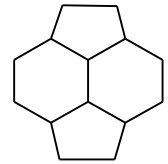
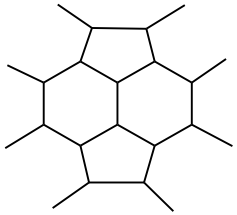
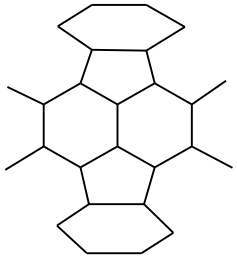
How to draw a C60?



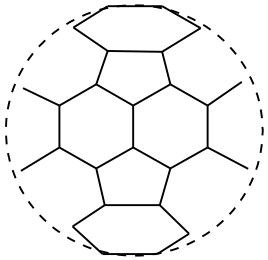
step 1



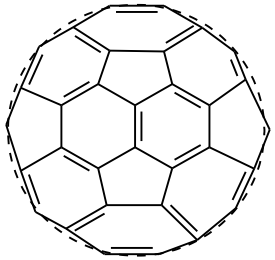
step 2



step 3

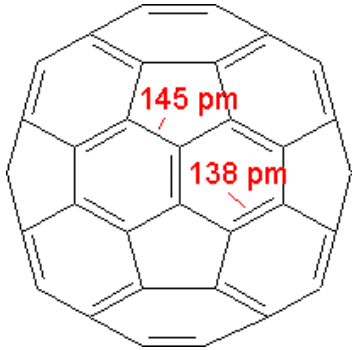


step 4



step 5

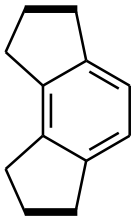
(no double bonds in pentagons)



The structure of C_{60} can be specifically described as having 12 pentagons and 20 hexagons with the pentagons sharing no common edge and the hexagons sharing edges with another hexagon or a pentagon. All the carbons are tricoordinate, pyramidal and all pentagons and hexagons are planar. Two types of C- C bonds are present in the molecule with differing bond lengths, 1.388 Å for a 6,6 bond (common for two hexagons) and 1.432 Å for a 5,6 bond (common for a hexagon and a pentagon).

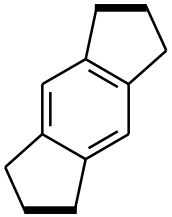
In contrast to C_{60} were all carbon atoms are identical, C_{70} has five different types of carbon atoms depending on the carbon environment. These are easily differentiated by ^{13}C NMR. C_{76}, another fullerene whose X ray structure has been solved belongs to D_2 point group, is chiral and occurs as a racemic mixture.

Stability of C_{60}



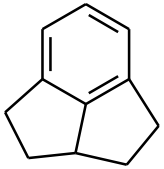
(a)

IPR



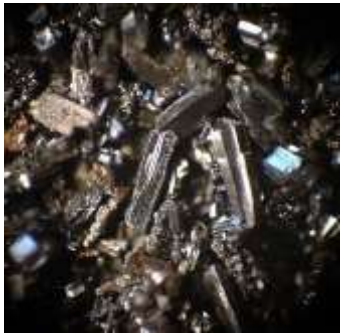
(b)

IPR



(c)

Not-IPR



The unusual stability of C_{60} compared to other higher / lower fullerenes has been explained. In the structure of C_{60} , all the twelve pentagons are isolated from each other. Again only in C_{60} we can see double bonds arranged in such a way that they are located only in six membered rings and none in five membered rings. This is favored as there will be less strain on the already strained five membered rings as a result of such an arrangement. The need to avoid double bonds in pentagons largely governs the stability of fullerenes as the five membered rings with five planar hexagons around are already strained and unsaturation is going to increase the strain further. C_{60} has only arrangement (a) in its structure while C_{70} and C_{84} has five and six of the (b) arrangements in their structures respectively.