

Atomic Clusters on the f.c.c. Lattice

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The manuscripts illustrate the 20 variants of placing 4 touching spheres centered on face-centered cubic lattice sites and the 131 variants of placing 5 touching spheres.

PACS numbers: 95.10.Km, 95.80.+p

I. OEIS A300812

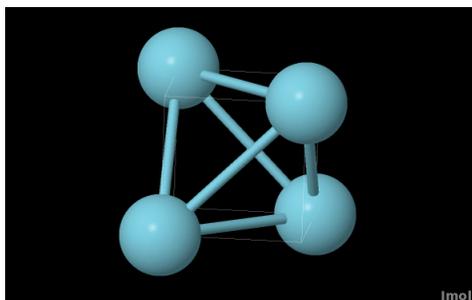
The atoms on cubic closed packed (face-centered cubic) lattice sites are represented by blue balls. The non-occupied lattice sites in the neighborhood are smaller white balls. Where occupied sites have the nearest-neighbor distance (half of the face diagonal of the f.c.c. lattice), bonds (contacts if the blue spheres are blown up to a diameter of half the face diagonal) are added in blue. Thin bounding boxes parallel to the unit vectors of the underlying simple cubic lattice are also drawn.

This helps to decipher how many clusters of size 4 and 5 exist with a given number of contacts [1, A300812].

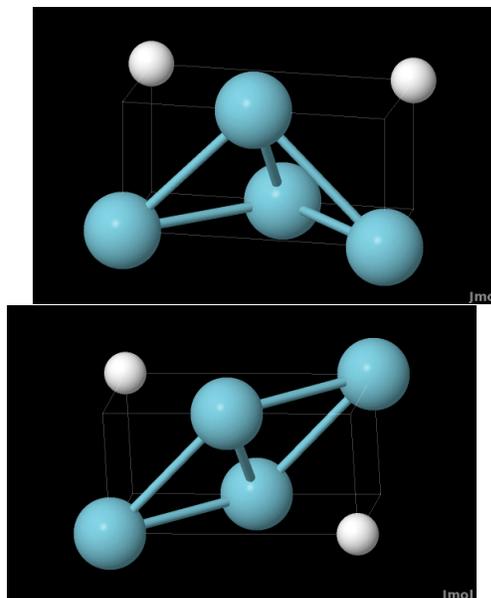
II. 20 CLUSTERS WITH 4 ATOMS

A. 1 Cluster with 6 contacts

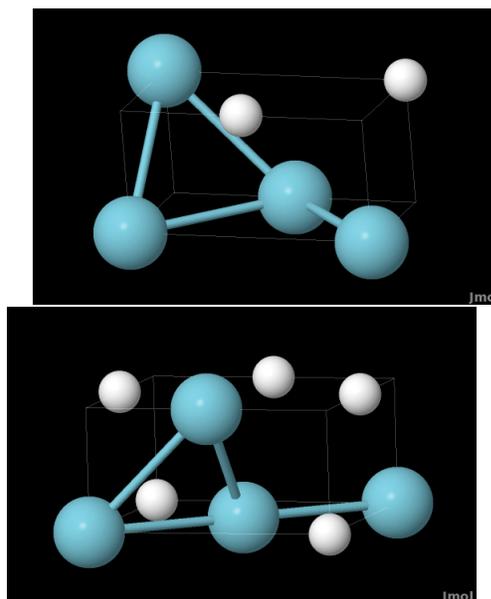
This is the tetrahedral graph.



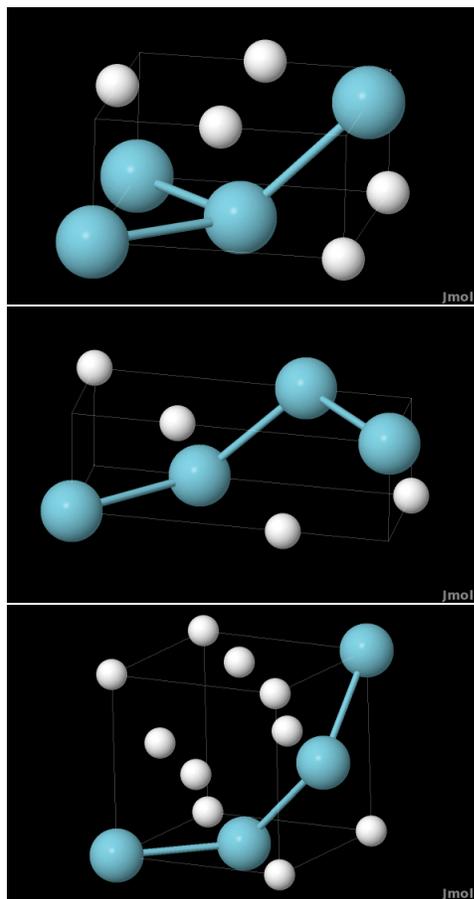
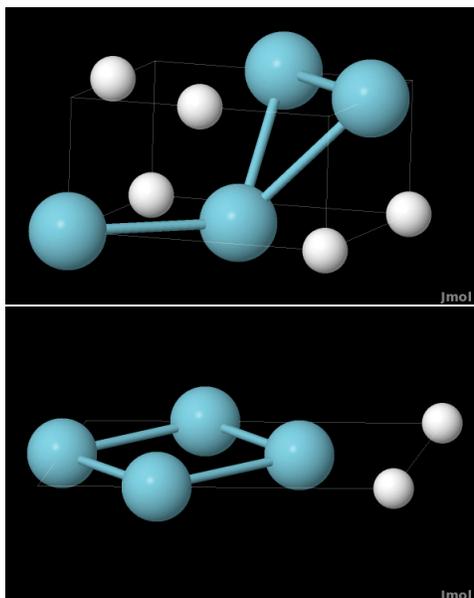
B. 2 Clusters with 5 contacts



