What is Symmetry in Chemistry?

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Part 1 H_2O & H_2O_2

1. H_2O :

a) Total Energy: -76.418 Hartree Point Group: C_{2v}

List the symmetry elements:

b) Identity E, Two Symmetry Planes σ, C_2 Axis of symmetry

2. 1.5 Å Stretched H_2O :

Total Energy: -76.319 Hartree Point Group C_s

List the symmetry elements:

E, One Symmetry Plane σ

3. Planar H_2O_2 :

a) Total Energy: -151.550 Hartree Point Group: C_{2h}

List the symmetry elements:

E, One Symmetry Plane σ, C_2 Axis of symmetry, and one point of symmetry i

4. Optimized H_2O_2 :

Total Energy: -151.551 Hartree Point Group: C_2

List the symmetry elements:

E, C_2

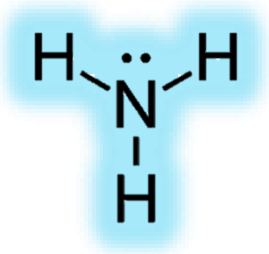
5. Why does the point group symmetry change when one of the O-H bond lengths in water is longer than the other and when hydrogen peroxide is not planar?

Because the symmetry elements have changed hence the point group symmetry.
In the water, we removed one symmetry plane and axis by stretching the bond.
In H2O2, we removed one point of symmetry and one axis of symmetry. Which resulted in changing the point group symmetry.

Part 2 Choose a molecule

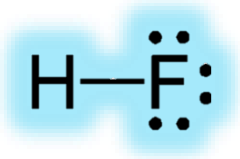
1. C_s Molecule: Ammonia

Total Energy: -56.554 Hartree Lewis Structure:



2. $C_{\infty v}$ Molecule: Hydrogen fluoride

Total Energy: -100.436 Hartree Lewis Structure:



3. D_{2h} Molecule: Oxalate ion

Total Energy: -377.037 Hartree Lewis Structure: