

Reaction Pathways, P-T Ranges, and Kinetic Constraints at the Core Mantle Boundary					
Reaction/Process	P-T Conditions	Reactants	Products	Key Details/Notes	Fate/Implications
Dehydration of deep-transported hydrous phases	Steep geothermal gradient near CMB	Hydrous minerals (e.g., δ -H, D, E, δ -H solid solution)	Fluids (water)	Hydrous minerals like δ -H solid solution are significant carriers of water to the base of the lower mantle. The steep geothermal profile at the CMB leads to their decomposition. Dissolution of the phase H component further lowers the decomposition temperature.	Release of water (fluids) at the base of the lower mantle, providing water for subsequent reactions with the core. This process is linked to the deep water cycle. Hydrated regions may create LLSVPs (Large Low Shear Velocity Provinces).
Reaction between iron (core) and water (mantle) at high P-T	Deep lower mantle / CMB conditions (~96-137 GPa, >2200 K)	Iron (Fe) from core, water (H_2O) released from mantle	Pyrite-structured FeO_2H_x (Py-phase), Iron Hydride (FeH or FeH_x)	At pressures significantly higher than ~5 GPa, water acts as a strong oxidizer, pushing iron oxidation beyond FeO to the oxygen-rich FeO_2H_x . This reaction is observed experimentally at conditions relevant to the deep lower mantle/CMB. The specific reaction is given as $4Fe + 2H_2O \rightarrow FeO_2H_x + 3FeH$. This reaction occurs where hydrated slab material touches the core.	Leads to the formation of an oxygen-rich interlayer (ORP) at the CMB. This interlayer includes FeO_2H_x and FeH. The growth of this layer depends on the available water supply. This reaction is potentially a mechanism for forming ULVZs and is frequently mentioned as a possible product at the CMB.
Alternative Iron-Water reaction at high pressure	Pressures > ~5 GPa (Lower mantle)	Iron (Fe), Water (H_2O)	Iron Hydride (FeH), Iron Oxide (FeO)	Proposed reaction: $3Fe + H_2O \rightarrow FeO + 2FeH$. Occurs at pressures above ~5 GPa. The resultant FeO can react with silicates or descend with FeH into the core. This reaction was proposed for primordial Earth but is also relevant to ongoing core-mantle interactions.	Sequesters hydrogen within the core as FeH. The resultant FeO can participate in partition reactions, forming (Mg,Fe)O and (Mg,Fe)SiO ₃ . This process is referred to as iron-water exchange and is initiated by water-induced iron oxidation.
Reaction between Fe-Si alloys (core) and water (mantle)	CMB conditions (~110-137 GPa, >3000 K)	Fe-Si alloy, Water (H_2O) from hydrous minerals	Iron Hydride (FeH _x or FeH), Silica (SiO ₂) phases	Experiments using Fe-Si alloys (e.g., Fe-9wt%Si) and hydrous silicates (e.g., lizardite+enstatite or $Al(OH)_3 + MgSiO_3$) show the formation of FeH _x and SiO ₂ phases. This indicates a chemical exchange where Si from the core is oxidized to form SiO ₂ (which may react with mantle minerals) while H from water is incorporated into the core as FeH _x . Redox reaction: $Si^0(metal) + 2H_2O \rightarrow 4H^+(metal) + SiO_2$.	Enables exchange of hydrogen and silicon between the mantle and the core. The resulting H-rich, Si-deficient layer at the topmost core is less dense and has lower seismic velocity, potentially contributing to the E' layer. SiO ₂ may react with ferropericlase to form bridgmanite or post-perovskite in the mantle.
