

Supplementary materials

Mechanism and Chemoselectivity of Mn-catalyzed Intramolecular Nitrene Transfer Reaction: C-H Amination vs. C=C Aziridination

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Optimized structures of the species in the reaction pathways of allylic C-H amination and C=C aziridination.

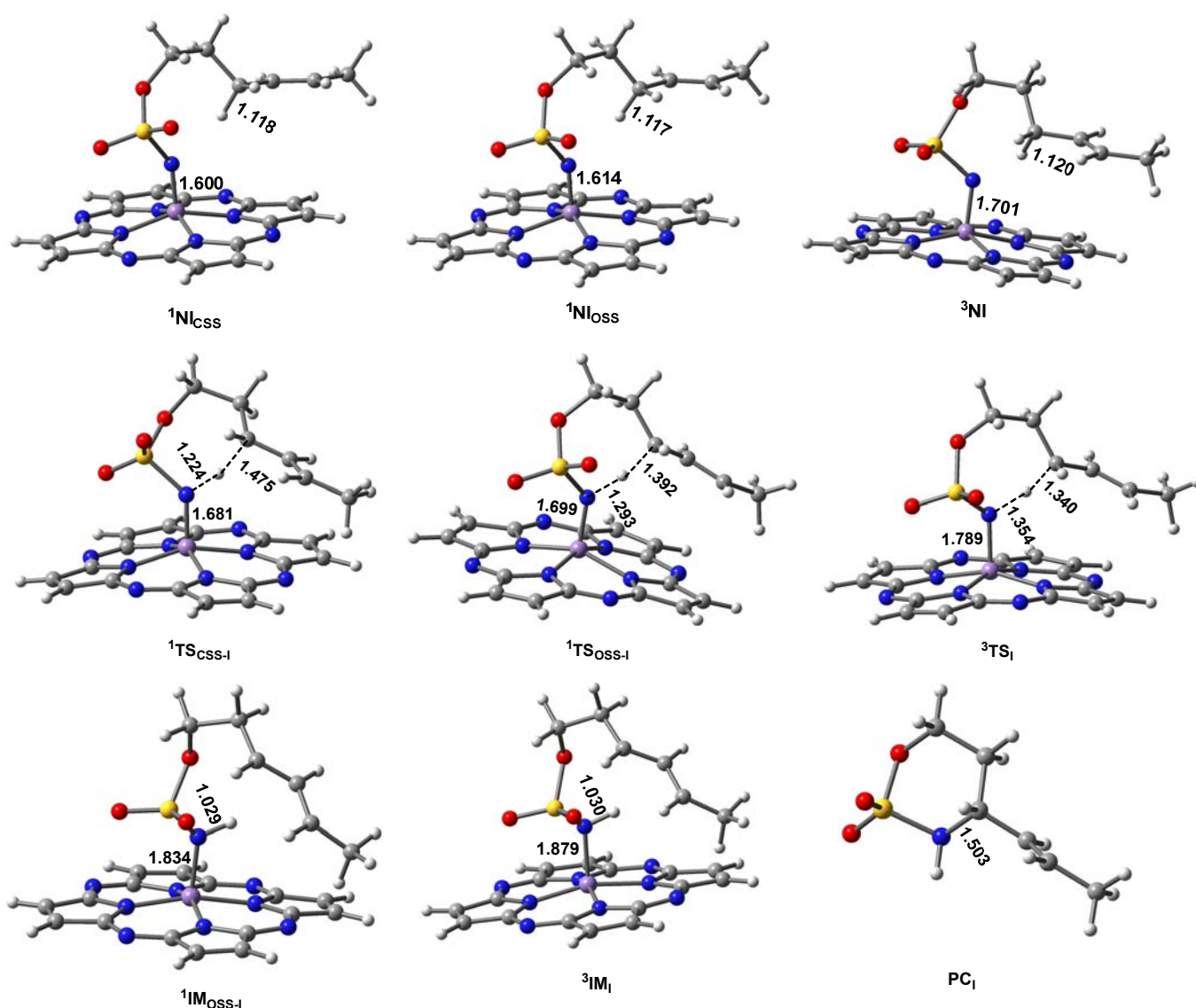


Figure S1(a). Optimized structures with important geometrical parameters (bond lengths in Å) of the species in the reaction pathways of allylic C-H amination.

