CHAPTER 5

CONCLUSION AND DISCUSSION

The final structure of Nb_3As was given from the last refinement of the least - squares method. A projection of Nb_3As structure along the c axis is illustrated in Fig.5.1. Plane layers of atoms are connected by full or broken lines.

The Nb_3As structure has four types of co-ordination polyhedra, which are densely packed.

By considering the arrangement of niobium atoms, these can be divided into three types.

The first type of the niobium atoms, Nb(1), is surrounded by 15 nearest atoms, of which eleven are niobium atoms and four are arsenic atoms. The arrangement is based on a polyhedra as shown in Fig.5.2. The co-ordinates, the interatomic distances and the interatomic angles of these atoms are given in Table 5.2(a), (b) and (c) respectively.

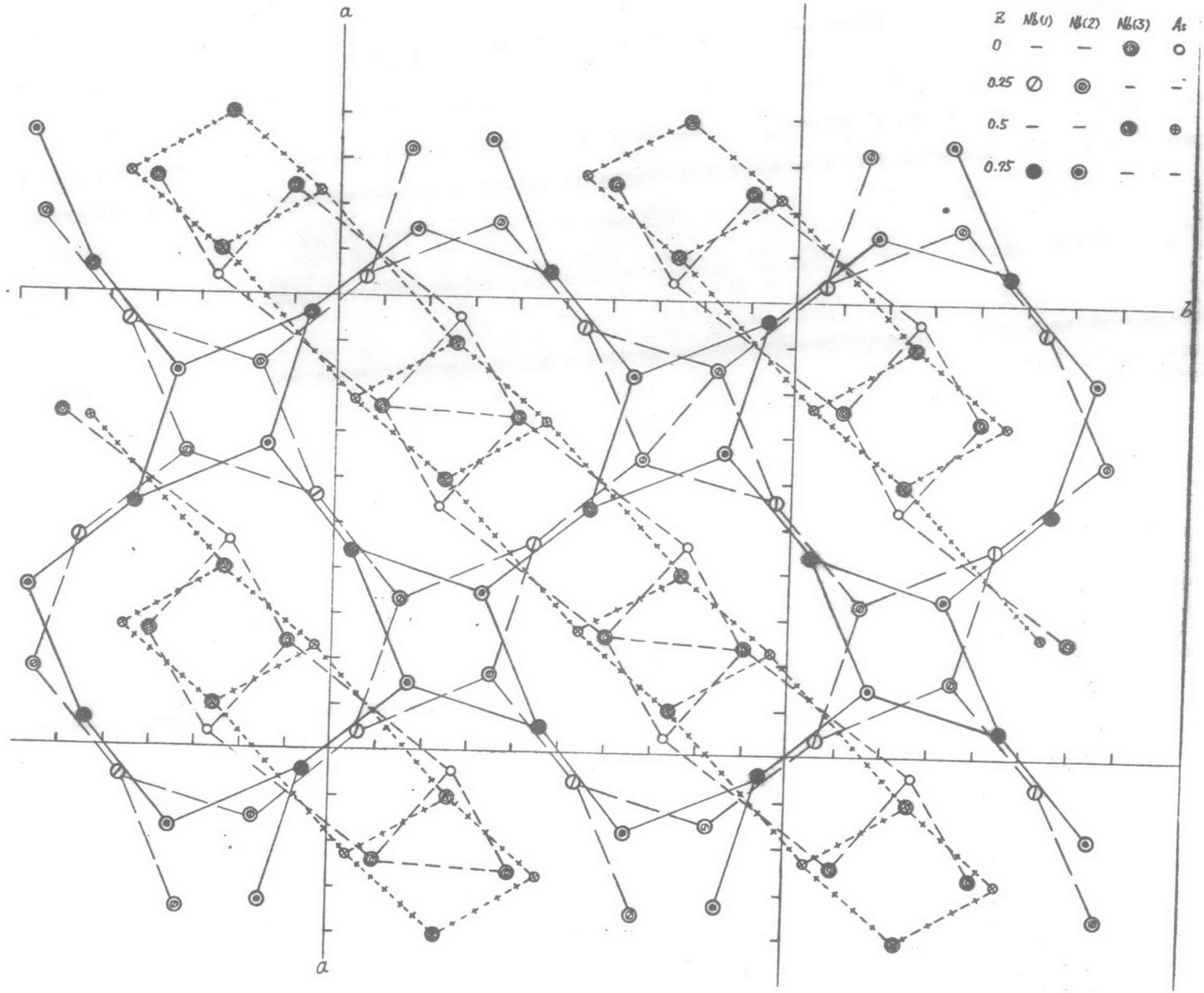
The second niobium atom, Nb(2), is surrounded by 12 niobium atoms and 2 arsenic atoms as shown in Fig.5.3. The co-ordinates, the interatomic distances and the interatomic angles of these atoms are given in Table 5.3(a), (b) and (c) respectively.

The third niobium atom, Nb(3), has 15 nearest neighbour atoms of which eleven are niobium atoms and the other four arsenic atoms. Four niobium atoms and two arsenic atoms approximately

form a triangular prism as shown in Fig.5.4. The Nb(3) is situated near to the prism edge formed by the two arsenic atoms. The co-ordinates, the interatomic distances and the interatomic angles of these atoms in Fig.5.4 are given in Table 5.4(a), (b) and (c) respectively.

The arsenic atoms in Nb_3As have 10 niobium neighbours as shown in Fig.5.5. The co-ordinates, the interatomic distances and the interatomic angles of these atoms are shown in Table 5.5 (a), (b) and (c) respectively.

Fig.5.1 Projection of Nb_3As structure in ab plane.



