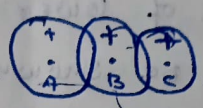
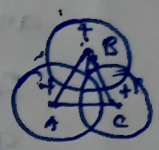
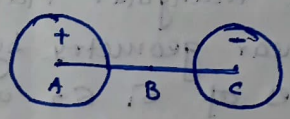
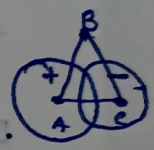
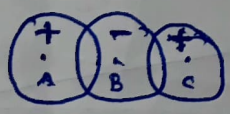
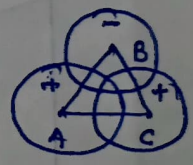
H_3^+ ion:- In H_3^+ ion three 1s orbitals of H_A, H_B, and H_C atoms can overlap with one another to produce equal number of molecular orbitals. The H_3^+ ion thus formed can either have a linear geometry or a triangular planar geometry leading to two different sets of sigma overlaps.

But in both cases the linear combinations of three 1s atomic orbitals can be represented by the same three ψMOs in the following manner:-

Various Combination of AOs of H_A H_B and H_C	Diagramatic Representation for Linear Geometry	Triangular Geometry
$\sigma_1 = \psi_1 MO$ $= \frac{1}{\sqrt{3}}[\psi_{1s(A)} + \psi_{1s(B)} + \psi_{1s(C)}]$		
$\sigma_2 = \psi_2 MO$ $= \frac{1}{\sqrt{2}}[\psi_{1s(A)} - \psi_{1s(C)}]$		
$\sigma_3 = \psi_3 MO$ $= \frac{1}{\sqrt{6}}[(\psi_{1s(A)} - 2\psi_{1s(B)} + \psi_{1s(C)})]$		

It is to be noted that each of the σ_1, σ_2 and σ_3 is a normalised function and that each ψ_{1s} is completely utilised while writing σ_1 σ_2 and σ_3. The sum of the squares of the coefficients of each of ψ_{1s} in σ_1, σ_2 and σ_3 is 1.

For H_3^+ ion having linear geometry, σ_1 which has positive overlaps between the three 1s orbitals, is obviously a bonding molecular orbital

The molecular orbital σ_2 in a linear geometry can not have any overlap and is, therefore non bonding.

while σ_3 having a negative overlap in this geometry is obviously antibonding.

The two electrons of H_3^+ will occupy the bonding Molecular Orbital σ_1 of its geometry is Linear.

For H_3^+ ion having triangular geometry, σ_1 is a bonding molecular orbital having positive overlaps as it is obvious from the figure but σ_2, for which H_A and H_C orbitals form a negative overlap, is antibonding and thus of higher energy than σ_2 of linear geometry.

The molecular orbital σ_3 of triangular geometry is bonding between H_A and H_C involving positive overlaps but is antibonding between H_A and H_B as also between H_B and H_C involving negative overlaps.

Therefore, σ_3 of triangular geometry, though antibonding, is of lower energy than σ_3 of linear geometry. Further it can be shown with the application of group theory that σ_2 and σ_3 of triangular geometry are of equal energy. It can be easily visualised that the triangular planar geometry can be obtained from linear geometry by bending $\angle ABC$ from 180° to 60°. The energies of σ_1 σ_2 and σ_3 as a function of $\angle ABC$ can be calculated if a correlation diagram is drawn for H_3^+ ion.

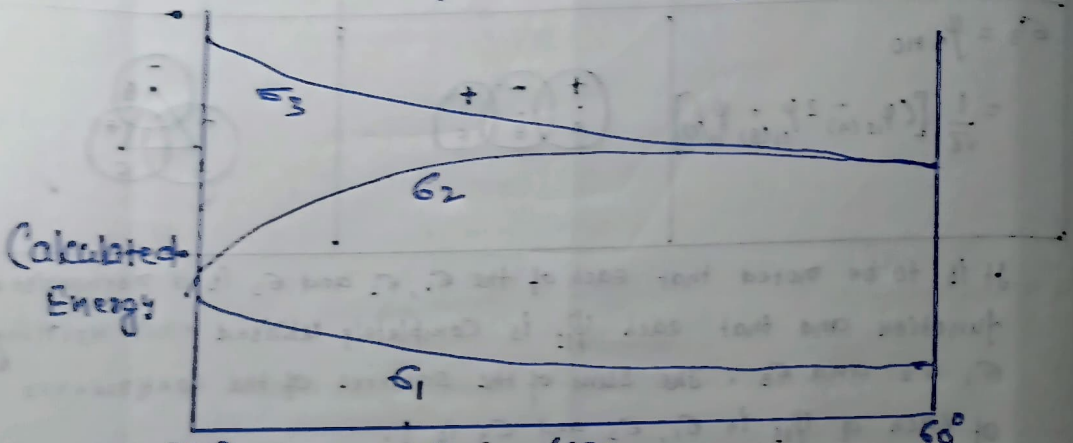


fig. 1

Plot of Calculated energies of molecular orbitals as a function of bond angle.

- By the help of diagram or plot it would be clearly indicate the a triangular geometry of H_3^+ ion is more stable than the linear geometry.

This is because σ_1 bonding molecular orbital which contains both the bonding electrons is of lower energy in the triangular geometry of H_3^+ ion because of greater overlaps amongst H_A, H_B and H_C than in its linear geometry as shown in the above figure.