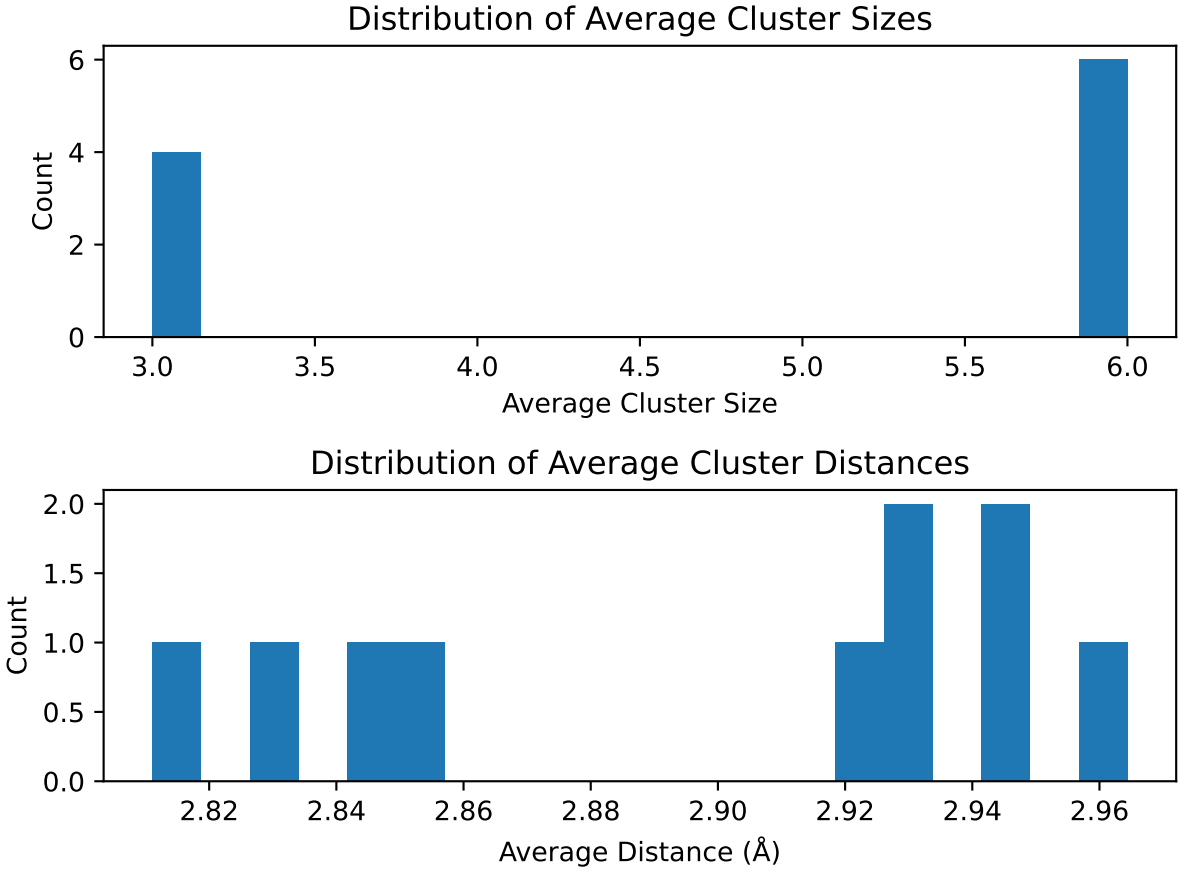
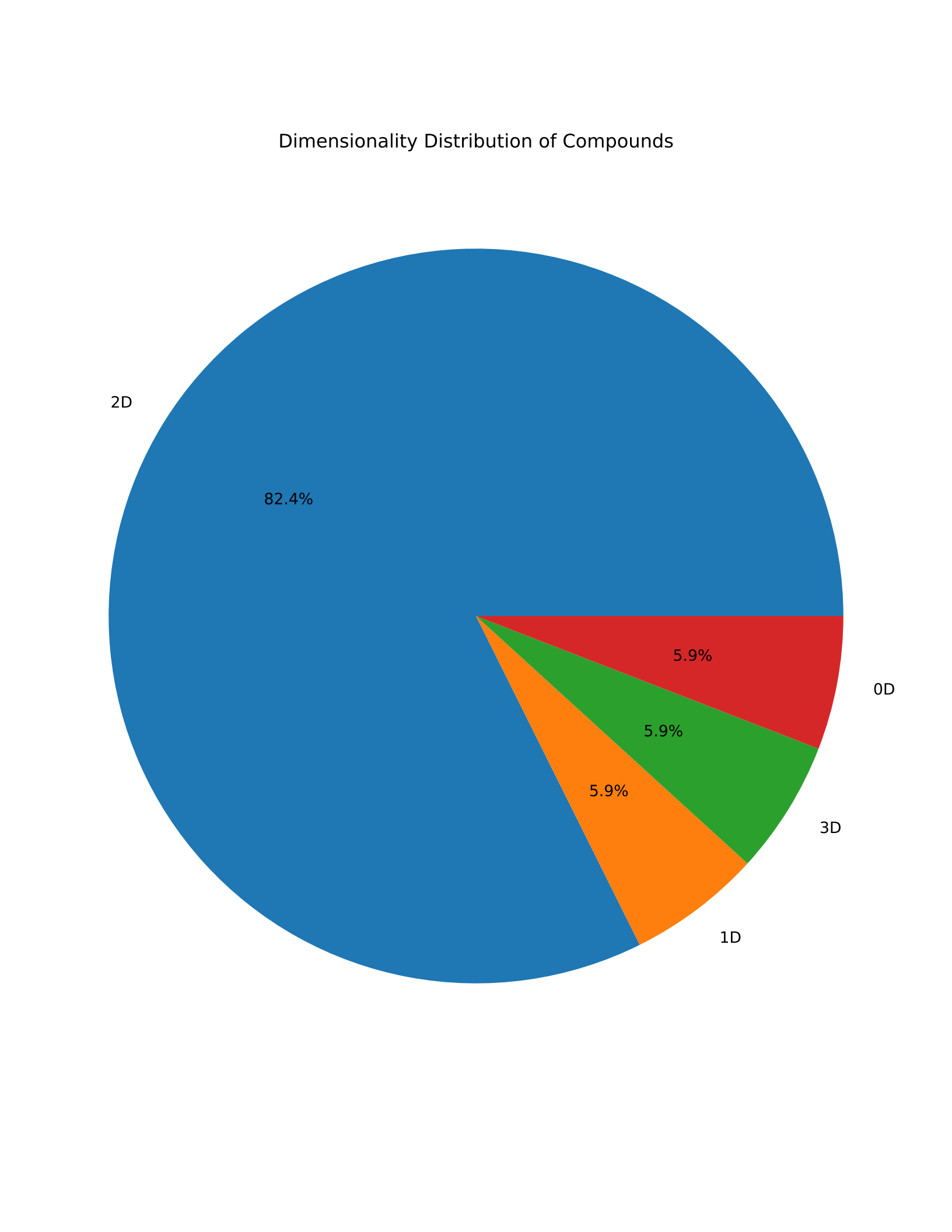
Analysis of Nb-Cl Compounds
Cluster Finder Results

Cluster Statistics Summary

Total compounds analyzed: 36

Number of compounds with clusters: 18


Distribution of Average Cluster Sizes
Count
0
2
4
6
3.0
3.5
4.0
4.5
5.0
5.5
6.0
Average Cluster Size
Distribution of Average Cluster Distances
Count
0.0
0.5
1.0
1.5
2.0
2.82
2.84
2.86
2.88
2.90
2.92
2.94
2.96
Average Distance (Å)


Dimensionality Distribution of Compounds
2D
82.4%
0D
5.9%
3D
5.9%
1D
5.9%

Top 10 Ranked Compounds

material_id	formula	predicted_dimentionality	rank_score
mp-29950	Nb3Cl8	2D	-1.9806265069071798
mp-570921	CsLu(NbCl3)6	2D	-2.0994011474262773
mp-778180	CsTi(NbCl3)6	2D	-2.148358084301869
mp-1224518	KGd(NbCl3)6	2D	-2.208505545183609
mp-29339	Lu(NbCl3)6	2D	-2.2426591533554276
mp-570972	K2Mn(NbCl3)6	2D	-2.27107955868046
mp-568478	Nb6Tl2VCl18	2D	-2.297078486655807
mp-680696	Nb3TlVCl11	2D	-2.765849960126188
mp-1213417	CsNb3VCl11	2D	-2.771325434745769
mp-1211867	KNb3VCl11	2D	-2.795648395150024

Compound Details: Nb3Cl8 (mp-29950)

Space Group: P6/mmm

Dimensionality: 2D

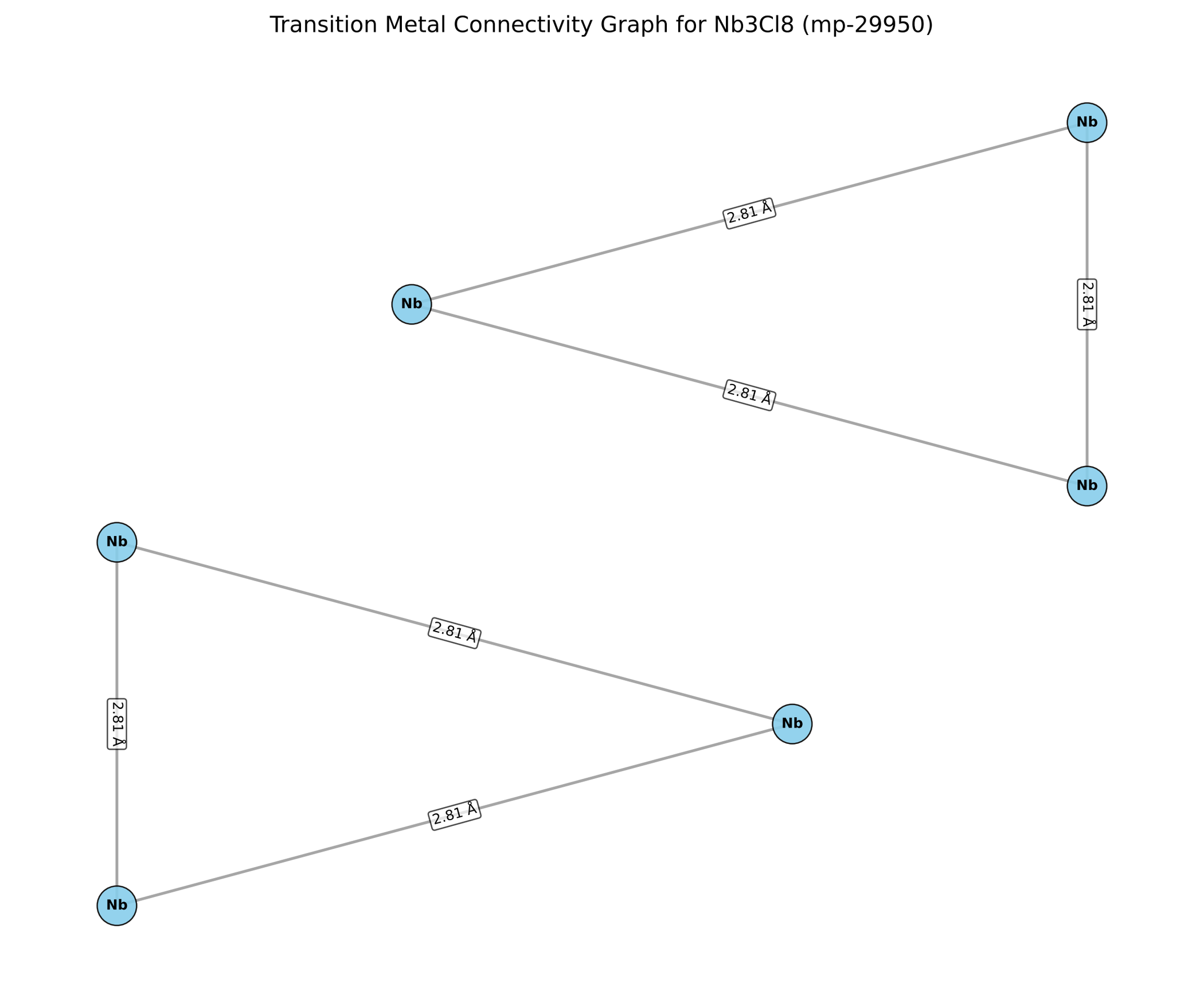
Energy Above Hull: 0.0 eV/atom

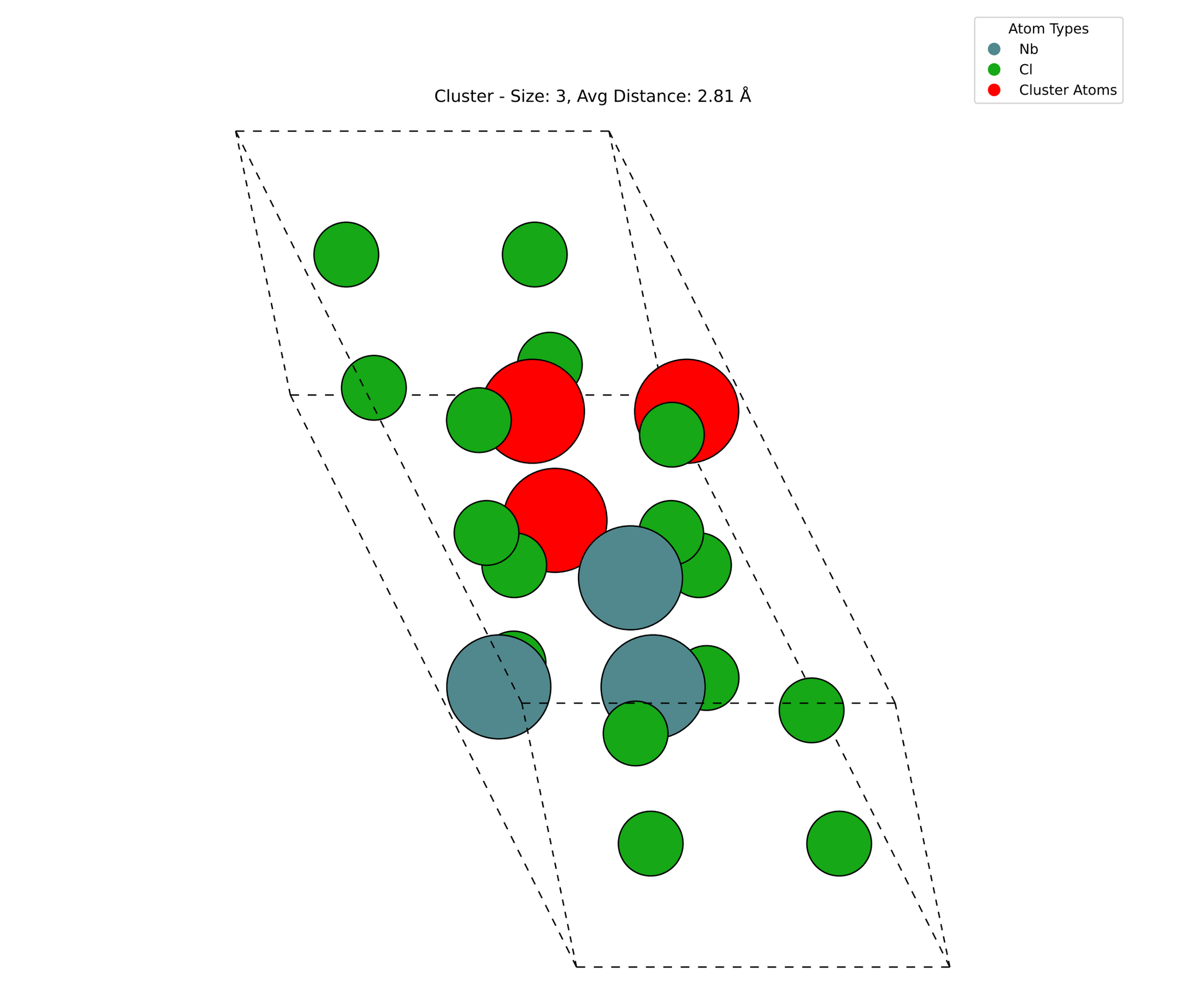
Rank Score: -1.9806

Cluster Statistics:

