

Chemical Processes under Extreme Conditions

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High pressure and temperature can significantly alter the electronic structure of a material. Chemical processes under these conditions may not be easily predicted or rationalized with conventional and intuitive chemical principles. In this study, we explore the reaction of H₂ and H₂O on several representative minerals over a broad pressure and temperature range, in the solid and molten state. The results unveil diverse chemical interactions and reaction products. An example is the observation on the formation of “diamondiods” coexist with molecular water was found in the simulation of the reaction of H₂ with CaCO₃. Subsequent experiment validation this prediction.