C. 4 Clusters with 4 contacts



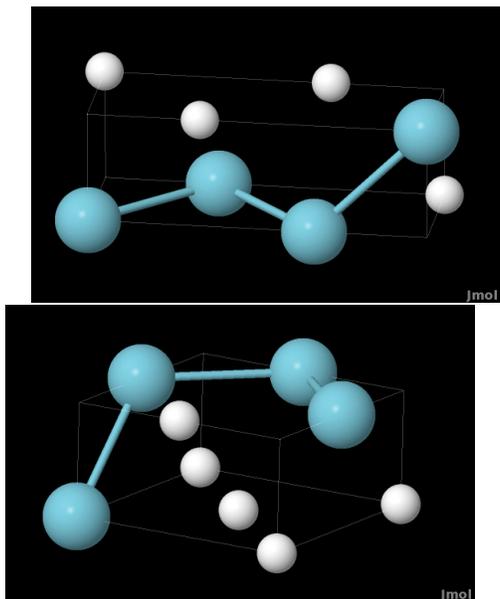
* <http://www.mpia.de/~mathar>



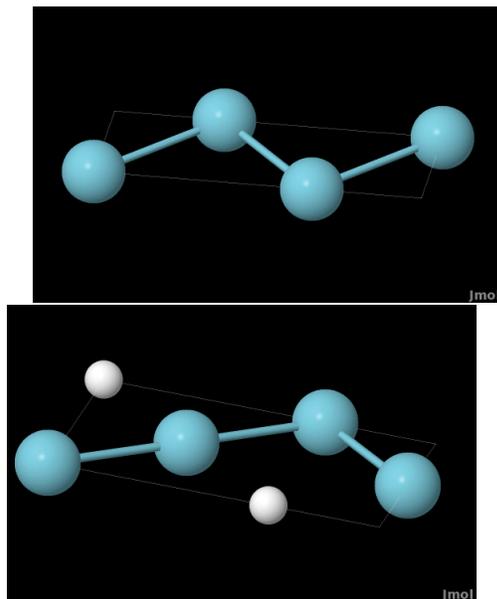
D. 13 Clusters with 3 contacts

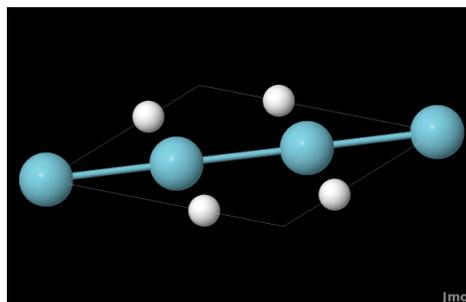
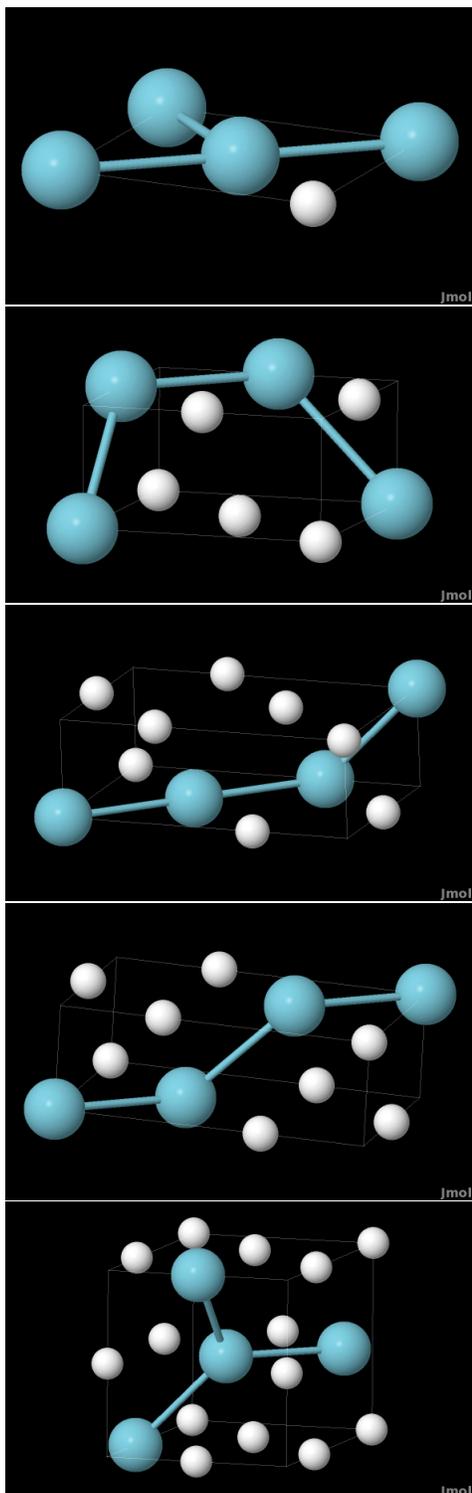
The 4-clusters with an underlying simple graph that is a tree. 5 of them are non-planar, 8 planar. (In this context *planar* means there is a plane that contains all sphere centers. It does not refer to the underlying simple graph representation.)

1. non-planar



2. planar

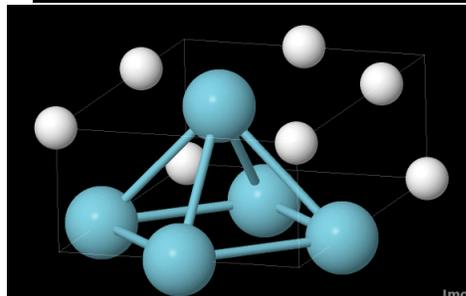
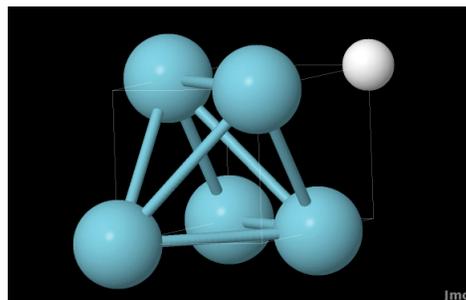




III. 131 CLUSTERS WITH 5 ATOMS

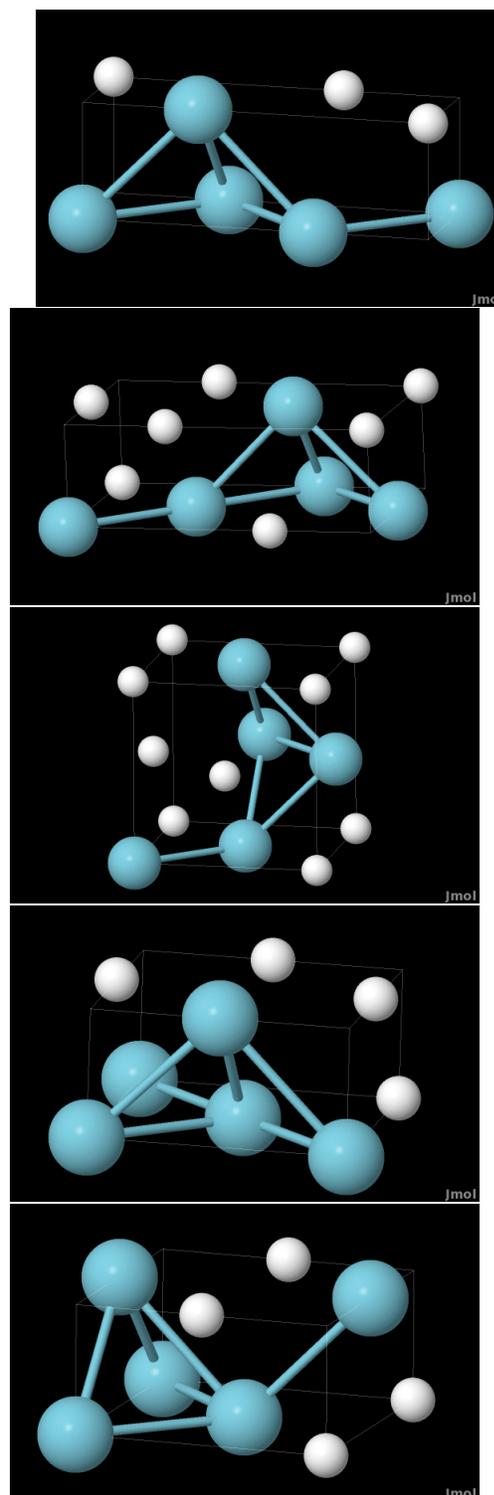
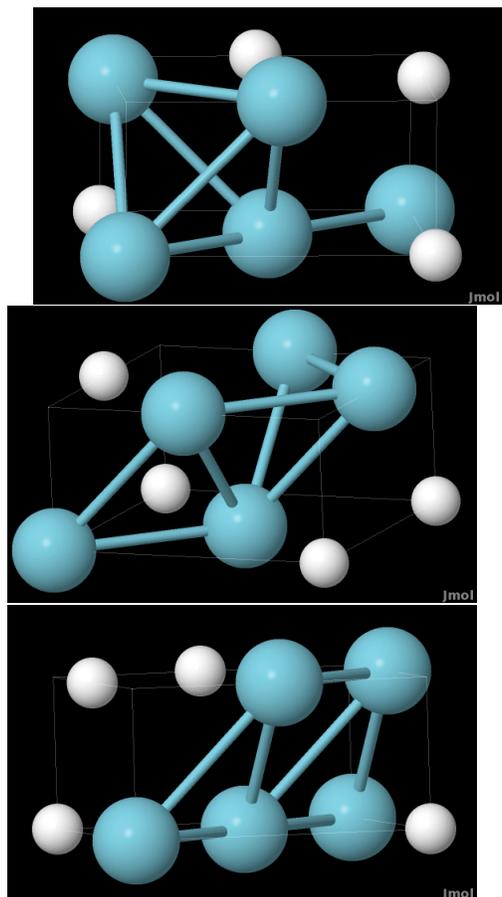
There is no cluster with 9 contacts because there is no choice to glue two tetrahedra face-to-face; that would require the hexagonal close lattice.

A. 2 Clusters with 8 contacts



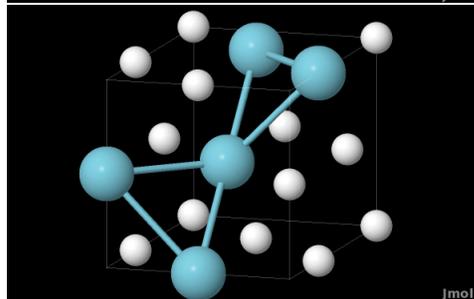
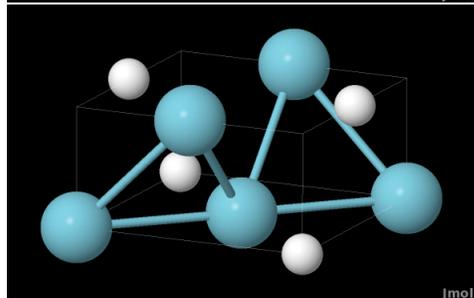
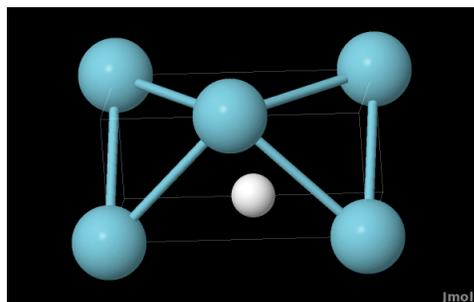
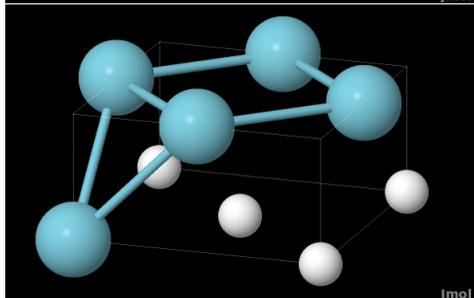
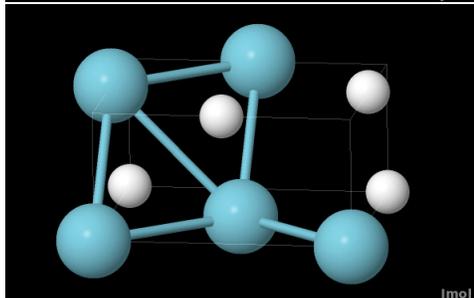
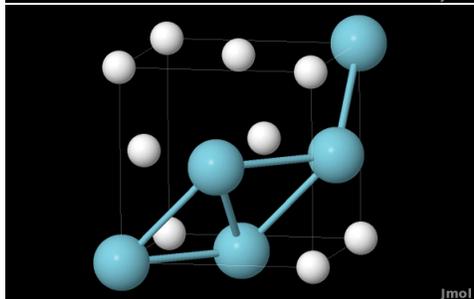
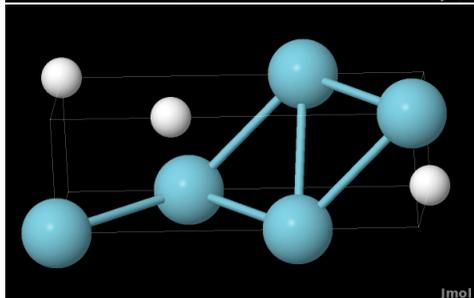
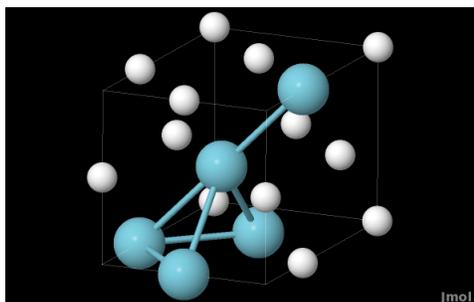
B. 3 Clusters with 7 contacts

