**Assignment 1- Atomic and electronic structure of materials**

**Bhuvanesh P – MM19B027**

**1 . Bravais Lattices**

1. Simple cubic

1.0

4.0000000000 0.0000000000 0.0000000000

0.0000000000 4.0000000000 0.0000000000

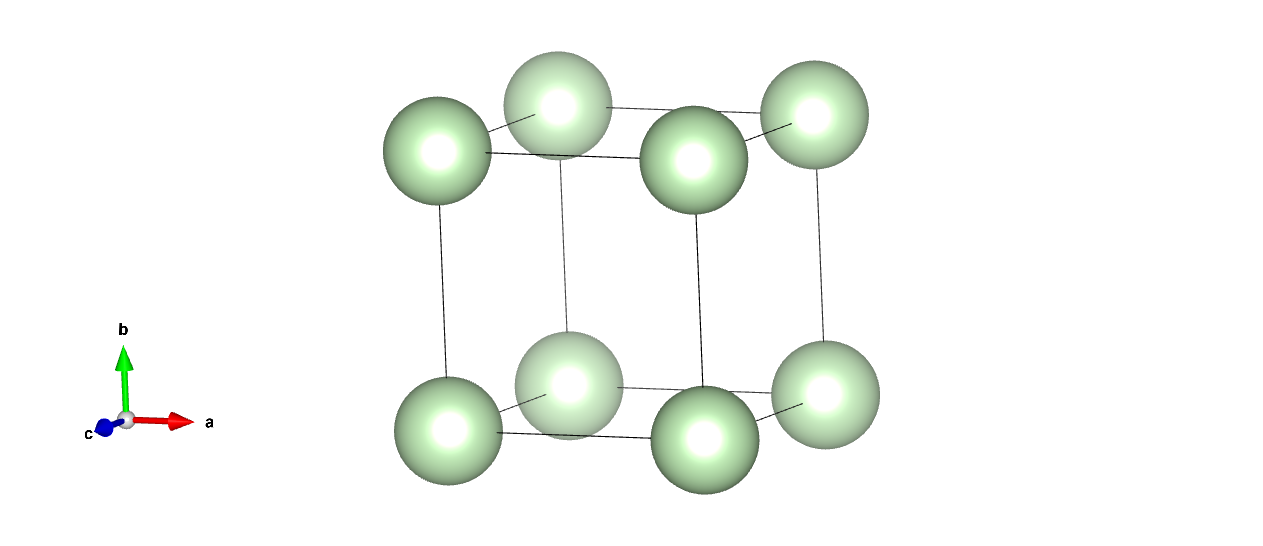
0.0000000000 0.0000000000 4.0000000000

Ar

1

Direct

0.000000000 0.000000000 0.000000000



2. Body centred cubic

1.0

4.0000000000 0.0000000000 0.0000000000

0.0000000000 4.0000000000 0.0000000000

0.0000000000 0.0000000000 4.0000000000

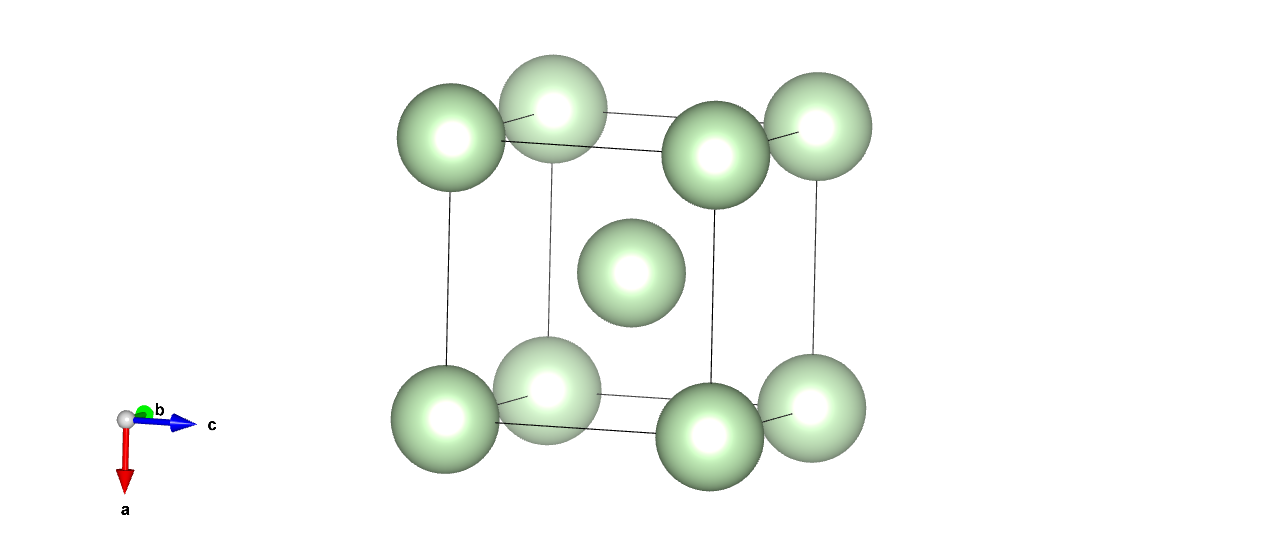
Ar

2

Direct

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0.500000000 0.500000000 0.500000000



