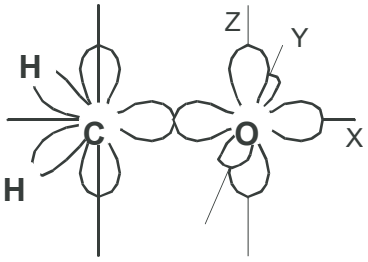
Formaldehyde

CH_2O

Updated 2/10/03



	Symmetry			
	yz	xz	xy	reflected through plane
	x	y	z	along axis
π	even	even	odd	
π^*	odd	even	odd	
n	even	odd	even	
	odd	even	even	μ_x
	even	odd	even	μ_y
	even	even	odd	μ_z

$$\langle \psi_i | \mu | \psi_f \rangle = \langle \psi_f | \mu_x | \psi_i \rangle + \langle \psi_f | \mu_y | \psi_i \rangle + \langle \psi_f | \mu_z | \psi_i \rangle$$

$$\int\int\int \psi_f \mu_x \psi_i \, dx\,dy\,dz + \int\int\int \psi_f \mu_y \psi_i \, dx\,dy\,dz + \int\int\int \psi_f \mu_z \psi_i \, dx\,dy\,dz$$

$\langle \psi^* | \mu | \psi \rangle = \langle \psi^* | \mu_x | \psi \rangle + \langle \psi^* | \mu_y | \psi \rangle + \langle \psi^* | \mu_z | \psi \rangle$

$\pi \rightarrow \pi^*$

$[(ooe)(eee)(oeo)]$ (even even even)

(non-zero)

$\neq 0$ **(allowed)**

$+ [(o\overset{0}{e}e)(e\overset{0}{o}e)(oeo)]$ (odd odd even)

$+ 0$

$+ [(o\overset{0}{e}e)(eee)(o\overset{0}{o}o)]$ (odd even odd)

0

along x along y along z

Example:

$[(oee)(eee)(ooo)]$

$\int_{odd}(oee)\partial x$

$\int_{even}(eee)\partial y$

$\int_{odd}(ooo)\partial z$

$\langle \psi^* | \mu | n \rangle = \langle \psi^* | \mu_x | n \rangle + \langle \psi^* | \mu_y | n \rangle + \langle \psi^* | \mu_z | n \rangle$

$n \rightarrow \pi^*$

$[(ooe)(e\overset{0}{e}o)(o\overset{0}{e}e)]$ (even odd odd)

0

$= 0$ **(forbidden)**

$+ [(oee)(eoo)(o\overset{0}{e}e)]$ (even even odd)

$+ 0$

$+ [(oee)(e\overset{0}{e}o)(ooe)]$ (even odd even)

$+ 0$

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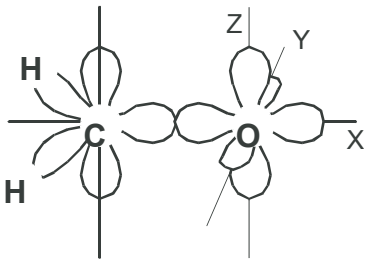
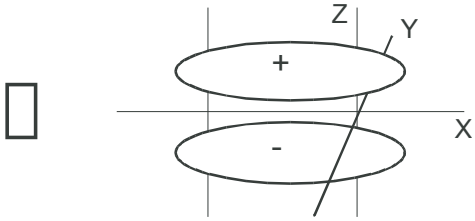
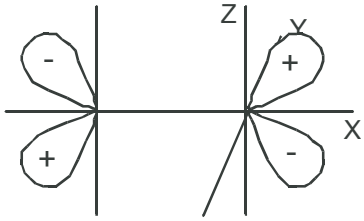


Symmetry

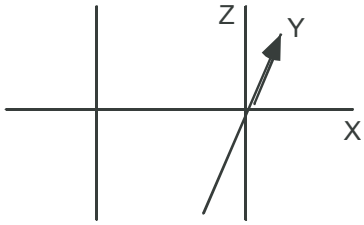
	yz	xz	xy	reflected through plane
	x	y	z	along axis



π



π*



even even odd

odd even odd

even odd even μ_y

$[(o\ e\ e)_{odd}\ (e\ o\ e)_{odd}\ (o\ e\ o)_{even}]$

$\left(\int\int\int \mu_y\, \partial x\right)\left(\int\int\int \mu_y\, \partial y\right)\left(\int\int\int \mu_y\, \partial z\right)$

$\left(\int\int\int \psi_f \mu_y \psi_i\, \partial x\right)\left(\int\int\int \psi_f \mu_y \psi_i\, \partial y\right)\left(\int\int\int \psi_f \mu_y \psi_i\, \partial z\right)$

$\langle \psi^* | \mu_y | \psi \rangle$

$\langle \psi_f | \mu_y | \psi_i \rangle$

$\int\int\int \psi_f \mu_y \psi_i\, \partial x \partial y \partial z$