Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

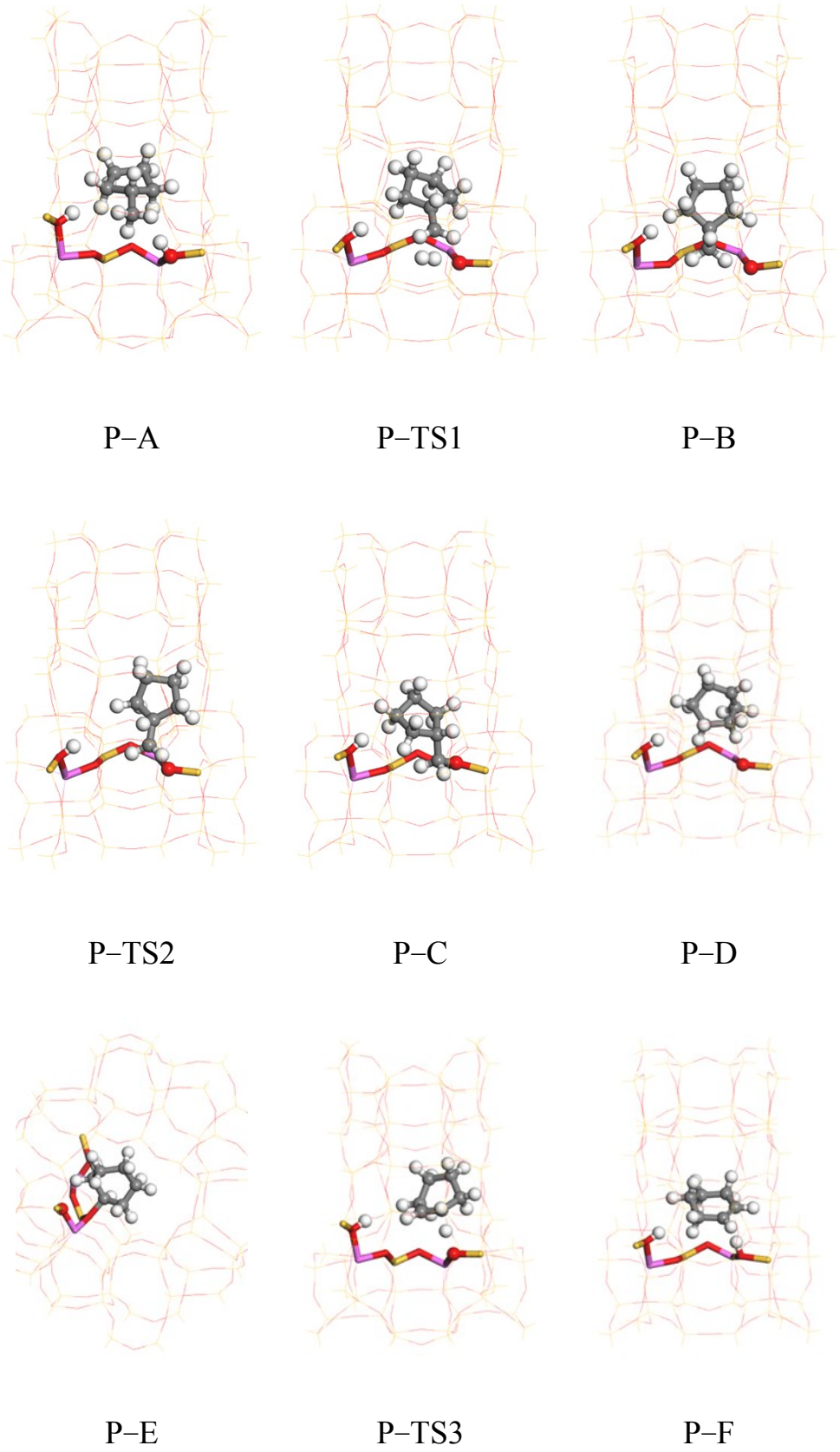


Fig. S1 The geometry structures of reactants, products, intermediates and transition states of

methylcyclopentane to cyclohexene through primary carbon mechanism on H−Z_1.