3. Face centred cubic

1.0

4.0000000000 0.0000000000 0.0000000000

0.0000000000 4.0000000000 0.0000000000

0.0000000000 0.0000000000 4.0000000000

Ar

4

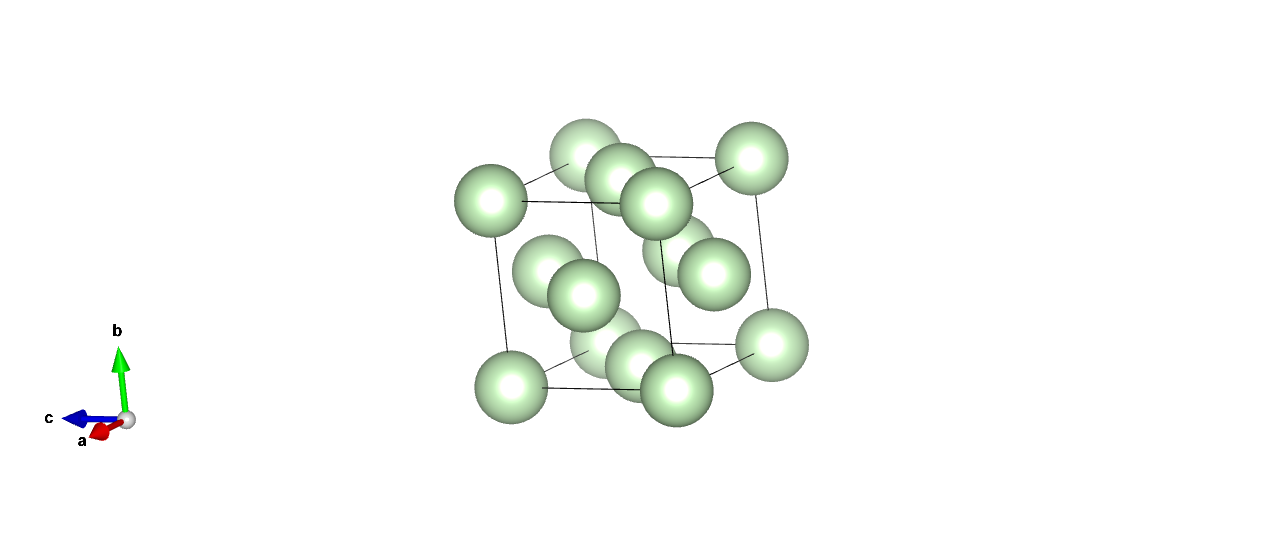
Direct

0.000000000 0.000000000 0.000000000

0.500000000 0.500000000 0.000000000

0.000000000 0.500000000 0.500000000

0.500000000 0.000000000 0.500000000



4. Primitive Tetragonal

1.0

4.0000000000 0.0000000000 0.0000000000

0.0000000000 4.0000000000 0.0000000000

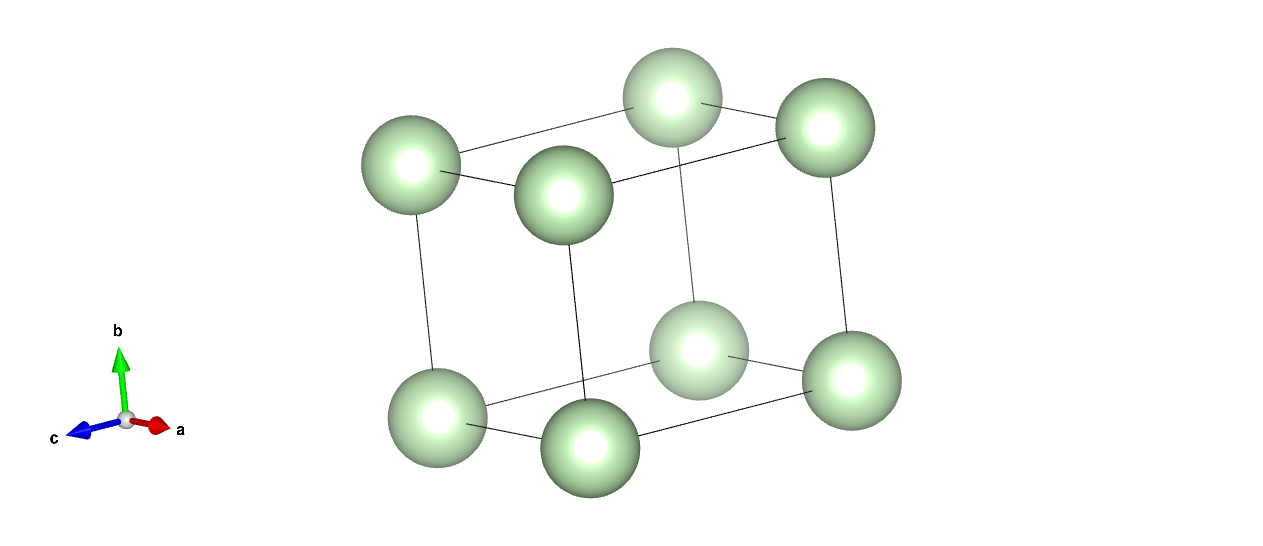
0.0000000000 0.0000000000 5.0000000000

Ar

1

Direct

0.000000000 0.000000000 0.000000000



5. Body centered tetragonal

1.0

4.0000000000 0.0000000000 0.0000000000

0.0000000000 4.0000000000 0.0000000000