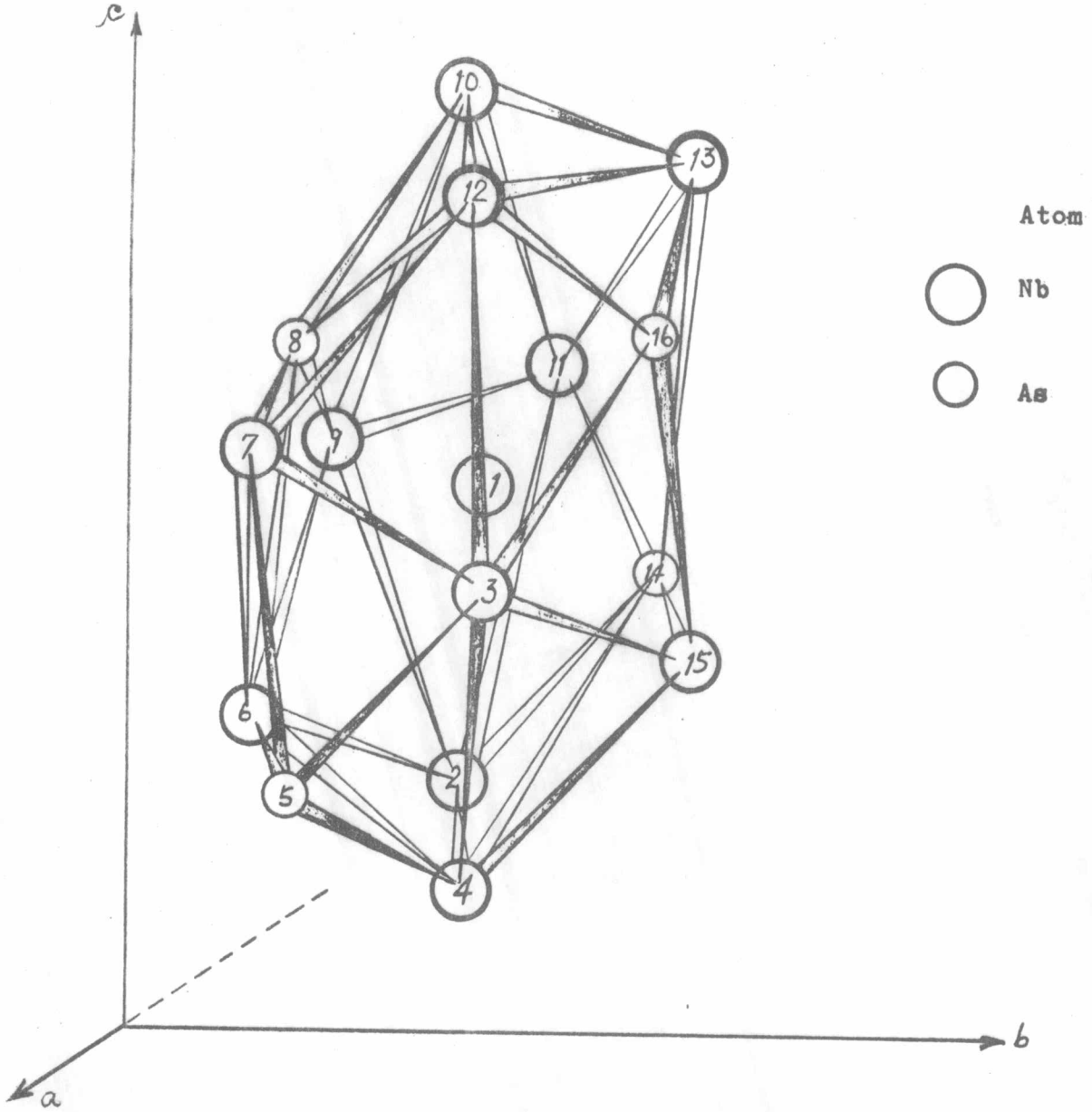


Fig.5.2 The Nb(1) atom and its nearest neighbours.

