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Electronic Supplementary Information

Theoretical Studies on Mechanism of Ru(II)-Catalyzed Regioselective C-H Allylation of Indoles with Allyl Alcohols

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1. SP calculation results through def2-tzvp and SDD+f basis sets for structures in Figure 1.

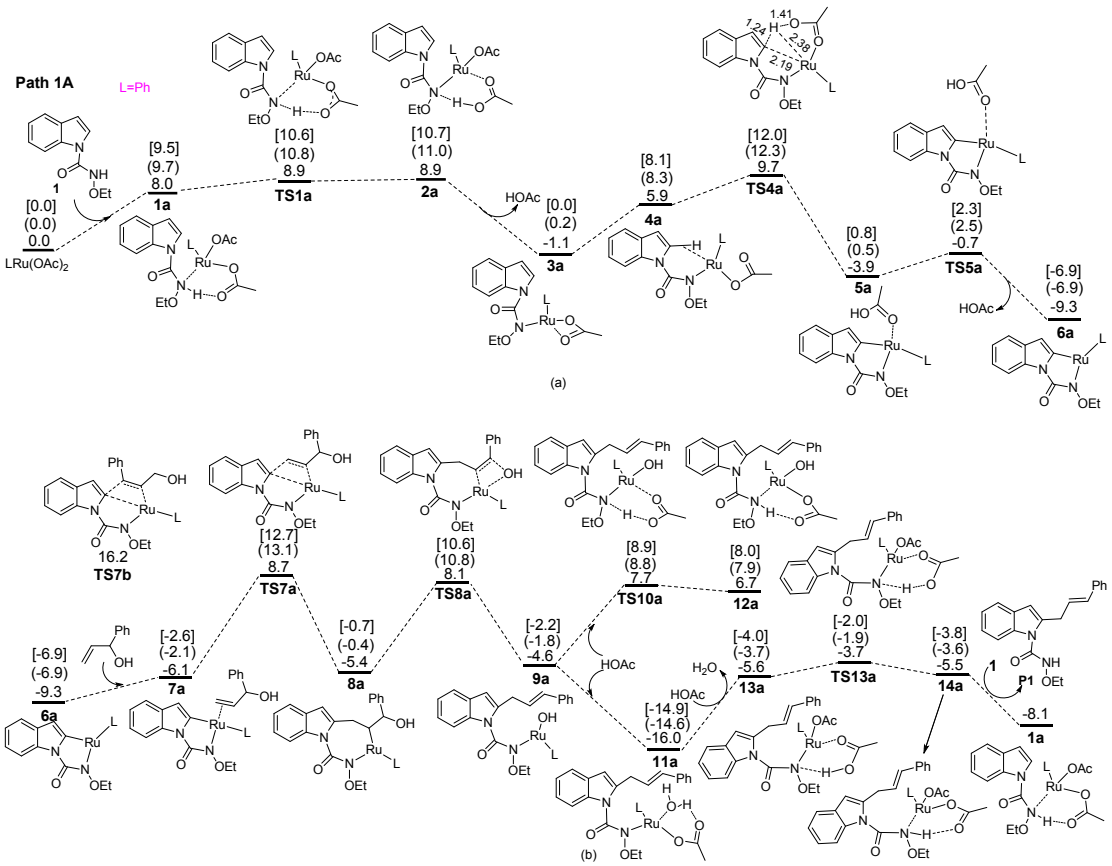

Fig. S1 Energy profile calculated for the C2-H allylation of indole through the C-Ru bond insertion. The solvation-corrected relative free energies are given in kcal/mol. SP calculation results through def2-tzvp and SDD+f basis sets for structures in Figure 1. The values in parentheses are computed with def2-tzvp basis set for Ru(II) and the values in square brackets are computed with SDD+f basis set for Ru(II).

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2. Fig. S2

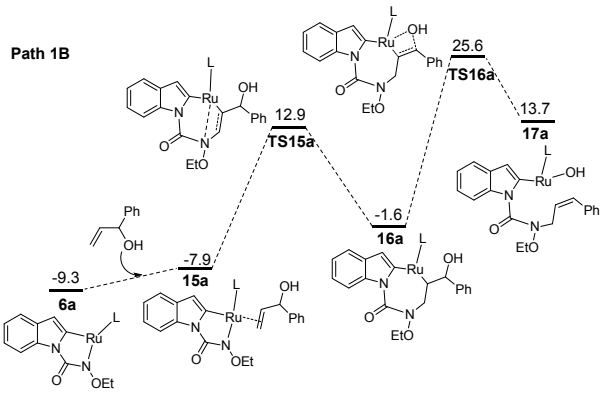

Fig. S2 Energy profile calculated for the N-Ru bond insertion via C2-H activation. The solvation-corrected relative free energies are given in kcal/mol.

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3. Fig. S3

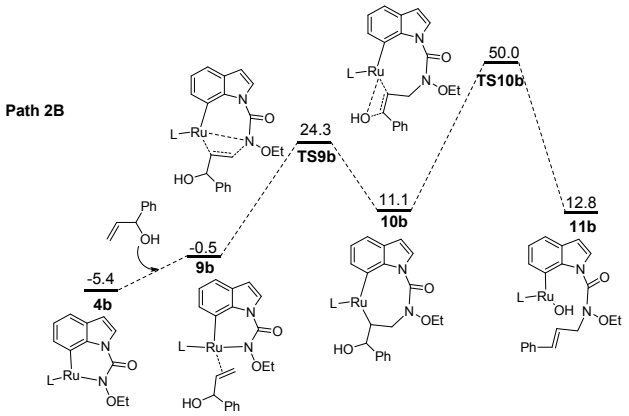

Fig. S3 Energy profile calculated for the N-Ru bond insertion via C7-H activation. The solvation-corrected relative free energies are given in kcal/mol.