0.0000000000 0.0000000000 5.0000000000

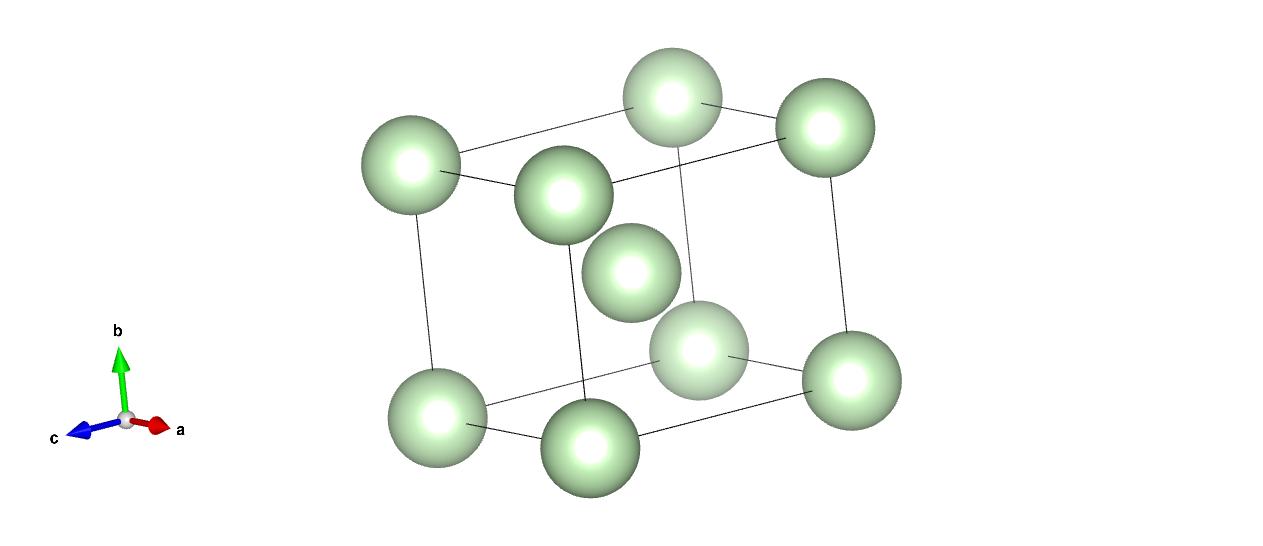
Ar

2

Direct

0.000000000 0.000000000 0.000000000

0.500000000 0.500000000 0.500000000



6. Primitive Orthorhombic

1.0

4.0000000000 0.0000000000 0.0000000000

0.0000000000 4.5000000000 0.0000000000

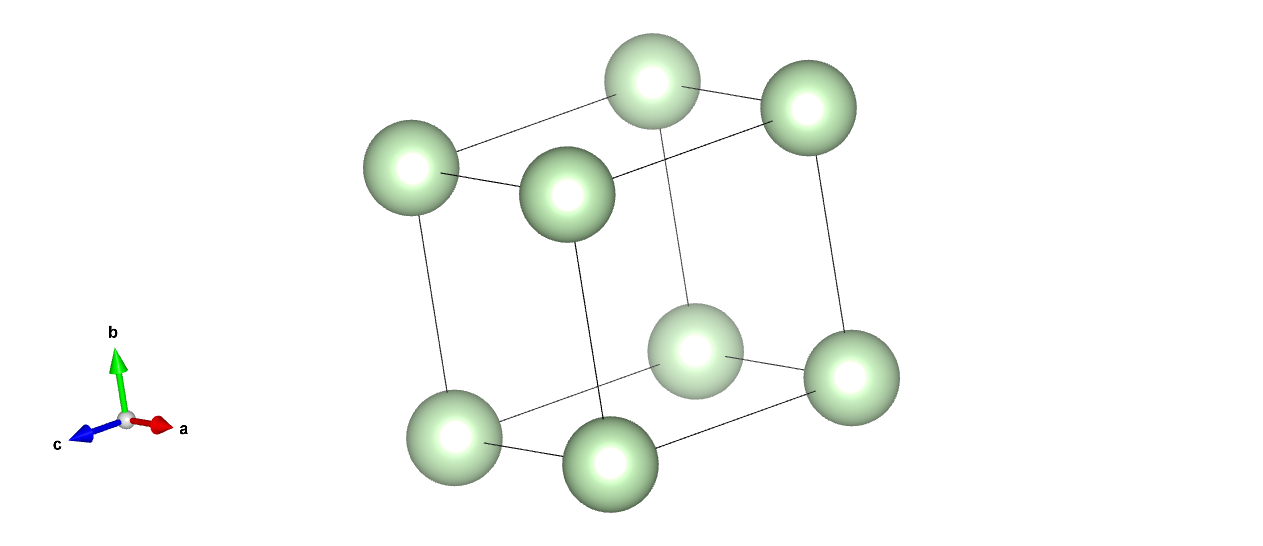
0.0000000000 0.0000000000 5.0000000000

Ar

1

Direct

0.000000000 0.000000000 0.000000000



7. Body Centered Orthorhombic

1.0

4.0000000000 0.0000000000 0.0000000000

0.0000000000 4.5000000000 0.0000000000

0.0000000000 0.0000000000 5.0000000000

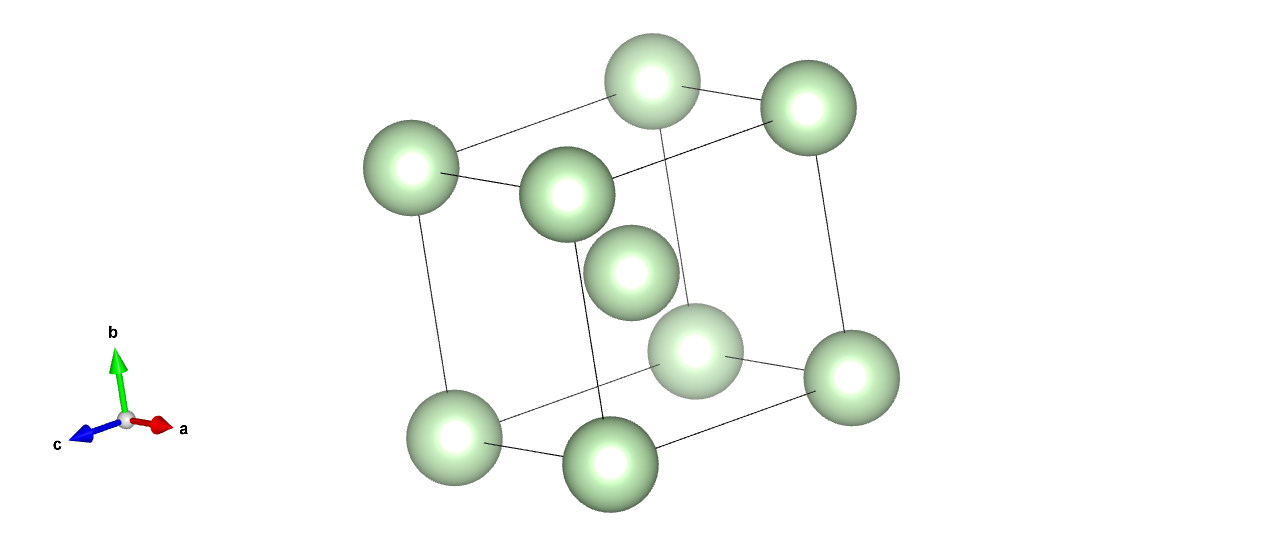
Ar

2

Direct

0.000000000 0.000000000 0.000000000

0.500000000 0.500000000 0.500000000



8. Base Centered Orthorhombic

1.0