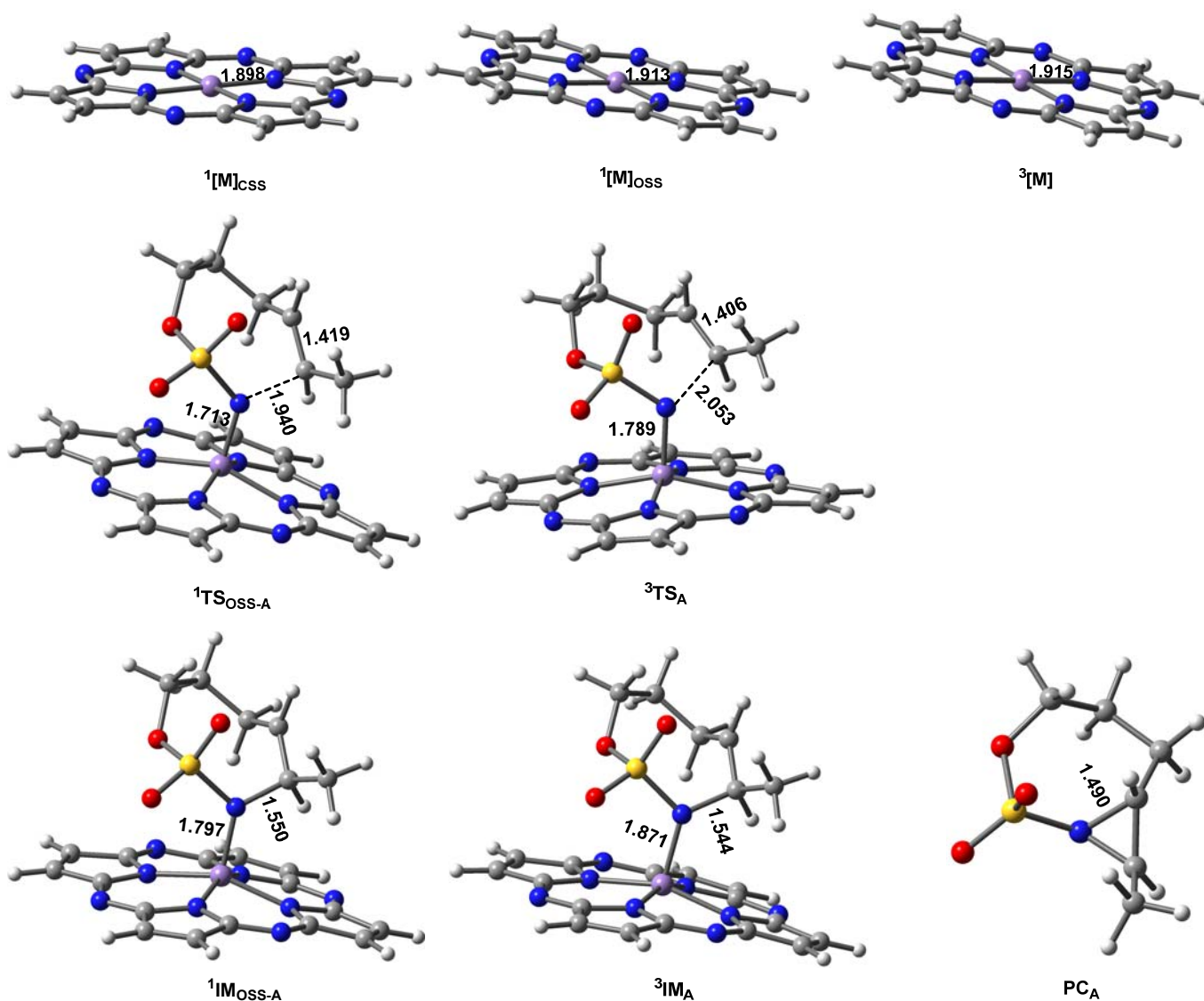


Figure S1(b). Optimized structures with important geometrical parameters (bond lengths in Å) of the species in the reaction pathways of allylic C=C aziridination.