Task#85323

Classify the following orbitals as gerade or ungerade: (i) 1s (ii) 2px (iii) 3dxy

Solution: The classification of orbitals into gerade and ungerade is based on centre of symmetry(i) .If the wave function does not change sign on inversion through centre of the orbital is called gerade(g) and if it is change ,is called ungerade(u).

(a)1S: S orbital is spherically symmetric in nature .So, centre of inversion is situated at centre of the sphere. So, inversion through origin(0,0,0) results no change in sign of wave function of 1S orbital So, it is gerade(g) in nature.

(b)2P_X: P orbital is dumbbell shaped.So,two lobes of $2P_X$ is placed along (+) & (-) ve X axis and lobes have opposite sign .So, inversion through origin(0,0,0) results change in sign of wave function of $2P_X$ orbital.So,it is ungerade(u) in nature.

(c) $3d_{xy}$: d orbital is dumbbell shaped. Four lobes are placed along XY plane, where if one lobe is (+)vely charged ,then adjacent lobes are (-)vely charged and vice versa such that two oppositely charged lobes are present at an angle 180° . So, inversion through origin(0,0,0) results no change in sign of wave function of $3d_{xy}$ orbital .So it is gerade(g) in nature.

See the picture of these three orbitals ,I think it is more understandable. Sorry my drawing is not very good but understandable.



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