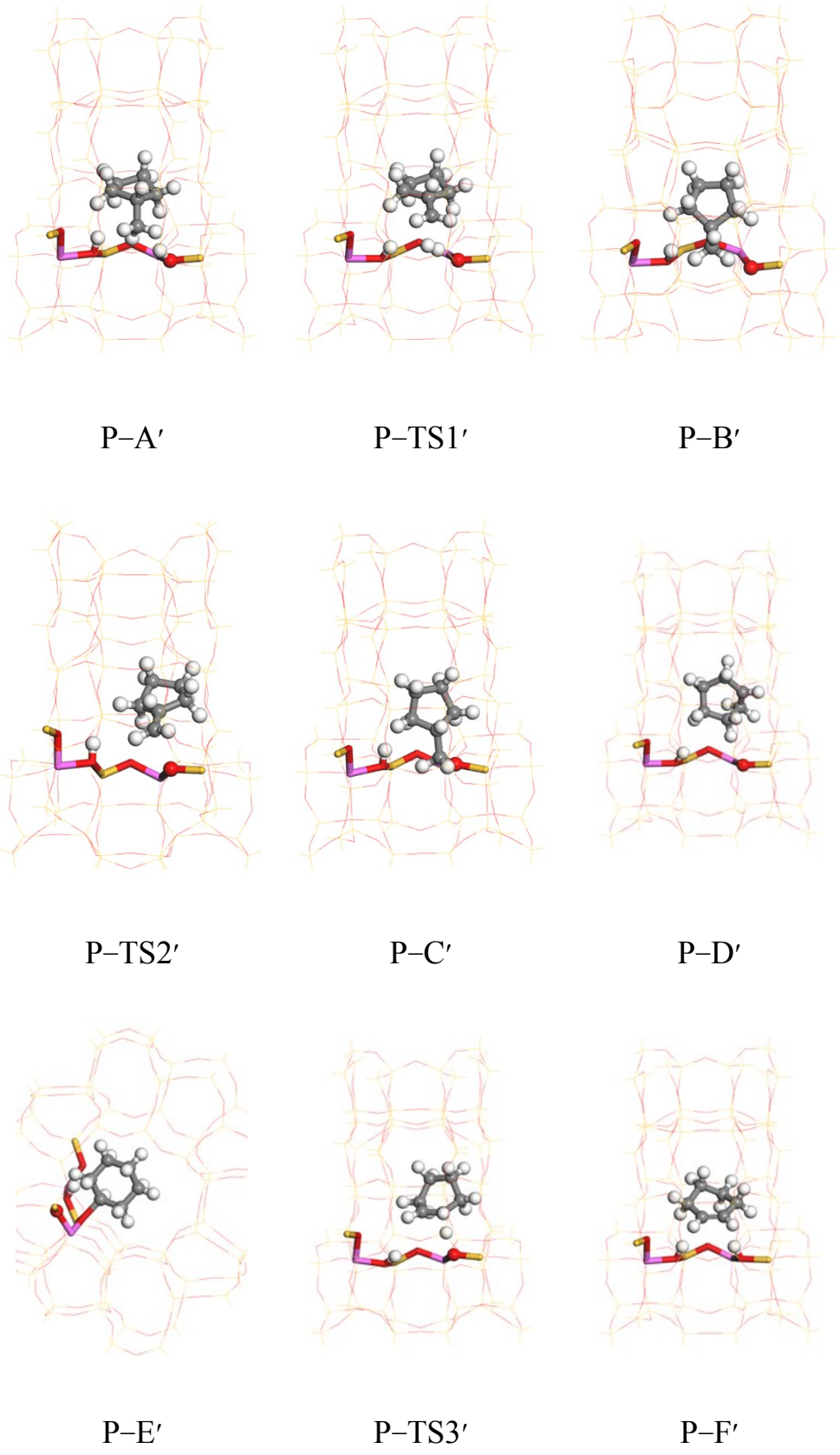


Fig. S2 The geometry structures of reactants, products, intermediates and transition states of

methylcyclopentane to cyclohexene through primary carbon mechanism on H−Z_2.

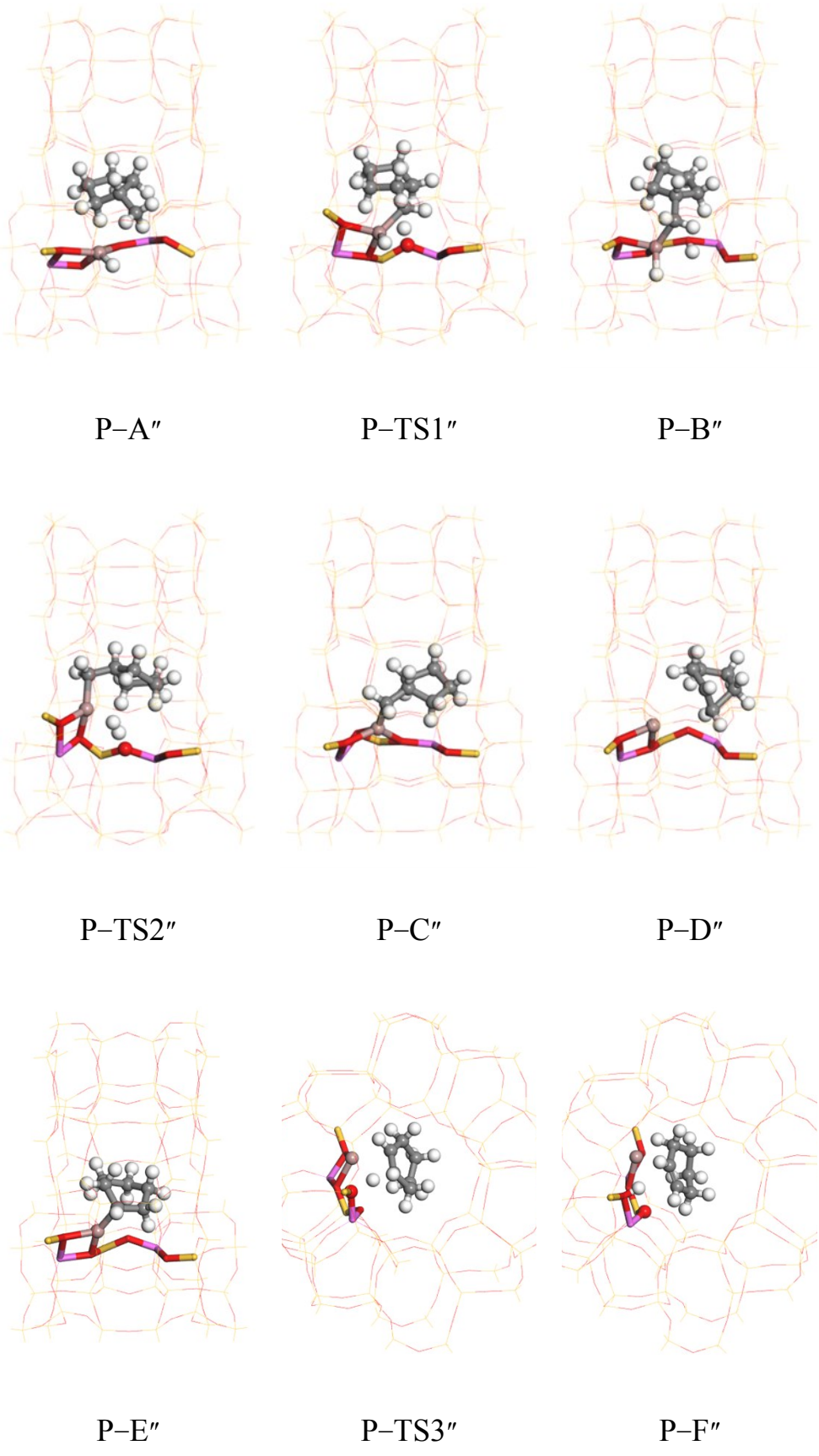


Fig. S3 The geometry structures of reactants, products, intermediates and transition states of

methylcyclopentane to cyclohexene through primary carbon mechanism on Ga−ZSM−5.