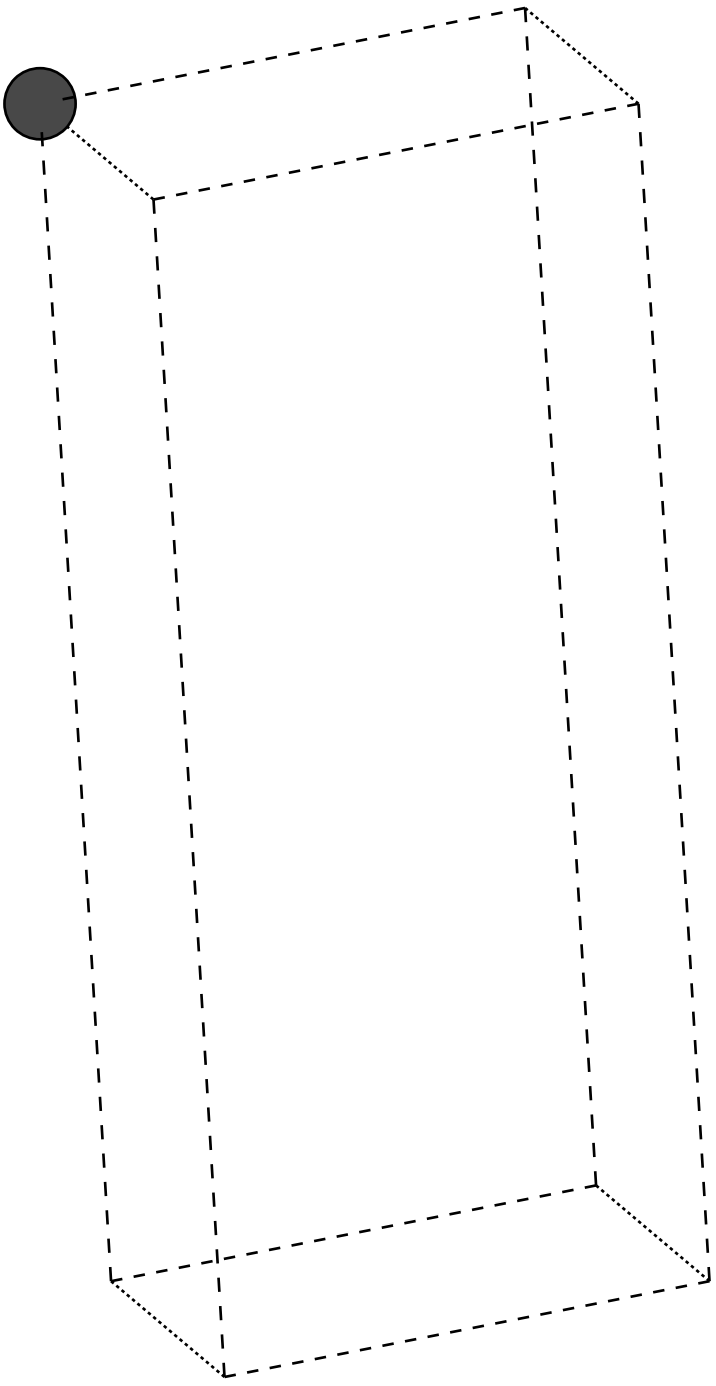
Number of Clusters: 2

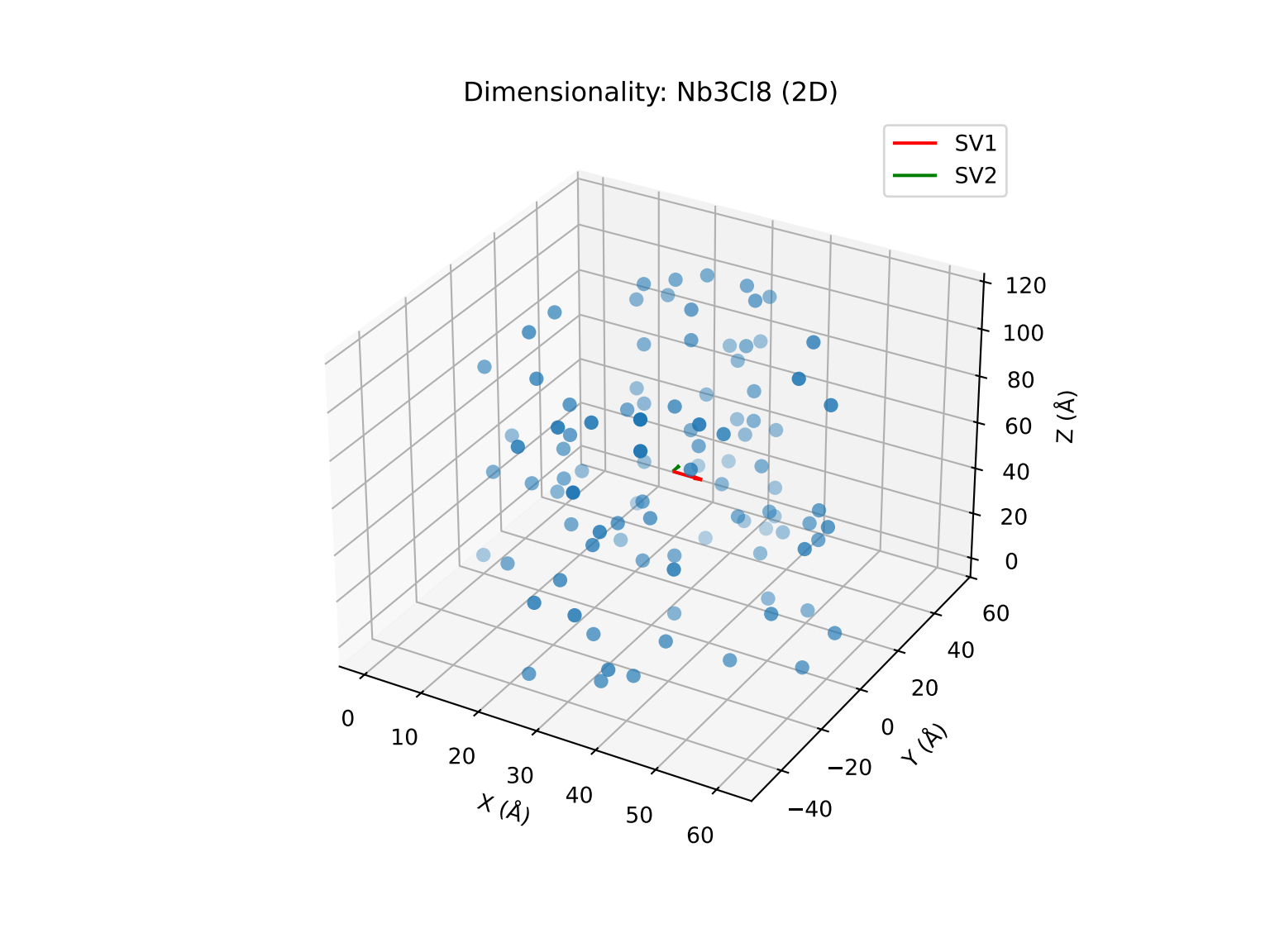
Average Cluster Size: 3.00 atoms
Average Distance: 2.811 Å


Transition Metal Connectivity Graph for Nb3Cl8 (mp-29950)
Nb
Nb
Nb
2.81 Å
2.81 Å
2.81 Å
Nb
Nb
Nb
2.81 Å
2.81 Å
2.81 Å


Atom Types
Nb
Cl
Cluster Atoms
Cluster - Size: 3, Avg Distance: 2.81 Å

Cluster Lattice for Nb3Cl8 (Space Group: P6/mmm)




Dimensionality: Nb3Cl8 (2D)
SV1
SV2
120
100
80
60
40
20
0
Z (Å)
60
40
20
0
−20
−40
Y (Å)
0
10
20
30
40
50
60
X (Å)

Compound Details: CsLu(NbCl3)6 (mp-570921)

Space Group: P6/mmm

Dimensionality: 2D

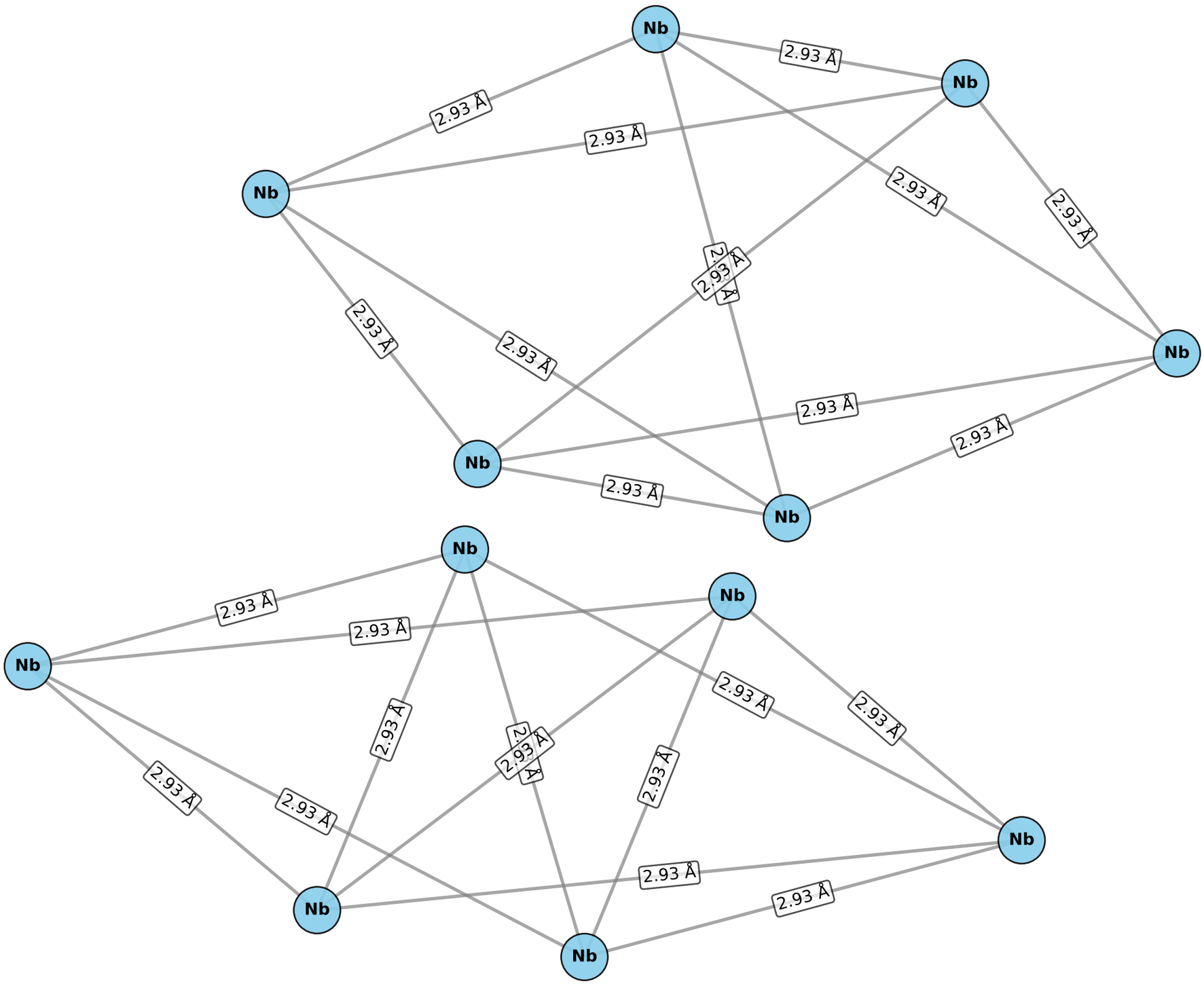
Energy Above Hull: 0.0 eV/atom

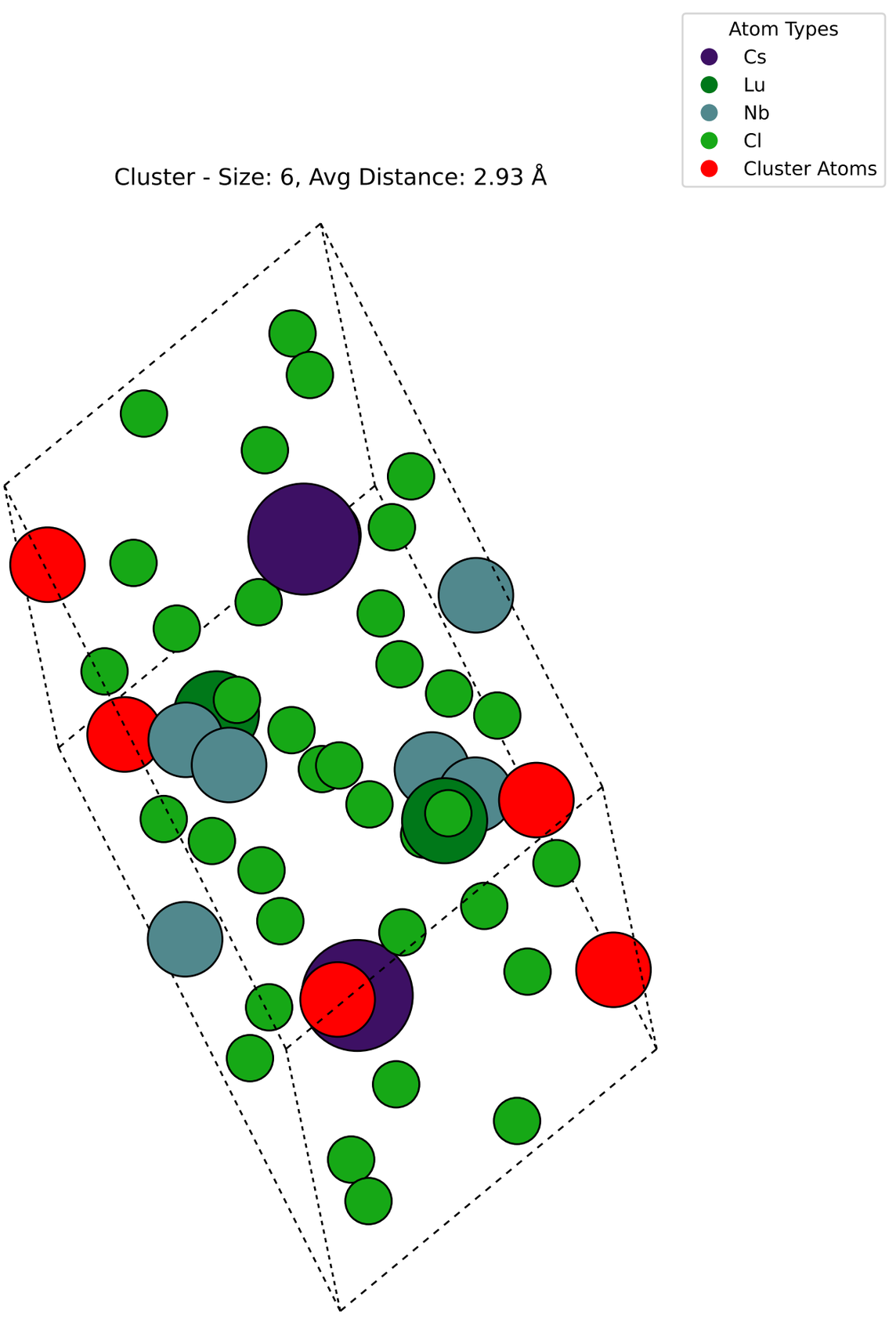
Rank Score: -2.0994

Cluster Statistics:

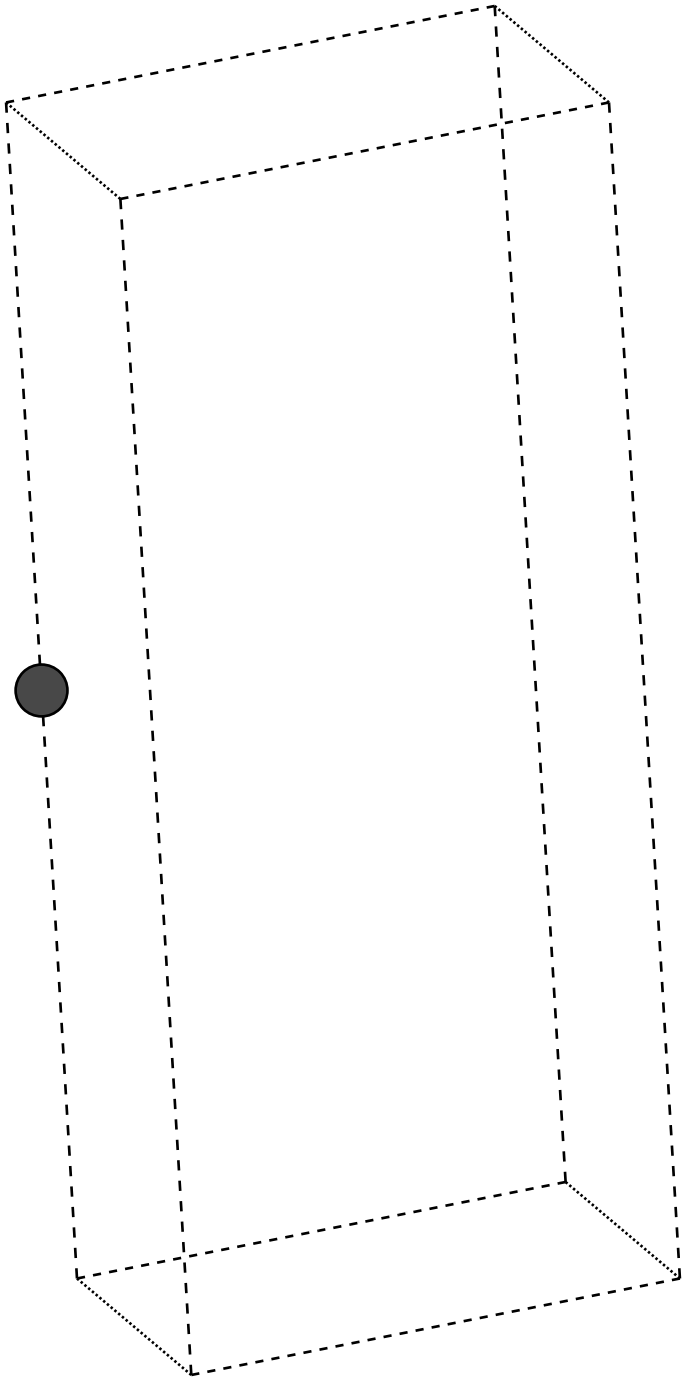
Number of Clusters: 2

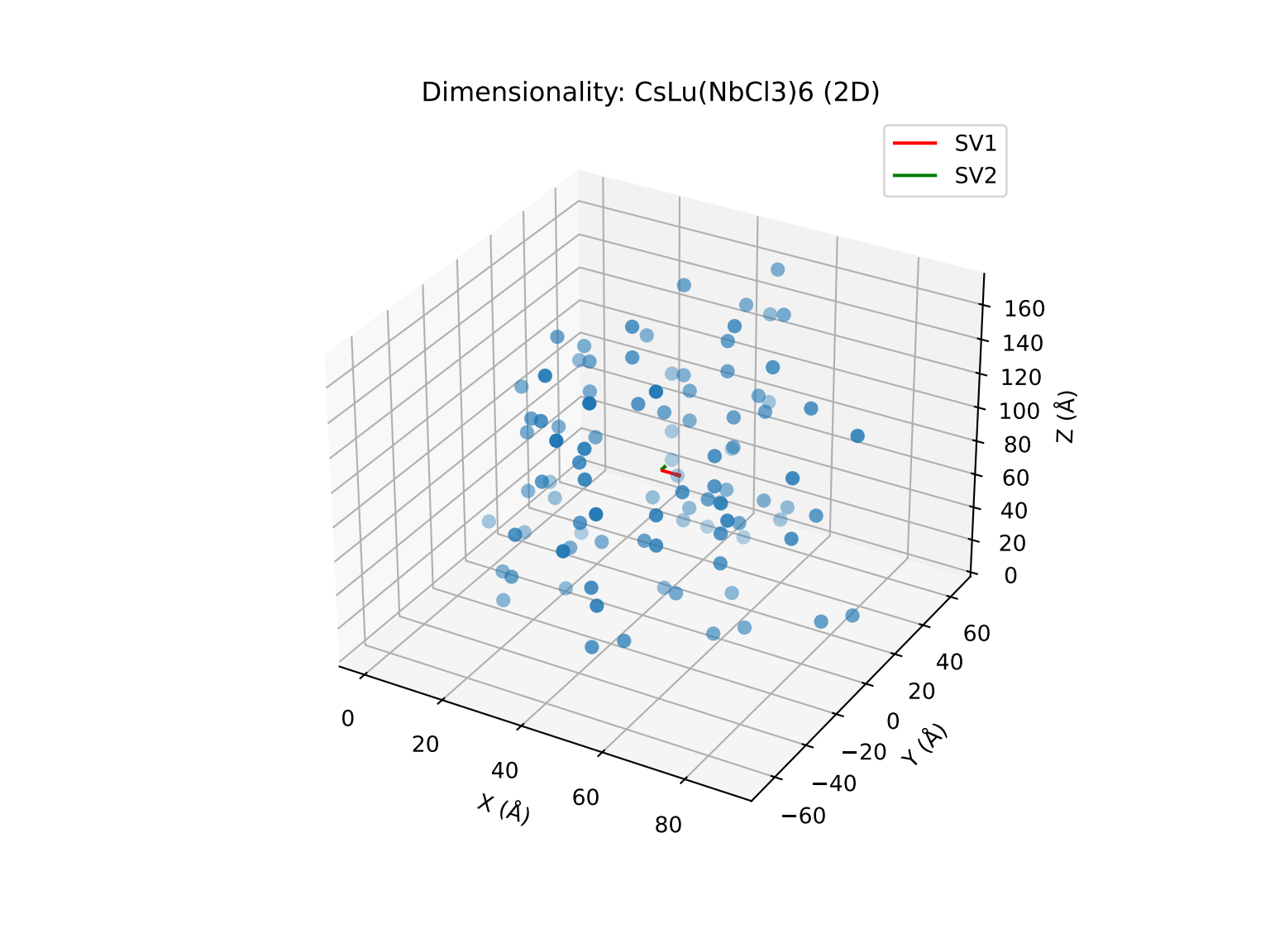
Average Cluster Size: 6.00 atoms
Average Distance: 2.930 Å


Transition Metal Connectivity Graph for CsLu(NbCl3)6 (mp-570921)
Nb
Nb
Nb
Nb
Nb
Nb
Nb
Nb
Nb
Nb
Nb
Nb
2.93 Å


Atom Types
Cs
Lu
Nb
Cl
Cluster Atoms
Cluster - Size: 6, Avg Distance: 2.93 Å

Cluster Lattice for CsLu(NbCl3)6 (Space Group: P6/mmm)




Dimensionality: CsLu(NbCl3)6 (2D)
SV1
SV2
160
140
120
100
80
60
40
20
0
Z (Å)
60
40
20
0
−20
−40
−60
Y (Å)
0
20
40
60
80
X (Å)

Compound Details: CsTi(NbCl3)6 (mp-778180)

