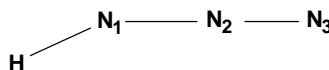


*Fundamentals of Molecular Symmetry*  
*Week 6/11*

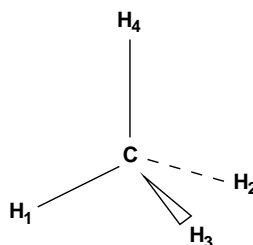
*Exercises*

6.1 Determine the molecular symmetry group (MS group) for the following molecules. When only one structure is indicated, you can assume that the corresponding minimum of the potential energy surface is separated by all other minima by very high barriers, and that no effects of tunneling through these barriers have been observed.

a)  $\text{HN}_3$



b)  $\text{CH}_4$



c) Projection operators for one-dimensional representations are constructed as follows:

$$P^{\Gamma_i} = \frac{1}{h} \sum_R \chi^{\Gamma_i}[R]^* R$$

Such an operator projects wavefunctions and coordinates into a sub-space of functions transforming according to the irreducible representation  $\Gamma_i$ . The wavefunctions/coordinates obtained by the projection have the symmetry  $\Gamma_i$ .

Consider again the methane molecule with its four bond lengths  $r_1, r_2, r_3, r_4$  (Problem 5.2).

Apply the projection operator for the totally symmetric representation ( $A_1$ ) to  $r_1$ . Which totally symmetric coordinate do you obtain?