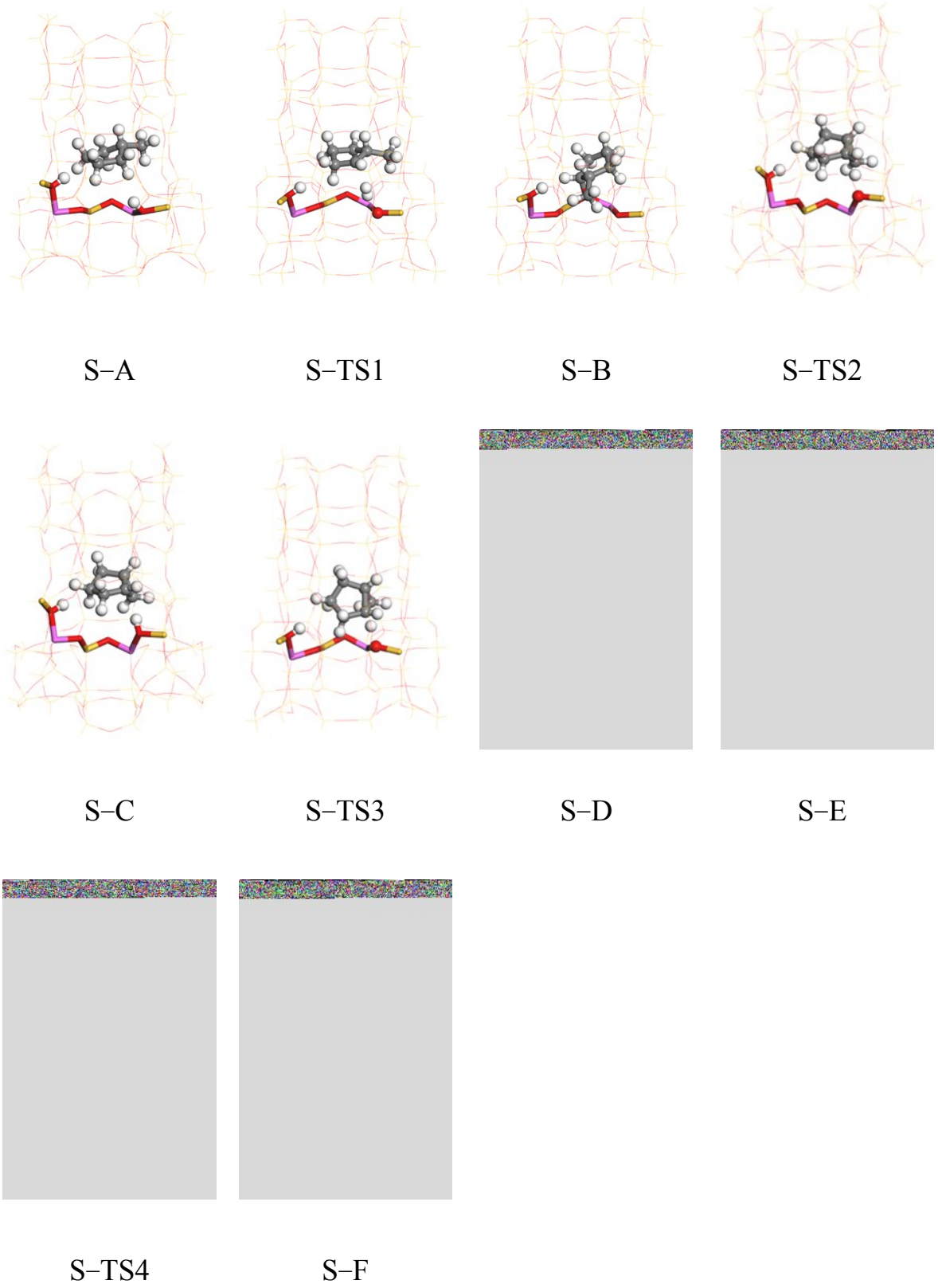


Fig. S4 The geometry structures of reactants, products, intermediates and transition states of methylcyclopentane to cyclohexene through secondary carbon mechanism on H−Z_1.