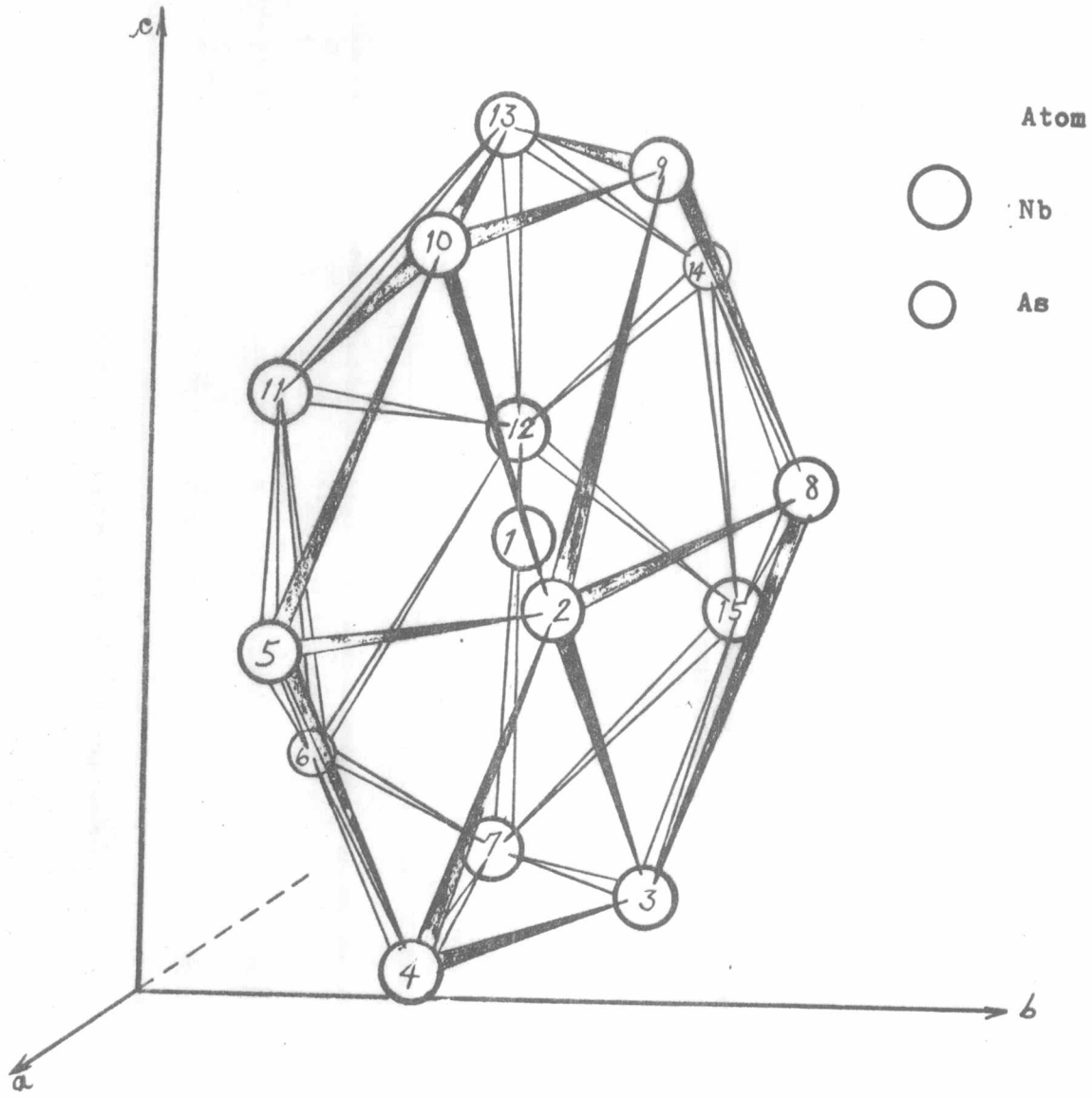


Fig.5.3 The Nb(2) atom and its nearest neighbours.

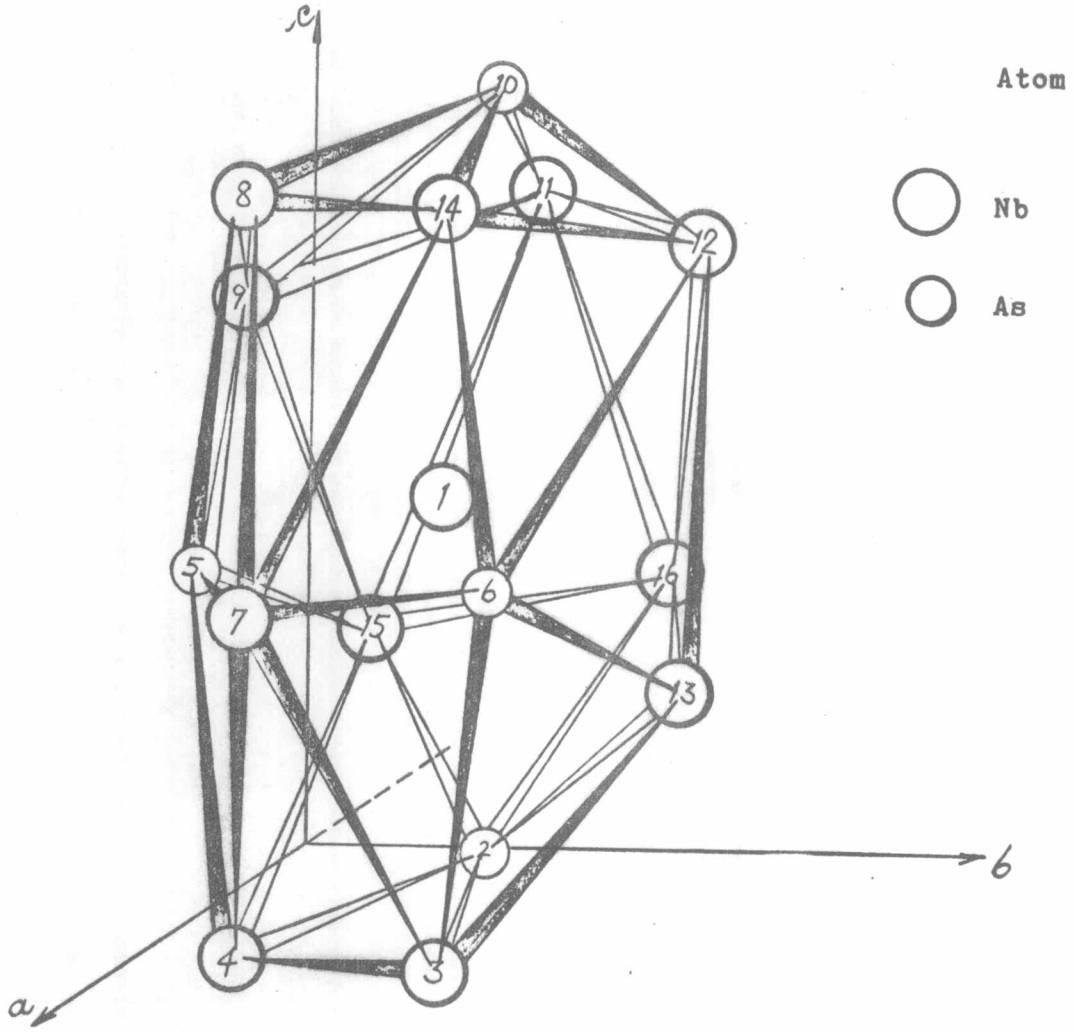


Fig.5.4 The Nb(3) atom and its nearest neighbours.