4.0000000000 0.0000000000 0.0000000000

0.0000000000 4.5000000000 0.0000000000

0.0000000000 0.0000000000 5.0000000000

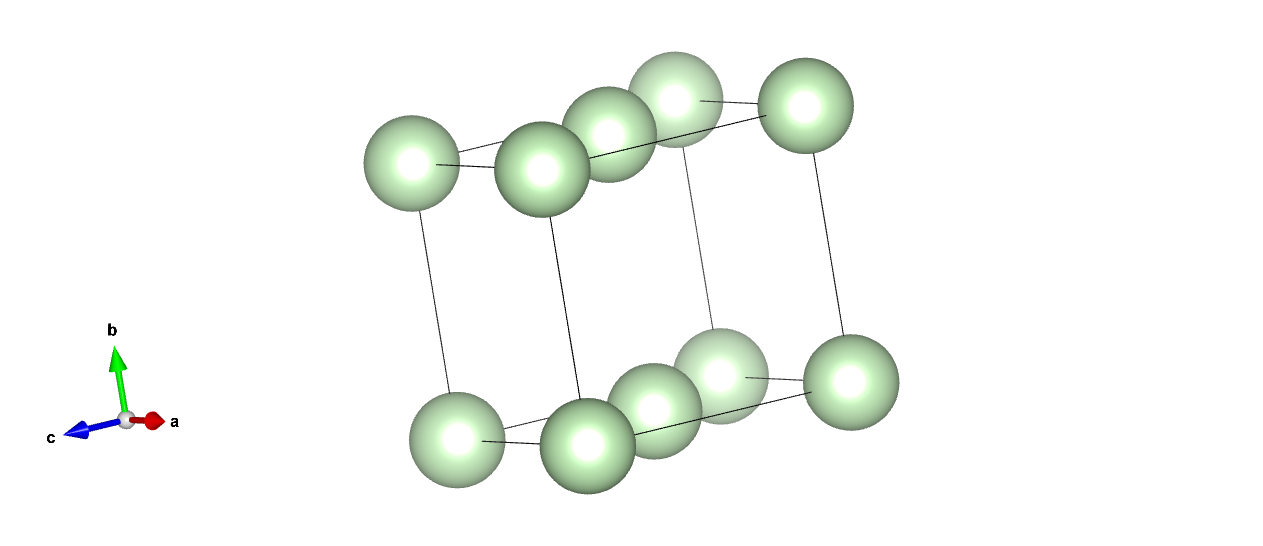
Ar

2

Direct

0.000000000 0.000000000 0.000000000

0.500000000 0.000000000 0.500000000



9. Face Centered Orthorhombic

1.0

4.0000000000 0.0000000000 0.0000000000

0.0000000000 4.5000000000 0.0000000000

0.0000000000 0.0000000000 5.0000000000

Ar

4

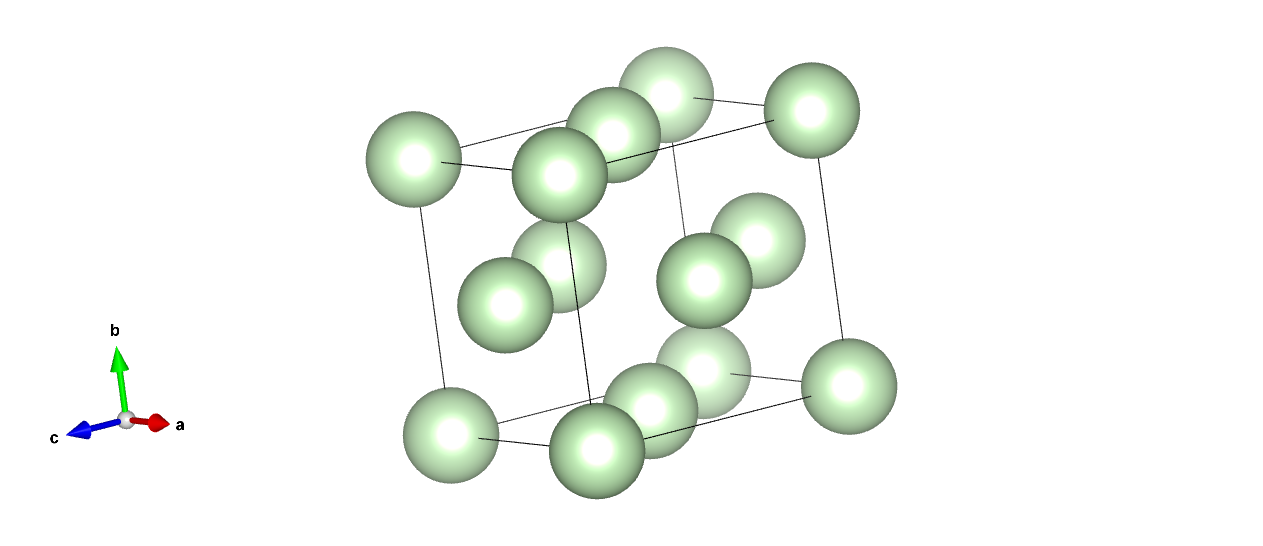
Direct

0.000000000 0.000000000 0.000000000

0.500000000 0.000000000 0.500000000

0.500000000 0.500000000 0.000000000

0.000000000 0.500000000 0.500000000



10. Primitive Hexagonal

1.0

4.0000000000 0.0000000000 0.0000000000

-2.0000000000 3.4641016151 0.0000000000