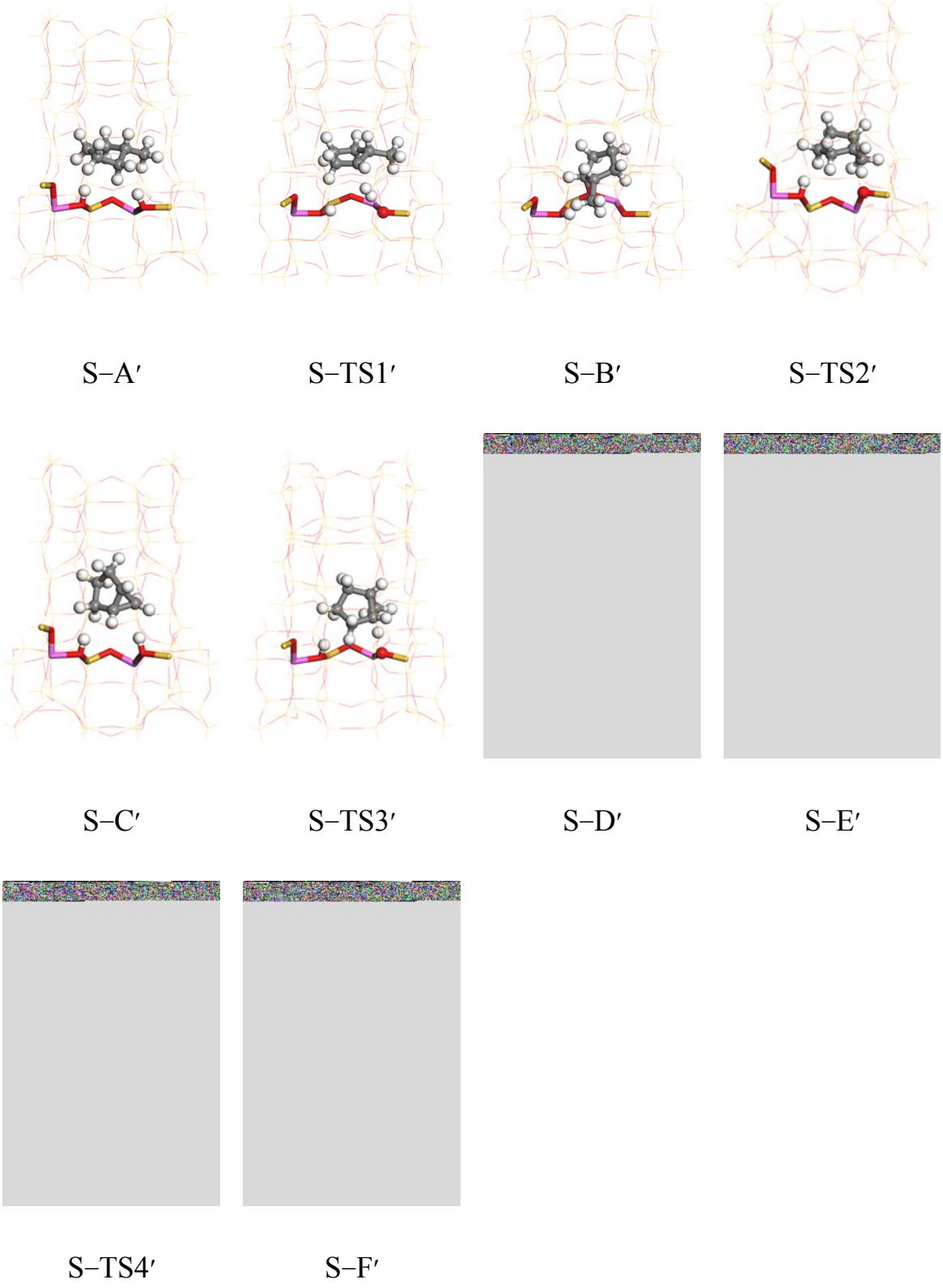


Fig. S5 The geometry structures of reactants, products, intermediates and transition states of methylcyclopentane to cyclohexene through secondary carbon mechanism on H−Z_2.

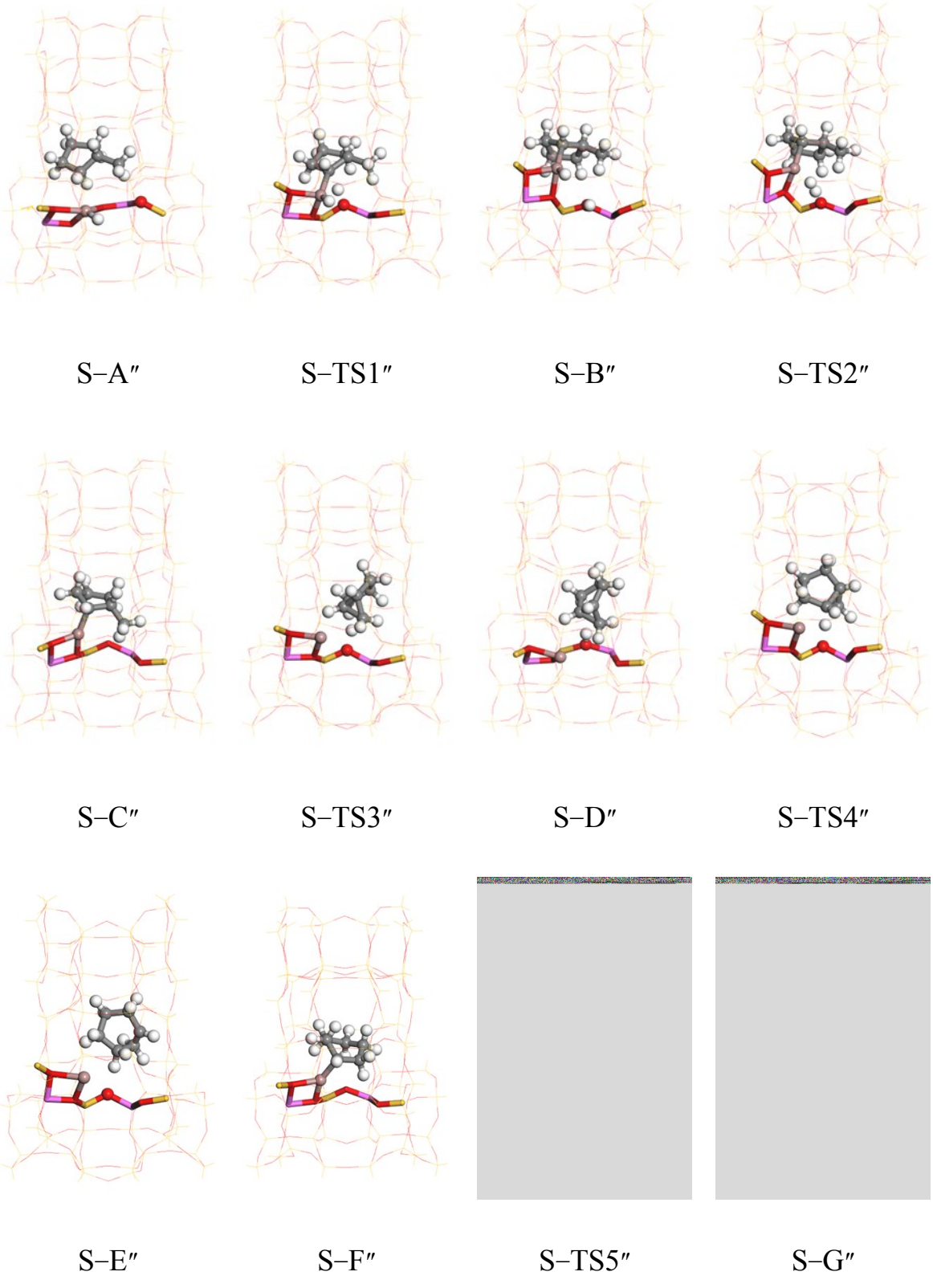


Fig. S6 The geometry structures of reactants, products, intermediates and transition states of methylcyclopentane to cyclohexene through secondary carbon mechanism on Ga−ZSM−5.