1. non-planar

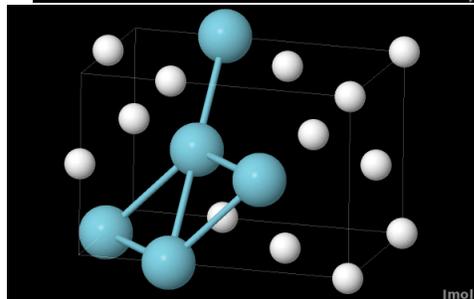
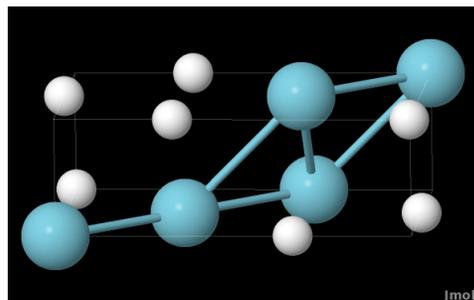


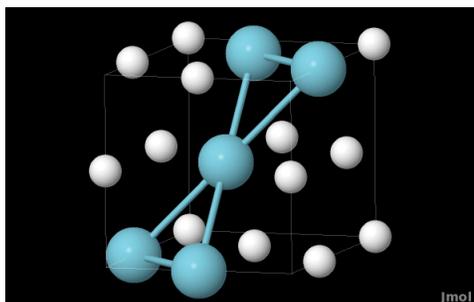
C. 16 Clusters with 6 contacts

Contains 13 non-planar and 3 planar geometries.



2. planar

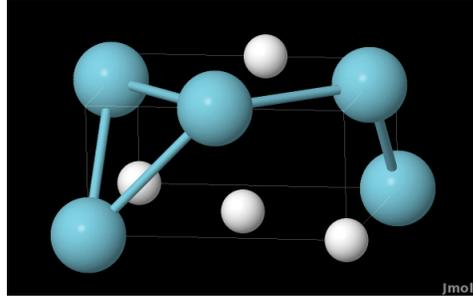
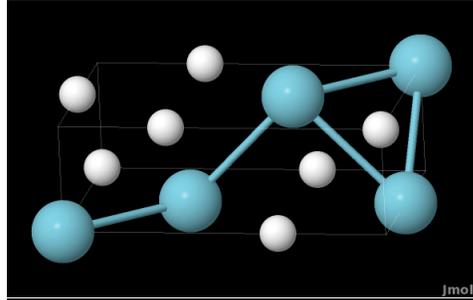
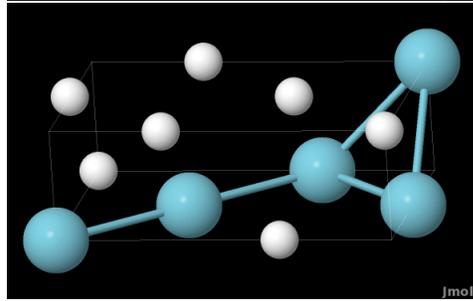
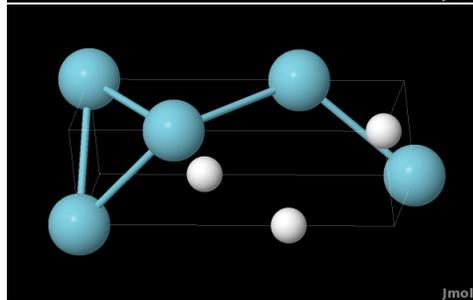
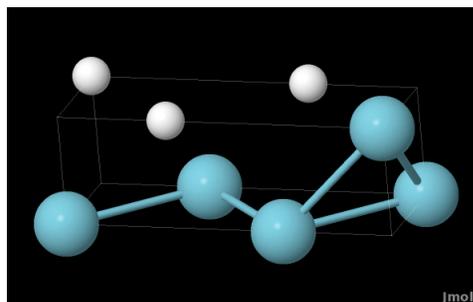
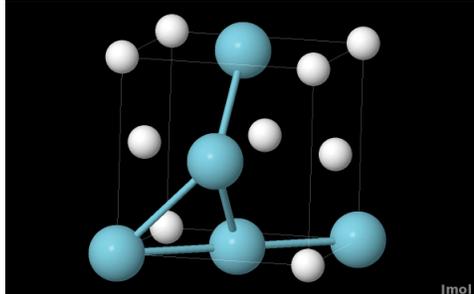
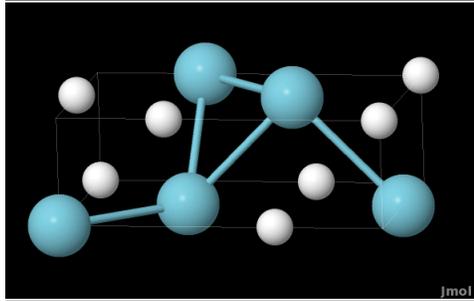
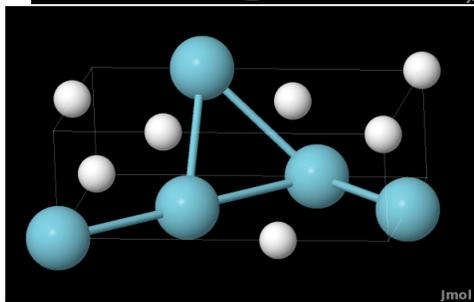
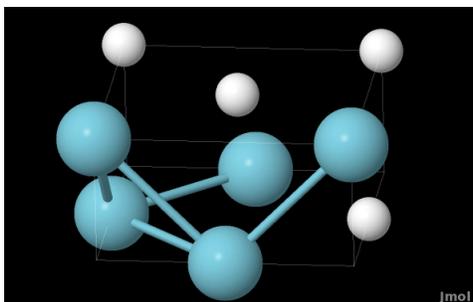


