

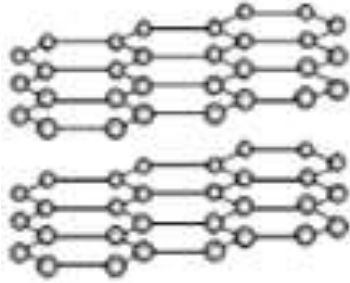
TOPIC- FULLERENES

UG PART I,
p- BLOCK ELEMENTS

By
Dr. PRIYANKA

The inorganic chemistry of Carbon

• Graphite



Layer structure

Application: electrode

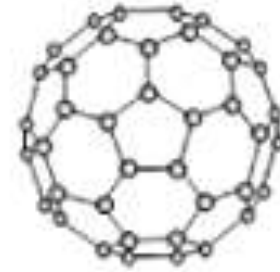
• Diamond



Hardest material in the world

Applications: jewel, cutter

• Fullerene(C60)

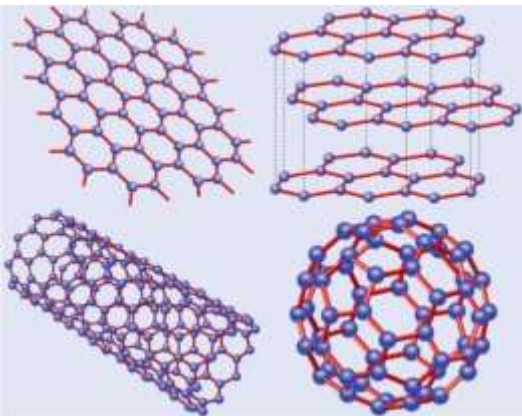


Soccer ball shape molecule

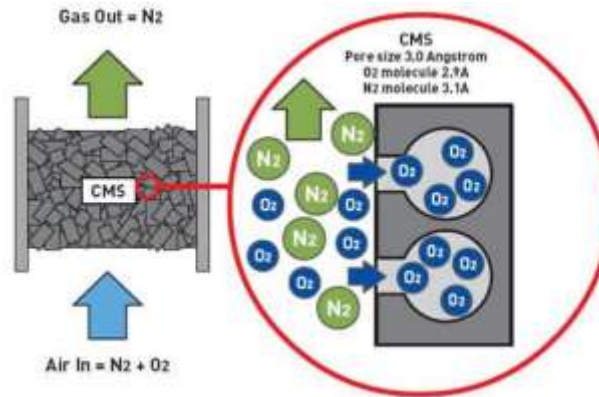
Applications: cosmetics

Diameter ; 0.7nm

Carbon Nano tubes & Graphene



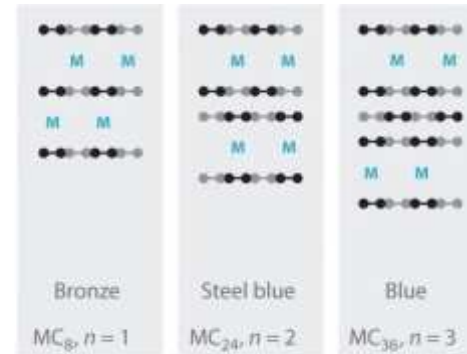
Carbon Molecular Sieves



Graphite intercalated compounds



(a) KC₈



(b) Layer arrangements and stoichiometries

Graphite vs Diamond

Graphite

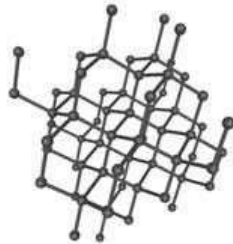
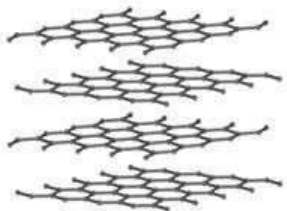


