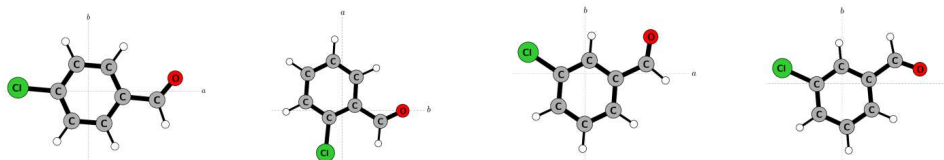


RA06: Microwave Study of Mono-Chlorobenzaldehydes

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Rotational study of four chlorobenzaldehyde species

Benchmarking

Methods: B2PLYP, B3LYP, B97, B97M, BP86

Dispersion corrections: D3, D4

Basis sets: def2-TZVPP, x2c-tzvppall-2c, x2c-tzvppall-s

Projection of quadrupolar coupling tensor into the principal axis system fails for ortho-chlorobenzaldehyde

