Rational Design on Methane Activation and Functionalization by Nickel-Borane Complex

Linlin Yang,[a] Kangqiao Fan,[a] Lei Zhang,*[b] Guixiang Zeng*[a]

[a] Kuang Yaming Honors School, Institute for Brain Sciences, Nanjing University, Nanjing 210023, China. E-mail: gxzeng@nju.edu.cn

[b] Institute of Theoretical and Computational Chemistry, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210023, China. E-mail: fly_zhanglei@163.com

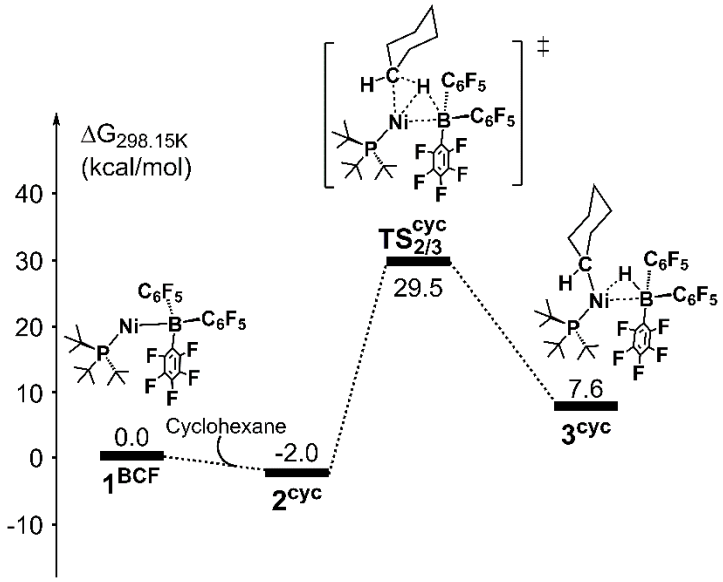

Figure S1. Gibbs energy profiles of the C-H σ-bond activation of Cyclohexane by $\mathbf{1}^{\mathbf{BCF}}$.

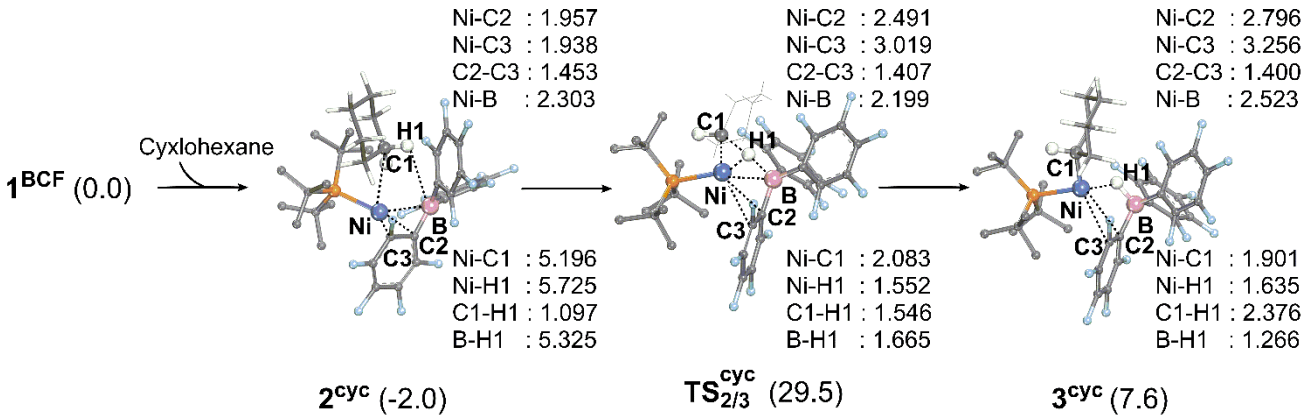

Figure S2. Optimized geometries of all species involved in the C-H σ-bond activation of Cyclohexane by $\mathbf{1}^{\mathbf{BCF}}$. Distances are in Å. The Gibbs energy changes are given in parentheses (kcal/mol).