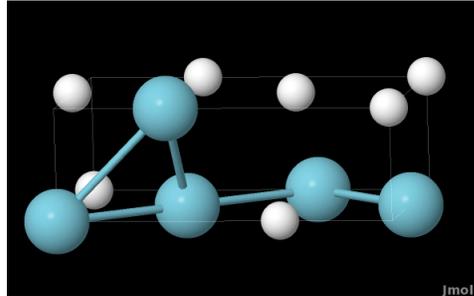
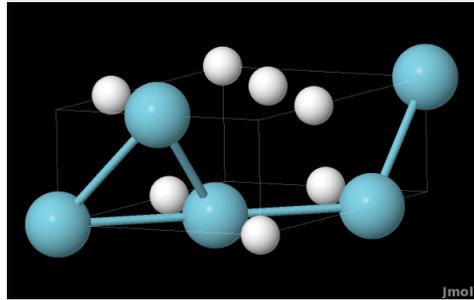
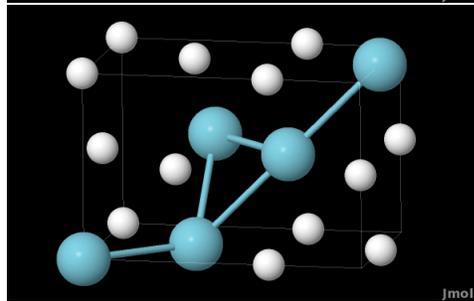
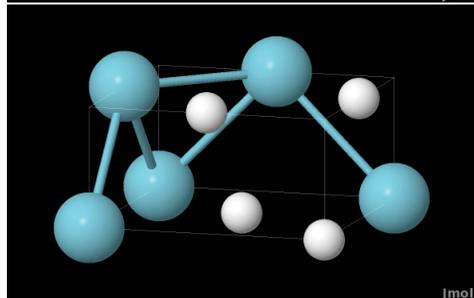
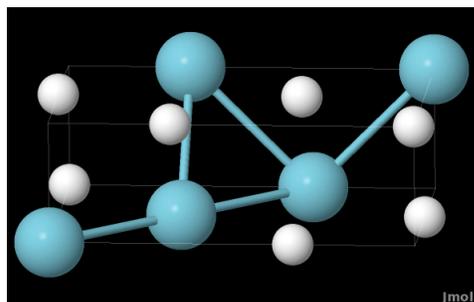
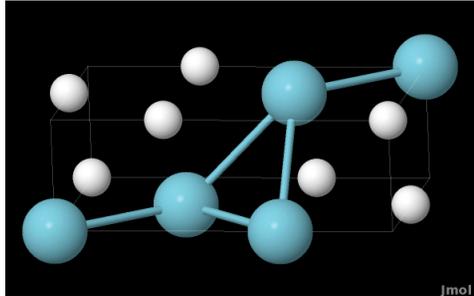
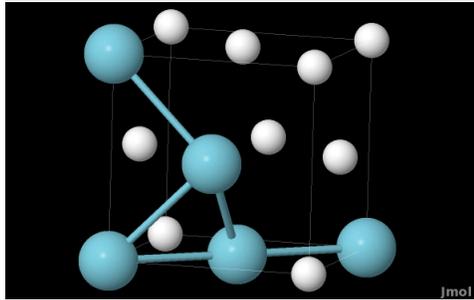
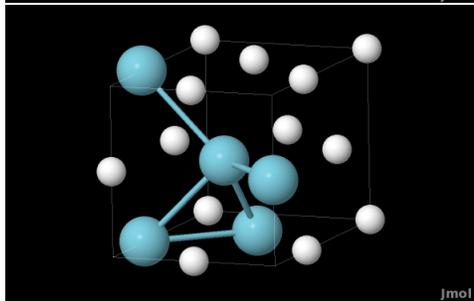
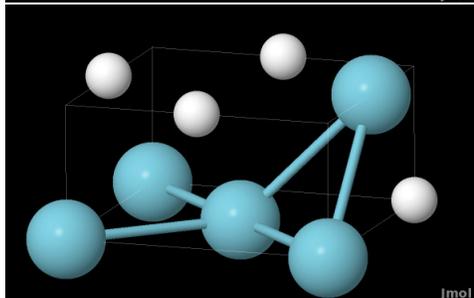
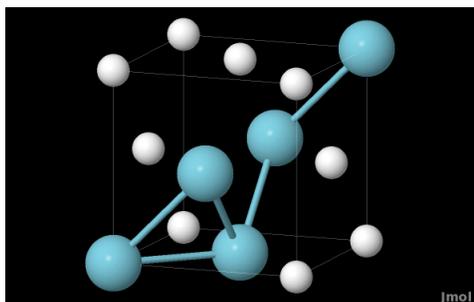


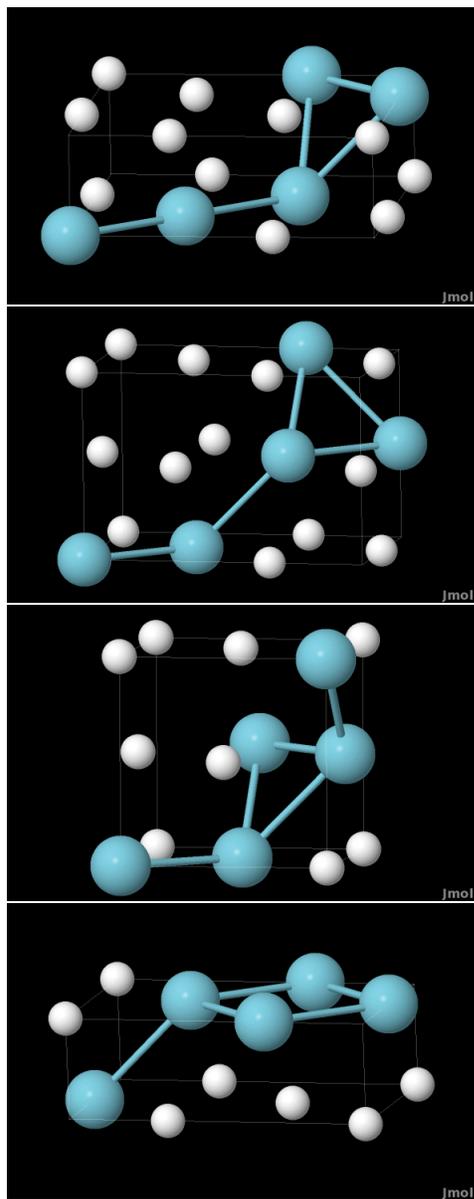
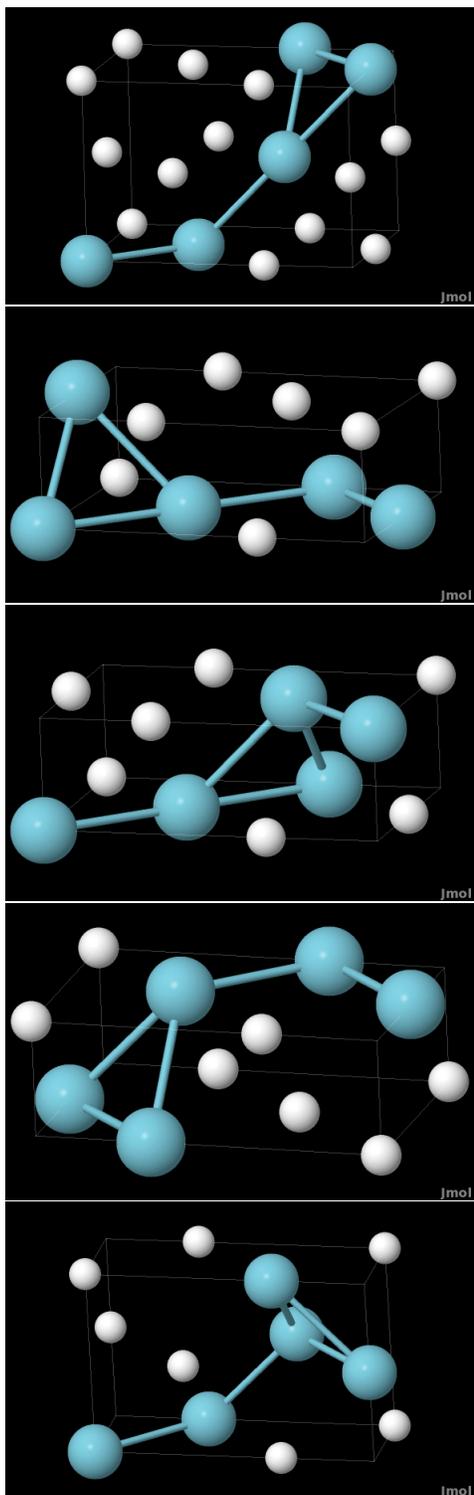
D. 35 Clusters with 5 contacts

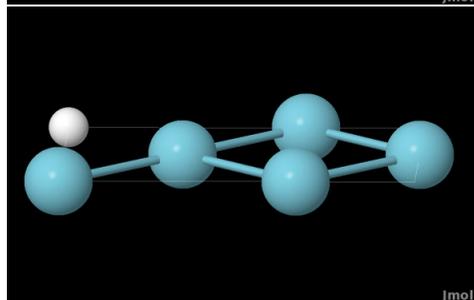
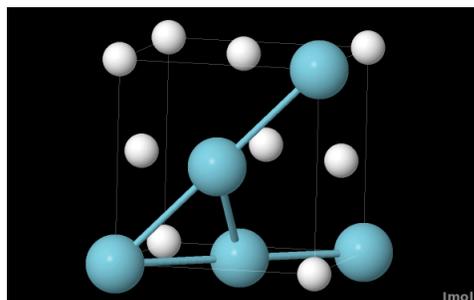
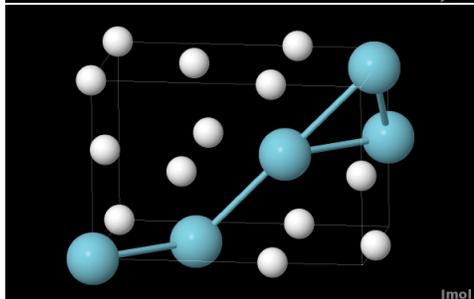
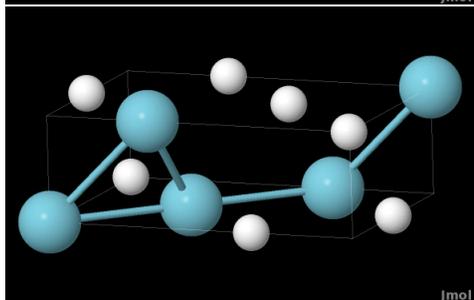
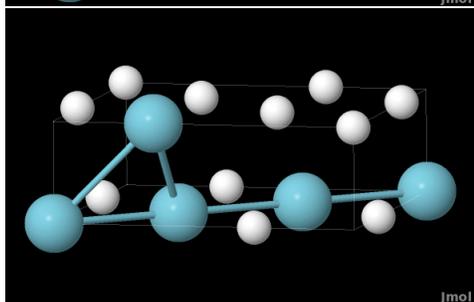
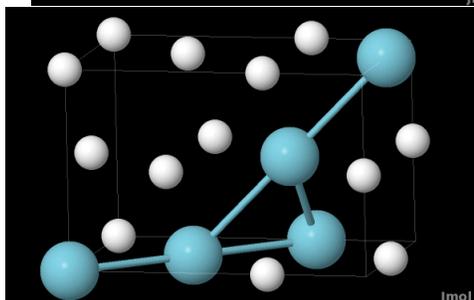
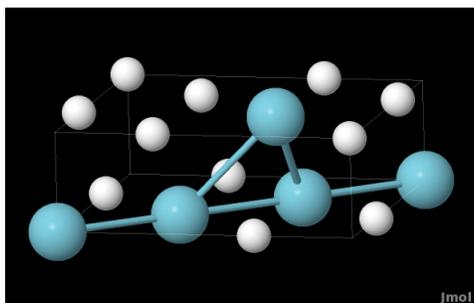
Contains 28 non-planar and 7 planar geometries.