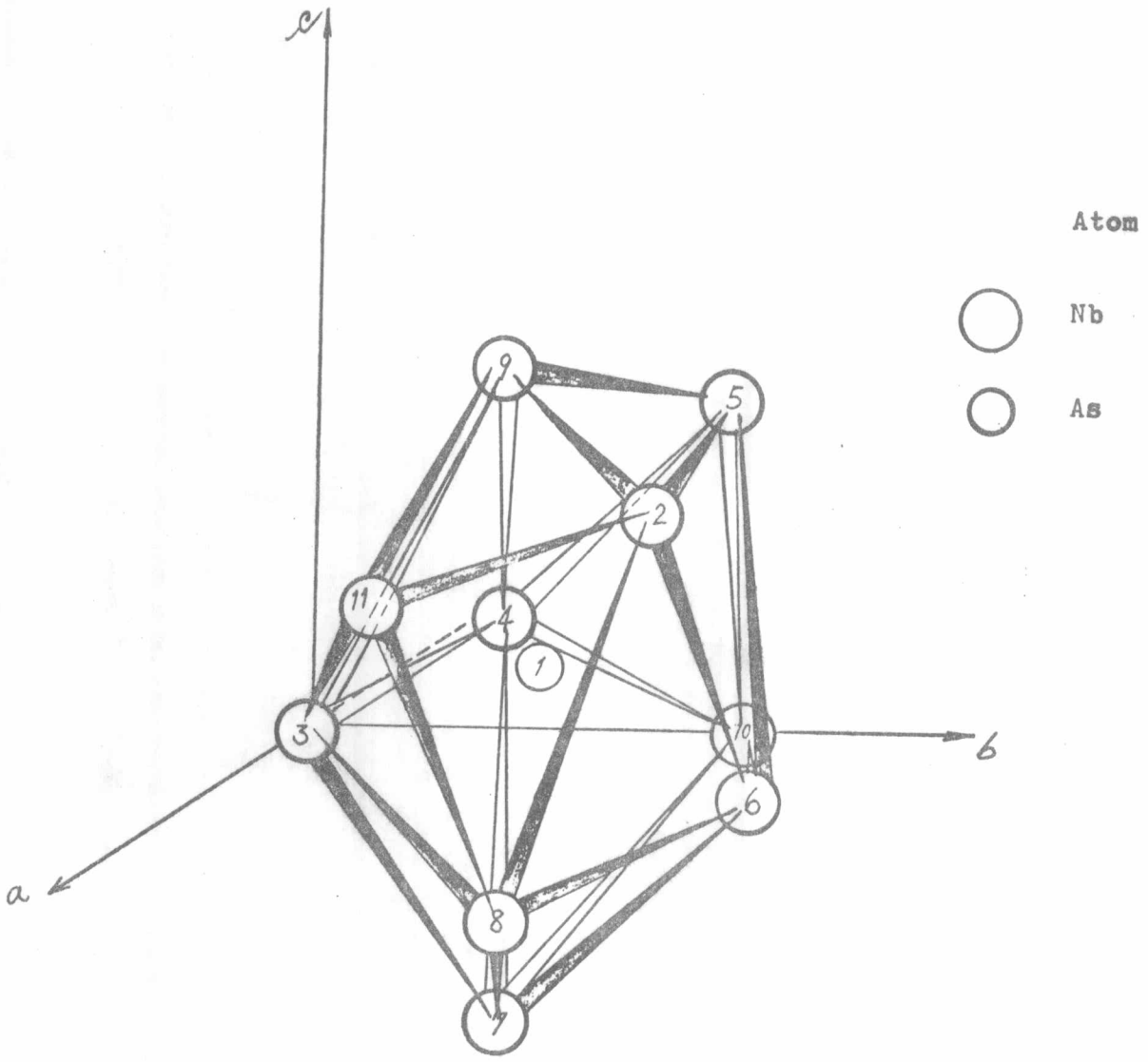


Fig.5.5 The As atom and its nearest neighbours.

Table 5.2(a) The co-ordinates of atoms of the Nb(1) co-ordination polyhedron in Fig.5.2.

	Atom	x	y	z
1	Nb(1)	- 0.057	0.464	0.761
2	Nb(2)	- 0.165	0.346	0.270
3	Nb(2)	0.165	0.654	0.730
4	Nb(1)	0.057	0.536	0.239
5	As	0.271	0.458	0.483
6	Nb(3)	0.102	0.262	0.516
7	Nb(3)	0.262	0.398	0.984
8	As	0.042	0.271	1.017
9	Nb(2)	- 0.154	0.165	0.770
10	Nb(2)	- 0.165	0.346	1.270
11	Nb(2)	- 0.346	0.335	0.770
12	Nb(1)	0.057	0.536	1.239
13	Nb(3)	- 0.262	0.602	1.016
14	As	- 0.271	0.542	0.517
15	Nb(3)	- 0.102	0.738	0.484
16	As	- 0.042	0.729	0.983

Table 5.2(b) Interatomic distances of atoms of the Nb(1) co-ordination polyhedron in Fig.5.2 and the standard deviation for the interatomic distances of the central atom only.

Bond	Distance, Å
1Nb(1)-2Nb(2)	3.041± 0.009
-3Nb(2)	3.014± 0.005
-4Nb(1)	3.047± 0.013
-5As	3.674± 0.007
-6Nb(3)	2.937± 0.007
-7Nb(3)	3.547± 0.006
-8As	2.593± 0.008
-9Nb(2)	3.237± 0.005
-10Nb(2)	3.116± 0.009
-11Nb(2)	3.257± 0.006
-12Nb(1)	2.841± 0.012
-13Nb(3)	2.873± 0.008
-14As	2.673± 0.009
-15Nb(3)	3.202± 0.008
-16As	2.962± 0.008
2Nb(2)-4Nb(1)	3.014
-6Nb(3)	3.155
-9Nb(2)	3.196
-11Nb(2)	3.196
-14As	2.632

Bond	Distance, Å
3Nb(2)-4Nb(1)	3.041
-5As	2.632
-7Nb(3)	3.118
-12Nb(1)	3.116
-15Nb(3)	3.155
-16As	2.618
4Nb(1)-5As	2.673
-6Nb(3)	3.202
-14As	3.674
-15Nb(3)	2.937
5As -6Nb(3)	2.670
-7Nb(3)	2.676
6Nb(3)-7Nb(3)	3.254
-8As	2.676
-9Nb(2)	3.118
7Nb(3)-8As	2.618
-12Nb(1)	2.873
8As -9Nb(2)	2.632
-10Nb(2)	2.618
-12Nb(1)	2.962

Table 5.2(b)

(continued)

Bond	Distance, Å
9Nb(2)-10Nb(2)	3.196
-11Nb(2)	2.640
10Nb(2)-11Nb(2)	2.633
-13Nb(3)	3.118
11Nb(2)-13Nb(3)	3.155
-14As	2.618
12Nb(1)-10Nb(2)	3.012
-13Nb(3)	3.547
-16As	2.593
13Nb(3)-14As	2.670
-16As	2.618
14As -15Nb(3)	2.670
15Nb(3)-16As	2.670

Table 5.2(c) Interatomic angles of atoms of the Nb(1) co-ordination polyhedron in Fig.5.2.

