

isotopologue

A molecular entity that differs only in isotopic composition (number of isotopic substitutions), e.g. CH₄, CH₃D, CH₂D₂.

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isotopomer

Isomers having the same number of each isotopic atom but differing in their positions. The term is a contraction of 'isotopic isomer'.

Isotopomers can be either constitutional isomers (e.g. CH₂DCH=O and CH₃CD=O) or isotopic stereoisomers [e.g. (*R*)- and (*S*)-CH₃CHDOH or (*Z*)- and (*E*)-CH₃CH=CHD].

1994, 66, 1132; 1996, 68, 2211