Decomposition/Instability of Pyrite-structured FeO_2H_x	Near the CMB, above a critical temperature (>2300 K for reaction with CO ₂), prolonged heating	FeO_2H_x	FeO-rich layers, release of hydrogen (H_2O or H_2), Oxygen (O ₂) release possible if $x \neq 1$	FeO_2H_x is thermally unstable and likely decomposes near the CMB. A recent study suggests that under realistic water supply, FeO_2H_x becomes unstable and loses hydrogen. The dissolved hydrogen in FeO_2H_x decreases with increasing temperature and prolonged heating. Carbonation by CO ₂ can also destabilize FeO_2H_x , yielding $Fe_4C_3O_{12}$ and H_2O .	FeO_2H_x cannot be the direct source of ULVZs due to its instability and likely decomposition near the CMB. Its decomposition leads to the local accumulation of FeO-rich layers at the bottom of the mantle. This process releases hydrogen, which can then escape and circulate upwards. Oxygen release could cause geodynamic instability.
Melting and Decomposition of Iron Hydride (FeH _x)	Melts at ~1000 K lower temperature than major lower mantle silicates/oxides, quenched from >1000 K above melting temp	FeH _x	Iron (Fe), Hydrogen (H)	FeH melts at a significantly lower temperature than surrounding mantle minerals. Higher temperature or melting enhances hydrogen solubility in liquid iron, but quenched samples show larger volume expansion if quenched from above melting, suggesting H is incorporated into the melt.	Melting of FeH leads to the release of hydrogen. This free hydrogen is light and mobile. Hydrogen escapes from FeH _x and ascends upwards, sustaining the hydrogen cycle. This process contributes to the overall movement of hydrogen back towards the surface.
Hydrogen Ascent Through the Mantle	Mantle conditions (grain boundaries, potentially forming hydrocarbons)	Free Hydrogen (H) from FeH _x melting/decomposition or FeO_2H_x decomposition	Hydrogen, potentially forming hydrocarbons	Hydrogen is light and mobile. It can infiltrate through grain boundaries of mantle minerals or react to form other volatiles. Carbonation reactions involving FeO_2H_x can also release H_2O into the deep mantle.	Completes the deep hydrogen cycle by moving hydrogen (or H-bearing fluids/volatiles) from the CMB region towards the surface. This ascent can impact mantle properties like viscosity and contribute to magma generation. Hydrogen can be oxidized to water primarily in the crust. Hydrogen returning to the surface via precipitation can re-enter the cycle.
Accumulation of FeO-rich layers at the CMB	Bottom of lower mantle	FeO from Fe-water reactions, potentially residual from FeO_2H_x decomposition	FeO-rich zones (potential ULVZ component)	FeO is a product of Fe-water reactions. The instability and decomposition of FeO_2H_x lead to local accumulation of FeO-rich layers. This accumulation is aided by the high mobility of water and strong partitioning of hydrogen into liquid iron. FeO enrichment increases density and decreases seismic velocities. High Fe diffusivity in ferropericlase (an FeO-bearing phase) aids the growth of these regions.	Accumulated FeO-rich layers are a strong candidate for explaining ULVZs. The increase in FeO content, especially in ferropericlase, leads to decreased seismic velocities and increased density consistent with ULVZ properties. FeO at the boundary can aid core-mantle coupling. Partial melting of these FeO-rich regions can also occur, which increases conductivity.
Reaction of FeO_2H_x with CO ₂ (carbonation)	Above 107 GPa, >2300 K (can occur as shallow as 1200 km in hot slabs)	FeO_2H_x , CO ₂	Tetrahedral carbonate $Fe_4C_3O_{12}$, H_2O	This reaction demonstrates interaction between carbon and hydrogen cycles in the deep mantle. The presence of CO ₂ can destabilize FeO_2H_x . Reaction can be schematized as $4FeOOH + 3CO_2 \Rightarrow Fe_4C_3O_{12} + 2H_2O$ or $4FeO_2H_x + 3CO_2 + 2(1-x)H_2 \Rightarrow Fe_4C_3O_{12} + 2H_2O$. $Fe_4C_3O_{12}$ is a candidate for a stable carbon host in the lower mantle.	Provides an additional mechanism for hydrogen release as H_2O within the deep lower mantle, adding to dehydration reactions and dehydrogenation. Highlights the complexity and interdependence of deep carbon and hydrogen cycles.