Bond	Angle (degree)
2Nb(2)-4Nb(1)-6Nb(3)	60.93
-14As	45.02
-6Nb(3)-4Nb(1)	56.60
-9Nb(2)	61.25
-9Nb(2)-6Nb(3)	59.94
-11Nb(2)	65.61
-11Nb(2)-9Nb(2)	65.61
-14As	52.70
-14As -4Nb(1)	54.10
-11Nb(2)	75.00
3Nb(2)-4Nb(1)-5As	54.40
-15Nb(3)	63.69
-5As -4Nb(1)	69.95
-7Nb(3)	71.94
-7Nb(3)-5As	53.37
-12Nb(1)	62.52
-12Nb(1)-7Nb(3)	62.60
-16As	53.64
-15Nb(3)-4Nb(1)	59.76
-16As	52.62
-16As -12Nb(1)	73.45
-15Nb(3)	73.25
4Nb(1)-2Nb(2)-6Nb(3)	62.49
-14As	80.89

Bond	Angle (degree)
4Nb(1)-3Nb(2)-5As	55.64
-15Nb(3)	97.95
-5As -6Nb(3)	73.64
-6Nb(3)-5As	53.22
-14As -15Nb(3)	52.29
-15Nb(3)-14As	81.73
5As -3Nb(2)-7Nb(3)	54.68
-4Nb(1)-6Nb(3)	53.14
-6Nb(3)-8As	100.75
-7Nb(3)-8As	102.13
6Nb(3)-2Nb(2)-9Nb(2)	58.80
-5As -7Nb(3)	74.99
-8As -9Nb(2)	71.94
-10Nb(2)	133.48
-9Nb(2)-8As	54.68
7Nb(3)-3Nb(2)-12Nb(1)	54.88
-8As -12Nb(1)	61.60
-12Nb(1)-8As	53.29
8As -6Nb(3)-9Nb(2)	53.38
-7Nb(3)-12Nb(1)	65.10
-9Nb(2)-10Nb(2)	52.30
-10Nb(2)-9Nb(2)	52.70
-12Nb(1)	63.17
-12Nb(1)-10Nb(2)	51.92

Table 5.2(c)

(continued)

Bond	Angle (degree)
9Nb(2)-2Nb(2)-11Nb(2)	48.79
-8As -10Nb(2)	75.00
-10Nb(2)-11Nb(2)	52.79
10Nb(2)-11Nb(2)-13Nb(3)	64.45
-13Nb(3)-11Nb(2)	49.63
11Nb(2)-13Nb(3)-14As	52.62
-14As -13Nb(3)	73.25
12Nb(1)-10Nb(2)-13Nb(3)	70.68
-13Nb(3)-10Nb(2)	53.26
-16As	46.81
13Nb(3)-10Nb(2)-11Nb(2)	65.92
-11Nb(2)-14As	54.13
-12Nb(1)-10Nb(2)	56.05
-16As	47.40
-14As -11Nb(2)	73.25
-15Nb(3)	82.16
-16As -12Nb(1)	73.45
-15Nb(3)	83.14

Table 5.3(a) The co-ordinates of atoms of the Nb(2) co-ordination polyhedron in Fig.5.3.

	Atom	x	y	z
1	Nb(2)	0.165	0.654	0.730
2	Nb(2)	0.335	0.846	0.730
3	Nb(2)	0.154	0.835	0.230
4	Nb(2)	0.346	0.665	0.230
5	Nb(1)	0.464	0.557	0.739
6	As	0.271	0.458	0.483
7	Nb(1)	0.057	0.536	0.239
8	Nb(1)	0.036	0.943	0.739
9	Nb(2)	0.154	0.835	1.230
10	Nb(2)	0.346	0.665	1.230
11	Nb(3)	0.262	0.398	0.984
12	Nb(1)	- 0.057	0.464	0.761
13	Nb(1)	0.057	0.536	1.239
14	As	- 0.042	0.729	0.983
15	Nb(3)	- 0.102	0.738	0.484

Table 5.3(b) Interatomic distances of atoms of the Nb(2) co-ordination polyhedron in Fig.5.3 and the standard deviation for the interatomic distances of the central atom only.

Bond	Distance, Å
1Nb(2)-2Nb(2)	2.633 ±0.008
-3Nb(2)	3.196 ±0.004
-4Nb(2)	3.196 ±0.004
-5Nb(1)	3.237 ±0.006
-6As	2.632 ±0.008
-7Nb(1)	3.041 ±0.009
-8Nb(1)	3.257 ±0.006
-9Nb(2)	3.196 ±0.004
-10Nb(2)	3.196 ±0.004
-11Nb(3)	3.118 ±0.007
-12Nb(1)	3.014 ±0.005
-13Nb(1)	3.116 ±0.009
-14As	2.618 ±0.006
-15Nb(3)	3.155 ±0.005
2Nb(2)-3Nb(2)	3.196
-4Nb(2)	3.196
-5Nb(1)	3.257
-8Nb(1)	3.237
-9Nb(2)	3.196
-10Nb(2)	3.196