1. non-planar



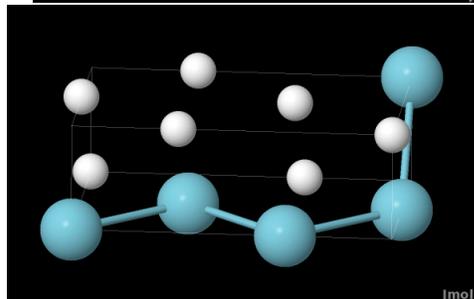
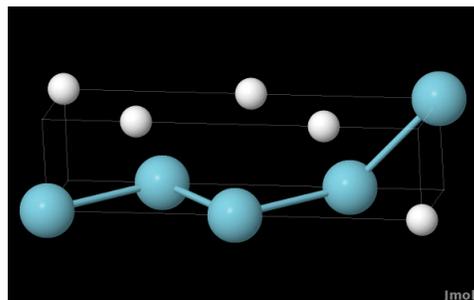


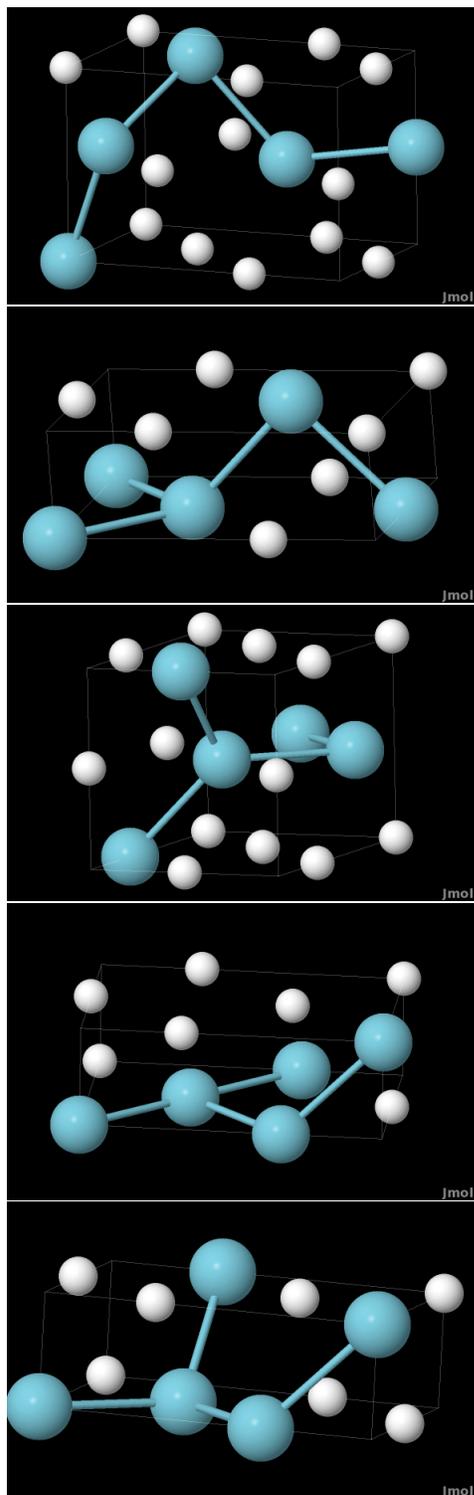
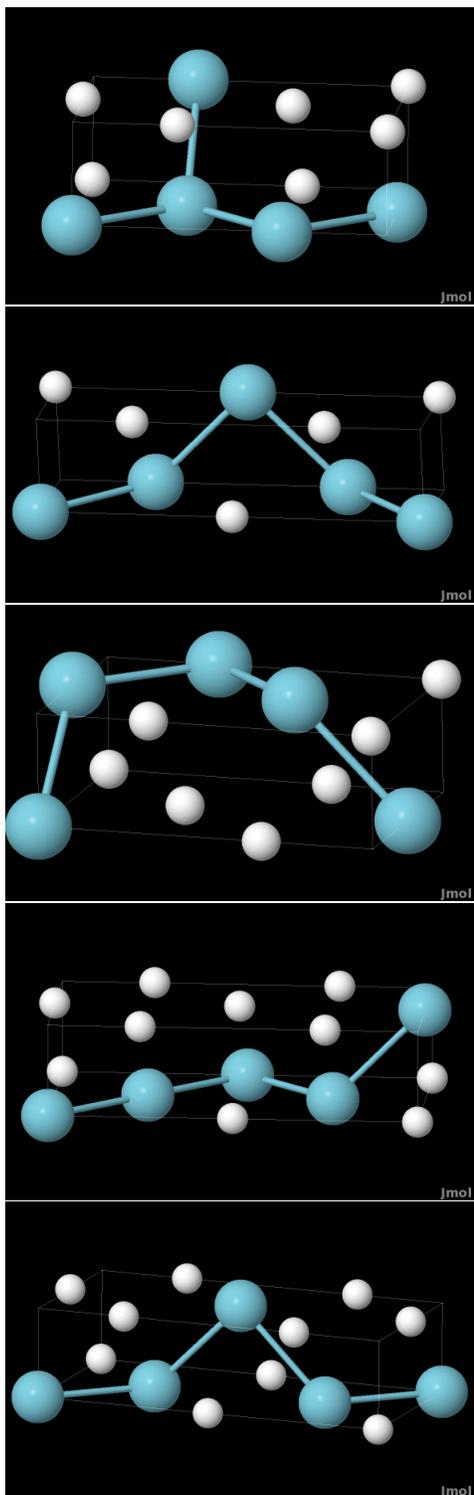


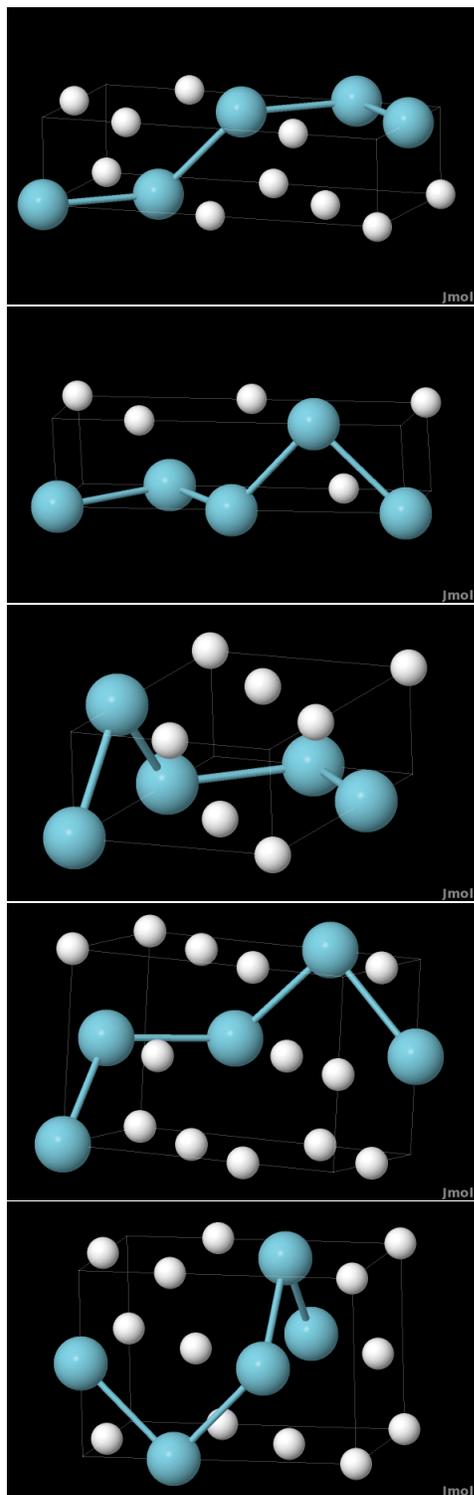
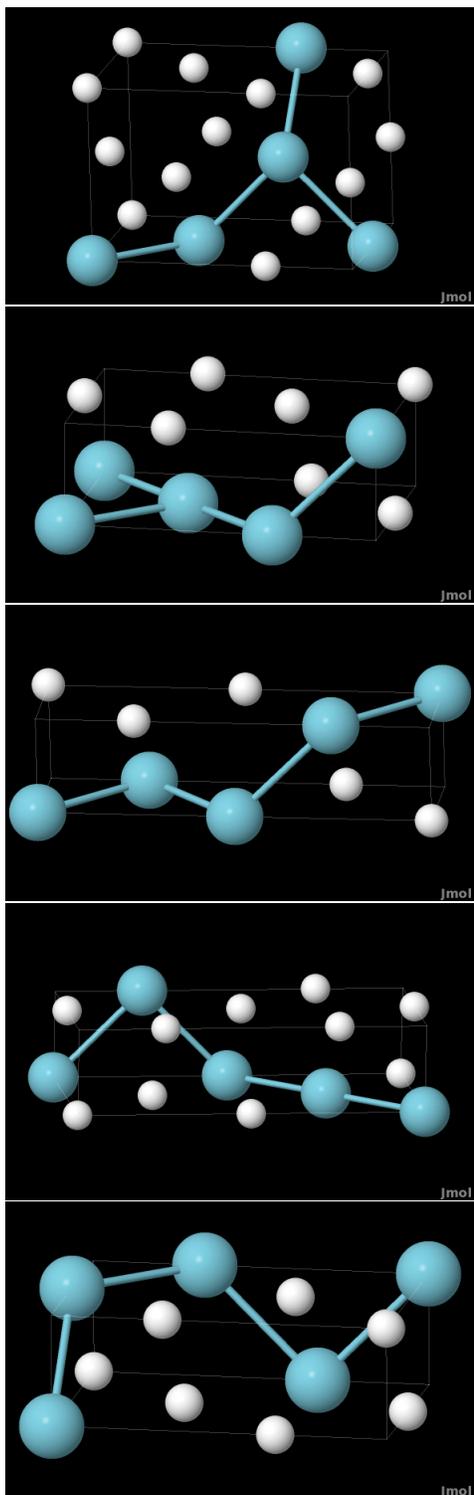
2. *planar*