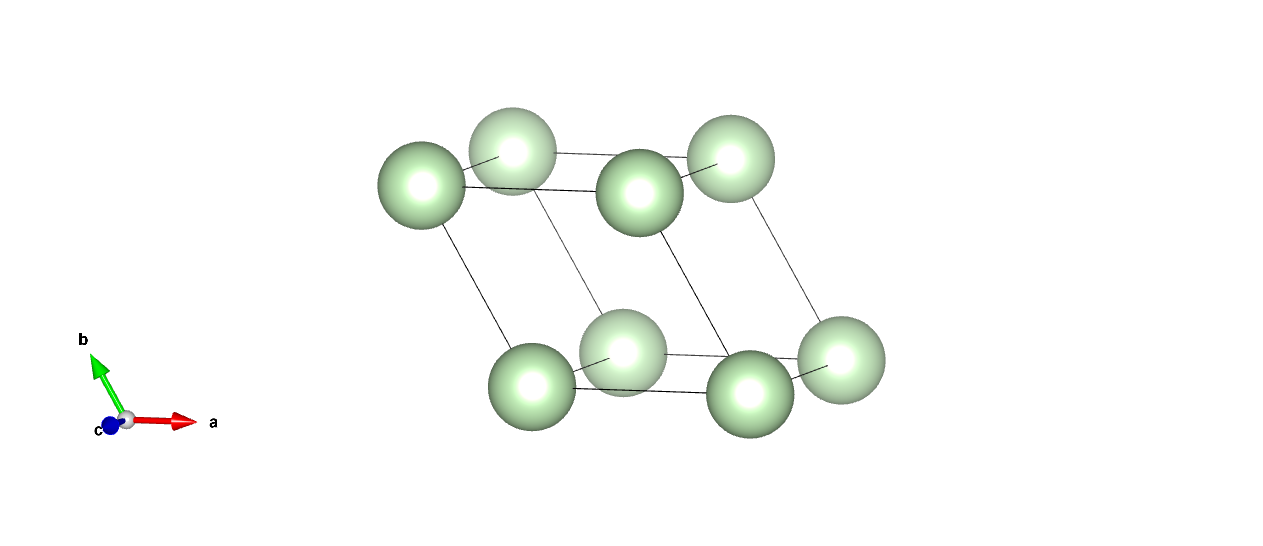
0.0000000000 0.0000000000 5.0000000000

Ar

1

Direct

0.000000000 0.000000000 0.000000000



11. Primitive Monoclinic

1.0

4.0000000000 0.0000000000 0.0000000000

0.0000000000 4.5000000000 0.0000000000

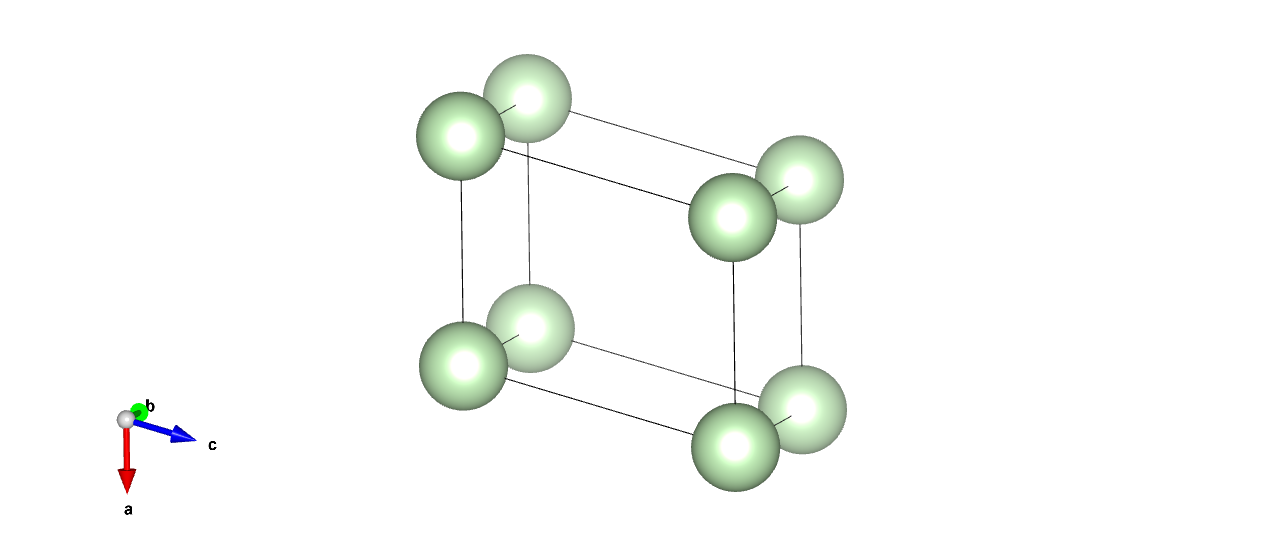
1.2940952255 0.0000000000 4.8296291314

Ar

1

Direct

0.000000000 0.000000000 0.000000000



12. Base Centered Monoclinic

1.0

4.0000000000 0.0000000000 0.0000000000

0.0000000000 4.5000000000 0.0000000000

1.2940952255 0.0000000000 4.8296291314

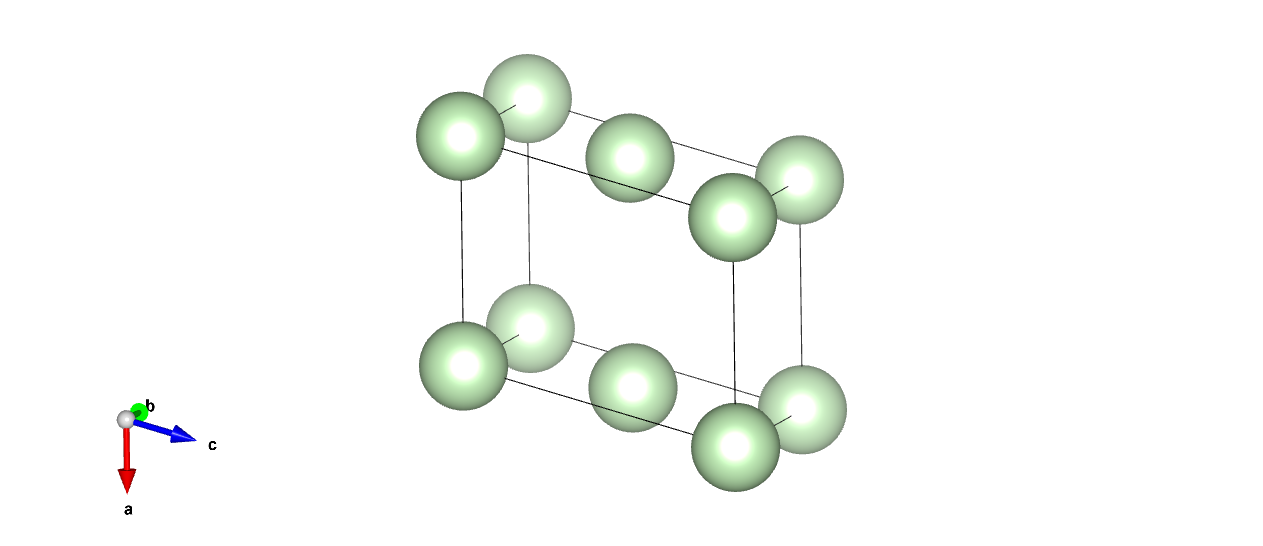
Ar

2

Direct

0.000000000 0.000000000 0.000000000

0.000000000 0.500000000 0.500000000



13. Trigonal Primitive

1.0

4.0000000000 0.0000000000 0.0000000000