Bond	Distance, Å
3Nb(2)-4Nb(2)	2.633
-7Nb(1)	3.237
-8Nb(1)	3.116
-15Nb(3)	3.118
4Nb(2)-5Nb(1)	3.116
-6As	2.618
-7Nb(1)	3.257
5Nb(1)-6As	2.592
-10Nb(2)	3.041
-11Nb(3)	2.937
6As -7Nb(1)	2.672
-11Nb(3)	2.677
-12Nb(1)	3.674
7Nb(1)-12Nb(1)	3.047
-15Nb(3)	<.937
8Nb(1)-9Nb(2)	3.041
-14As	2.672
-15Nb(3)	2.873
9Nb(2)-10Nb(2)	2.633
-13Nb(1)	3.237
-14As	2.632

Table 5.3(b)

(continued)

Bond	Distance, Å
10Nb(2)-11Nb(3)	3.155
-13Nb(1)	3.257
11Nb(3)-12Nb(1)	3.546
-13Nb(1)	2.873
12Nb(1)-13Nb(1)	2.841
-14As	2.962
-15Nb(3)	3.202
13Nb(1)-14As	2.592
14As -15Nb(3)	2.670

Table 5.3(c) Interatomic angles of atoms of the Nb(2) co-ordination polyhedron in Fig.5.3.

Bond	Angle (degree)
2Nb(2)-3Nb(2)-4Nb(2)	65.67
-8Nb(1)	61.69
-4Nb(2)-3Nb(2)	65.67
-5Nb(1)	62.11
-5Nb(1)-4Nb(2)	60.15
-10Nb(2)	60.88
-8Nb(1)-3Nb(2)	60.37
-9Nb(2)	61.11
-9Nb(2)-8Nb(1)	62.47
-10Nb(2)	65.67
-10Nb(2)-5Nb(1)	62.90
-9Nb(2)	65.67
3Nb(2)-2Nb(2)-4Nb(2)	48.65
-8Nb(1)	57.94
-4Nb(2)-7Nb(1)	65.68
-7Nb(1)-4Nb(2)	47.84
-15Nb(3)	103.10
-8Nb(1)-15Nb(3)	62.59
-15Nb(3)-7Nb(1)	64.55
-8Nb(1)	62.52
4Nb(2)-2Nb(2)-5Nb(1)	57.74
-3Nb(2)-7Nb(1)	66.48

Bond	Angle (degree)
-5Nb(1)-6As	53.65
-6As -5Nb(1)	73.46
-7Nb(1)	76.00
-7Nb(1)-6As	51.25
5Nb(1)-2Nb(2)-10Nb(2)	56.22
-4Nb(2)-6As	52.89
-6As -12Nb(1)	119.83
-10Nb(2)-11Nb(3)	56.55
-11Nb(3)-10Nb(2)	59.76
-12Nb(1)	114.06
6As -4Nb(2)-7Nb(1)	52.75
-7Nb(1)-12Nb(1)	79.65
-12Nb(1)-7Nb(1)	45.68
-11Nb(3)	43.48
7Nb(1)-3Nb(2)-15Nb(3)	55.01
-6As -12Nb(1)	54.67
-12Nb(1)-15Nb(3)	54.54
-15Nb(3)-12Nb(1)	59.33
8Nb(1)-2Nb(2)-9Nb(2)	77.80
-3Nb(2)-15Nb(3)	54.89
-9Nb(2)-14As	55.64
-14As -9Nb(2)	69.96
-15Nb(3)	65.07

Table 5.3(c)

(continued)

Bond	Angle (degree)
9Nb(2)-2Nb(2)-10Nb(2)	48.65
-10Nb(2)-13Nb(1)	65.68
-13Nb(1)-10Nb(2)	47.84
-14As	52.27
-14As -13Nb(1)	41.43
10Nb(2)-9Nb(2)-13Nb(1)	66.48
-11Nb(3)-13Nb(1)	65.21
-13Nb(1)-11Nb(3)	61.59
11Nb(3)-5Nb(1)-6As	57.51
-10Nb(2)	63.68
-10Nb(2)-13Nb(1)	53.21
-12Nb(1)-13Nb(1)	52.05
-13Nb(1)-12Nb(1)	76.73
12Nb(1)-7Nb(1)-15Nb(3)	64.66
-11Nb(3)-13Nb(1)	51.24
-13Nb(1)-14As	65.89
-14As -13Nb(1)	61.10
-15Nb(3)	69.07
-15Nb(3)-14As	59.77
13Nb(1)-9Nb(2)-14As	51.16
-12Nb(1)-14As	53.01
14As -12Nb(1)-15Nb(3)	51.16

Table 5.4(a) The co-ordinates of atoms of the Nb(3) co-ordination polyhedron in Fig.5.4.

	Atom	x	y	z
1	Nb(3)	0.102	0.262	0.516
2	As	0.042	0.271	0.017
3	Nb(3)	0.262	0.398	-0.016
4	Nb(3)	0.238	0.102	-0.016
5	As	0.229	0.042	0.483
6	As	0.271	0.458	0.483
7	Nb(3)	0.398	0.238	0.516
8	Nb(3)	0.238	0.102	0.984
9	Nb(1)	0.036	-0.057	0.739
10	As	0.042	0.271	1.017
11	Nb(2)	-0.154	0.165	0.770
12	Nb(1)	-0.057	0.464	0.761
13	Nb(1)	0.057	0.536	0.239
14	Nb(3)	0.262	0.398	0.984
15	Nb(1)	-0.036	0.057	0.261
16	Nb(2)	-0.165	0.346	0.270

Table 5.4(b) Interatomic distances of atoms of the Nb(3) co-ordination polyhedron in Fig.5.4 and the standard deviation for the interatomic distances of the central atom only.

