Walsh Diagram

Walsh diagram is a correlation diagram and predict about geometry of small molecules. This theory introduce in 1953. In this diagram orbital binding energies are plotted against bond angle.

Total energy is the sum of all the orbitals binding energies. Therefore by considering the stabilization or distabilization of all the orbitals by a change in the angle, we can predict the equilibrium bond angle for a given state of a molecule. Only valence ~~electron~~ orbitals are used in plotting walsh diagram because core orbitals are very low in energy.

To understand walsh diagram we will study correlation diagram of BeH_2 and H_2O.

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Thus Walsh diagram is a correlation diagram of change of energy of molecular orbital as molecule distorted from reference molecule. When molecule distorted bond angle changed and bond energy change.

From the desk of DATE

As we know that in MO diagram of BeH_2 four Molecular orbitals are formed.

σ^*_{1s}
σ_{1s} > by overlapping of $2s + Y_1$

$\sigma^*_{2p_x}$
σ_{2p_x} > by overlapping of $2p_x + Y_2$

2 orbital p_y and p_z remains as non bonding. their orbitals are represented as $2\sigma_g, 1\sigma_u, 1\pi_u, 3\sigma_g, 2\sigma_u$

From M.O diagram of H_2O 5 molecular orbitals are formed and one remains as ndn bonding. their molecular orbitals are represented by $2a_1, 3a_1, 1b_2, 1b_1, 4a_1, 2b_2$

Now these molecular orbitals are arranged according to their energies.

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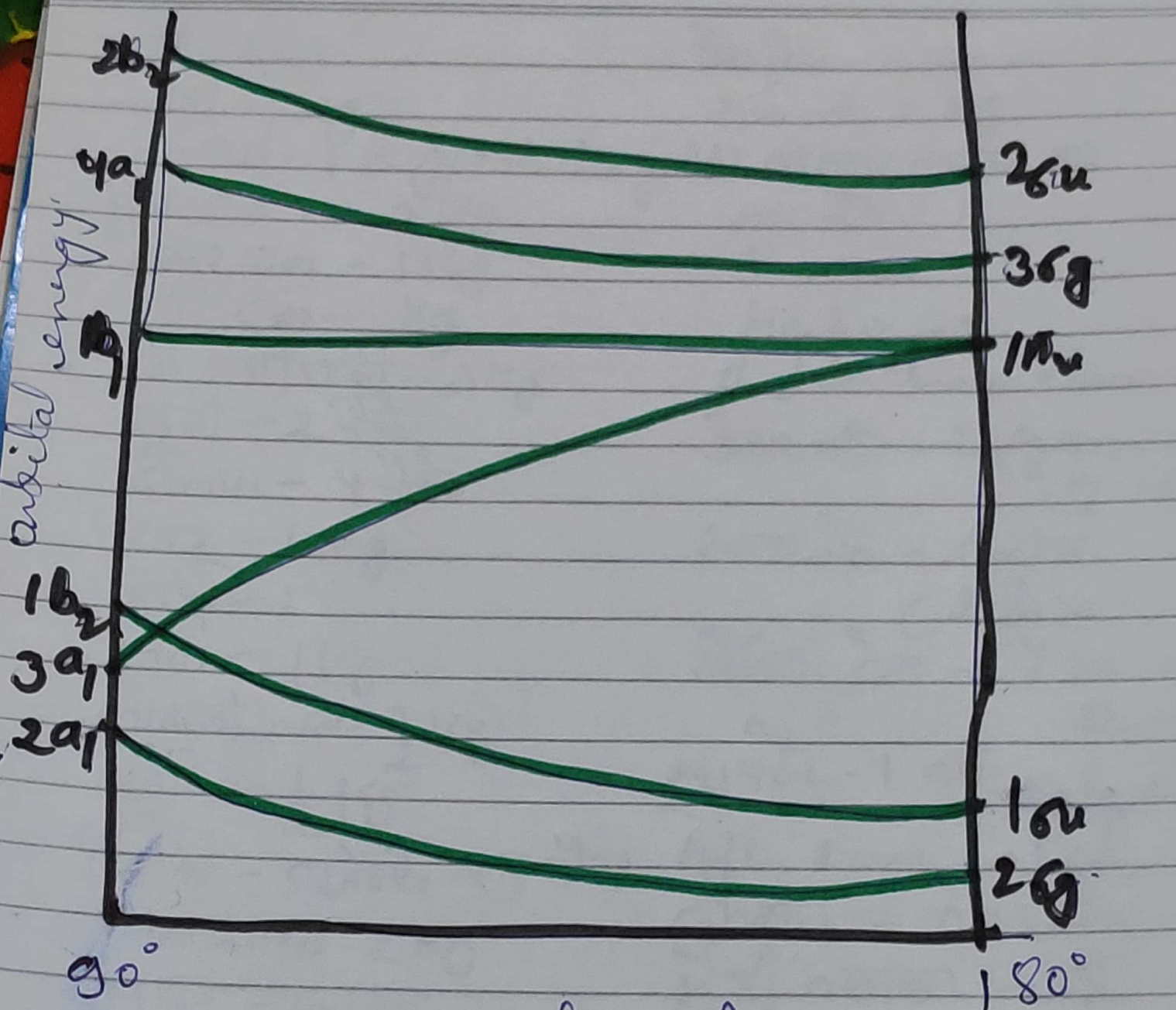

H_2O Bond angle- BeH_2

Walsh diagram for XH_2 molecul

From this diagram it has been observed that - when distortion takes place in H_2O molecule and bond angle changed from 90° to 180° then energy of a_1 orbital slight decreasing but energy of $3a_1$ orbital abnormally increases due to sp mixing and destabilized $1b_2$ orbital is stabilized by slightly decreasing their energies $1b_1$ orbital is non bonding does not change in energy and $4a_1$ and $2b_2$ orbital stabilized by decreasing their energy but all these decreases does not affect as it affected by increasing energy of $3a_1$ orbital therefore. When H_2O molecule mave from bent to linear get distorted. Therefore it prefers bent structure. Similar condition takes place with BeH_2 as it move from 180° to 90° therefore it prefers linear structure

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