Space Group: P6/mmm

Dimensionality: 2D

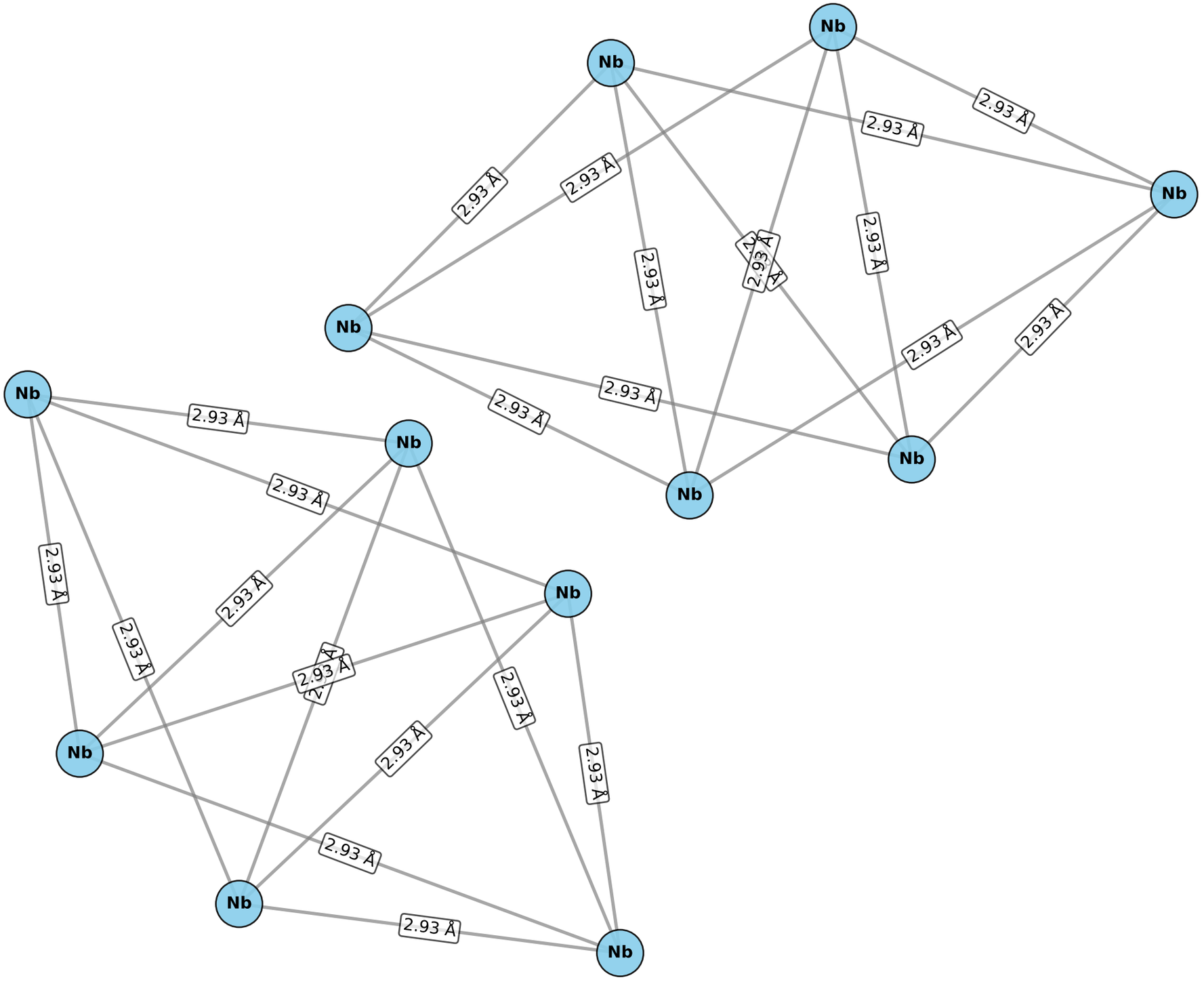
Energy Above Hull: 0.017678687596136 eV/atom

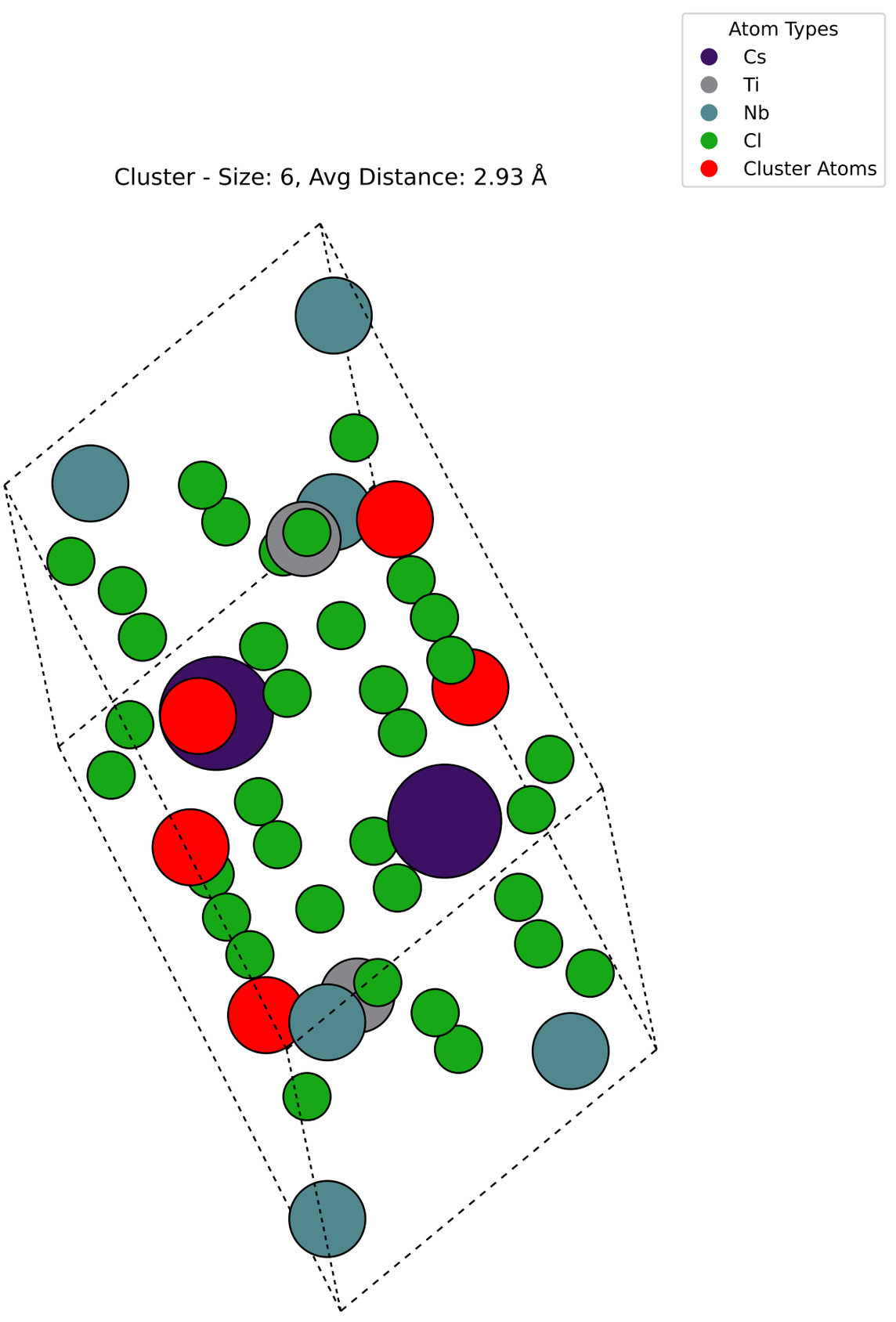
Rank Score: -2.1484

Cluster Statistics:

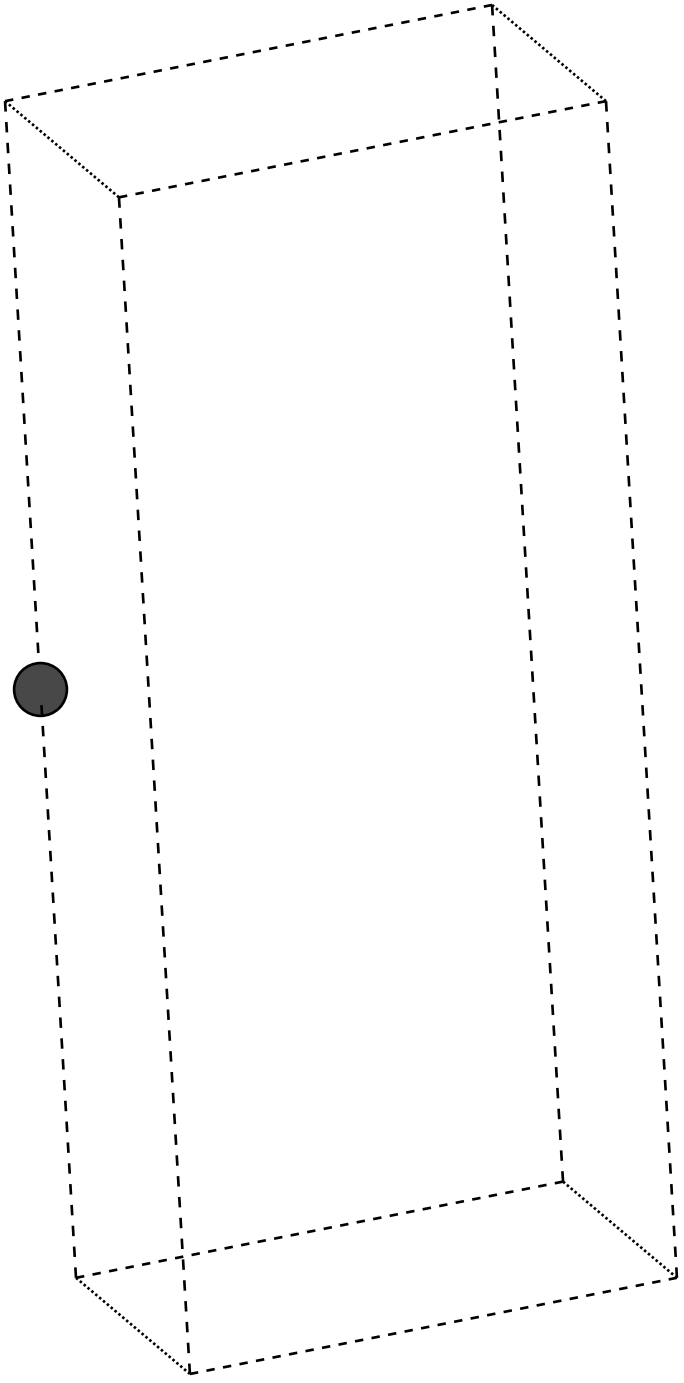
Number of Clusters: 2

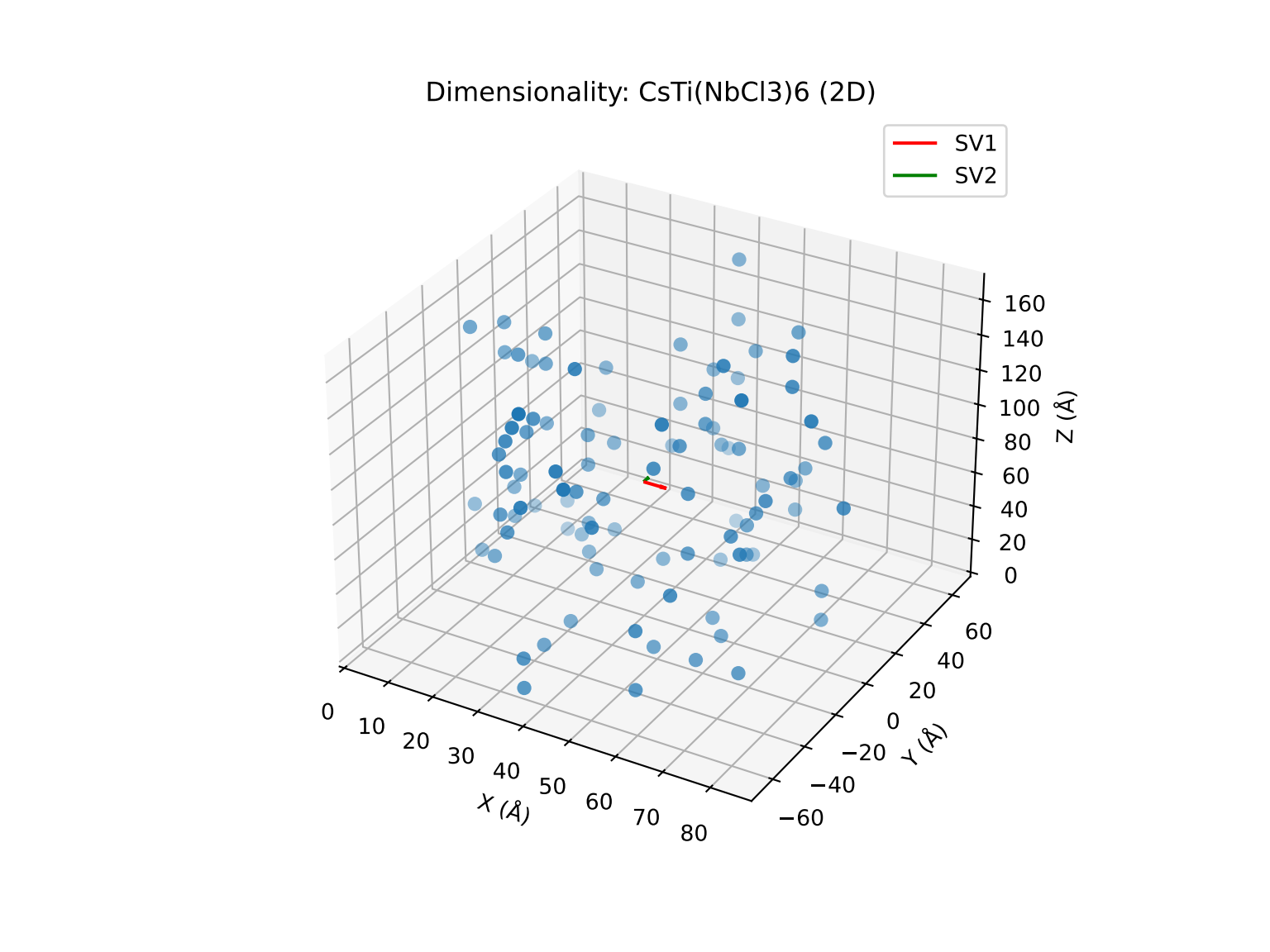
Average Cluster Size: 6.00 atoms
Average Distance: 2.926 Å


Transition Metal Connectivity Graph for CsTi(NbCl3)6 (mp-778180)
Nb
2.93 Å


Atom Types
Cs
Ti
Nb
Cl
Cluster Atoms
Cluster - Size: 6, Avg Distance: 2.93 Å

Cluster Lattice for CsTi(NbCl3)6 (Space Group: P6/mmm)




Dimensionality: CsTi(NbCl3)6 (2D)
SV1
SV2
X (Å)
Y (Å)
Z (Å)
0
10
20
30
40
50
60
70
80
−60
−40
−20
0
20
40
60
0
20
40
60
80
100
120
140
160

Compound Details: KGd(NbCl3)6 (mp-1224518)

Space Group: R-3m

Dimensionality: 2D

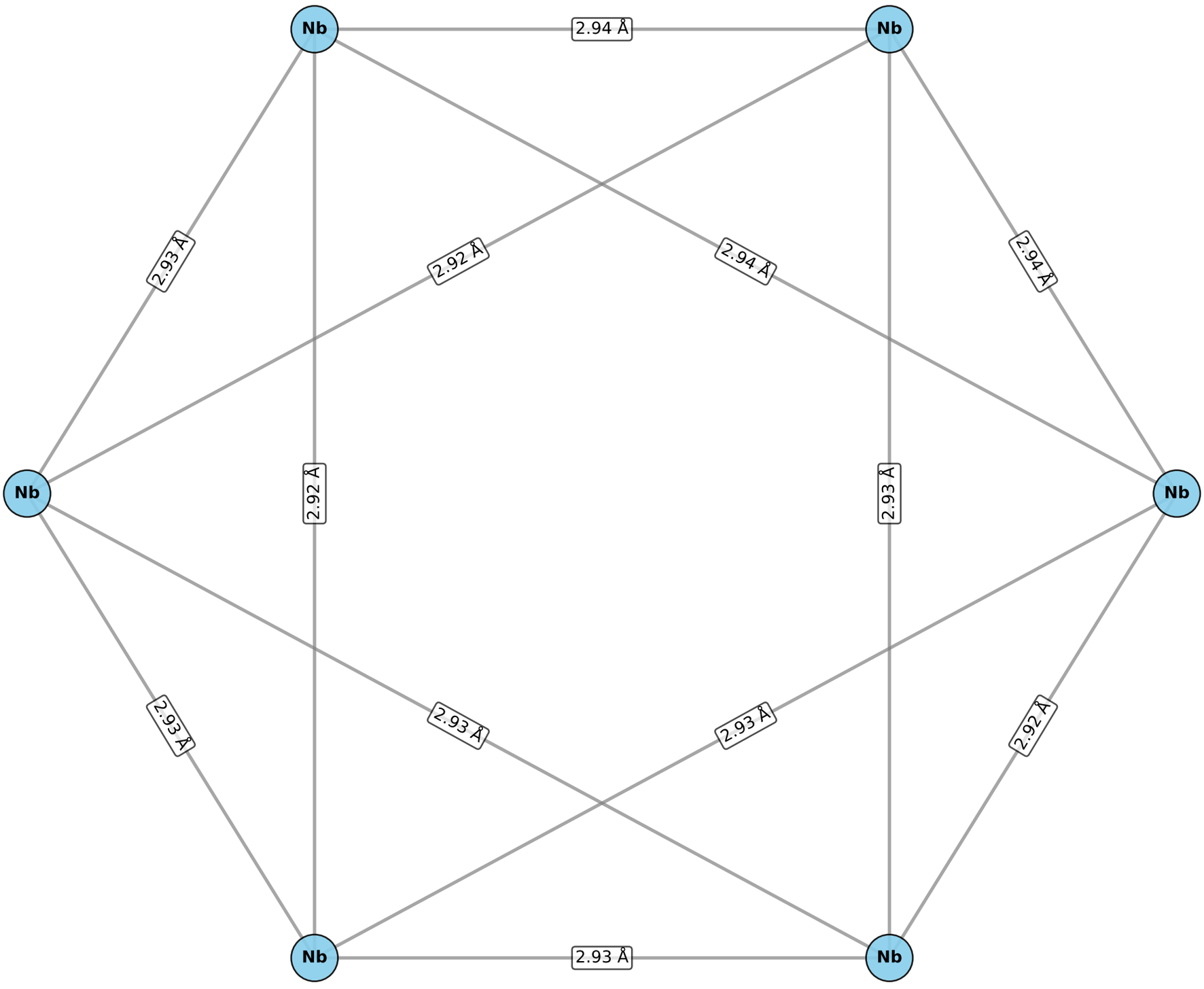
Energy Above Hull: 0.0 eV/atom

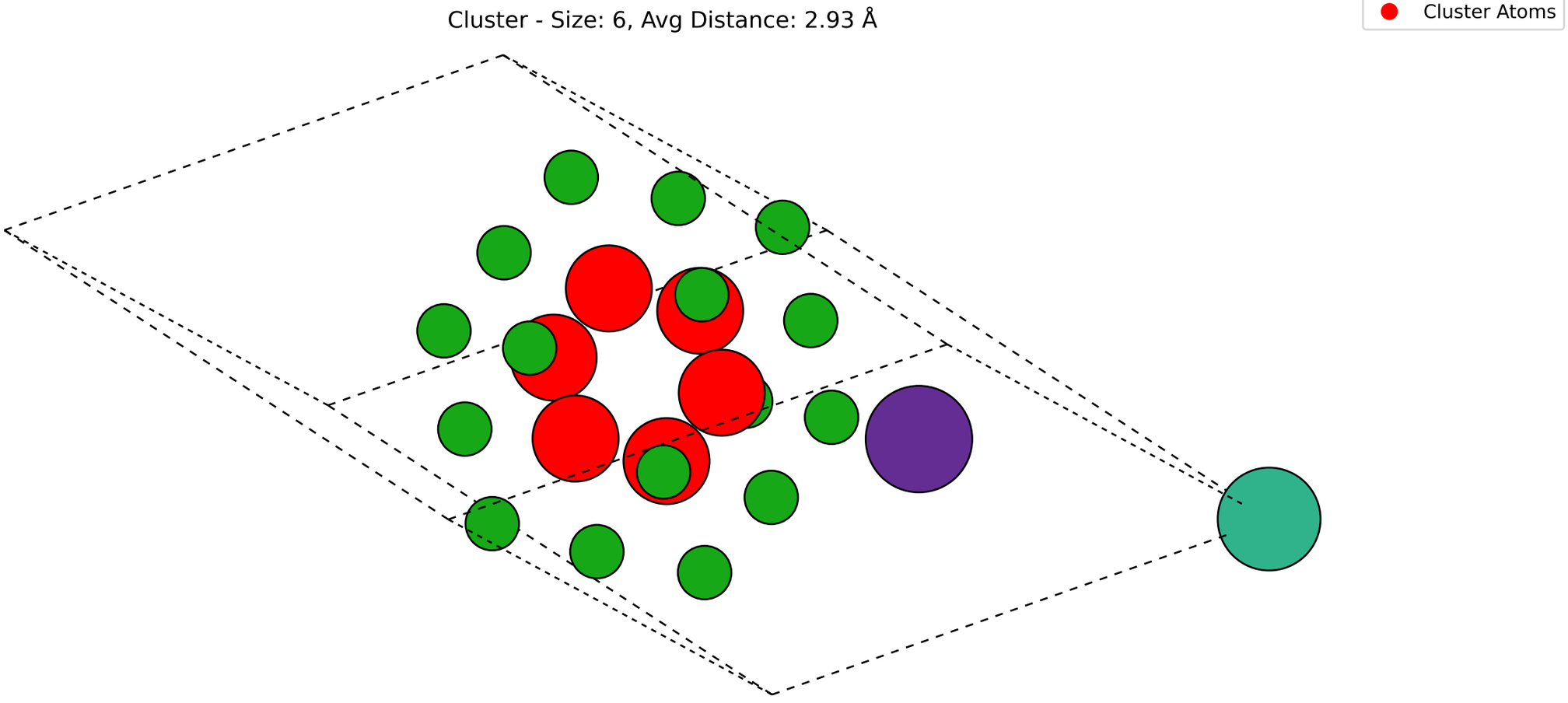
Rank Score: -2.2085

Cluster Statistics:

