

TiC

1.0

4.3312997818	0.0000000000	0.0000000000
0.0000000000	4.3312997818	0.0000000000
0.0000000000	0.0000000000	4.3312997818

C Ti

4 4

Cartesian

0.0000000000	0.0000000000	0.0000000000
0.0000000000	2.165649891	2.165649891
2.165649891	0.0000000000	2.165649891
2.165649891	2.165649891	0.0000000000
2.165649891	2.165649891	2.165649891
2.165649891	0.0000000000	0.0000000000
0.0000000000	2.165649891	0.0000000000
0.0000000000	0.0000000000	2.165649891

TiN

1.0

4.2463002205	0.0000000000	0.0000000000
0.0000000000	4.2463002205	0.0000000000
0.0000000000	0.0000000000	4.2463002205

N Ti

4 4

Cartesian

0.0000000000	0.0000000000	0.0000000000
0.0000000000	2.123150110	2.123150110
2.123150110	0.0000000000	2.123150110
2.123150110	2.123150110	0.0000000000
2.123150110	2.123150110	2.123150110
2.123150110	0.0000000000	0.0000000000
0.0000000000	2.123150110	0.0000000000
0.0000000000	0.0000000000	2.123150110

TiC0.75N0.25

1.0

4.3074998856	0.0000000000	0.0000000000
0.0000000000	4.3074998856	0.0000000000
0.0000000000	0.0000000000	4.3074998856

N	C	Ti
1	3	4

Cartesian

0.0000000000	0.0000000000	0.0000000000
0.0000000000	2.153749943	2.153749943
2.153749943	0.0000000000	2.153749943
2.153749943	2.153749943	0.0000000000
2.153749943	2.153749943	2.153749943
2.153749943	0.0000000000	0.0000000000
0.0000000000	2.153749943	0.0000000000
0.0000000000	0.0000000000	2.153749943

Ti<sub>0.75</sub>Al<sub>0.25</sub>C

1.0

4.3220000267	0.0000000000	0.0000000000
0.0000000000	4.3220000267	0.0000000000
0.0000000000	0.0000000000	4.3220000267

C	Al	Ti
4	1	3

Cartesian

0.0000000000	0.0000000000	0.0000000000
0.0000000000	2.161000013	2.161000013
2.161000013	0.0000000000	2.161000013
2.161000013	2.161000013	0.0000000000
2.161000013	2.161000013	2.161000013
2.161000013	0.0000000000	0.0000000000
0.0000000000	2.161000013	0.0000000000
0.0000000000	0.0000000000	2.161000013

Ti0.75Al0.25C0.75N0.25

1.0

4.2916998863	0.0000000000	0.0000000000
0.0000000000	4.2916998863	0.0000000000
0.0000000000	0.0000000000	4.2916998863

N	C	Al	Ti
1	3	1	3

Cartesian

0.0000000000	0.0000000000	0.0000000000
0.0000000000	2.145849943	2.145849943
2.145849943	0.0000000000	2.145849943
2.145849943	2.145849943	0.0000000000
2.145849943	2.145849943	2.145849943
2.145849943	0.0000000000	0.0000000000
0.0000000000	2.145849943	0.0000000000
0.0000000000	0.0000000000	2.145849943