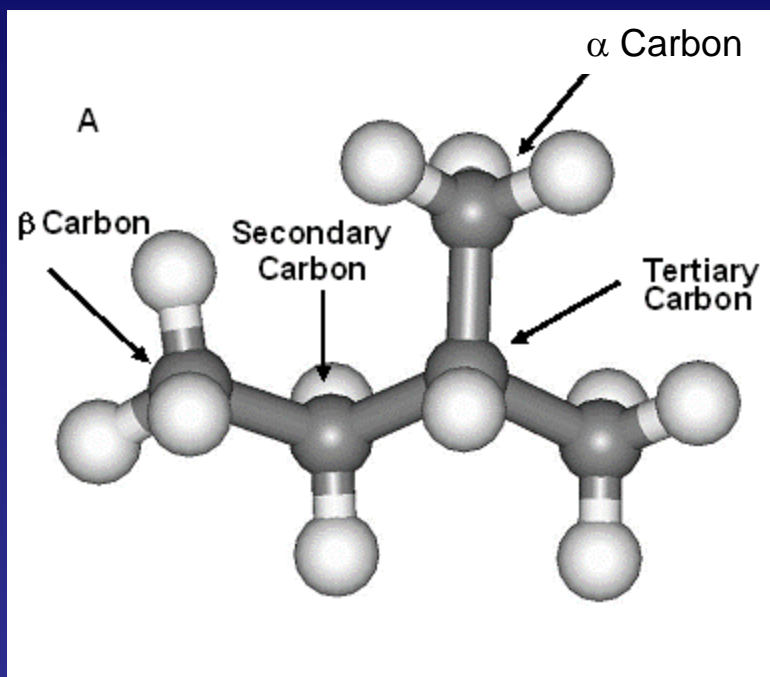


Quantum Mechanical Calculation of Hydrogen Isotope Exchange Thermodynamics and Kinetics on Petroleum Model Compounds

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The H-D exchange reaction of various sites on alkanes has been predicted to be significantly faster with aluminol (i.e., Al-OH and Al-OH₂) that exist on mineral surfaces than with H₂O.

Various sites on kerogen/petroleum components are modeled for the thermodynamics and kinetics of H-D exchange with water & minerals.