Diamond



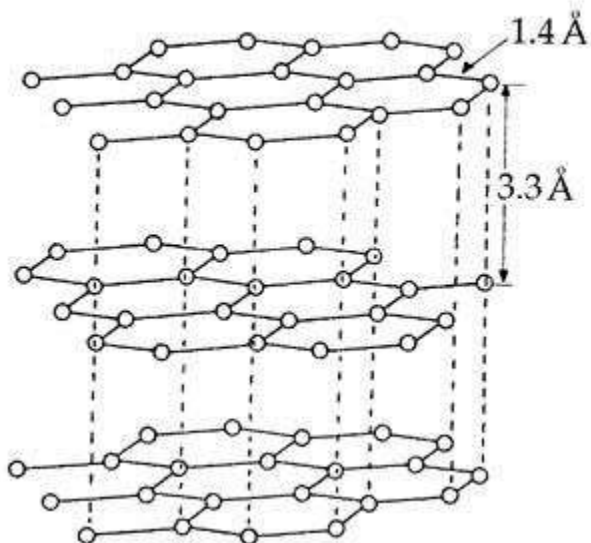
Dull, opaque, soft, common

Brilliant, transparent, hard, rare

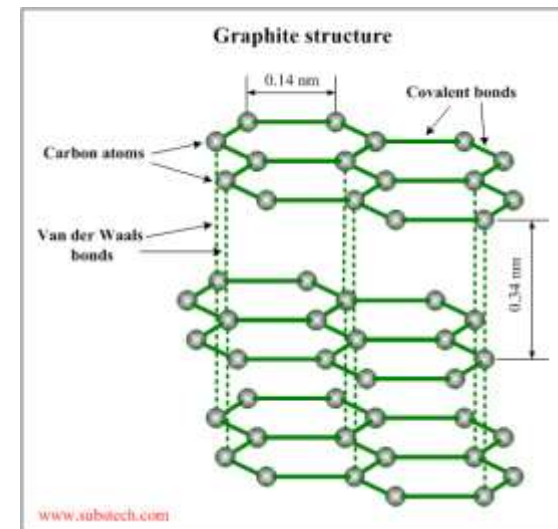
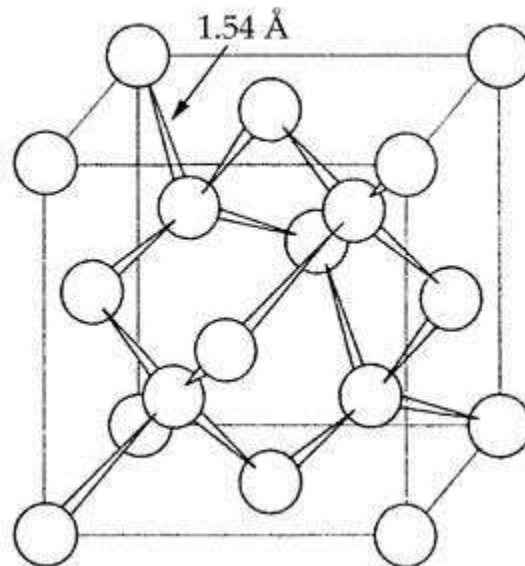


Diamond	Graphite
It occurs naturally in free state	It occurs naturally and is manufactured artificially
It is the hardest natural substance known	It is soft and greasy to touch
It has high relative density (about 3.5)	Its relative density is 2.3
It is transparent and has high refractive index (2.45)	It is black in colour and opaque
It is non-conductor of heat and electricity	Graphite is a good conductor of heat and electricity
It burns in air at 900°C to give CO ₂	It burns in air at 700-800°C to give CO ₂
It occurs as octahedral crystals	It occurs as hexagonal crystals
It is insoluble in all solvents	It is insoluble in all ordinary solvents