Bond	Distance, Å
1Nb(3)-2As	2.670± 0.011
-3Nb(3)	3.507± 0.011
-4Nb(3)	3.507± 0.011
-5As	2.618± 0.006
-6As	2.670± 0.007
-7Nb(3)	3.049± 0.001
-8Nb(3)	3.249± 0.011
-9Nb(1)	3.547± 0.006
-10As	2.676± 0.011
-11Nb(2)	3.118± 0.008
-12Nb(1)	2.937± 0.007
-13Nb(1)	3.202± 0.008
-14Nb(3)	3.249± 0.011
-15Nb(1)	2.873± 0.007
-16Nb(2)	3.155± 0.005
2As -3Nb(3)	2.618
-4Nb(3)	2.670
-13Nb(1)	2.962
-15Nb(1)	2.673
-16Nb(2)	2.618

Bond	Distance, Å
3Nb(3)-4Nb(3)	3.049
-6As	2.670
-7Nb(3)	3.507
-13Nb(1)	2.873
4Nb(3)-5As	2.670
-7Nb(3)	3.507
-15Nb(1)	3.202
5As -7Nb(3)	2.670
-8Nb(3)	2.676
-9Nb(1)	2.592
-15Nb(1)	2.962
6As -7Nb(3)	2.618
-12Nb(1)	3.674
-13Nb(1)	2.672
-14Nb(3)	2.676
7Nb(3)-8Nb(3)	3.249
8Nb(3)-9Nb(1)	2.937
-10As	2.670
-14Nb(3)	3.049

Table 5.4(b)

(continued)

Bond	Distance, Å
9Nb(1)-10As	3.674
-11Nb(2)	3.014
-15Nb(1)	2.841
10As -11Nb(2)	2.632
-12Nb(1)	2.592
-14Nb(3)	2.618
11Nb(2)-12Nb(1)	3.237
-15Nb(1)	3.116
-16Nb(2)	3.196
12Nb(1)-13Nb(1)	3.047
-14Nb(3)	3.546
-16Nb(2)	3.041
13Nb(1)-16Nb(2)	3.014
15Nb(1)-16Nb(2)	3.257

Table 5.4(c) Interatomic angles of atoms of the Nb(3) co-ordination polyhedron in Fig.5.4.

Bond	Angle (degree)
2As -3Nb(3)-4Nb(3)	55.59
-13Nb(1)	65.10
-4Nb(3)-15Nb(1)	53.22
-13Nb(1)-16Nb(2)	51.94
-15Nb(1)-4Nb(3)	53.14
-16Nb(2)	51.25
-16Nb(2)-13Nb(1)	63.00
-15Nb(1)	52.77
3Nb(3)-4Nb(3)-2As	53.99
-7Nb(3)	64.23
-6As -7Nb(3)	83.08
-13Nb(1)	65.07
-7Nb(3)-4Nb(3)	51.53
-6As	49.09
-13Nb(1)-2As	53.29
-6As	57.44
4Nb(3)-3Nb(3)-7Nb(3)	64.23
-5As -7Nb(3)	82.10
-15Nb(1)	69.07
-7Nb(3)-5As	48.95
-15Nb(1)-5As	51.16
5As -4Nb(3)-7Nb(3)	48.95
-15Nb(1)	59.77

Bond	Angle (degree)
5As -7Nb(3)-8Nb(3)	52.66
-8Nb(3)-7Nb(3)	52.49
-9Nb(1)	54.77
-9Nb(1)-8Nb(3)	57.49
-15Nb(1)	65.89
-15Nb(1)-9Nb(1)	53.01
6As -3Nb(3)-7Nb(3)	47.82
-13Nb(1)	57.50
-7Nb(3)-14Nb(3)	52.88
-12Nb(1)-13Nb(1)	45.68
-14Nb(3)	43.46
-13Nb(1)-12Nb(1)	79.65
-14Nb(3)-7Nb(3)	51.27
-12Nb(1)	70.81
7Nb(3)-6As -14Nb(3)	75.85
-8Nb(3)-14Nb(3)	62.12
-14Nb(3)-8Nb(3)	61.96
9Nb(1)-8Nb(3)-10As	81.73
-10As -11Nb(2)	54.09
-11Nb(2)-10As	80.89
-15Nb(1)	55.19
-15Nb(1)-11Nb(2)	60.58

Table 5.4(c)

(continued)

Bond	Angle (degree)
10As -8Nb(3)-14Nb(3)	53.99
-9Nb(1)-11Nb(2)	45.02
-11Nb(2)-12Nb(1)	51.16
-12Nb(1)-11Nb(2)	52.27
-14Nb(3)	47.42
11Nb(2)-9Nb(1)-15Nb(1)	64.23
-10As -12Nb(1)	76.57
-12Nb(1)-16Nb(2)	62.63
-15Nb(1)-16Nb(2)	60.15
-16Nb(2)-12Nb(1)	62.47
-15Nb(1)	57.74
12Nb(1)-10As -14Nb(3)	85.79
-11Nb(2)-16Nb(2)	56.42
-13Nb(1)-16Nb(2)	60.22
-14Nb(3)-10As	46.80
-16Nb(2)-13Nb(1)	60.42
13Nb(1)-2As -16Nb(2)	65.04
-6As -12Nb(1)	54.67
-12Nb(1)-16Nb(2)	59.35
-16Nb(2)-15Nb(1)	128.74
15Nb(1)-11Nb(2)-16Nb(2)	62.11
-16Nb(2)-2As	52.77

Table 5.5(a) The co-ordinates of atoms of the As co-ordination polyhedron in Fig.5.5.

	Atom	x	y	z
1	As	0.771	0.958	0.517
2	Nb(2)	0.846	1.165	0.770
3	Nb(3)	0.898	0.738	0.484
4	Nb(3)	0.602	0.762	0.484
5	Nb(1)	0.557	1.036	0.761
6	Nb(2)	0.665	1.154	0.270
7	Nb(3)	0.762	0.898	0.016
8	Nb(1)	0.964	1.057	0.261
9	Nb(3)	0.762	0.898	1.016
10	Nb(1)	0.443	0.964	0.239
11	Nb(1)	1.036	0.943	0.739

Table 5.5(b) Interatomic distances of atoms of the As co-ordination polyhedron in Fig.5.5 and the standard deviation for the interatomic distances of the central atom only.

