

Symmetry in Chemistry - Assignment 1

Due date: April 11, 2021

(For each solution, show your work through a set of important steps)

1. Identify the symmetry elements in cubane (assume all H atoms are along the body diagonals). (3 Pts)

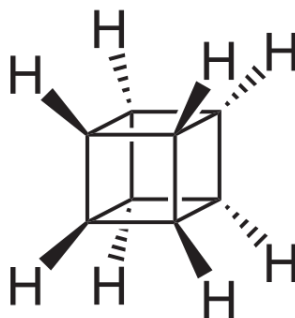


Fig 1. Molecular structure of cubane

2. For an improper rotation with an *odd* order, how many unique symmetry operations can be generated? (2 Pts)
 3. What do these combination of symmetry operations represent? (4 pts)
 - (a) $S_4^2(z) \cdot i$
 - (b) $C_8^2(z) \cdot C_4^1(z) \cdot \sigma_{xy}$
 - (c) $\sigma_{xy} \cdot \sigma_{yz} \cdot \sigma_{xz} \cdot C_8^1(z)$
 - (d) $C_4^1(z) \cdot C_2^1(z) \cdot S_2^1(x)$
 4. Verify the validity of all five commutation rules using specific examples of symmetry operations. (5pts)
 5. Derive a general matrix representation of a reflection operation that is carried out using a mirror plane containing the z-axis; the mirror plane can be arbitrarily oriented w.r.t to the x and y-axis. (4 pts)
 6. A point (1,-1,2) in a 3D Cartesian space is subjected to a clockwise rotation about the y-axis by an angle of 45° followed by a reflection about the xz-plane. Locate the point in the space. Also, check if the transformation represents any of symmetry operations. (2 pts)
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