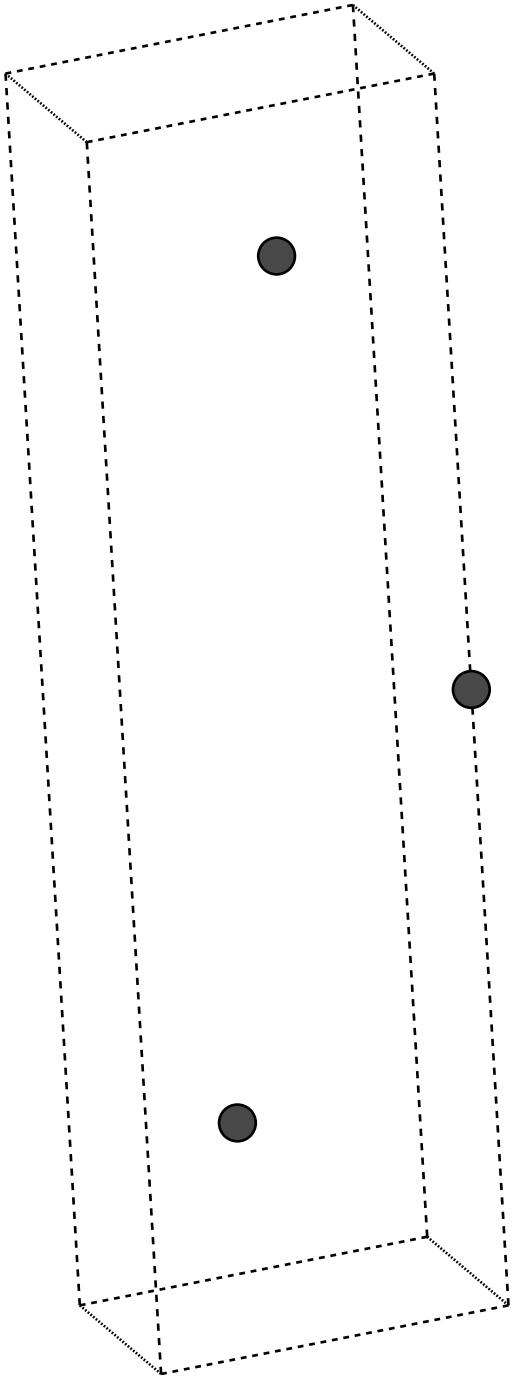
Number of Clusters: 1

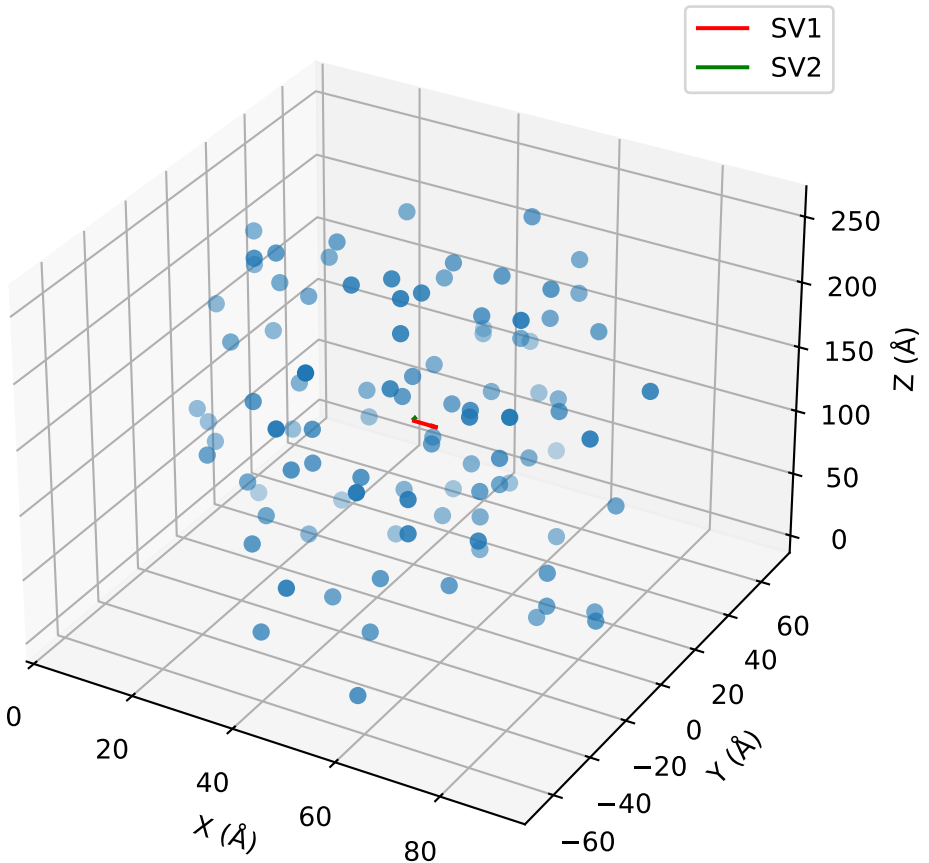
Average Cluster Size: 6.00 atoms
Average Distance: 2.930 Å


Transition Metal Connectivity Graph for KGd(NbCl3)6 (mp-1224518)
Nb
Nb
Nb
Nb
Nb
Nb
2.94 Å
2.93 Å
2.92 Å
2.94 Å
2.94 Å
2.92 Å
2.93 Å
2.93 Å
2.93 Å
2.93 Å
2.92 Å
2.93 Å


Cluster - Size: 6, Avg Distance: 2.93 Å
Atom Types
K
Gd
Nb
Cl
Cluster Atoms

Cluster Lattice for KGd(NbCl3)6 (Space Group: R-3m)




Dimensionality: KGd(NbCl3)6 (2D)
SV1
SV2
250
200
150
100
50
0
Z (Å)
60
40
20
0
−20
−40
−60
Y (Å)
0
20
40
60
80
X (Å)

Compound Details: Lu(NbCl3)6 (mp-29339)

Space Group: R-3m

Dimensionality: 2D

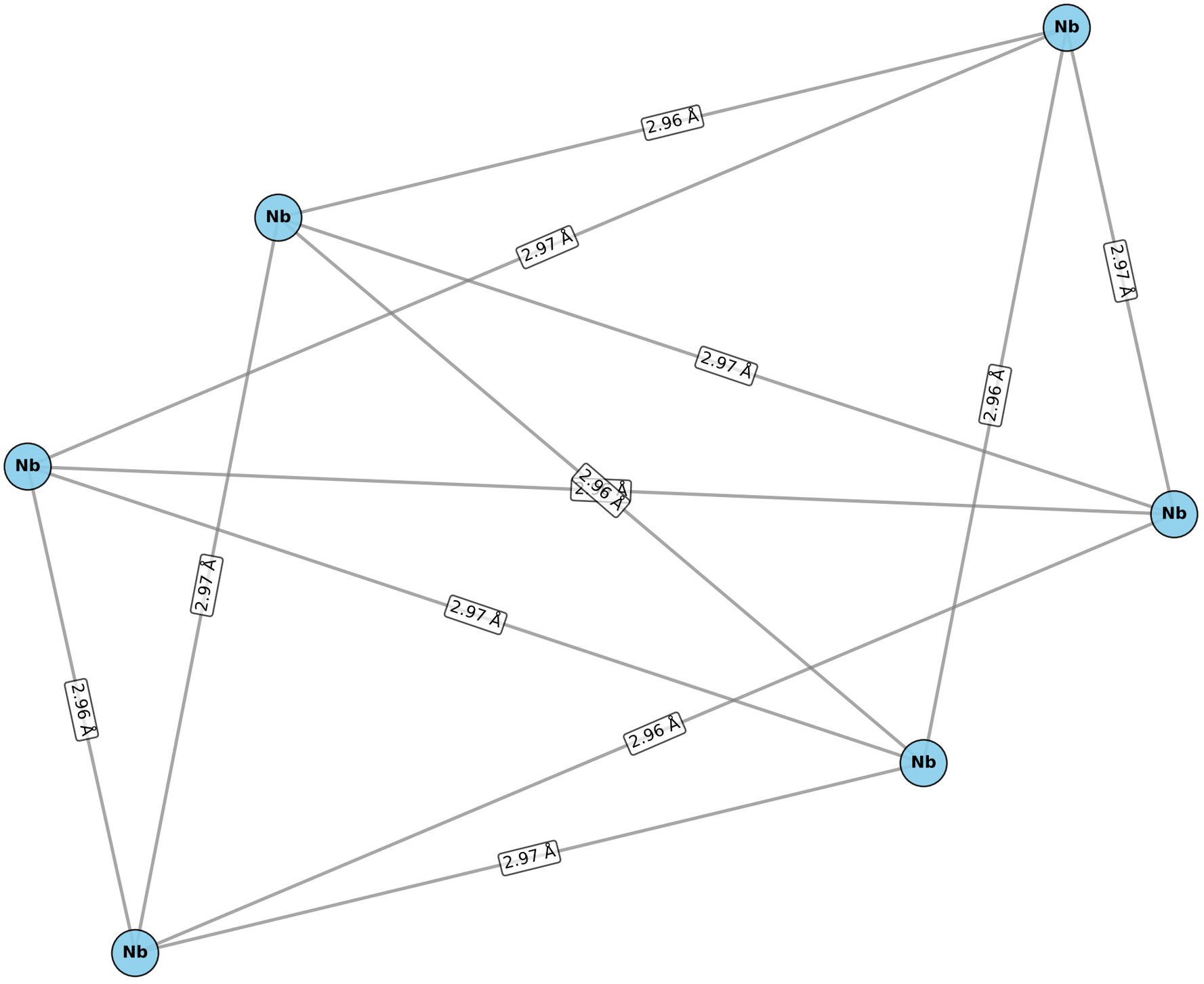
Energy Above Hull: 0.0 eV/atom

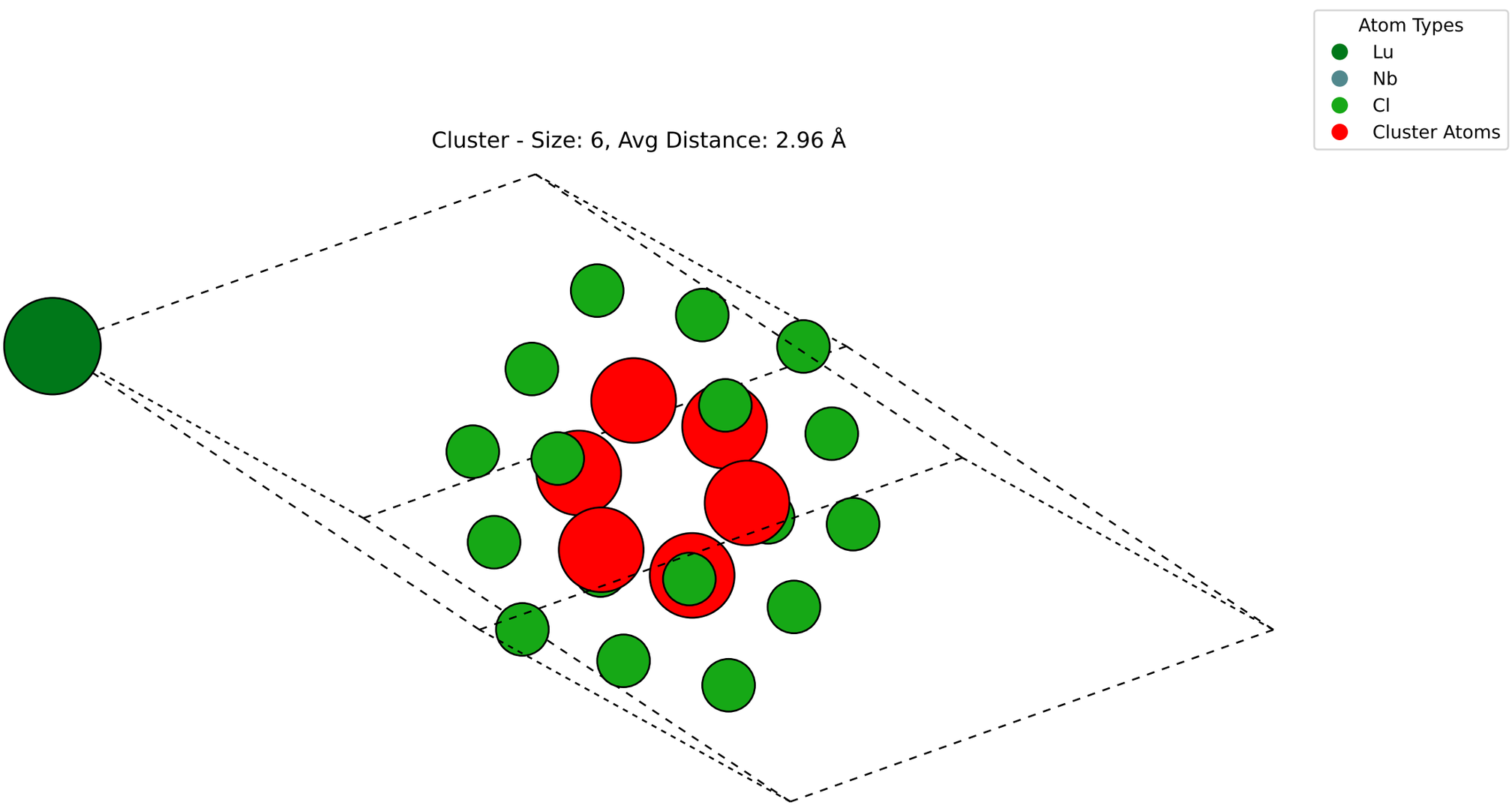
Rank Score: -2.2427

Cluster Statistics:

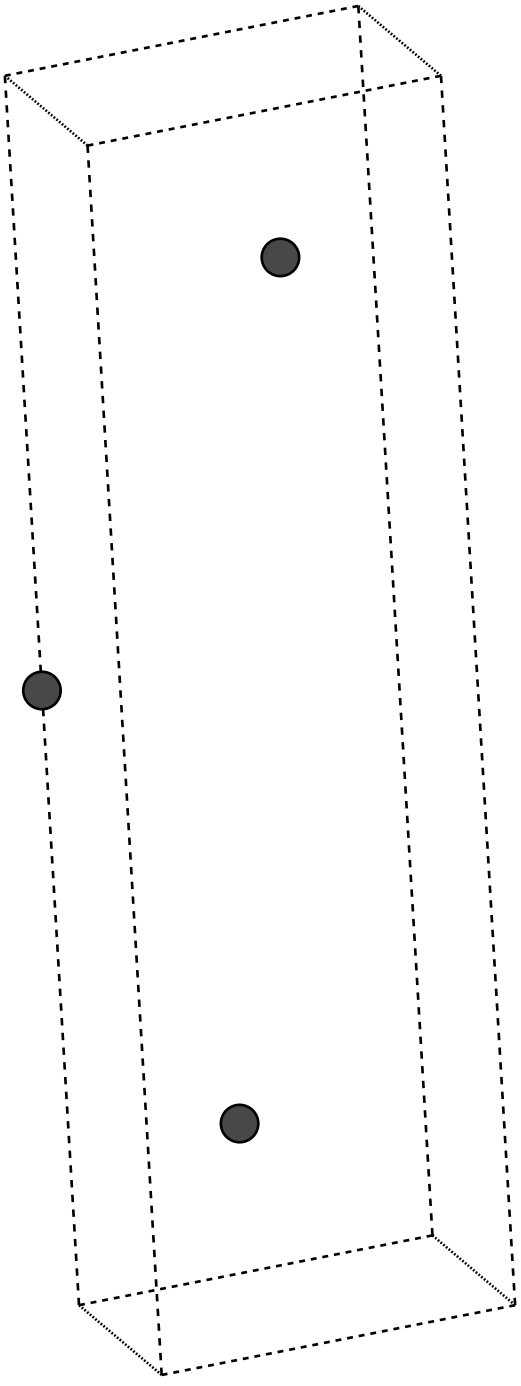
Number of Clusters: 1

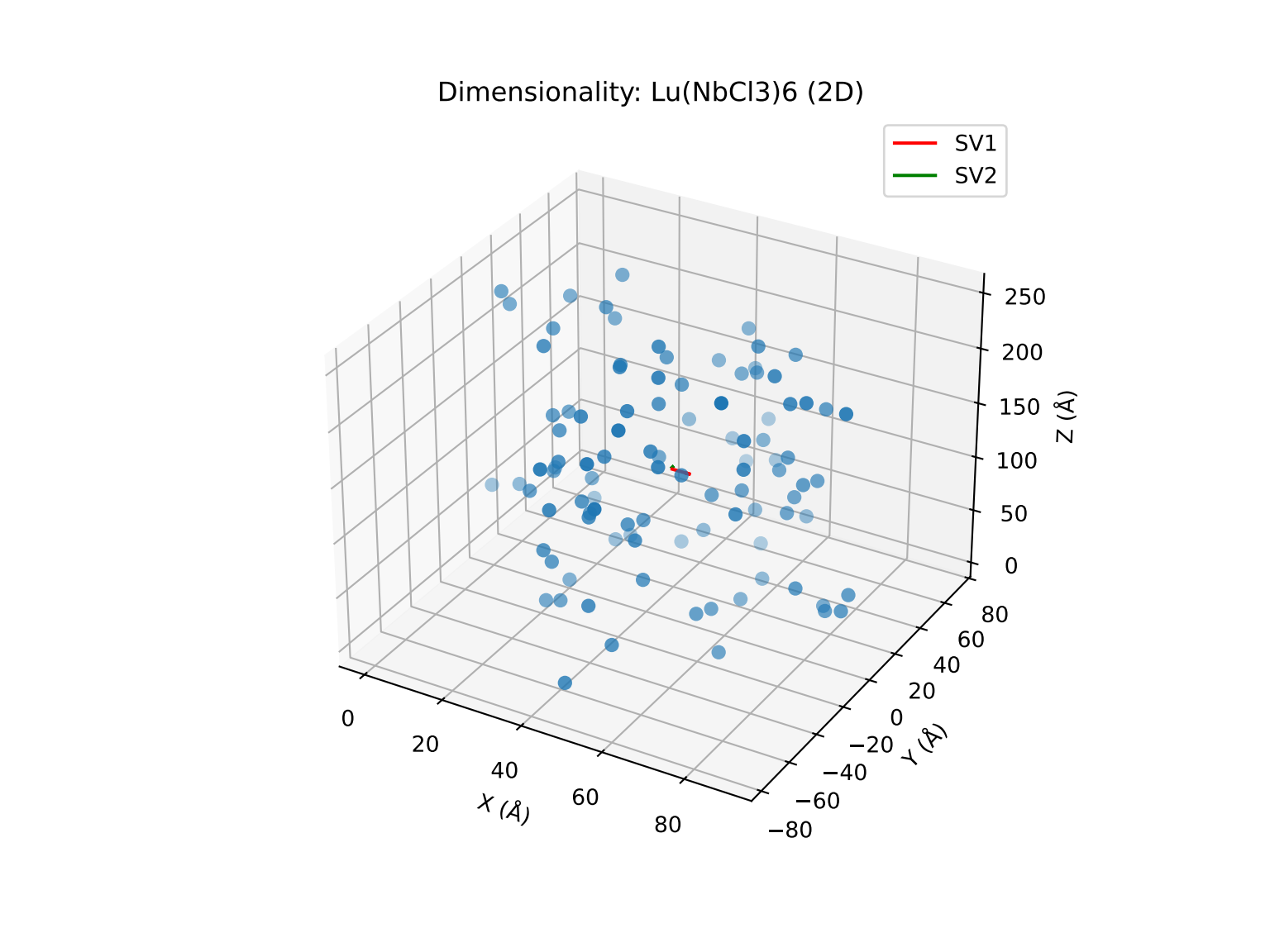
Average Cluster Size: 6.00 atoms
Average Distance: 2.964 Å