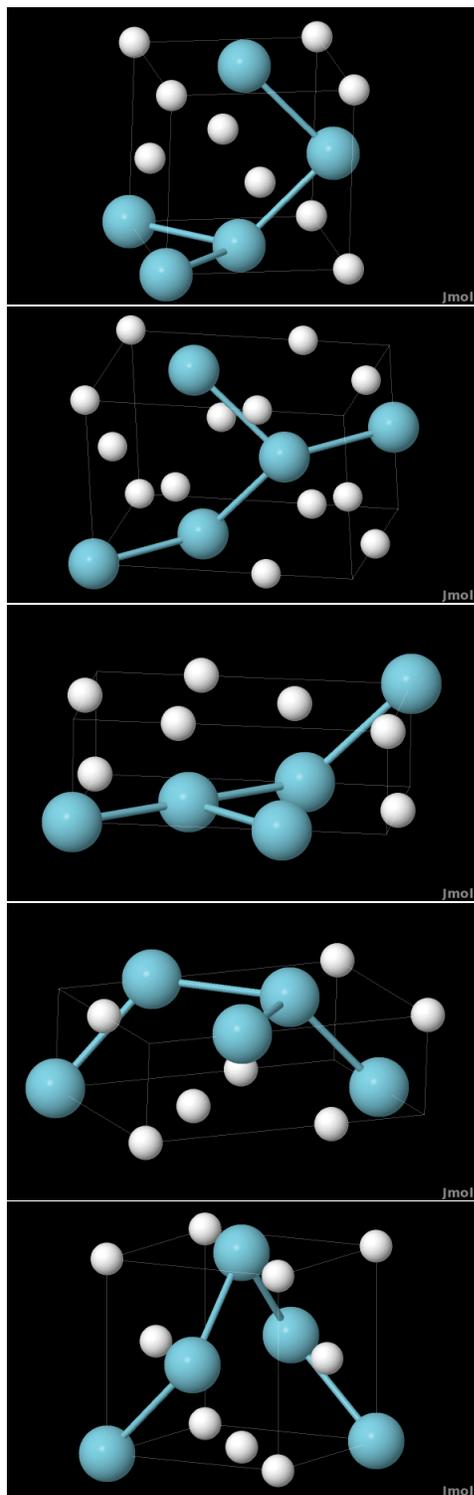
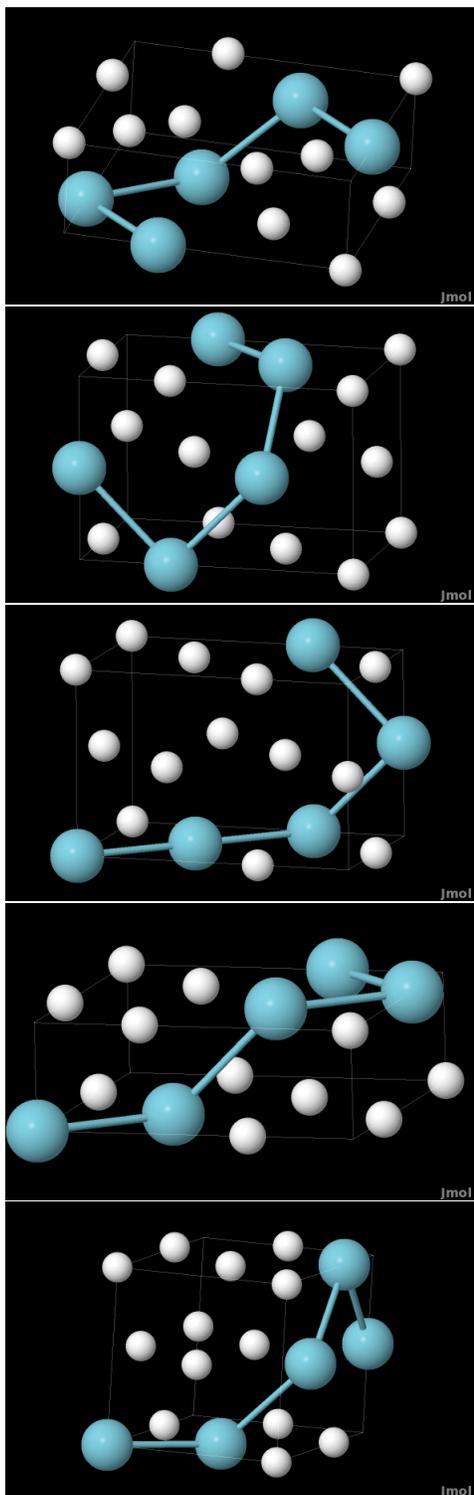
E. 75 Clusters with 4 contacts