2.2943057454 3.2766081772 0.0000000000

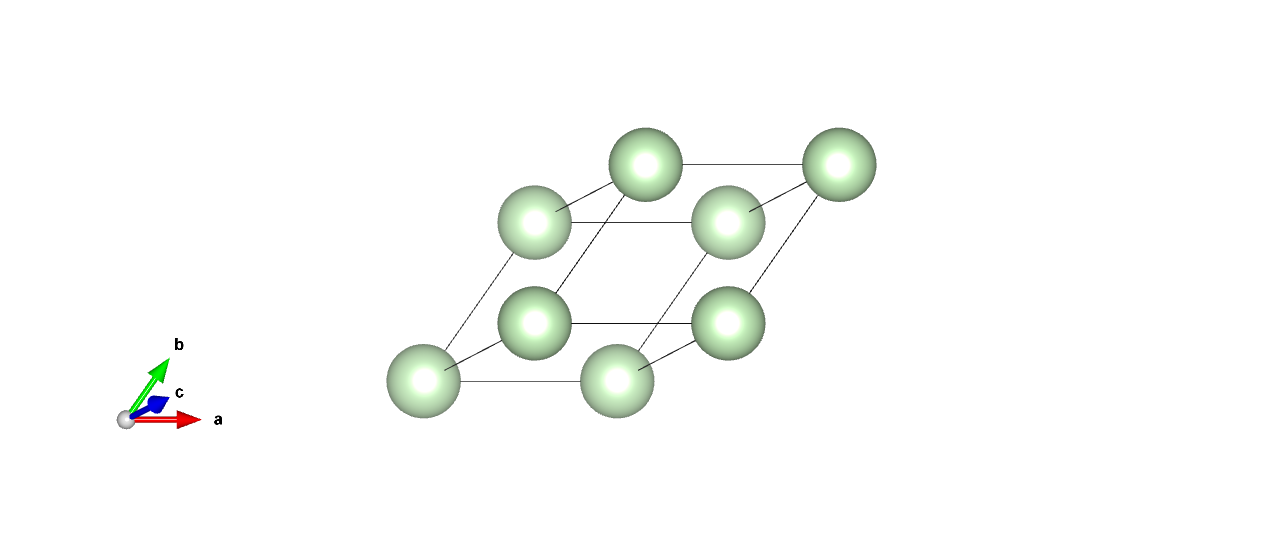
2.2943057454 1.1943399749 3.0511822579

Ar

1

Direct

0.000000000 0.000000000 0.000000000



14. Primitive Triclinic

1.0

4.0000000000 0.0000000000 0.0000000000

0.7814167995 4.4316348886 0.0000000000

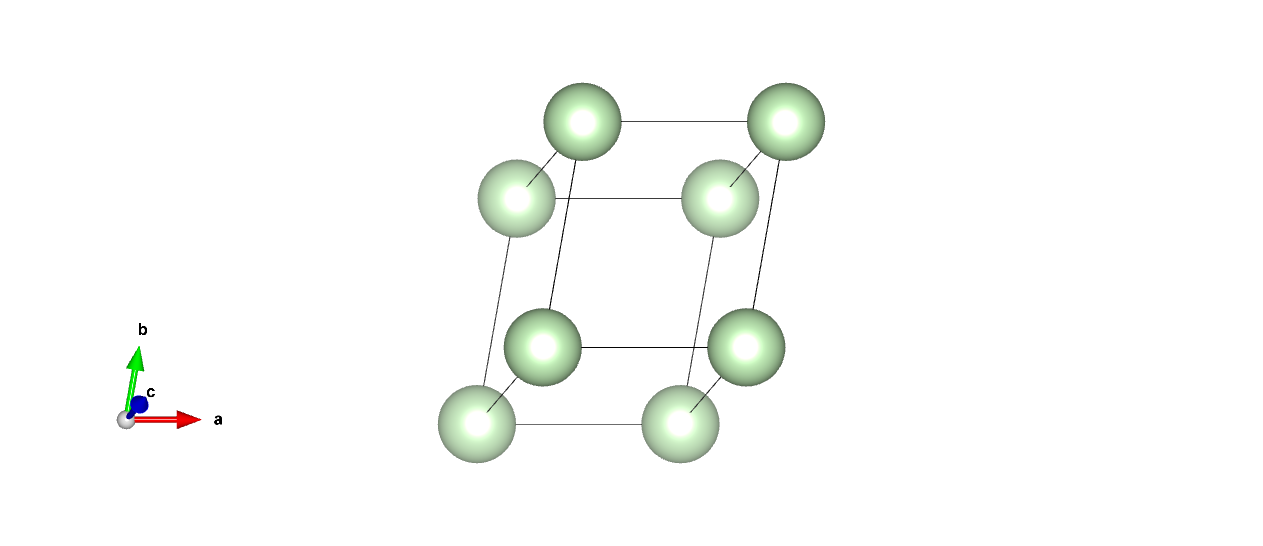
1.2940952255 1.5082978728 4.5880665944

Ar

1

Direct

0.000000000 0.000000000 0.000000000



**2. Unit cells of atoms and molecules**

a. Al

1.0

4.0399999619 0.0000000000 0.0000000000

0.0000000000 4.0399999619 0.0000000000

0.0000000000 0.0000000000 4.0399999619

Al

4

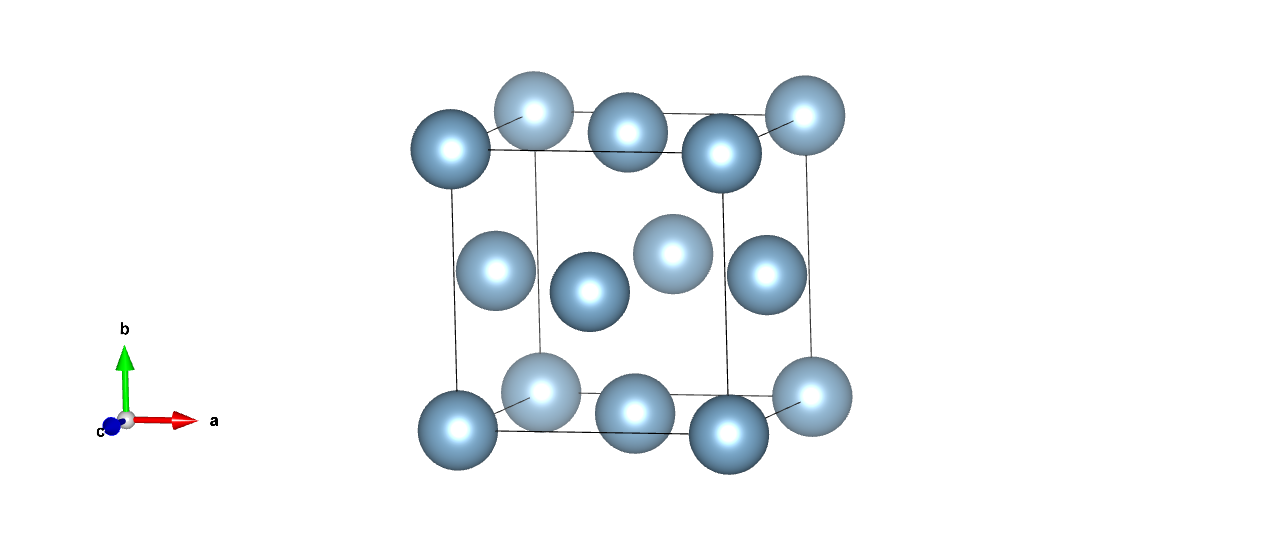
Direct

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0.000000000 0.500000000 0.500000000