Transition Metal Connectivity Graph for Lu(NbCl3)6 (mp-29339)
Nb
Nb
Nb
Nb
Nb
Nb
2.96 Å
2.97 Å
2.97 Å
2.97 Å
2.96 Å
2.96 Å
2.97 Å
2.97 Å
2.96 Å
2.96 Å
2.97 Å


Cluster - Size: 6, Avg Distance: 2.96 Å
Atom Types
Lu
Nb
Cl
Cluster Atoms

Cluster Lattice for Lu(NbCl3)6 (Space Group: R-3m)




Dimensionality: Lu(NbCl3)6 (2D)
SV1
SV2
X (Å)
Y (Å)
Z (Å)
0
20
40
60
80
−80
−60
−40
−20
0
20
40
60
80
100
150
200
250

Compound Details: K2Mn(NbCl3)6 (mp-570972)

Space Group: R-3m

Dimensionality: 2D

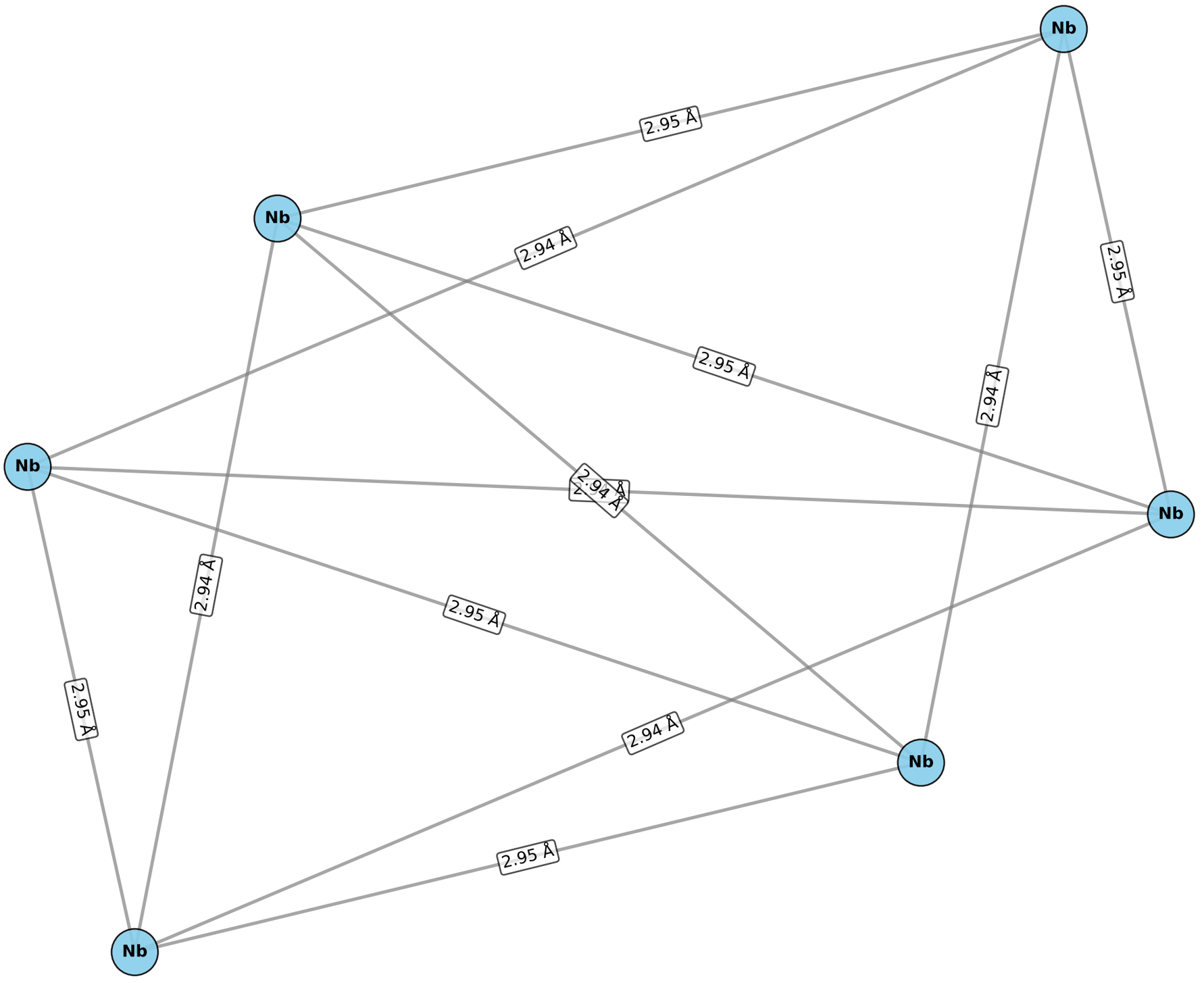
Energy Above Hull: 0.015942826319365 eV/atom

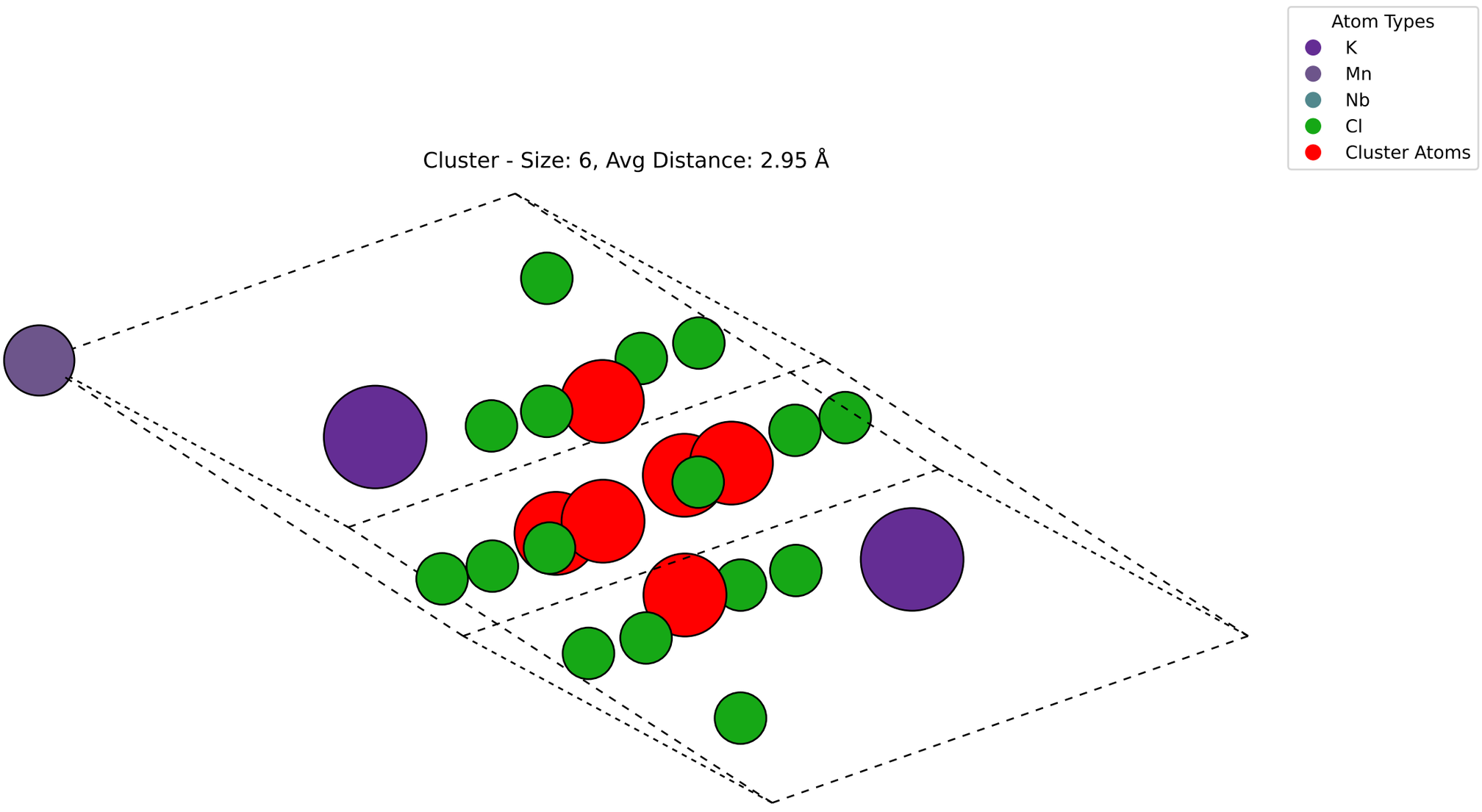
Rank Score: -2.2711

Cluster Statistics:

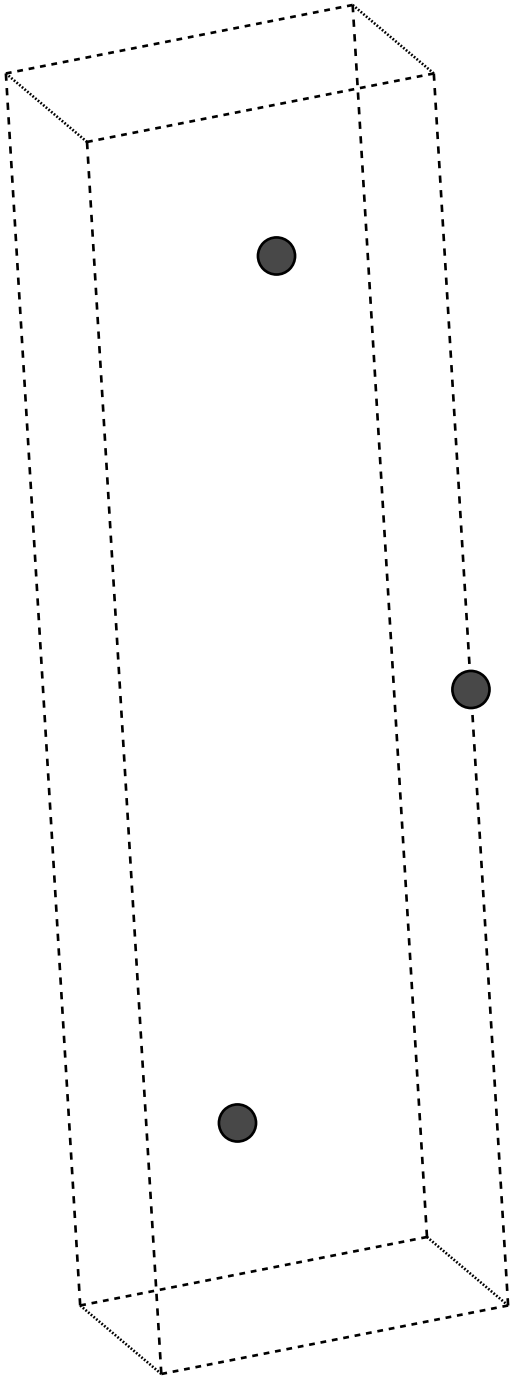
Number of Clusters: 1

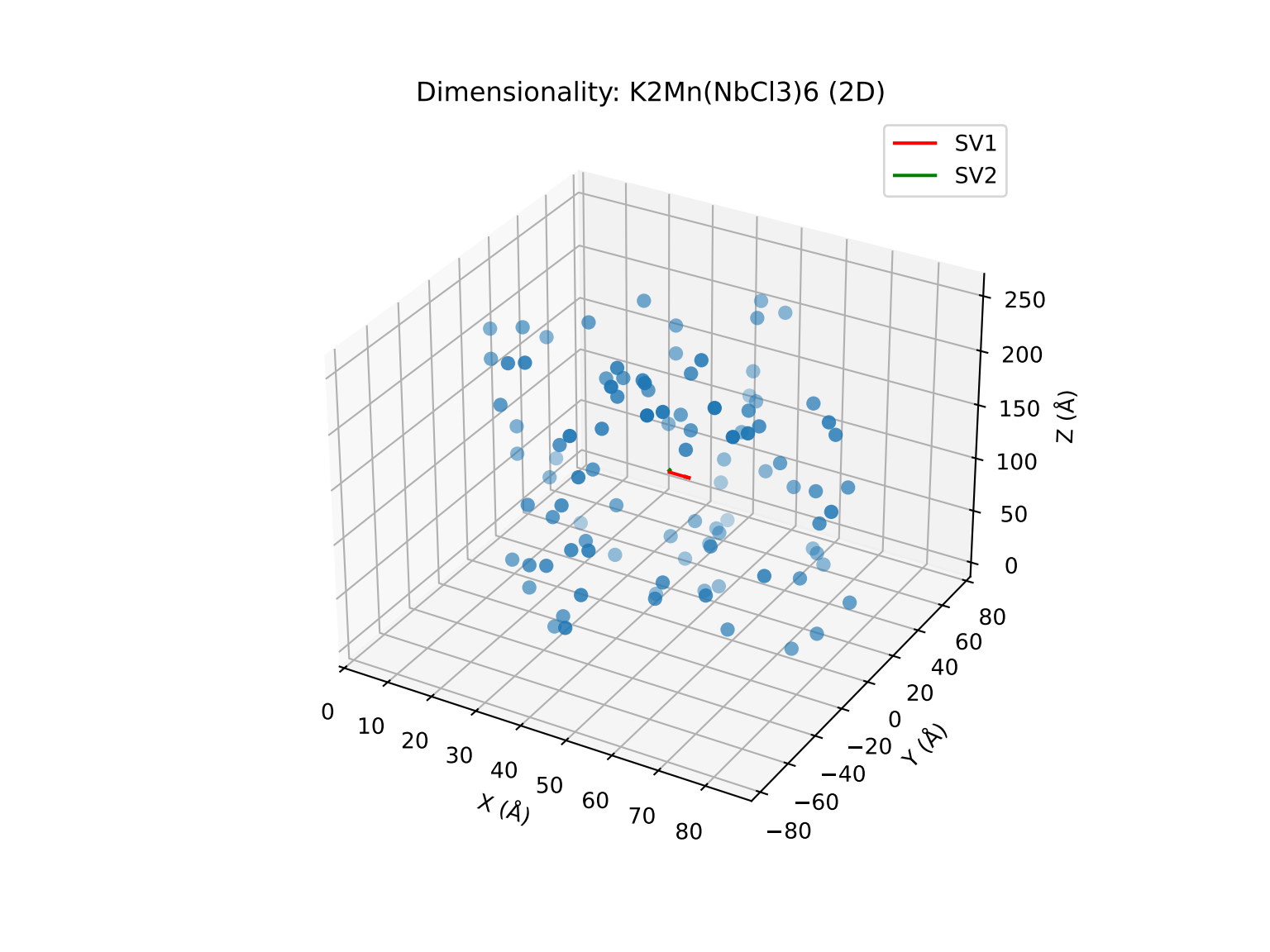
Average Cluster Size: 6.00 atoms
Average Distance: 2.945 Å


Transition Metal Connectivity Graph for K2Mn(NbCl3)6 (mp-570972)
Nb
Nb
Nb
Nb
Nb
Nb
2.95 Å
2.94 Å
2.95 Å
2.95 Å
2.94 Å
2.94 Å
2.94 Å
2.95 Å
2.95 Å
2.94 Å
2.95 Å


Cluster - Size: 6, Avg Distance: 2.95 Å
Atom Types
K
Mn
Nb
Cl
Cluster Atoms

Cluster Lattice for K2Mn(NbCl3)6 (Space Group: R-3m)




Dimensionality: K2Mn(NbCl3)6 (2D)
SV1
SV2
X (Å)
Y (Å)
Z (Å)
0
10
20
30
40
50
60
70
80
−80
−60
−40
−20
0
20
40
60
80
0
50
100
150
200
250

Compound Details: Nb6Tl2VCl18 (mp-568478)

Space Group: R-3m

Dimensionality: 2D

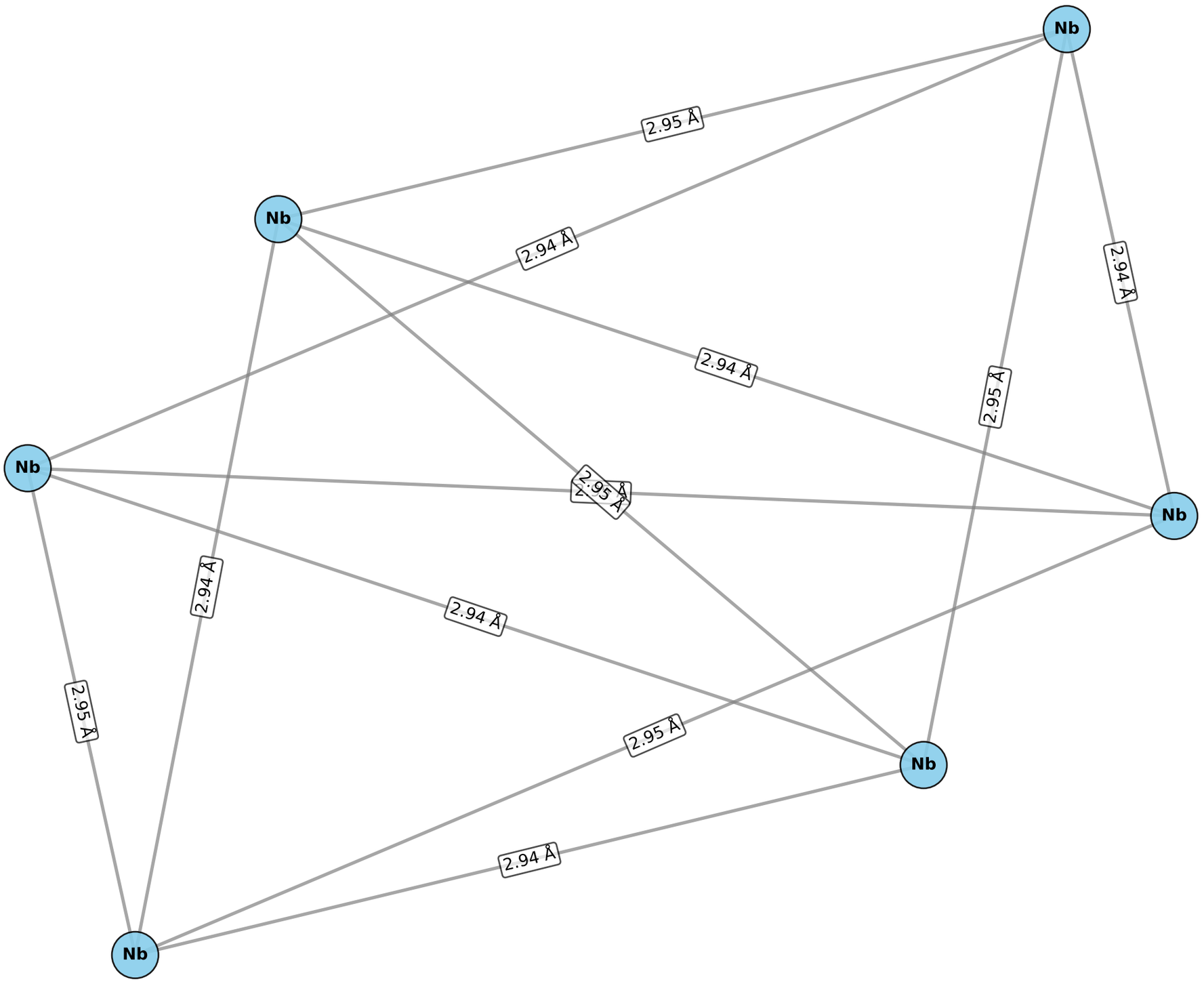
Energy Above Hull: 0.023889087962968 eV/atom