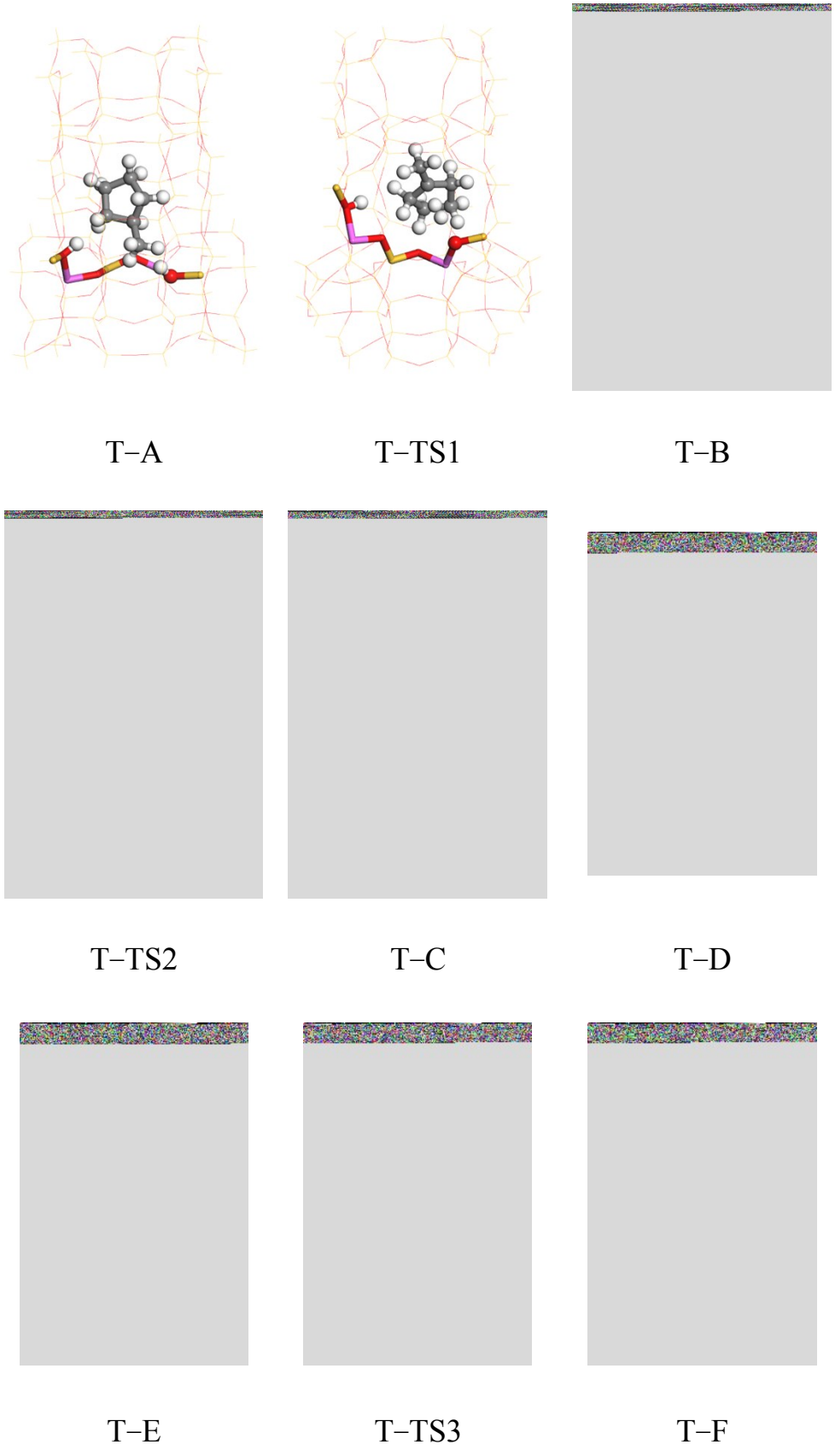
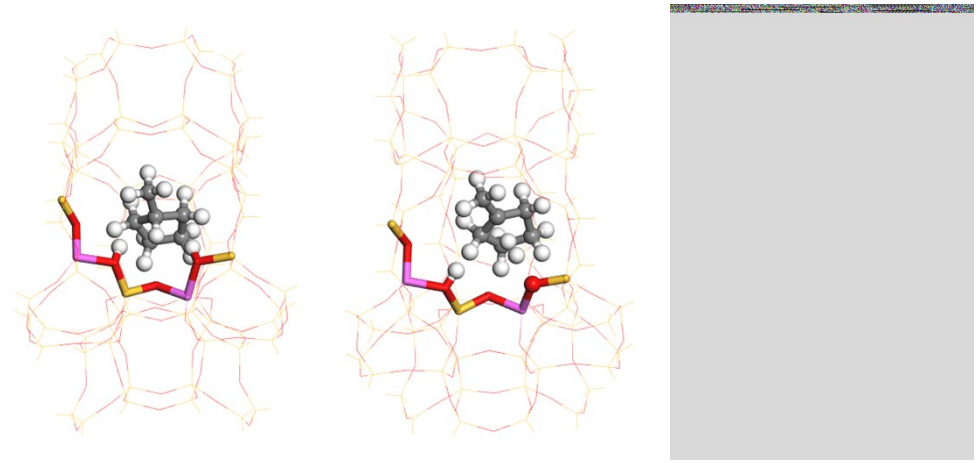
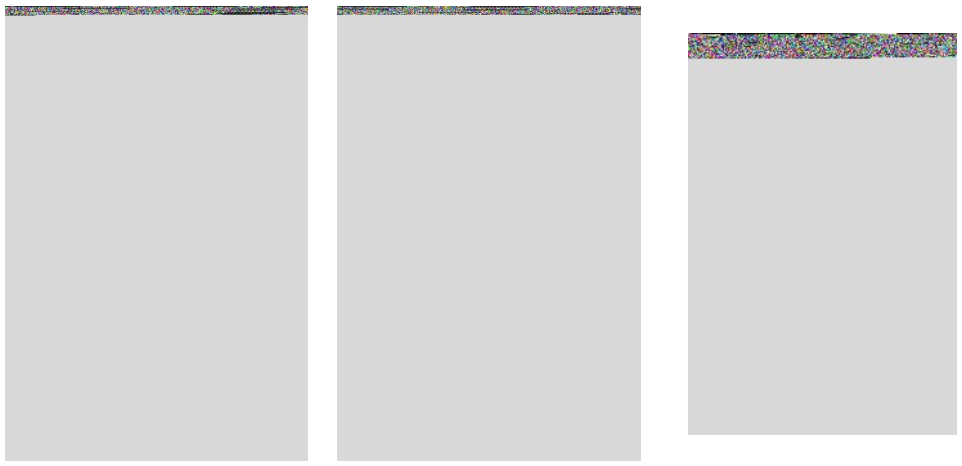


Fig. S7 The geometry structures of reactants, products, intermediates and transition states of

methylcyclopentane to cyclohexene through tertiary carbon mechanism on $H{-}Z_1$.