0.500000000 0.000000000 0.500000000

0.500000000 0.500000000 0.000000000



b. Ti

1.0

2.9300000668 0.0000000000 0.0000000000

-1.4650000334 2.5374544909 0.0000000000

0.0000000000 0.0000000000 4.6599998474

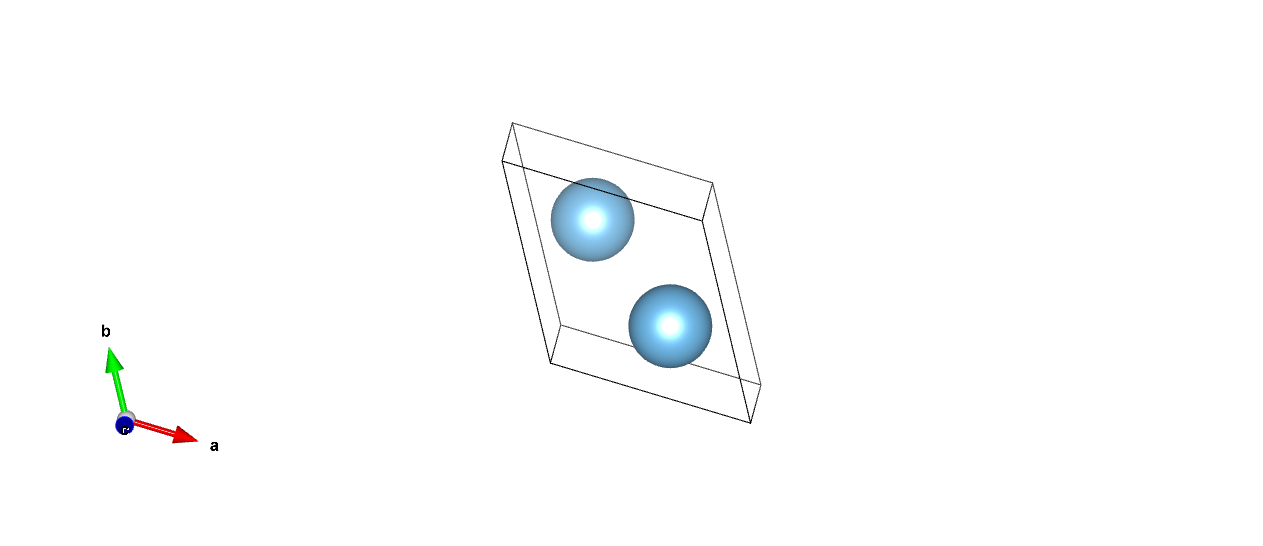
Ti

2

Direct

0.333333343 0.666666687 0.250000000

0.666666627 0.333333313 0.750000000



c. Ti4N3

1.0

9.9300003052 0.0000000000 0.0000000000

0.0000000000 3.0199999809 0.0000000000

-8.9469050362 0.0000000000 5.1032239028

Ti N

8 6

Direct

0.266000003 0.500000000 0.633000016

0.733999968 0.500000000 0.366999984

0.766000032 0.000000000 0.633000016

0.233999997 0.000000000 0.366999984

0.257999986 0.000000000 0.884999990

0.741999984 0.000000000 0.115000010

0.758000016 0.500000000 0.884999990

0.242000014 0.500000000 0.115000010

0.001000000 0.500000000 0.749000013

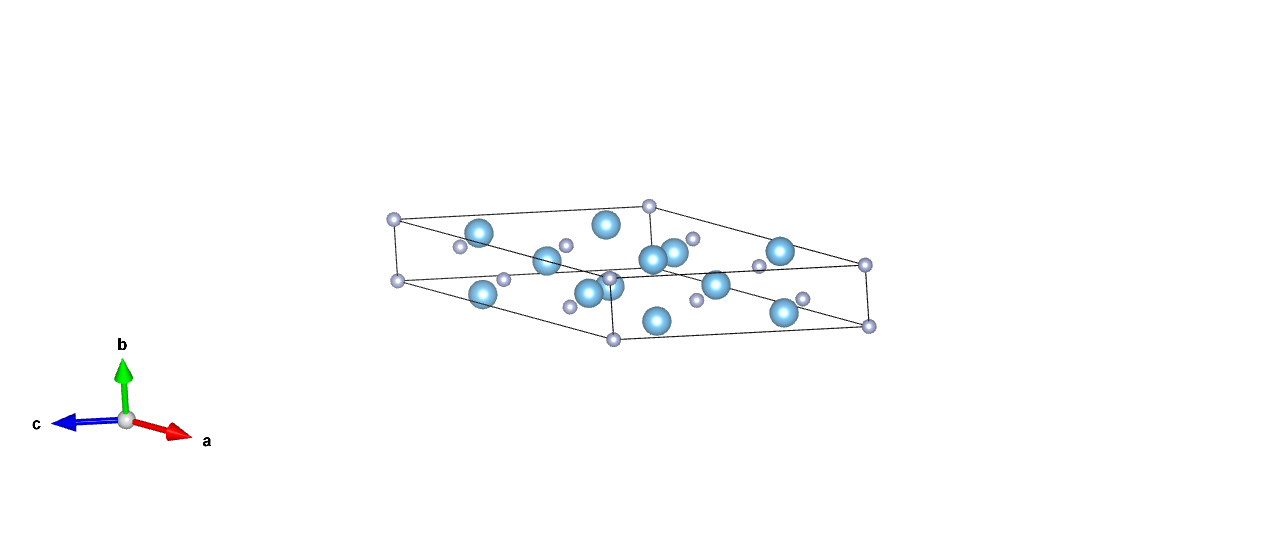
0.999000013 0.500000000 0.250999987

0.500999987 0.000000000 0.749000013

0.499000013 0.000000000 0.250999987

0.000000000 0.000000000 0.000000000

0.500000000 0.500000000 0.000000000



d.ZnS

1.0

5.4499998093 0.0000000000 0.0000000000

0.0000000000 5.4499998093 0.0000000000

0.0000000000 0.0000000000 5.4499998093

Zn S

4 4

Direct

0.000000000 0.000000000 0.000000000

0.000000000 0.500000000 0.500000000

0.500000000 0.000000000 0.500000000

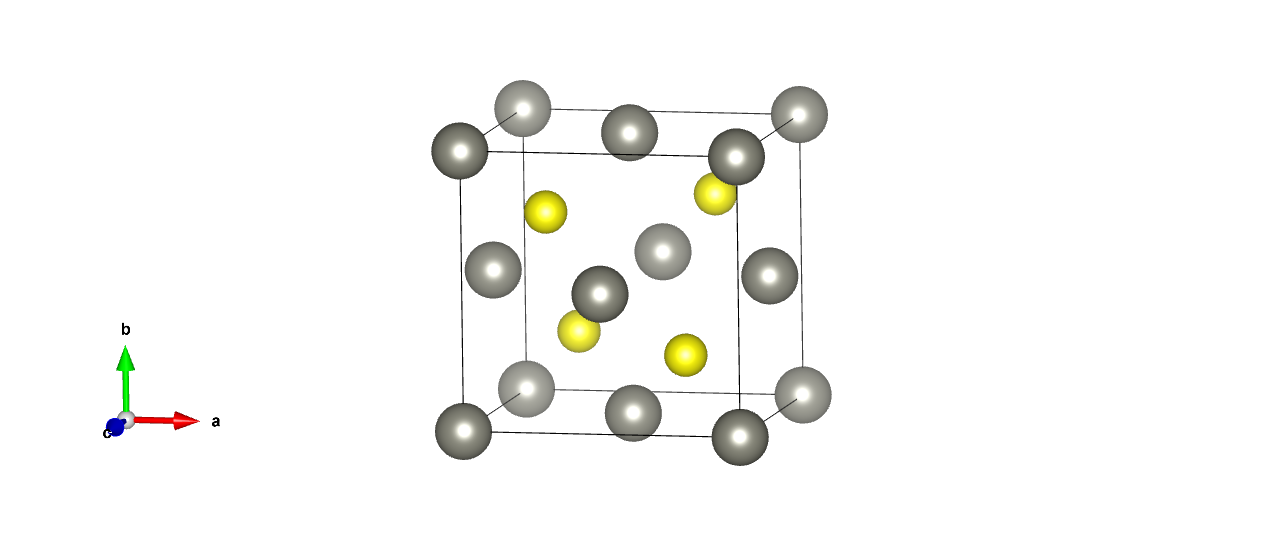
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0.250000000 0.250000000 0.250000000

0.750000000 0.750000000 0.250000000

0.750000000 0.250000000 0.750000000

0.250000000 0.750000000 0.750000000



e.ZnO

1.0

3.2899999619 0.0000000000 0.0000000000

-1.6449999809 2.8492235454 0.0000000000

0.0000000000 0.0000000000 5.3099999428

Zn O

2 2

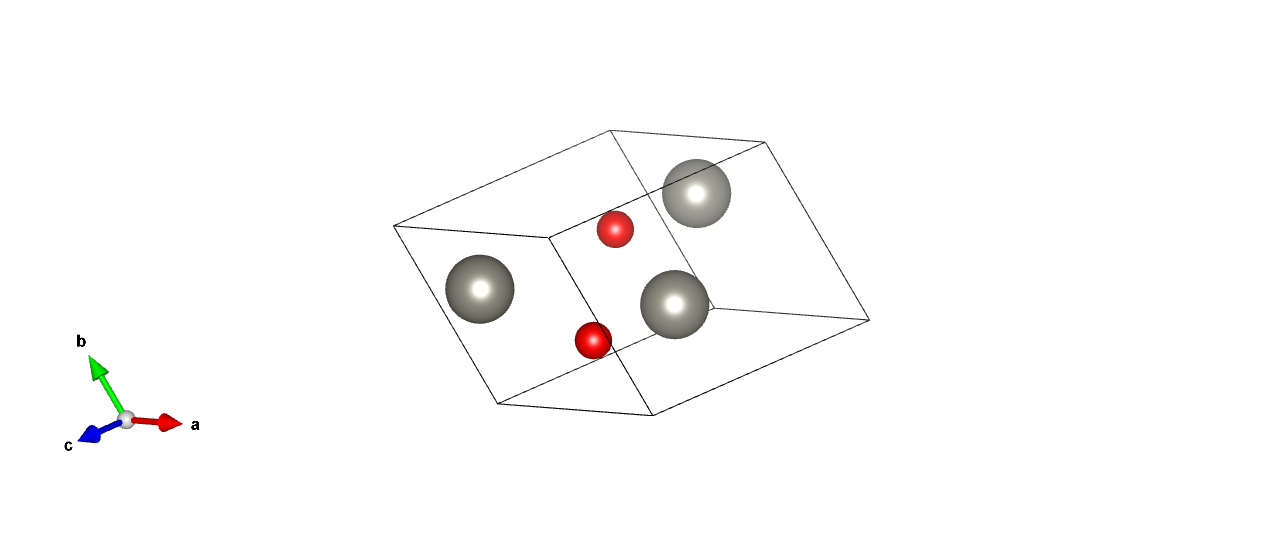
Direct

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0.666666627 0.333333313 0.500000000

0.333333343 0.666666687 0.375000000

0.666666627 0.333333313 0.875000000



f.Lu3Al5O12

1.0

11.9700002670 0.0000000000 0.0000000000

0.0000000000 11.9700002670 0.0000000000

0.0000000000 0.0000000000 11.9700002670

Lu Al O

24 40 96

Direct

0.000000000 0.250000000 0.125000000

0.000000000 0.750000000 0.875000000

0.500000000 0.750000000 0.625000000

0.500000000 0.250000000 0.375000000