graphite



diamond



Fullerenes

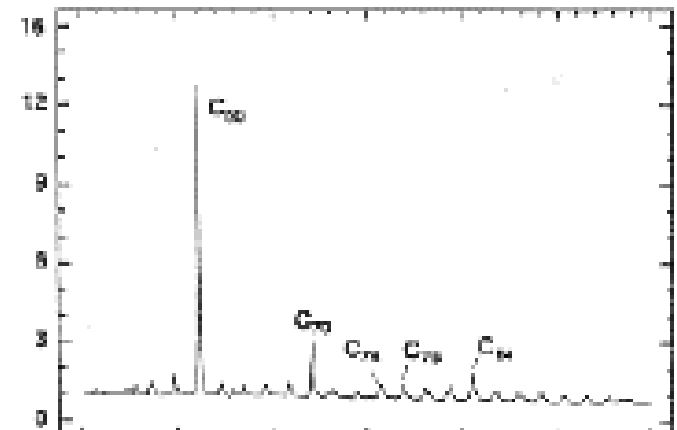
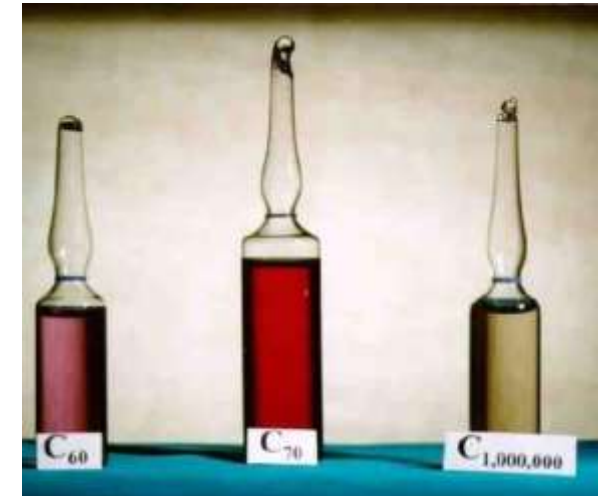
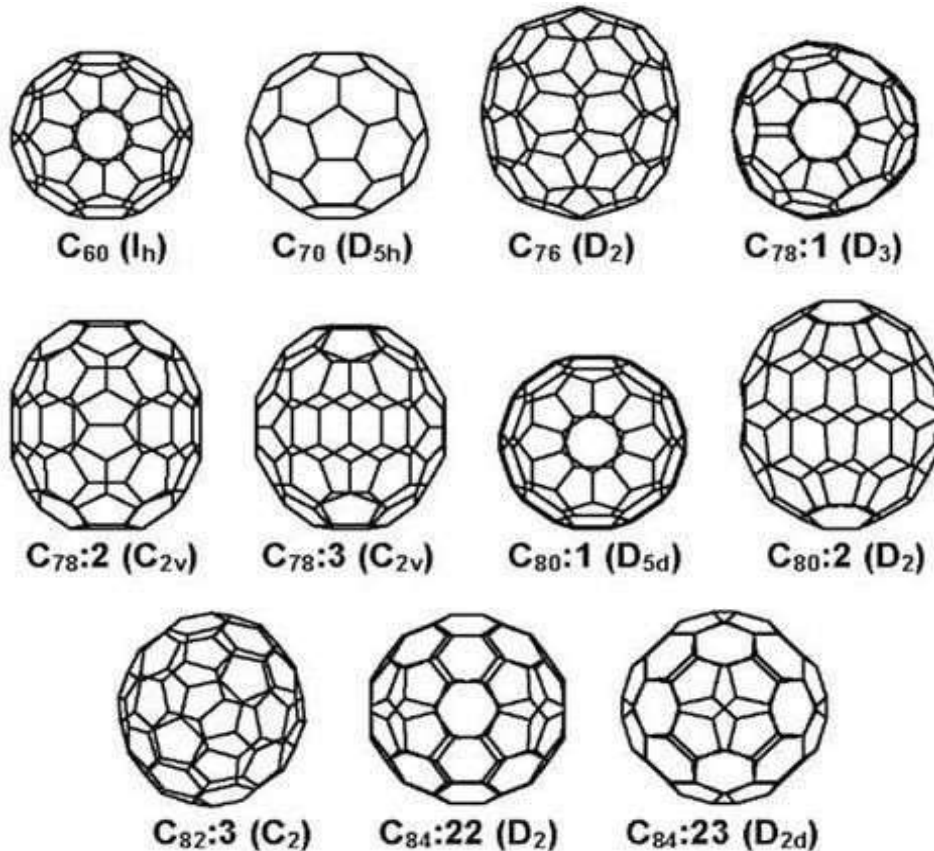
In 1985, Harold Kroto (Sussex), Robert Curl and Richard Smalley, (Rice University,) discovered C_{60} , and shortly thereafter came to discover the fullerenes. Kroto, Curl, and Smalley were awarded the 1996 Nobel Prize in Chemistry for their roles in the discovery of this class of molecules. C_{60} and other fullerenes were later noticed occurring outside the laboratory (for example, in normal candle-soot)..