Bond	Distance, Å
1As -2Nb(2)	2.618 ± 0.006
-3Nb(3)	2.618 ± 0.007
-4Nb(3)	2.670 ± 0.007
-5Nb(1)	2.672 ± 0.007
-6Nb(2)	2.632 ± 0.009
-7Nb(3)	2.676 ± 0.011
-8Nb(1)	2.592 ± 0.008
-9Nb(3)	2.670 ± 0.011
-10Nb(1)	3.674 ± 0.007
-11Nb(1)	2.966 ± 0.008
2Nb(2)-5Nb(1)	3.258
-6Nb(2)	3.199
-8Nb(1)	2.875
-9Nb(3)	3.152
-11Nb(1)	3.012
3Nb(3)-4Nb(3)	3.049
-7Nb(3)	3.249
-8Nb(1)	3.546
-9Nb(3)	3.507
-11Nb(1)	2.868

Bond	Distance, Å
4Nb(3)-5Nb(1)	3.200
-7Nb(3)	3.249
-9Nb(3)	3.507
-10Nb(1)	2.937
5Nb(1)-6Nb(2)	3.036
-9Nb(3)	2.868
-10Nb(1)	3.047
6Nb(2)-7Nb(3)	3.112
-8Nb(1)	3.236
-10Nb(1)	3.012
7Nb(3)-8Nb(1)	2.937
-10Nb(1)	3.548
8Nb(1)-11Nb(1)	2.845
9Nb(3)-11Nb(1)	3.200

Table 5.5(c) Interatomic angles of atoms of the As co-ordination polyhedron in Fig.5.5.

Bond	Angle (Degree)
2Nb(2)-5Nb(1)-6Nb(2)	60.98
-9Nb(3)	61.54
-6Nb(2)-5Nb(1)	62.94
-8Nb(1)	53.07
-8Nb(1)-6Nb(2)	62.81
-11Nb(1)	63.55
-9Nb(3)-5Nb(1)	65.33
-11Nb(1)	56.61
3Nb(3)-4Nb(3)-7Nb(3)	62.02
-9Nb(3)	64.23
-7Nb(3)-4Nb(3)	55.97
-8Nb(1)	69.74
-8Nb(1)-7Nb(3)	59.27
-11Nb(1)	51.93
-9Nb(3)-4Nb(3)	51.53
-11Nb(1)	50.38
4Nb(3)-3Nb(3)-7Nb(3)	62.02
-9Nb(3)	64.23
-5Nb(1)-9Nb(3)	63.38
-10Nb(1)	56.02
-7Nb(3)-10Nb(1)	50.97
-9Nb(3)-5Nb(1)	59.25
-10Nb(1)-5Nb(1)	64.22
-7Nb(3)	59.24

Bond	Angle (Degree)
5Nb(1)-2Nb(2)-6Nb(2)	52.73
-9Nb(3)	53.13
-6Nb(2)-10Nb(1)	60.50
-10Nb(1)-6Nb(2)	60.14
6Nb(2)-2Nb(2)-8Nb(1)	64.12
-5Nb(1)-10Nb(1)	59.36
-7Nb(3)-8Nb(1)	64.61
-10Nb(1)	53.29
-10Nb(1)-7Nb(3)	55.92
7Nb(3)-3Nb(3)-8Nb(1)	50.99
-4Nb(3)-10Nb(1)	69.79
-6Nb(2)-8Nb(1)	55.08
-10Nb(1)	70.79
8Nb(1)-3Nb(3)-11Nb(1)	51.34
-2Nb(2)-11Nb(1)	57.74

The interatomic distances shorter than 4.0 Å were listed in Table 5.2(b), 5.3(b), 5.4(b) and 5.5(b).

In the Ti_3P-type structure, the nearest neighbours of the metal atom of the compound, Nb_3As , Nb_3P and Zr_3P range between 12 to 15 atoms and the number of the nearest neighbours of the non-metal is 9 and 10 atoms.

The comparison of the interatomic distances between the metal atom and non-metal atom from the central atom of these compounds is shown in Table 5.6 , where

d_M = average distance between the central atom and its metal neighbours ;

d_N = average distance between the central atom and its non-metal neighbours ;

and M-M distances shorter than 3.6 Å and M-N distances shorter than 3.7 Å were taken into account.

In Nb_3P , each phosphorus atom has eight near niobium neighbours at distances between 2.53 and 2.64 Å while a ninth niobium atom is situated as far as 2.89 Å from the central phosphorus atom. The packing of the metal atoms in Nb_3P is dense, each niobium atom having 11-12 niobium neighbours at an average distance of 3.09 Å .

In Nb_3As, there are 14 to 15 neighbouring atoms to each metal atom and 10 atoms to each non-metal atom. The distance of about 2.7 Å between non-metal atom and metal atom is shorter than the distance between metal atom and metal atom that is about 3.4 Å . The non-metallic atoms are relatively far apart at the shortest distance of 3.893 Å .

Although in Nb_3As the average distance of niobium to niobium atoms is marginally large at 3.12 Å than **that** in Nb_3P, but there are also more niobium neighbours to each central atom, in this respect the packing of the metal atoms in Nb_3As may be regarded just as dense.

Table 5.6 Comparison between d_M and d_N.

Compound	Central atom	Co-ordination number	d_M(Å)	d_N(Å)
Nb_3As	Nb(1)	15	3.101±0.0007	2.976±0.002
	Nb(2)	14	3.113±0.0005	2.625±0.004
	Nb(3)	15	3.218±0.0007	2.659±0.002
	As	10	2.779±0.0008	-
Nb_3P	Nb(1)	15	3.050±0.0002	2.686±0.001
	Nb(2)	14	3.065±0.0001	2.581±0.003
	Nb(3)	15	3.155±0.0002	2.604±0.0006
	P	9	2.626±0.0006	-
Zr_3P	Zr(1)	13	3.187± 0.0004	2.785±0.003
	Zr(2)	14	3.282±0.0003	2.750±0.004
	Zr(3)	12	3.065±0.0005	2.762±0.002
	P	9	2.766± 0.0009	-