0.000000000 0.750000000 0.375000000

0.000000000 0.250000000 0.625000000

0.500000000 0.250000000 0.875000000

0.500000000 0.750000000 0.125000000

0.125000000 0.000000000 0.250000000

0.875000000 0.000000000 0.750000000

0.625000000 0.500000000 0.750000000

0.375000000 0.500000000 0.250000000

0.375000000 0.000000000 0.750000000

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0.250000000 0.125000000 0.000000000

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0.750000000 0.375000000 0.000000000

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0.000000000 0.000000000 0.500000000

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0.471000016 0.552999973 0.644999981

0.528999984 0.446999997 0.355000019

0.971000016 0.947000027 0.355000019

0.028999999 0.053000003 0.644999981

0.528999984 0.053000003 0.855000019

0.471000016 0.947000027 0.144999996

0.144999996 0.028999999 0.446999997

0.855000019 0.971000016 0.552999973

0.644999981 0.471000016 0.552999973

0.355000019 0.528999984 0.446999997

0.355000019 0.971000016 0.947000027

0.644999981 0.028999999 0.053000003

0.855000019 0.528999984 0.053000003

0.144999996 0.471000016 0.947000027

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0.552999973 0.855000019 0.971000016

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0.053000003 0.855000019 0.528999984

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0.303000003 0.778999984 0.105000004

0.802999973 0.778999984 0.394999981

0.196999997 0.221000001 0.605000019

0.778999984 0.394999981 0.802999973

0.221000001 0.605000019 0.196999997

0.221000001 0.894999981 0.697000027

0.778999984 0.105000004 0.303000003

0.721000016 0.605000019 0.303000003

0.278999984 0.394999981 0.697000027

0.278999984 0.105000004 0.196999997

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0.894999981 0.697000027 0.221000001

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0.644999981 0.528999984 0.947000027

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0.355000019 0.028999999 0.552999973

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0.053000003 0.355000019 0.471000016

0.053000003 0.144999996 0.971000016

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