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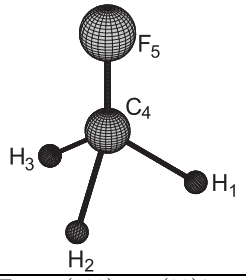
Fundamentals of Molecular Symmetry ***Exercises***

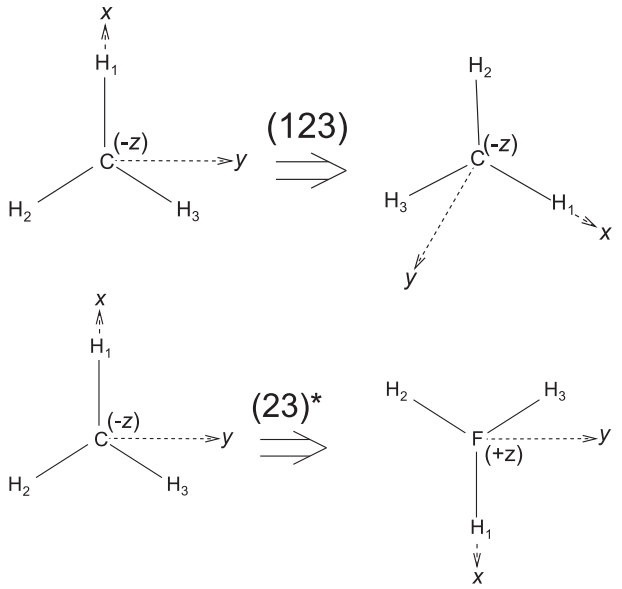
Week 11/11

11.1 We consider the molecule CH_3F discussed in the lecture; the numbering of the nuclei and the character table of the molecular symmetry group $\boldsymbol{C}_{3v}(M)$ are as follows:



	E	(123)	$(23)^*$		
$\boldsymbol{C}_{3v}(M)$:	1	2	3		
$\boldsymbol{C}_{3v}$:	E	$2C_3$	$3\sigma_v$		
Equiv. rot.:	R^0	${R_z}^{2\pi/3}$	${R_{\pi/2}}^{\pi}$		
A_1:	1	1	1	:	T_z
A_2:	1	1	-1	:	R_z, Γ^*
E:	2	-1	0	:	$(T_x, T_y), (R_x, R_y)$

The right-handed molecule-fixed axis system xyz for CH_3F is chosen such that the z axis lies along the CF bond, pointing from C towards F, and the x axis lies in the plane defined by the nuclei C, F, and proton H_1, and pointing from the CF axis towards H_1. The following two sketches show how the xyz axis system is affected by the (123) and $(23)^*$ operations, respectively. "$(-z)$" indicates that the z axis points into the plane of the paper; "$(+z)$" that it points out of the paper plane.



a) Consider a point in space with coordinates (x, y, z) in the molecule-fixed axis system. Determine the coordinates (x', y', z') of this point in the new molecule-fixed axis systems resulting from the application of (123) and $(23)^*$, respectively.

b) Use Cartesian displacement coordinates to determine the representation Γ_Q of $\boldsymbol{C}_{3v}(\mathrm{M})$ (expressed in terms of the irreducible representations) generated by the normal coordinates Q_r of CH_3F.

c) Determine the representation of $\boldsymbol{C}_{3v}(\mathrm{M})$ generated by the dipole moment components (μ_x, μ_y, μ_z) along the molecule-fixed axes for CH_3F. Determine also the symmetrized linear combinations of (μ_x, μ_y, μ_z).