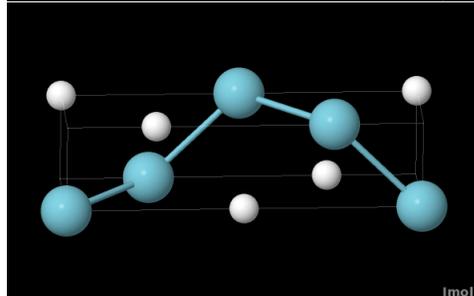
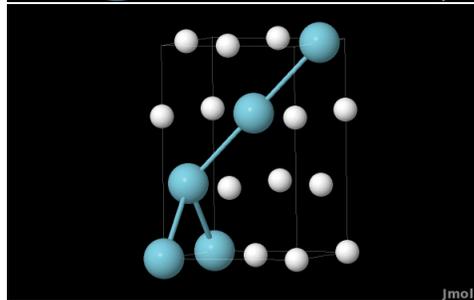
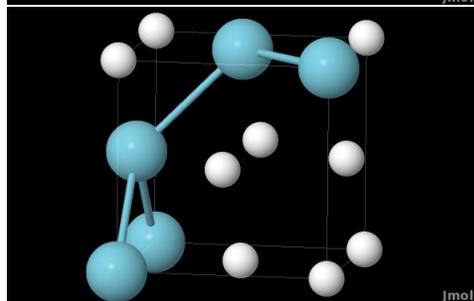
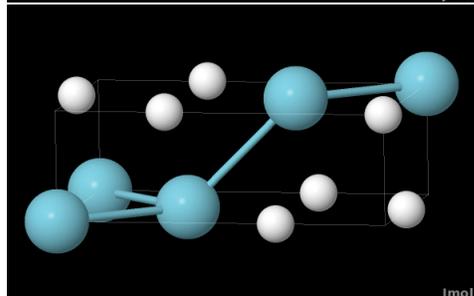
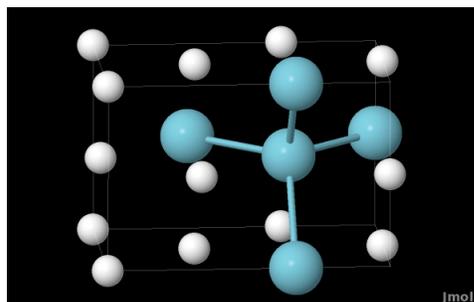
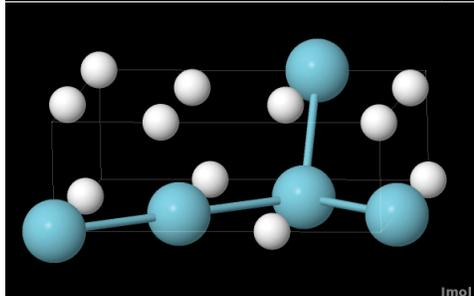
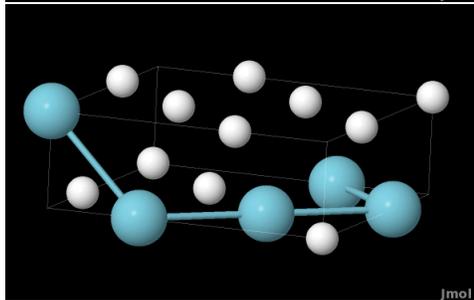
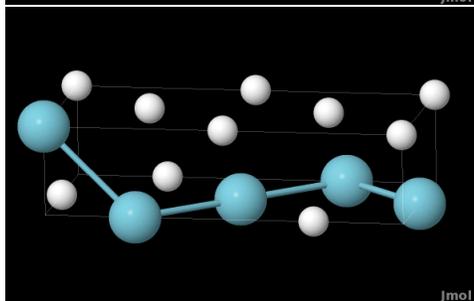
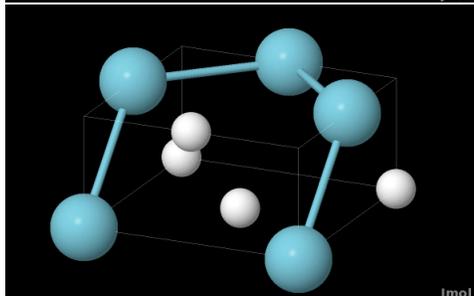
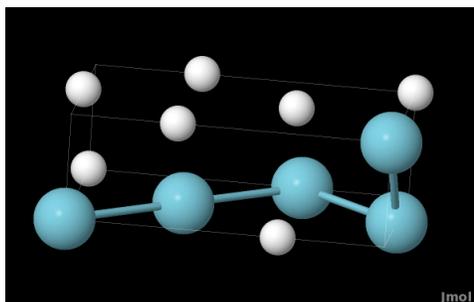
The 5-clusters with an underlying simple graph that is a tree. Classified as 54 non-planar and 21 planar geometries.