T−A′ T−TS1′ T−B′

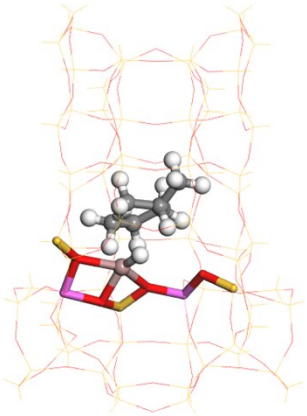


T−TS2′ T−C′ T−D′

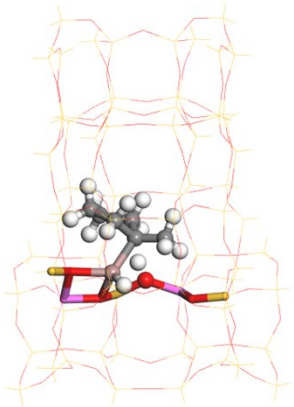
T−E′ T−TS3′ T−F′

Fig. S8 The geometry structures of reactants, products, intermediates and transition states of

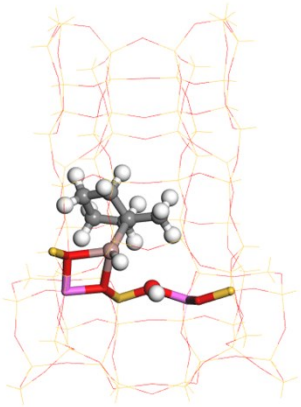
methylcyclopentane to cyclohexene through tertiary carbon mechanism on $H{-}Z_2$.



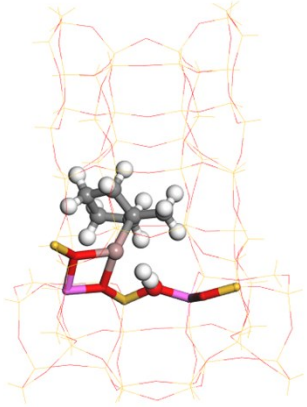
T−A"



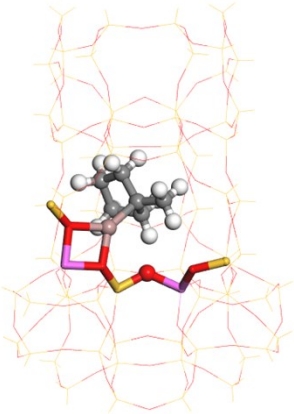
T−TS1"



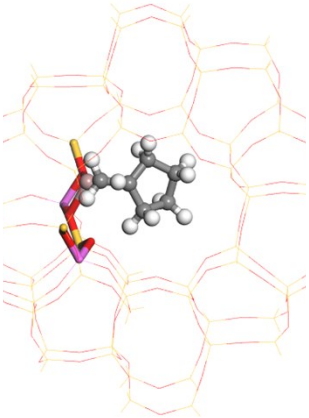
T−B"



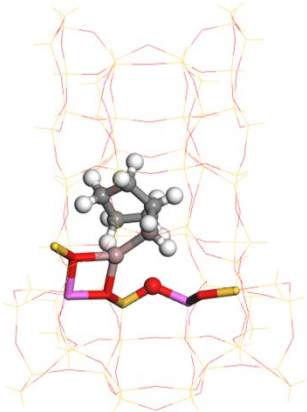
T−TS2"



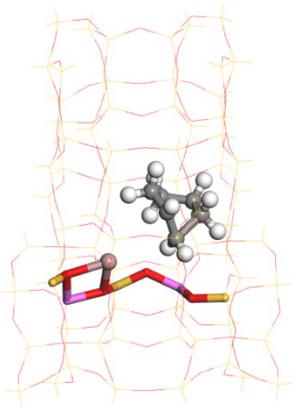
T−C"



T−TS3"



T−D"



T−E"

T−F"

T−TS4"　　T−G"

Fig. S9 The geometry structures of reactants, products, intermediates and transition states of methylcyclopentane to cyclohexene through tertiary carbon mechanism on Ga−ZSM−5.