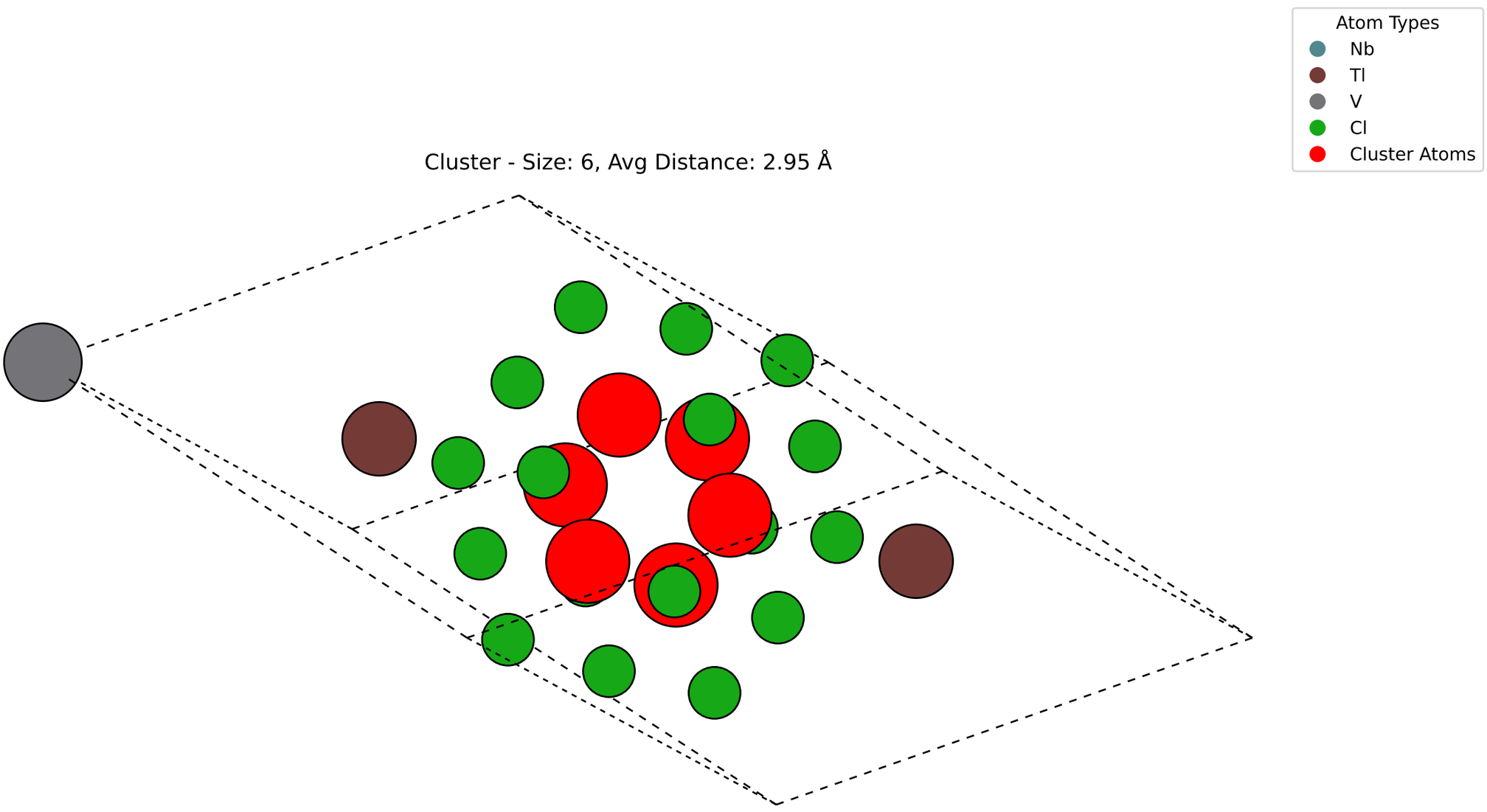
Rank Score: -2.2971

Cluster Statistics:

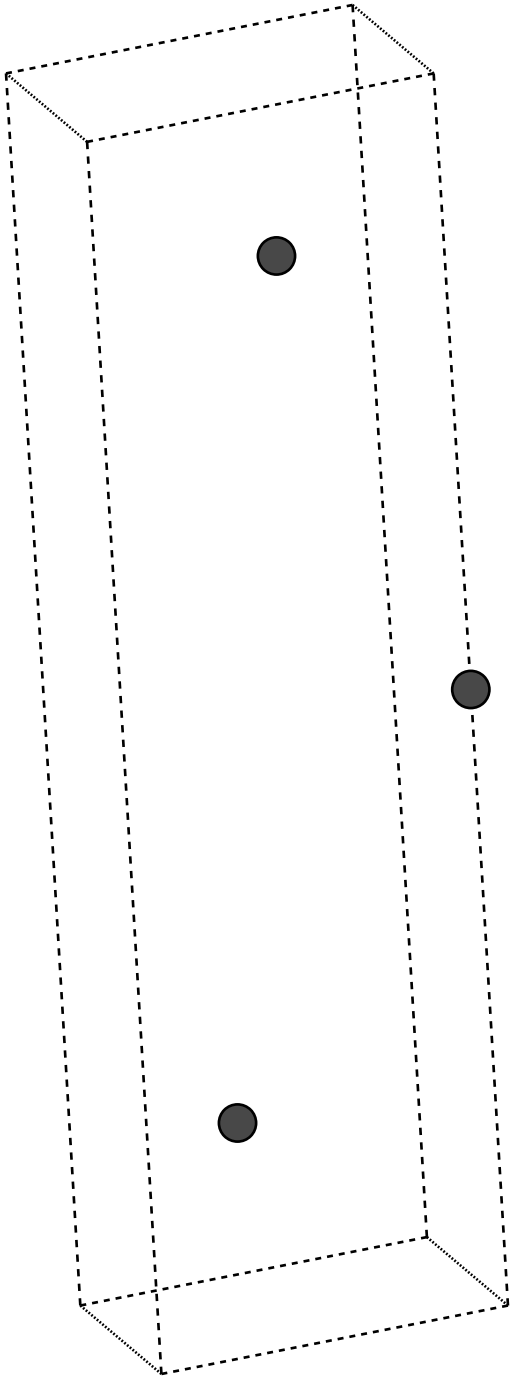
Number of Clusters: 1

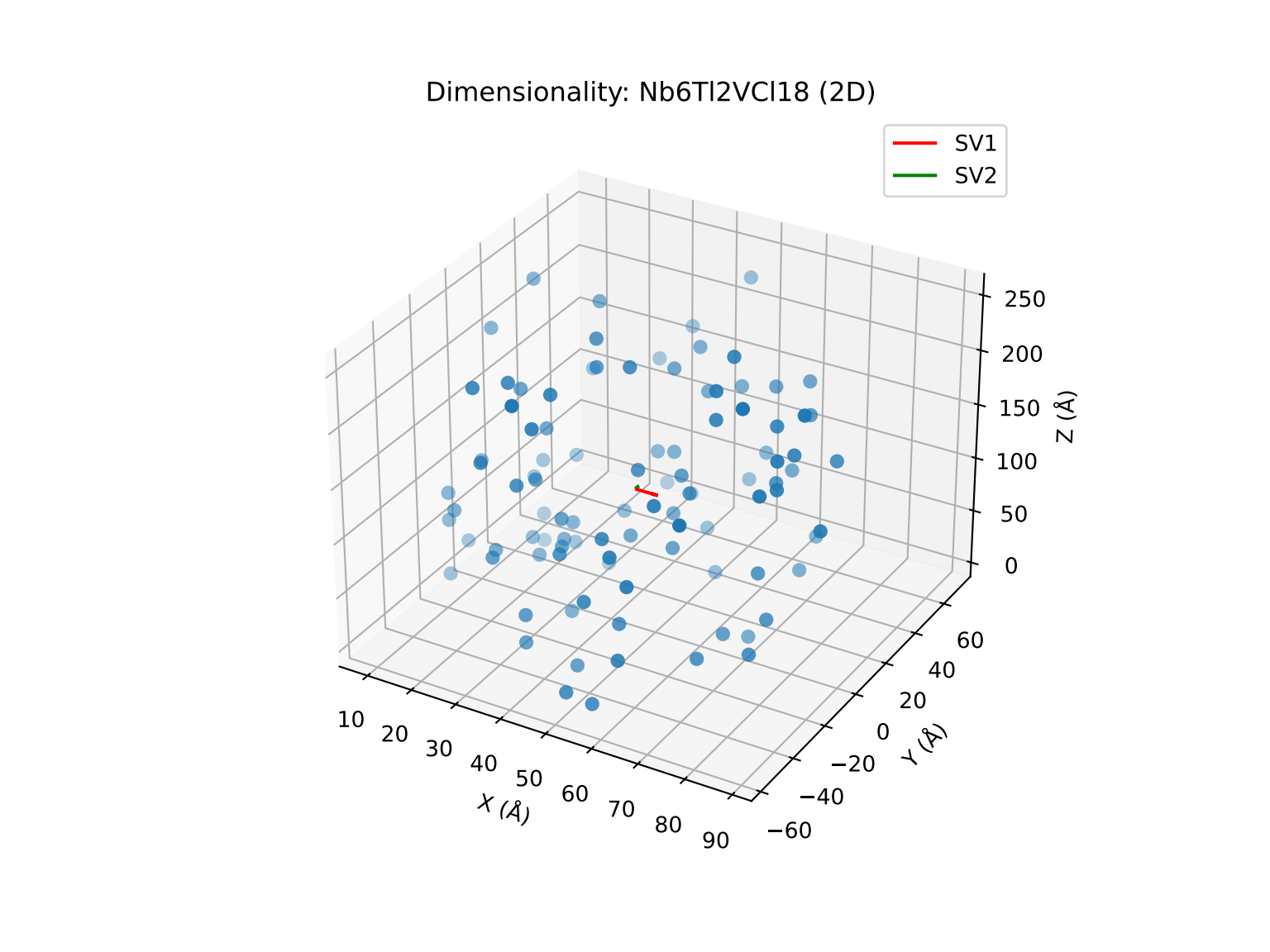
Average Cluster Size: 6.00 atoms
Average Distance: 2.947 Å


Transition Metal Connectivity Graph for Nb6Tl2VCl18 (mp-568478)
Nb
Nb
Nb
Nb
Nb
Nb
2.95 Å
2.94 Å
2.94 Å
2.94 Å
2.95 Å
2.95 Å
2.95 Å
2.94 Å
2.94 Å
2.95 Å
2.95 Å
2.94 Å


Cluster - Size: 6, Avg Distance: 2.95 Å
Atom Types
Nb
Tl
V
Cl
Cluster Atoms

Cluster Lattice for Nb6Tl2VCl18 (Space Group: R-3m)




Dimensionality: Nb6Tl2VCl18 (2D)
SV1
SV2
X (Å)
Y (Å)
Z (Å)
10
20
30
40
50
60
70
80
90
−60
−40
−20
0
20
40
60
0
50
100
150
200
250

Compound Details: Nb3TlVCl11 (mp-680696)

Space Group: Pmmm

Dimensionality: 2D

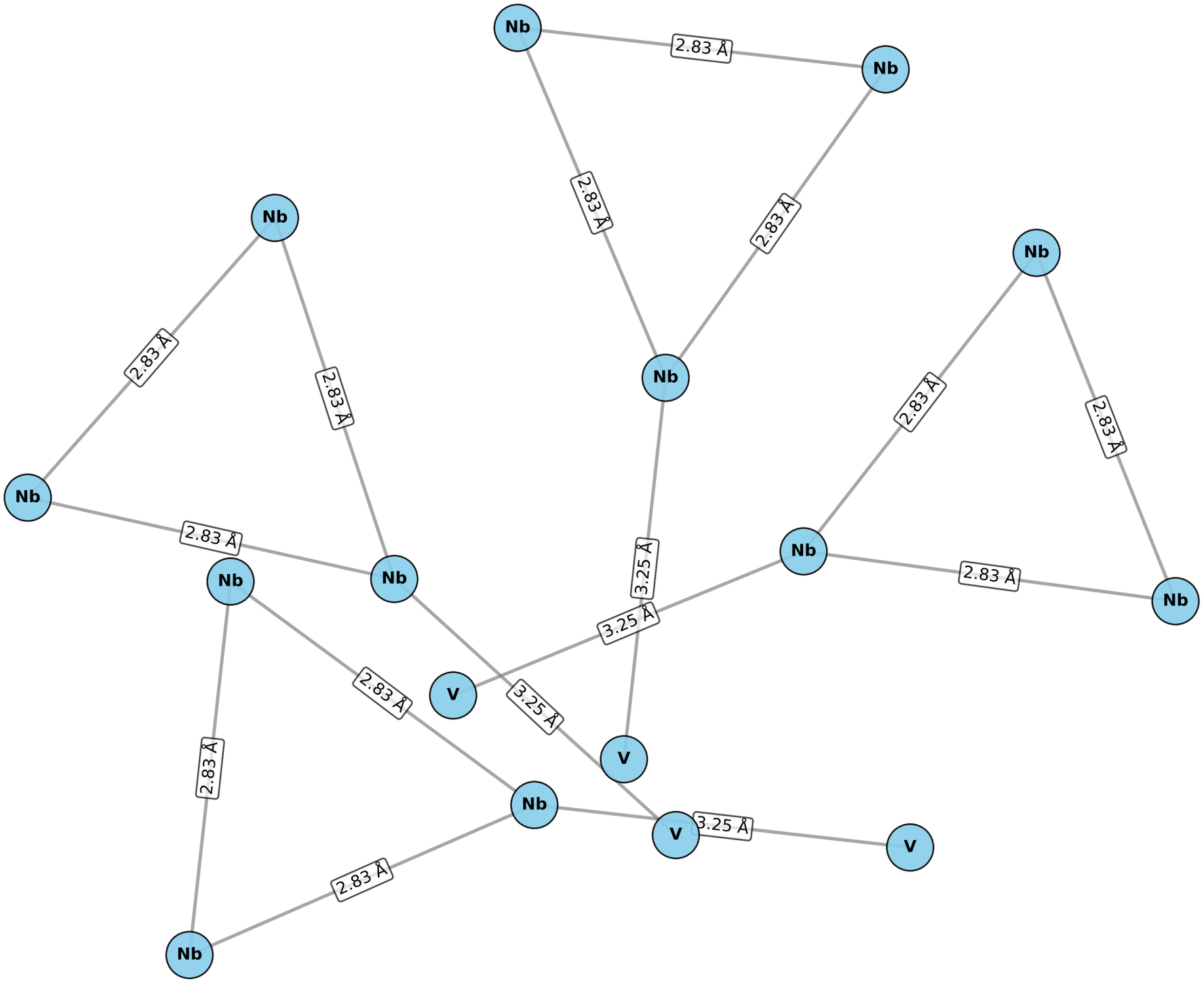
Energy Above Hull: 0.0464517493750000004 eV/atom