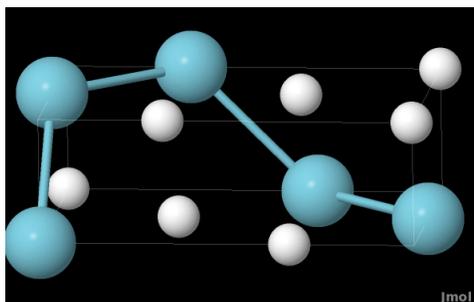
1. *non-planar*



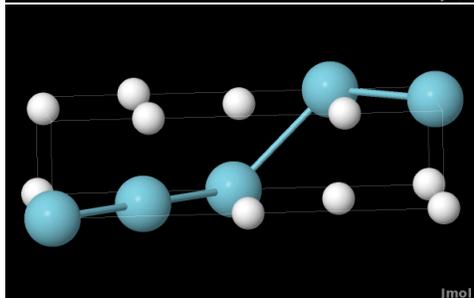




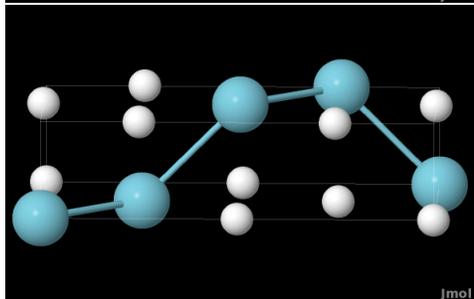




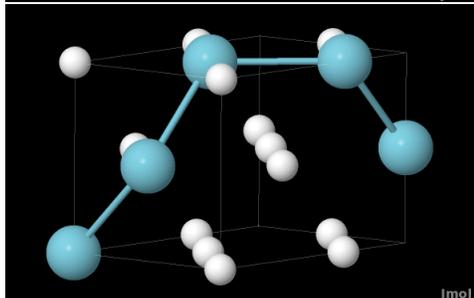
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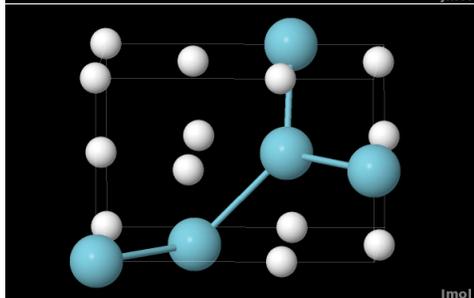
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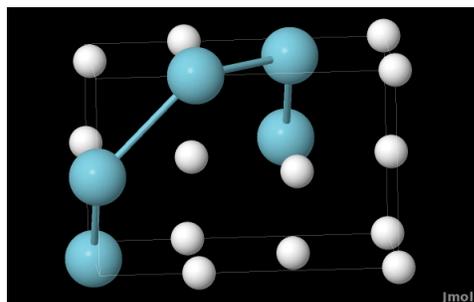
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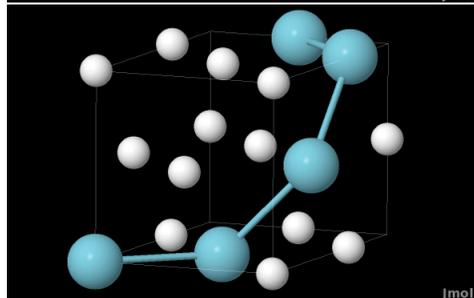
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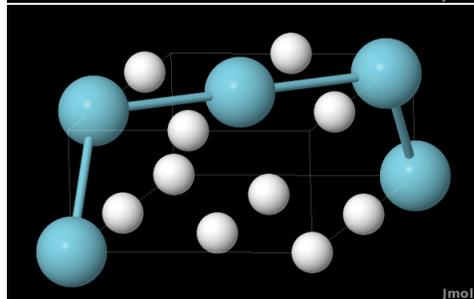
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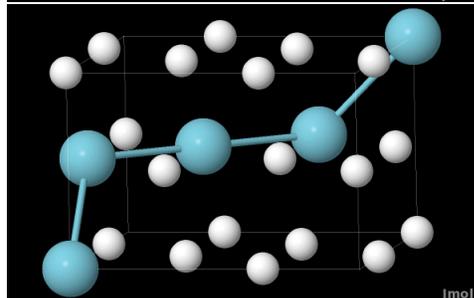
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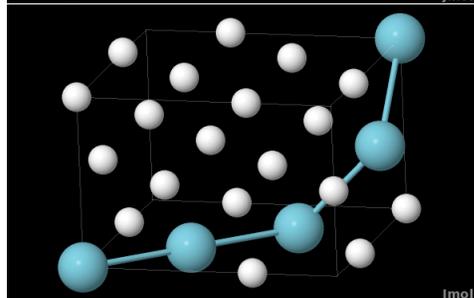
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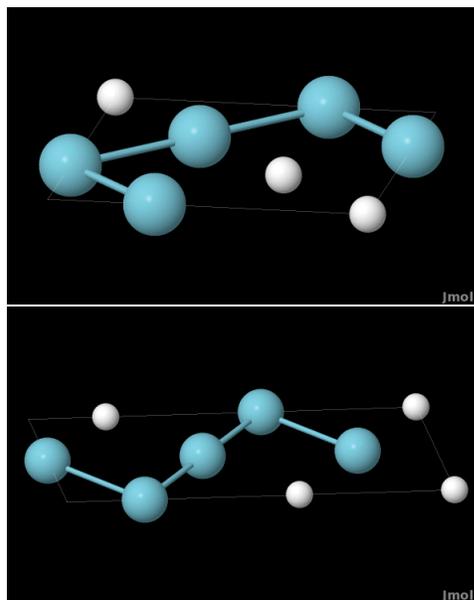
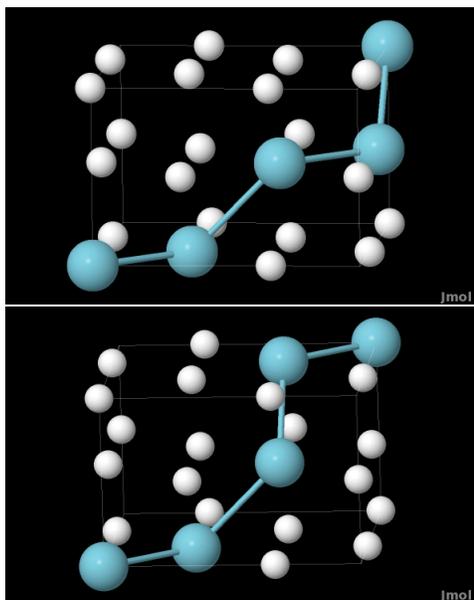
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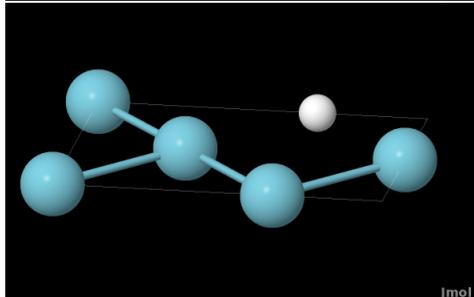
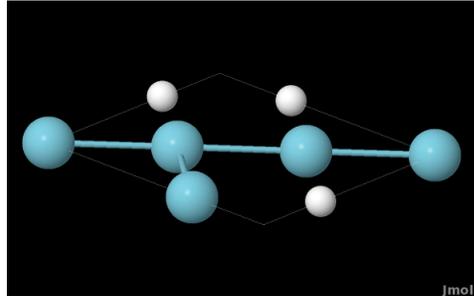
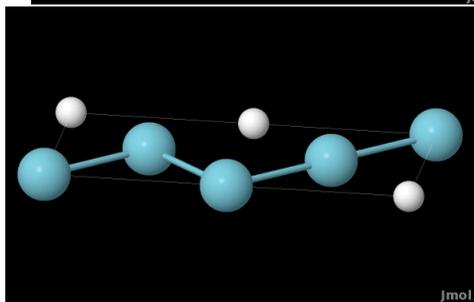
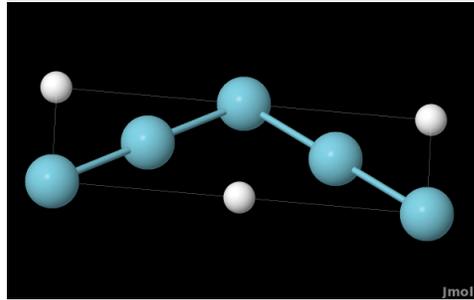
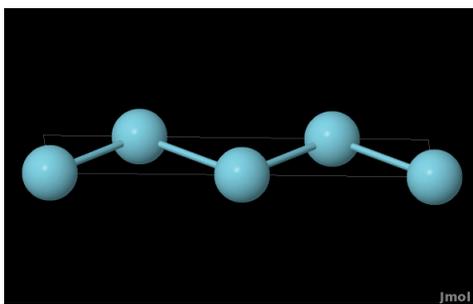
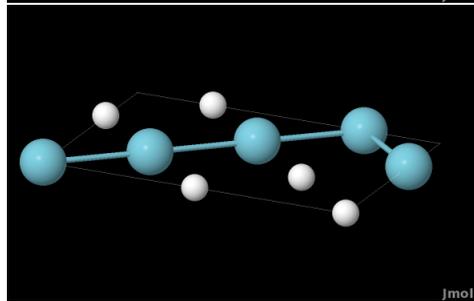
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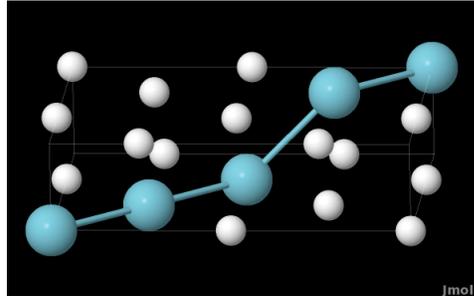
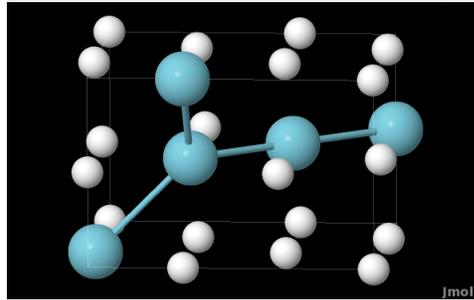
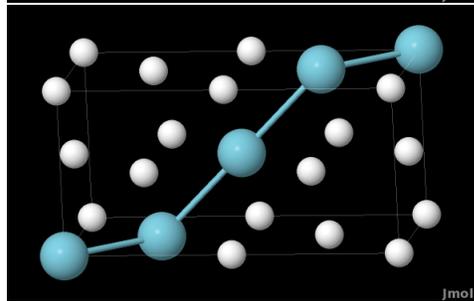
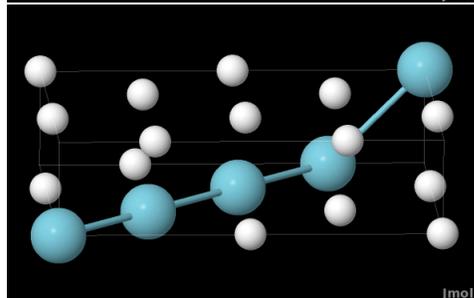
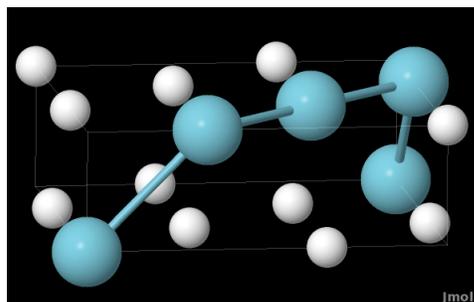
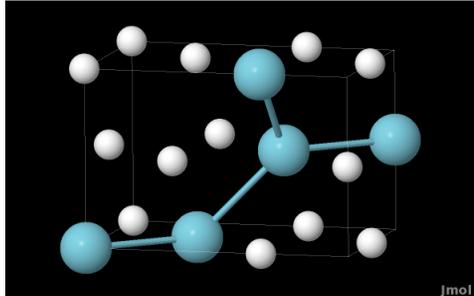
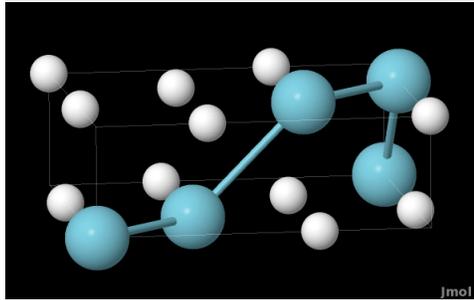
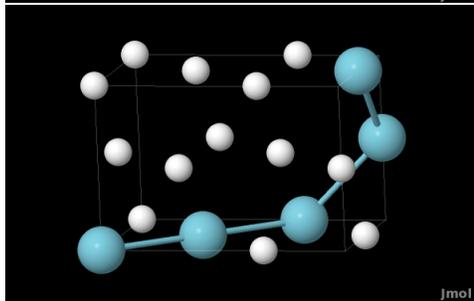
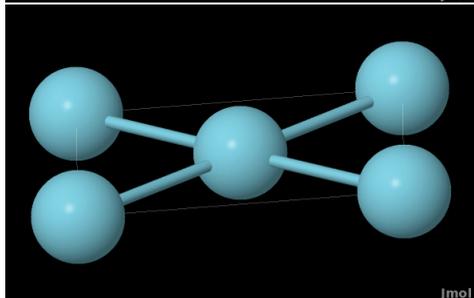
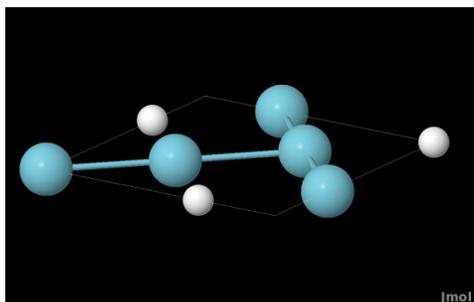


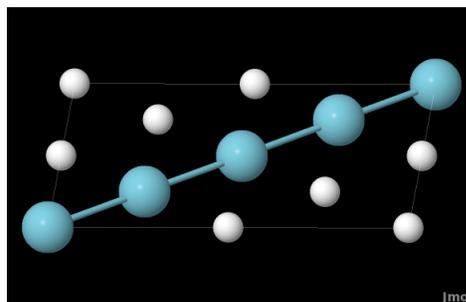
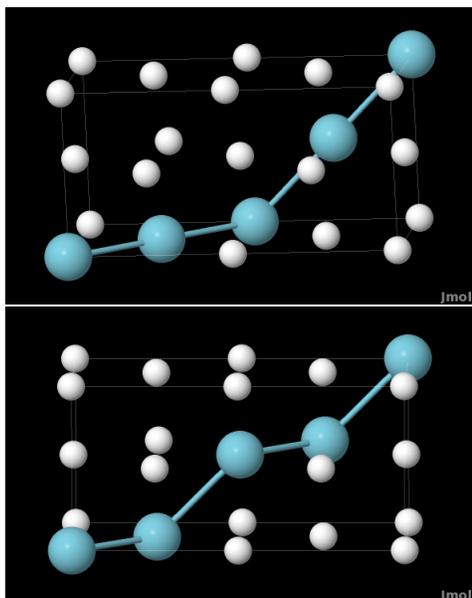
Jmol



2. *planar*







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- [1] N. J. A. Sloane, *Notices Am. Math. Soc.* **50**, 912 (2003),
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