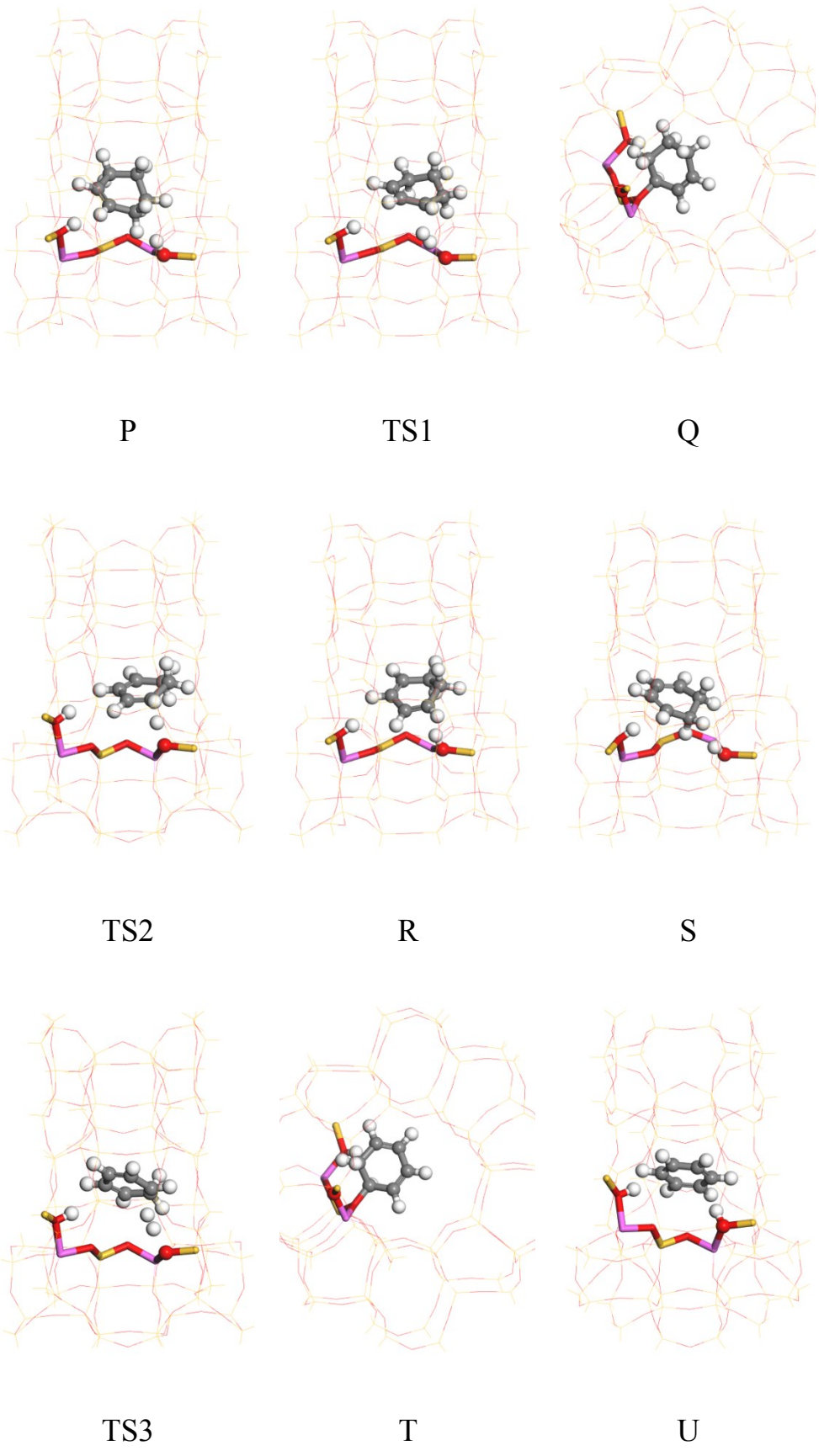


Fig. S10 The geometry structures of reactants, products, intermediates and transition states of

cyclohexene to benzene on $H{-}Z_1$.

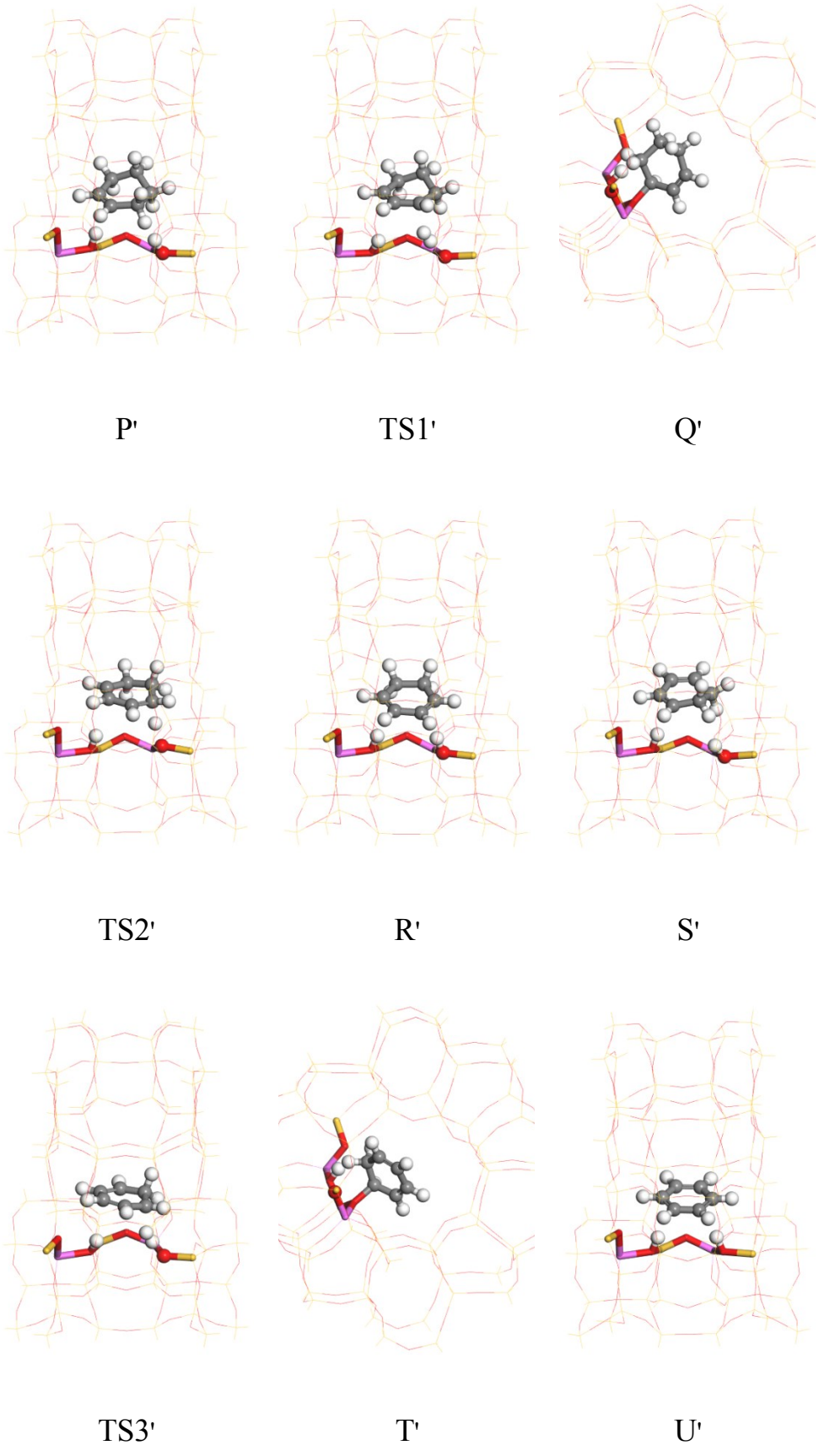
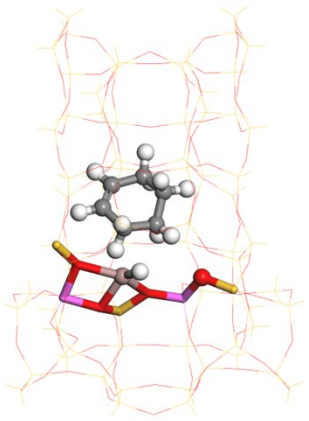
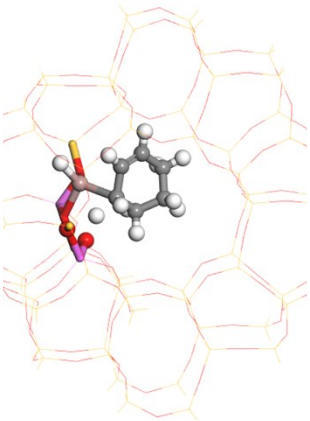


Fig. S11 The geometry structures of reactants, products, intermediates and transition states of

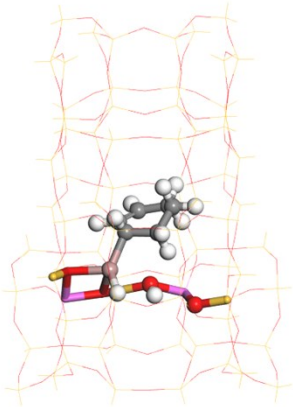
cyclohexene to benzene on H−Z_2.