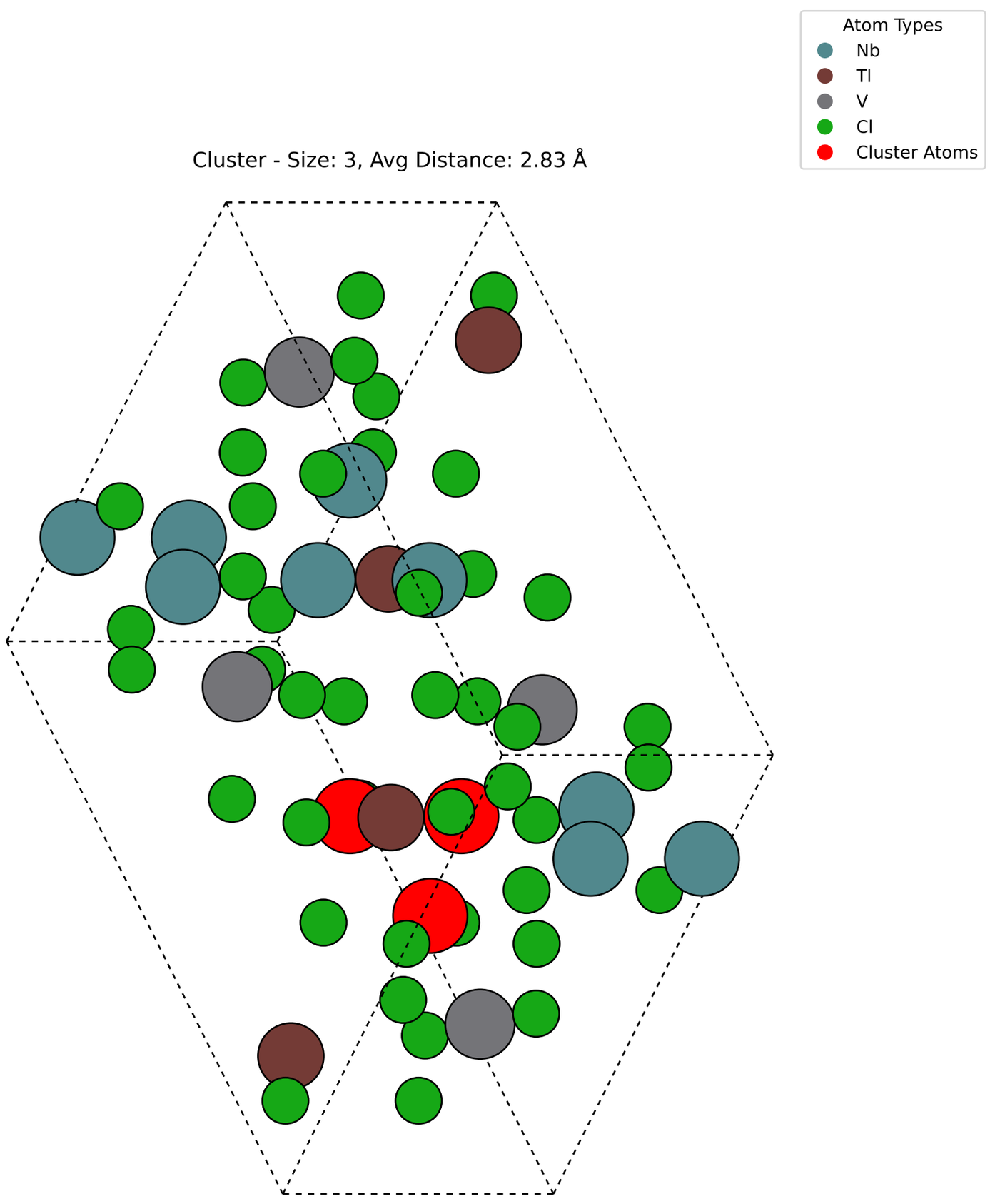
Rank Score: -2.7658

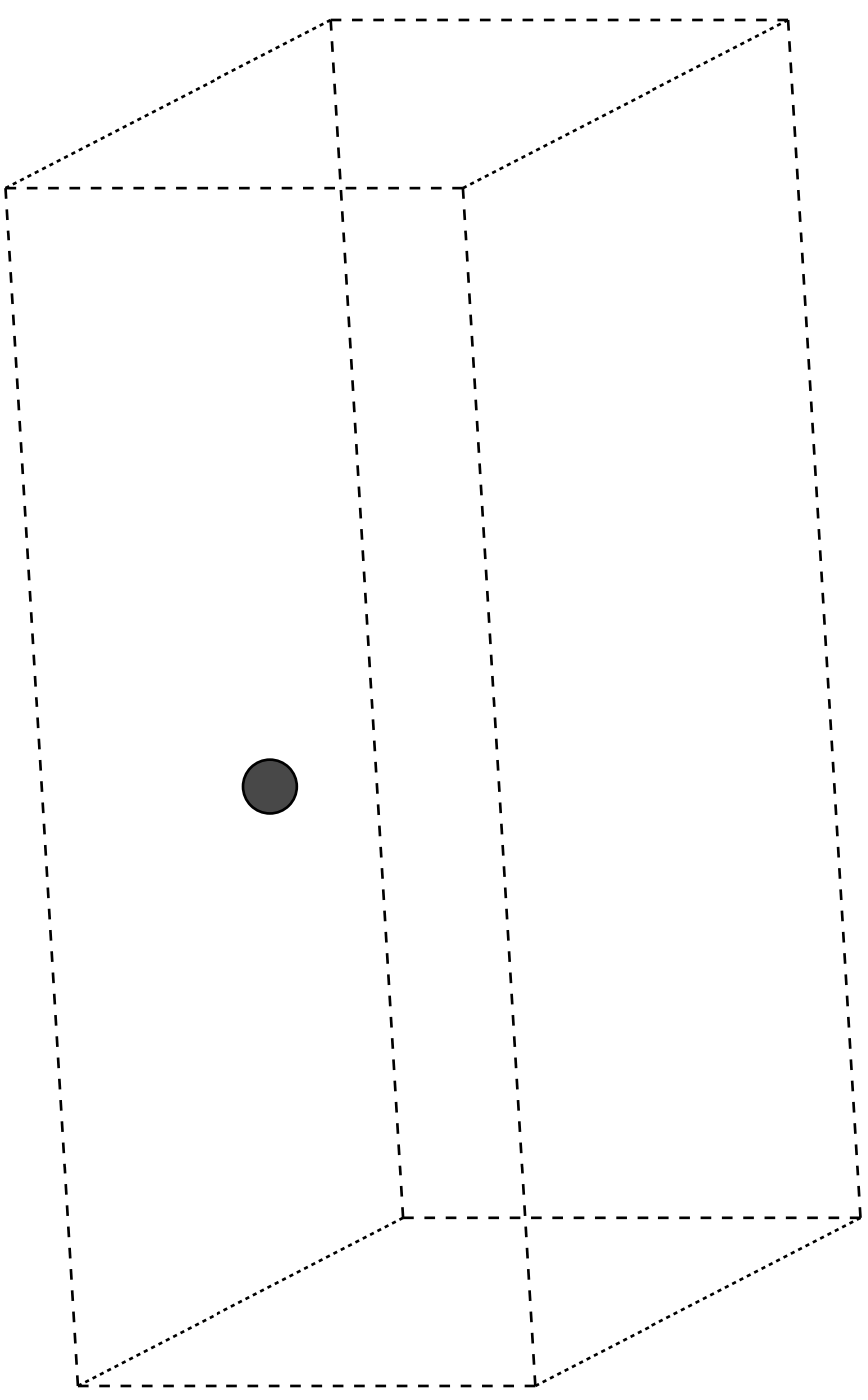
Cluster Statistics:

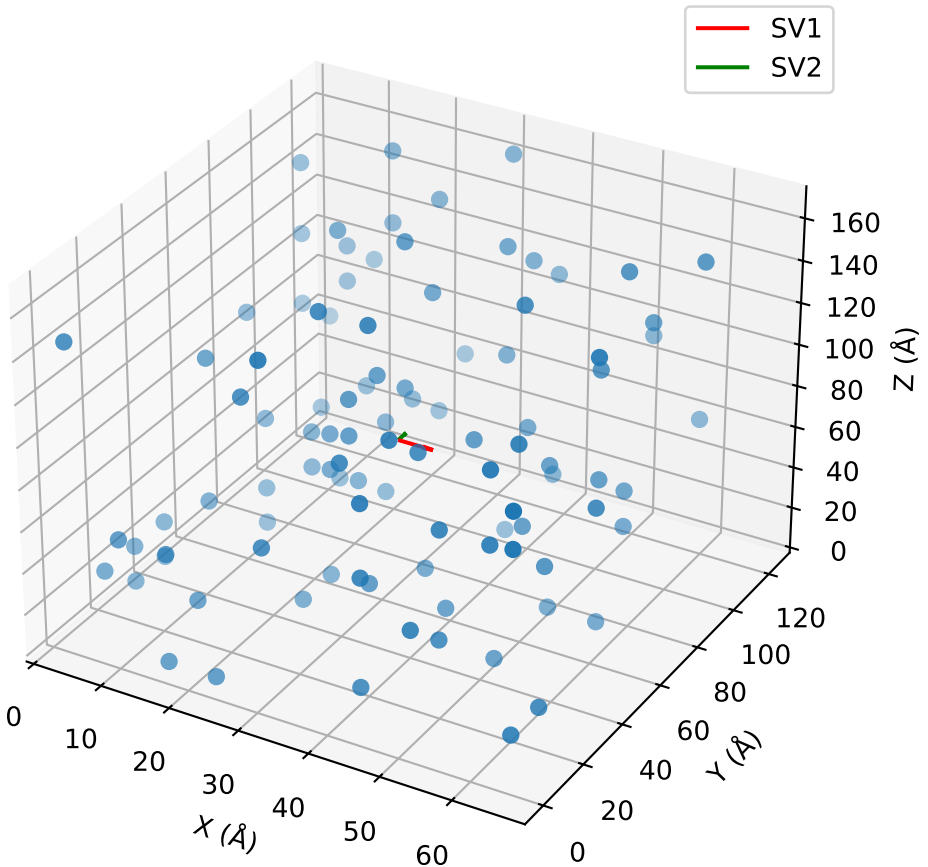
Number of Clusters: 4

Average Cluster Size: 3.00 atoms
Average Distance: 2.831 Å


Transition Metal Connectivity Graph for Nb3TlVCl11 (mp-680696)
Nb
Nb
Nb
Nb
Nb
Nb
Nb
Nb
Nb
V
V
V
V
2.83 Å
2.83 Å
2.83 Å
2.83 Å
2.83 Å
2.83 Å
2.83 Å
2.83 Å
2.83 Å
3.25 Å
3.25 Å
3.25 Å
3.25 Å


Atom Types
Nb
Tl
V
Cl
Cluster Atoms
Cluster - Size: 3, Avg Distance: 2.83 Å


Cluster Lattice for Nb3TlVCl11 (Space Group: Pmmm)


Dimensionality: Nb3TlVCl11 (2D)
SV1
SV2
0
10
20
30
40
50
60
X (Å)
0
20
40
60
80
100
120
Y (Å)
0
20
40
60
80
100
120
140
160
Z (Å)

Compound Details: CsNb3VCl11 (mp-1213417)

Space Group: Pmmm

Dimensionality: 2D

Energy Above Hull: 0.0397345357031220 06 eV/atom

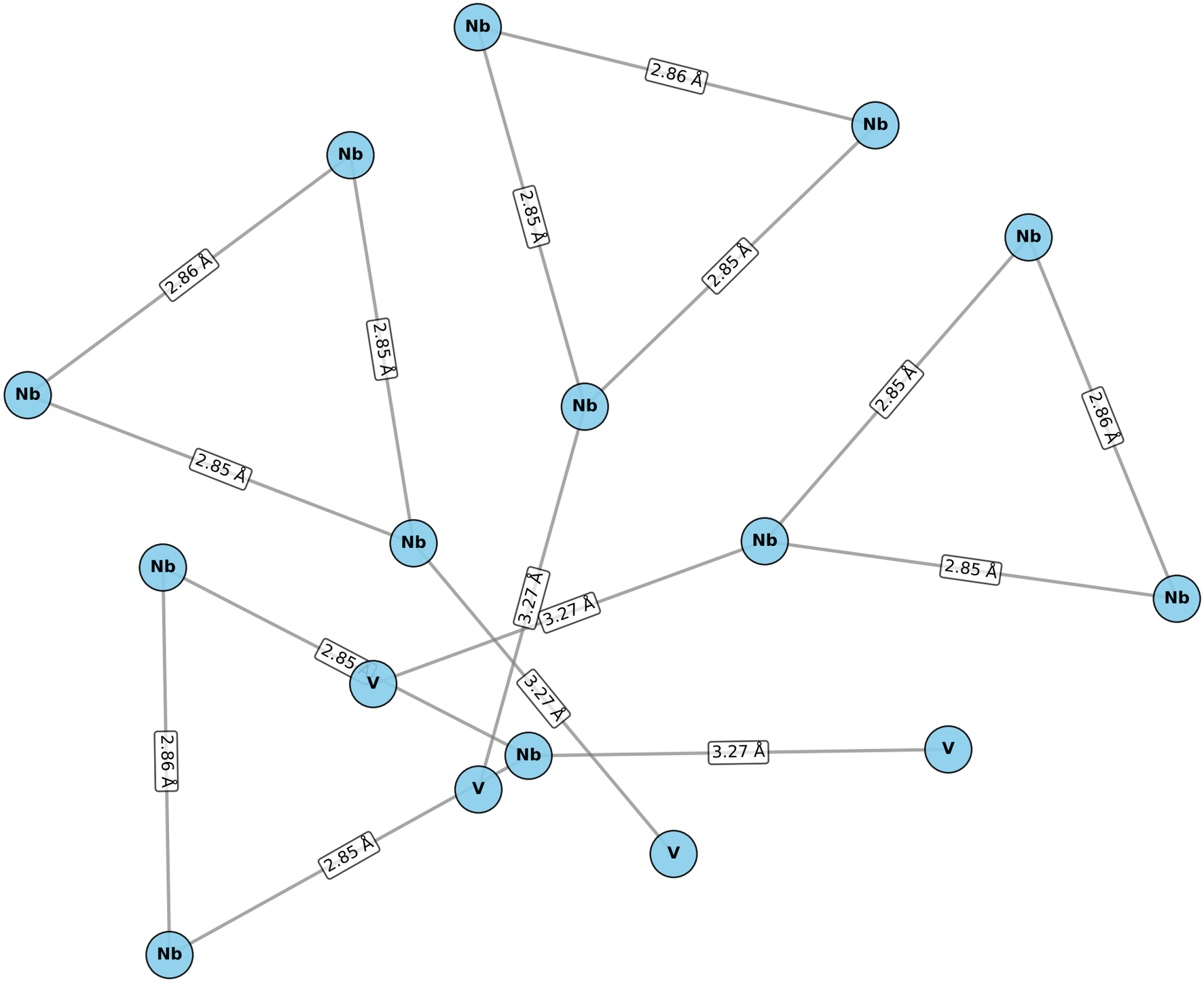
Rank Score: -2.7713

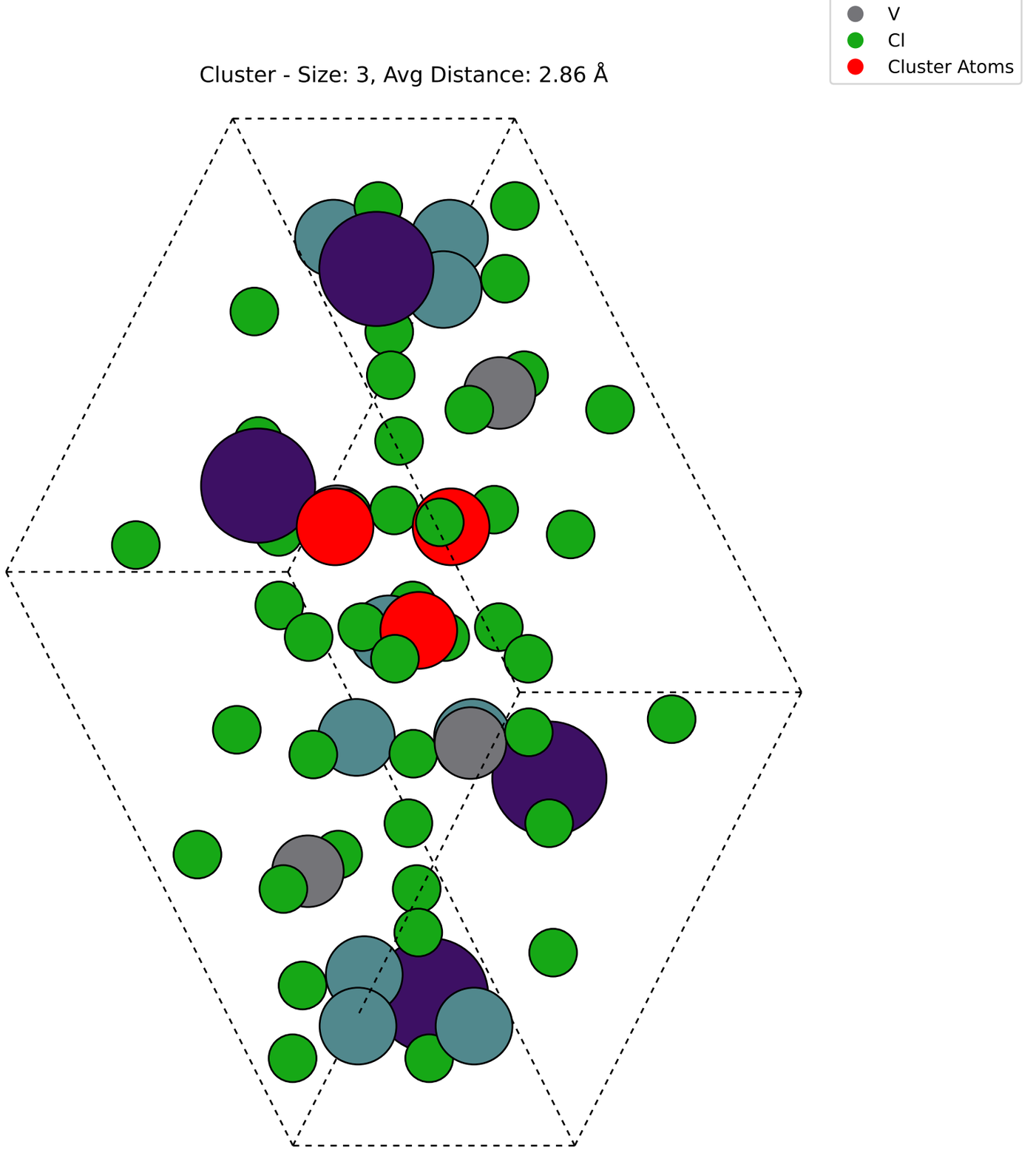
Cluster Statistics:

