261	.102	.262	.516	.238	.102	.984
N31	N33	AS	57.51	.20	2.873	2.670	2.672	-0.036	.057	.261	.102	.262	.516	.042	.271	.017
N31	N33	AS	111.84	.23	2.873	2.676	4.575	-0.036	.057	.251	.102	.262	.516	.042	.271	1.017
N31	N33	AS	148.21	.35	2.873	2.670	5.331	-0.036	.057	.251	.102	.262	.516	.271	.456	.483
N31	N33	AS	65.11	.24	2.873	2.618	2.962	-0.036	.057	.261	.102	.262	.516	.229	.042	.483
N32	N33	N32	61.25	.13	3.155	3.118	3.135	-0.165	.346	.270	.102	.262	.516	-0.154	.165	.770
N32	N33	N33	153.10	.28	3.155	3.049	6.035	-0.165	.346	.270	.102	.262	.516	.398	.238	.516
N32	N33	N33	88.90	.27	3.155	3.507	4.672	-0.165	.346	.270	.102	.262	.516	.262	.398	-0.016
N32	N33	N33	128.90	.32	3.155	3.249	5.775	-0.165	.346	.270	.102	.262	.516	.262	.398	.984
N32	N33	N33	98.91	.29	3.155	3.507	5.003	-0.165	.346	.270	.102	.262	.516	.238	.102	-0.016
N32	N33	N33	144.68	.36	3.155	3.249	6.133	-0.165	.346	.270	.102	.262	.516	.238	.102	.984
N32	N33	AS	52.60	.15	3.155	2.670	2.613	-0.165	.346	.270	.102	.262	.516	.042	.271	.017
N32	N33	AS	140.46	.18	3.155	2.676	4.492	-0.165	.346	.270	.102	.262	.516	.042	.271	1.017
N32	N33	AS	109.09	.27	3.155	2.670	4.771	-0.165	.346	.270	.102	.262	.516	.271	.456	.483
N32	N33	AS	129.97	.30	3.155	2.618	5.237	-0.165	.346	.270	.102	.262	.516	.229	.042	.483
N32	N33	N33	144.96	.24	3.118	3.049	5.881	-0.154	.165	.770	.102	.262	.516	.398	.238	.516
N32	N33	N33	149.12	.29	3.118	3.507	6.385	-0.154	.165	.770	.102	.262	.516	.262	.398	-0.016
N32	N33	N33	104.50	.32	3.118	3.249	5.035	-0.154	.165	.770	.102	.262	.516	.262	.398	.984
N32	N33	N33	121.36	.24	3.118	3.507	5.773	-0.154	.165	.770	.102	.262	.516	.238	.102	-0.016
N32	N33	N33	83.44	.28	3.118	3.249	4.238	-0.154	.165	.770	.102	.262	.516	.238	.102	.984
N32	N33	AS	102.48	.17	3.118	2.670	4.539	-0.154	.165	.770	.102	.262	.516	.042	.271	.017
N32	N33	AS	53.38	.16	3.118	2.676	2.632	-0.154	.165	.770	.102	.262	.516	.042	.271	1.017
N32	N33	AS	145.25	.28	3.118	2.670	5.525	-0.154	.165	.770	.102	.262	.516	.271	.456	.483
N32	N33	AS	99.84	.24	3.118	2.618	4.430	-0.154	.165	.770	.102	.262	.516	.229	.042	.483
N33	N33	N33	64.23	.12	3.049	3.507	3.507	.398	.238	.515	.102	.262	.516	.262	.398	-0.016
N33	N33	N33	62.01	.13	3.049	3.249	3.249	.398	.238	.516	.102	.262	.516	.262	.398	.984
N33	N33	N33	64.23	.12	3.049	3.507	3.507	.398	.238	.516	.102	.262	.516	.238	.102	-0.015
N33	N33	N33	62.01	.13	3.049	3.249	3.249	.398	.238	.516	.102	.262	.516	.238	.102	.984
N33	N33	AS	103.61	.06	3.049	2.670	4.501	.398	.238	.516	.102	.262	.516	.042	.271	.017
N33	N33	AS	103.58	.06	3.049	2.676	4.504	.398	.238	.516	.102	.262	.516	.042	.271	1.017
N33	N33	AS	53.99	.19	3.049	2.670	2.613	.399	.238	.515	.102	.262	.516	.271	.456	.483
N33	N33	AS	55.58	.22	3.049	2.618	2.670	.398	.236	.516	.102	.262	.516	.229	.042	.483
N33	N33	N33	100.48	.11	3.507	3.249	5.135	.262	.398	-0.016	.102	.262	.516	.262	.398	.984
N33	N33	N33	51.54	.18	3.507	3.507	3.049	.262	.398	-0.016	.102	.262	.516	.238	.102	-0.016
N33	N33	N33	126.15	.03	3.507	3.249	6.024	.262	.398	-0.016	.102	.262	.516	.238	.102	.984
N33	N33	AS	47.83	.21	3.507	2.670	2.618	.262	.398	-0.015	.102	.262	.516	.042	.271	.017
N33	N33	AS	149.46	.23	3.507	2.676	5.968	.262	.398	-0.015	.102	.262	.516	.042	.271	1.017
N33	N33	AS	46.96	.19	3.507	2.670	2.670	.262	.398	-0.015	.102	.262	.516	.271	.456	.483
N33	N33	AS	93.47	.25	3.507	2.618	4.501	.262	.398	-0.016	.102	.262	.516	.229	.042	.483
N33	N33	N33	126.15	.03	3.249	3.507	6.024	.262	.398	.984	.102	.262	.516	.238	.102	-0.016
N33	N33	N33	55.97	.20	3.249	3.249	3.049	.262	.398	.984	.102	.262	.516	.238	.102	.984
N33	N33	AS	146.34	.24	3.249	2.670	5.654	.262	.398	.994	.102	.262	.516	.042	.271	.017
N33	N33	AS	51.34	.23	3.249	2.676	2.618	.262	.398	.994	.102	.262	.516	.042	.271	1.017
N33	N33	AS	52.66	.19	3.249	2.670	2.675	.262	.398	.984	.102	.262	.516	.271	.456	.483