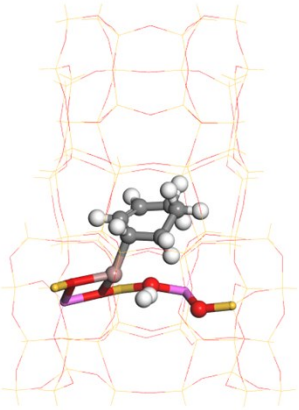
P"



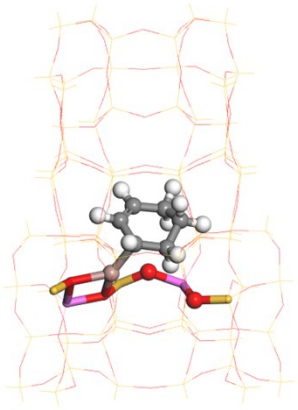
TS1"



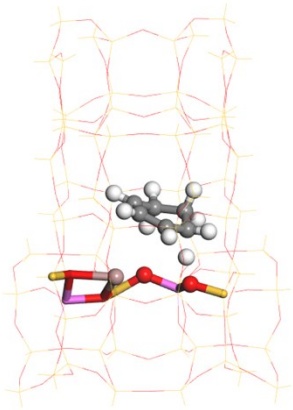
Q"



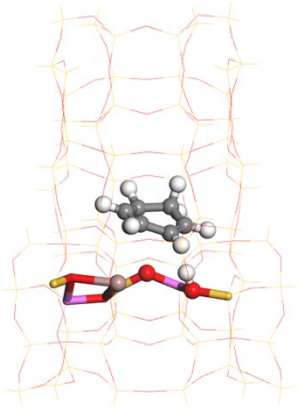
TS2"



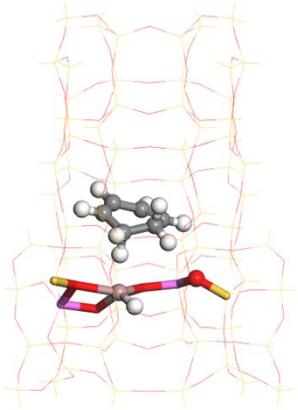
R"



TS3"



S"



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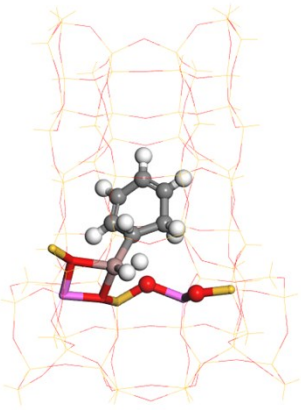

TS4"

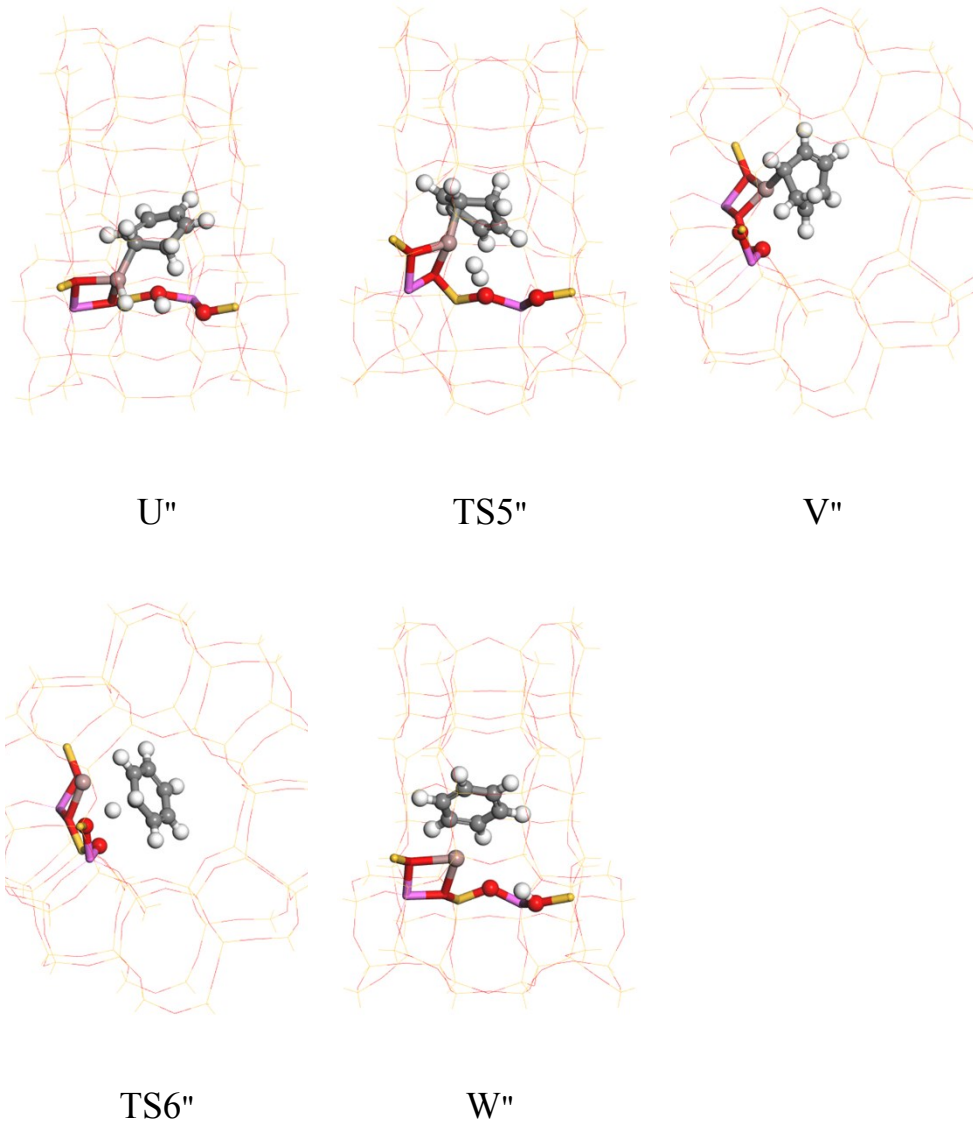

Fig. S12 The geometry structures of reactants, products, intermediates and transition states of cyclohexene to benzene on Ga−ZSM−5.