H. Kroto



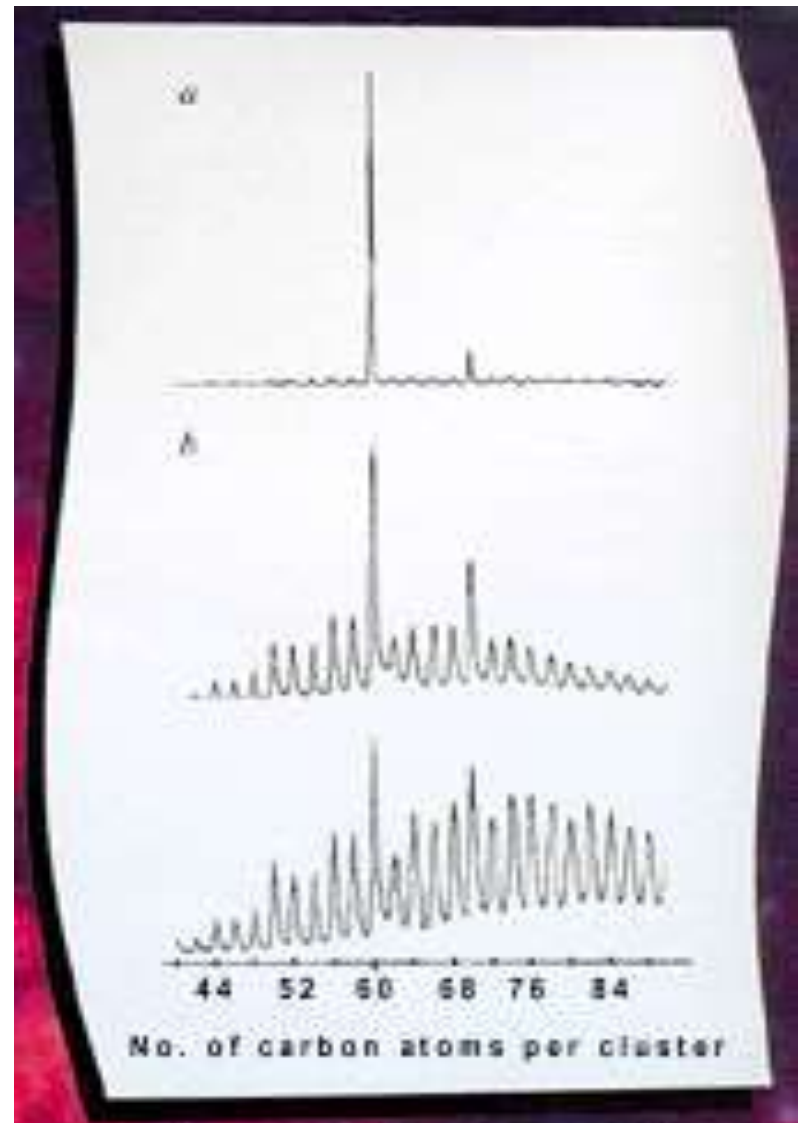
R. Smalley



Fullerenes

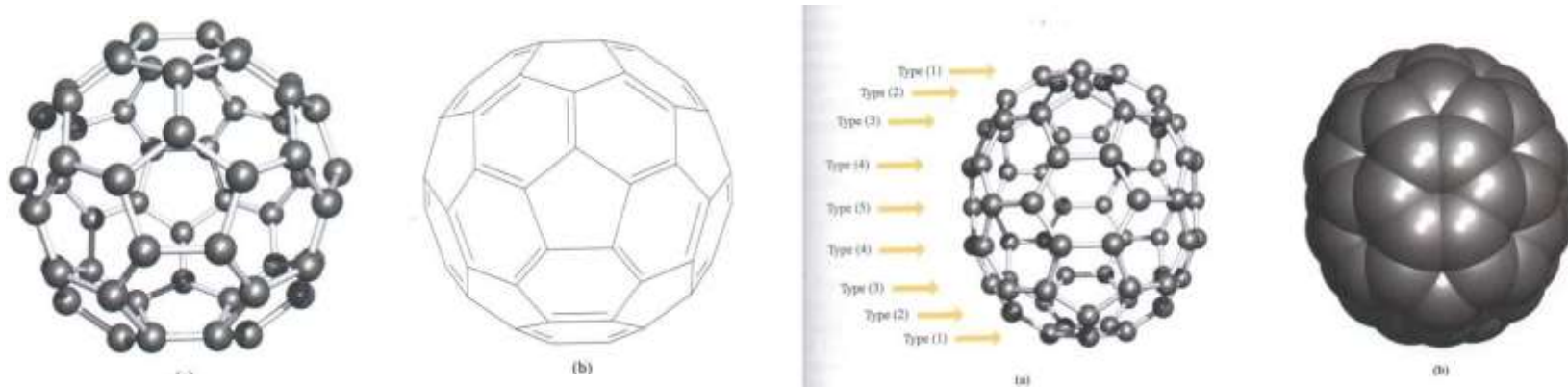
An idea from outer space

Kroto's special interest in red giant stars rich in carbon led to the discovery of the fullerenes. For years, he had had the idea that long-chained molecules of carbon could form near such giant stars. To mimic this special environment in a laboratory, **Curl** suggested contact with **Smalley** who had built an apparatus which could evaporate and analyze almost any material with a laser beam. During the crucial week in Houston in 1985 the Nobel laureates, together with their younger co-workers J. R. Heath and J. C. O'Brien, starting from graphite, managed to produce clusters of carbon consisting mainly of 60 or 70 carbon atoms. These clusters proved to be stable and more interesting than long-chained molecules of carbon. Two questions immediately arose. How are these clusters built? Does a new form of carbon exist besides the two well-known forms graphite and diamond?



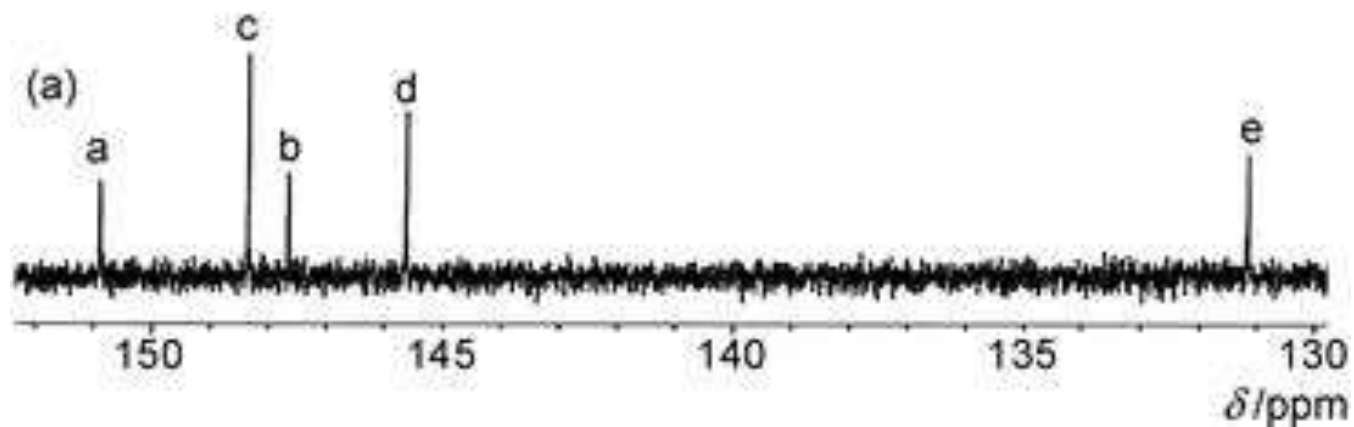
The read-out from the mass spectrometer shows how the peaks corresponding to C_{60} and C_{70} become more distinct when the experimental conditions are optimized.

C_{60} is soccer-ball-shaped or I_h with 12 pentagons and 20 hexagons. According to Euler's theorem these 12 pentagons are required for closure of the carbon network consisting of n hexagons and C_{60} is the first stable fullerene because it is the smallest possible to obey this rule (higher ones C 180, 540). **In this structure none of the pentagons make contact with each other.** Both C_{60} and its relative C_{70} obey this so-called **isolated pentagon rule (IPR)**. Non-IPR fullerenes have thus far only been isolated as endohedral fullerenes such as $Tb_3N@C_{84}$



The double bonds in fullerene are not all the same. Two groups can be identified: 30 so-called [6,6] double bonds connect two hexagons and 60 [5,6] bonds connect a hexagon and a pentagon. Of the two the [6,6] bonds are shorter with more double-bond character and therefore a hexagon is often represented as a cyclohexatriene and a pentagon as a pentalene or [5]radialene. In other words, although the carbon atoms in fullerene are all conjugated the superstructure is not a super aromatic compound. The X-ray diffraction bond length values are 135.5 pm for the [6,6] bond and 146.7 pm for the [5,6] bond.

^{13}C NMR of C_{60} and C_{70}



C_{70} ($\delta = 150.91, 148.36, 147.67, 145.64,$ and 131.15)

