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3. External Nuclear Motions

3.2 External rotation

Rotational symmetry number

[examples]

H₂O (C_{2v}): $\sigma = 2 \cdot 1 = 2$

SF₆ (O_h): $\sigma = 6 \cdot 4 = 24$

C₂H₆ (D_{3d}): $\sigma = 6 \cdot 1 = 6$

C₆H₆ (D_{6h}): $\sigma = 6 \cdot 2 = 12$

[Exercise-3.1] Count rotational symmetry number of following molecules.

(1) CO₂

(2) CH₄

(3) C₂H₄

(4) NO₃ (planar)

(5) CH₃I

(6) CHF₂Cl

Number of isomers (chirality)

[examples]

HFCO (C_s): achiral ($n_{\text{isom}} = 1$)

CHFClBr (C_1): chiral ($n_{\text{isom}} = 2$)

NH₂F (C_s): achiral ($n_{\text{isom}} = 1$)

H₂O₂ (C_2): chiral ($n_{\text{isom}} = 2$)

[Exercise-3.2] Determine whether the molecule is chiral ($n_{\text{isom}} = 2$) or achiral ($n_{\text{isom}} = 1$).

(1) HDO

(2) SF₆

(3) NHDF

(4) CH₃OH

(5) *gauche*-CH₂Cl-CH₂Cl (*gauche*-1,2-dichloroethane)