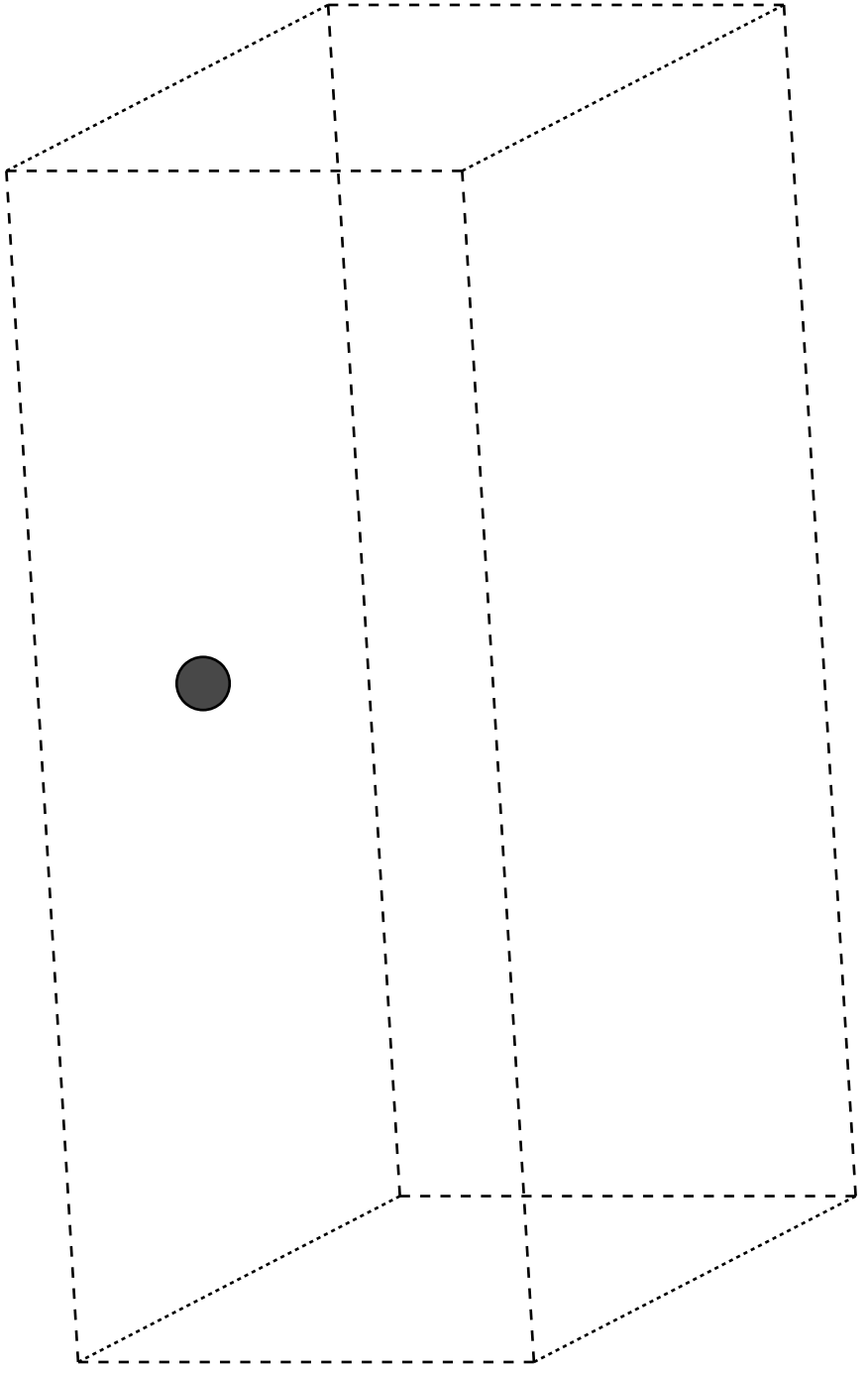
Number of Clusters: 4

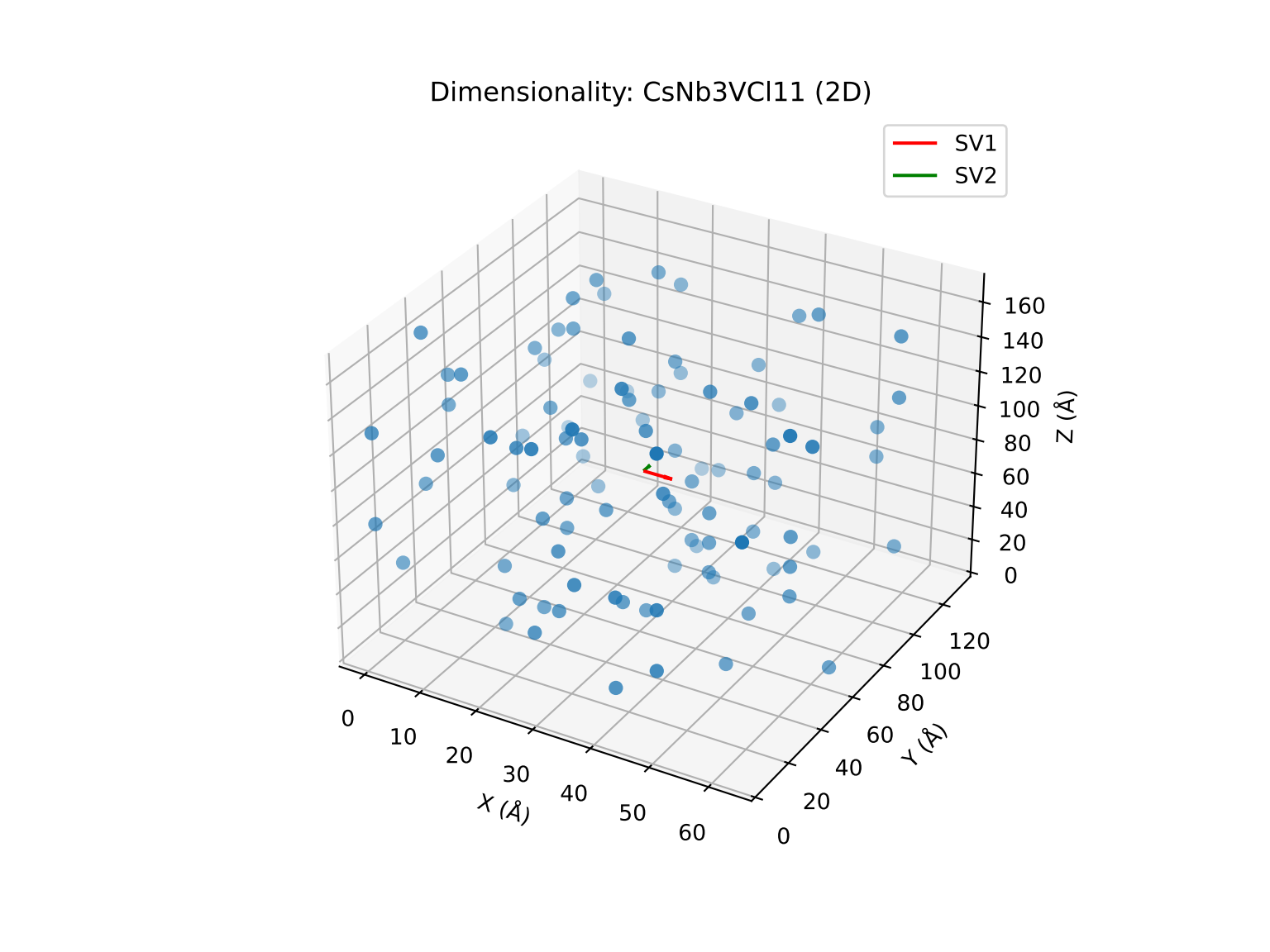
Average Cluster Size: 3.00 atoms
Average Distance: 2.857 Å

Transition Metal Connectivity Graph for CsNb3VCl11 (mp-1213417)




Cluster - Size: 3, Avg Distance: 2.86 Å
Atom Types
Cs
Nb
V
Cl
Cluster Atoms


Cluster Lattice for CsNb3VCl11 (Space Group: Pmmm)


Dimensionality: CsNb3VCl11 (2D)
SV1
SV2
X (Å)
Y (Å)
Z (Å)
0
10
20
30
40
50
60
0
20
40
60
80
100
120
0
20
40
60
80
100
120
140
160

Compound Details: KNb3VCl11 (mp-1211867)

Space Group: Pmmm

Dimensionality: 2D

Energy Above Hull: 0.052237557860579 eV/atom

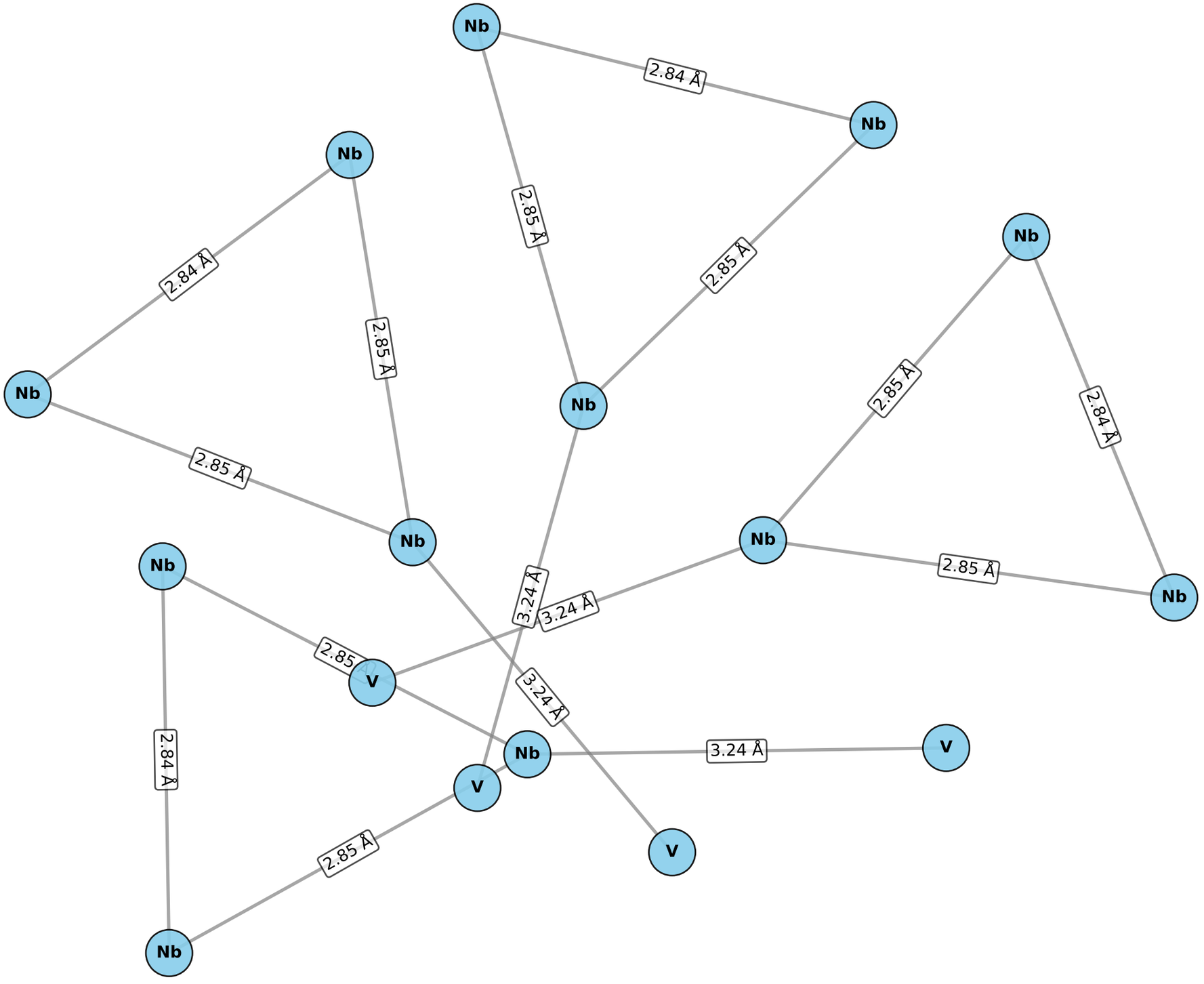
Rank Score: -2.7956

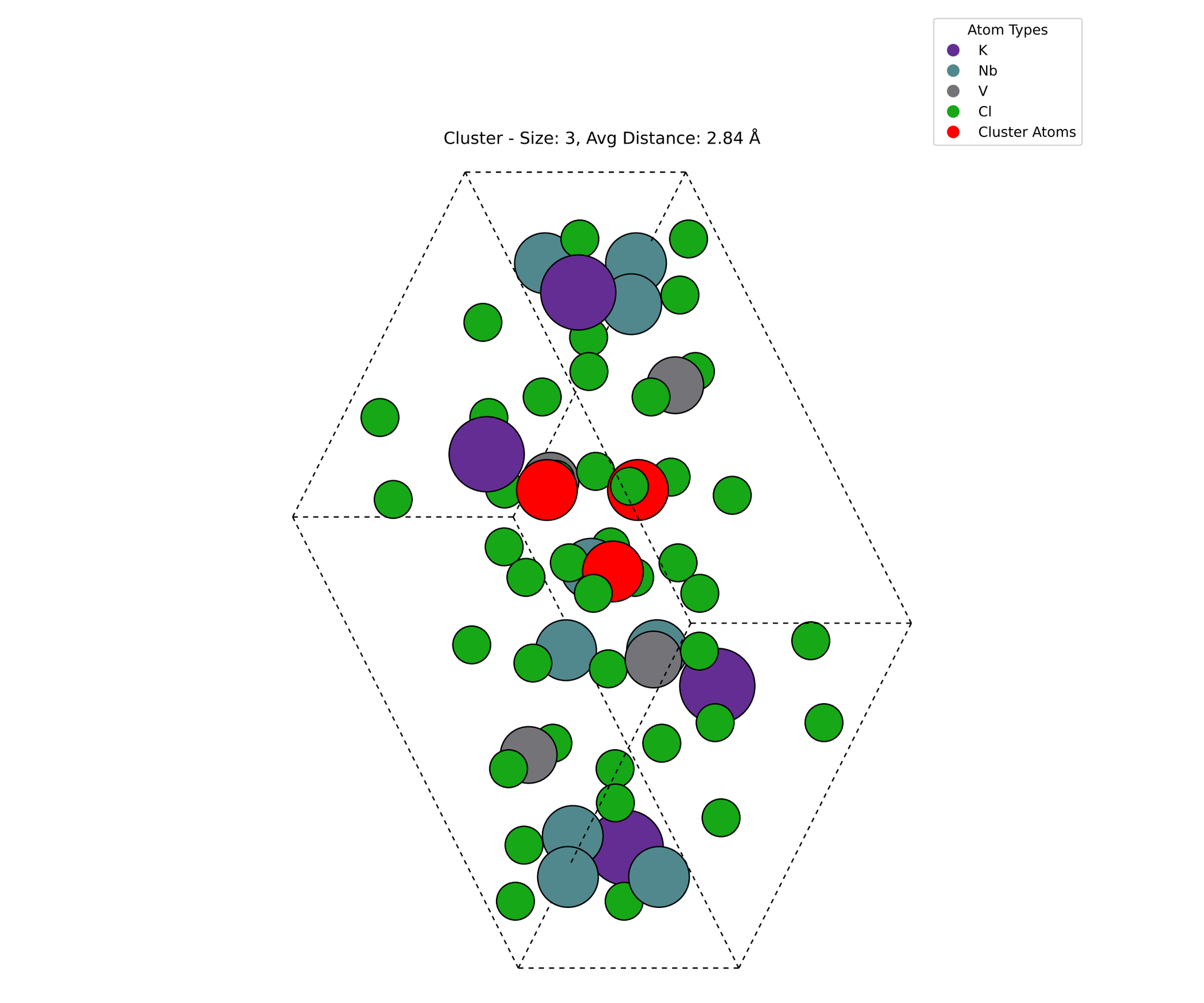
Cluster Statistics:

Number of Clusters: 4

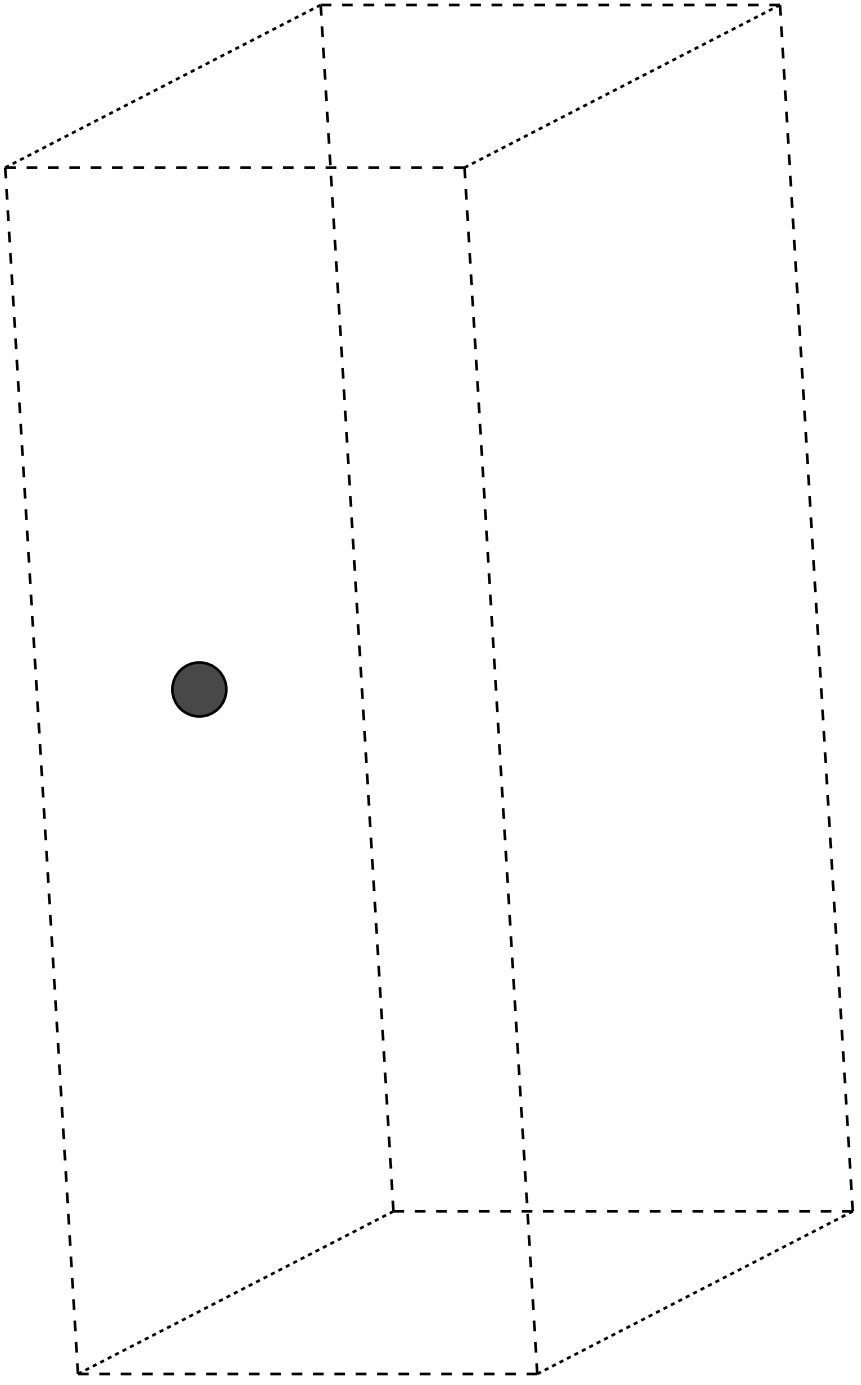
Average Cluster Size: 3.00 atoms
Average Distance: 2.844 Å

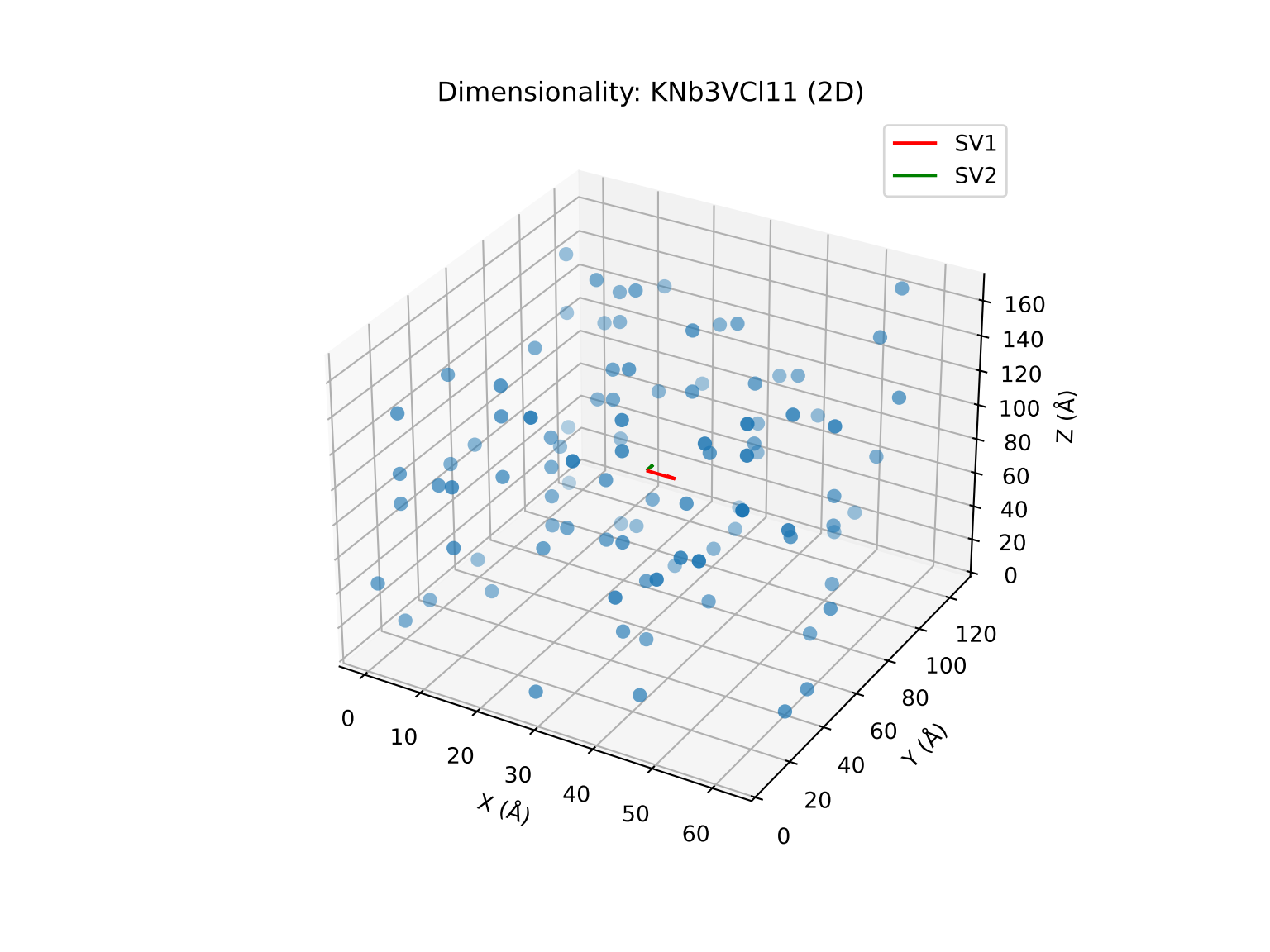
Transition Metal Connectivity Graph for KNb3VCl11 (mp-1211867)




Atom Types
K
Nb
V
Cl
Cluster Atoms
Cluster - Size: 3, Avg Distance: 2.84 Å

Cluster Lattice for KNb3VCl11 (Space Group: Pmmm)




Dimensionality: KNb3VCl11 (2D)
SV1
SV2
0
10
20
30
40
50
60
X (Å)
0
20
40
60
80
100
120
Y (Å)
0
20
40
60
80
100
120
140
160
Z (Å)