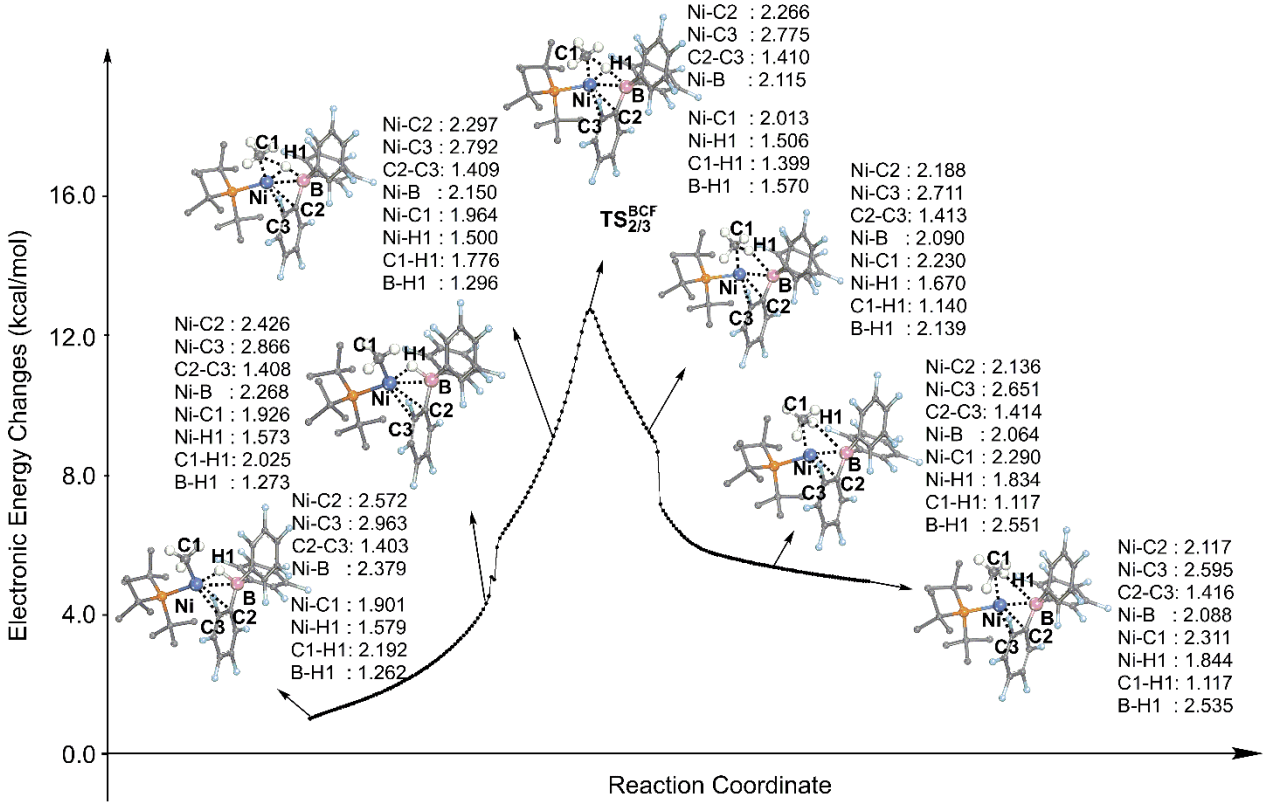

Figure S3. The intrinsic reaction coordinate of $\mathbf{TS}_{2/3}^{\mathbf{BCF}}$.

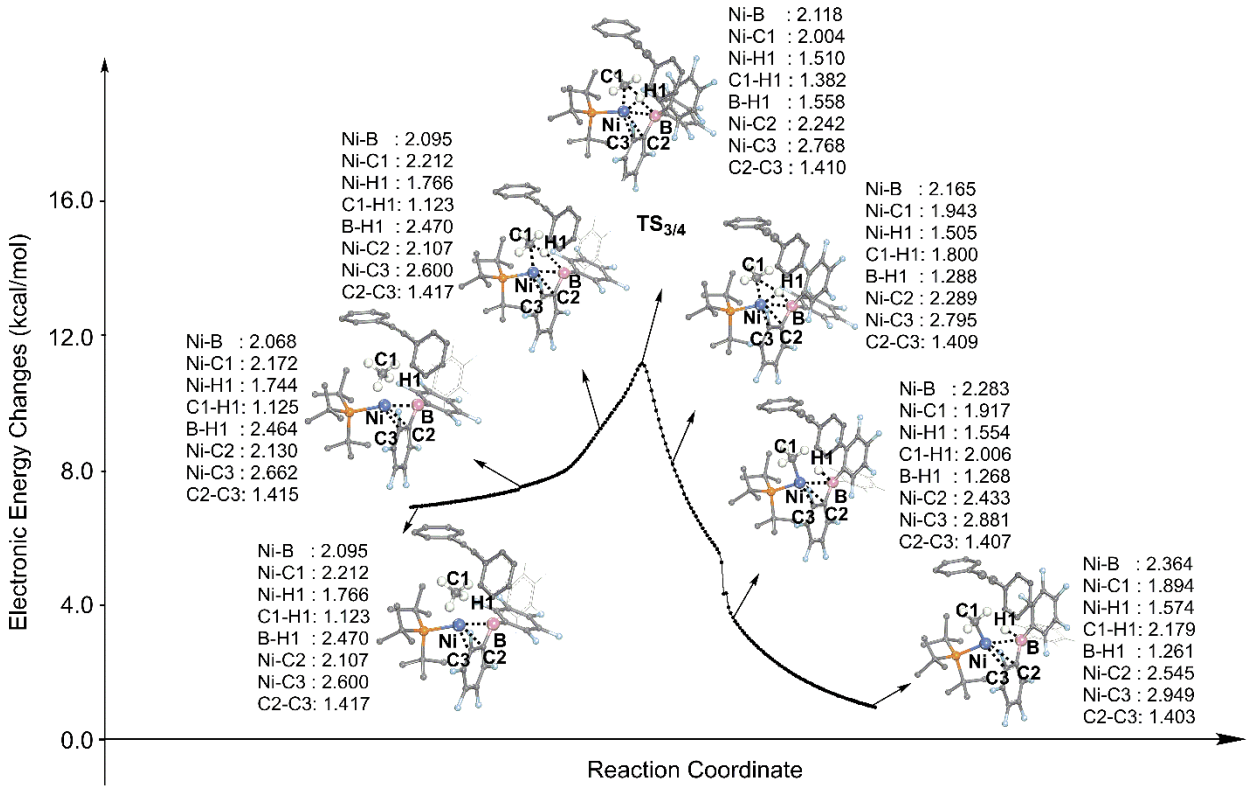

Figure S4. The intrinsic reaction coordinate of **TS3/4**.

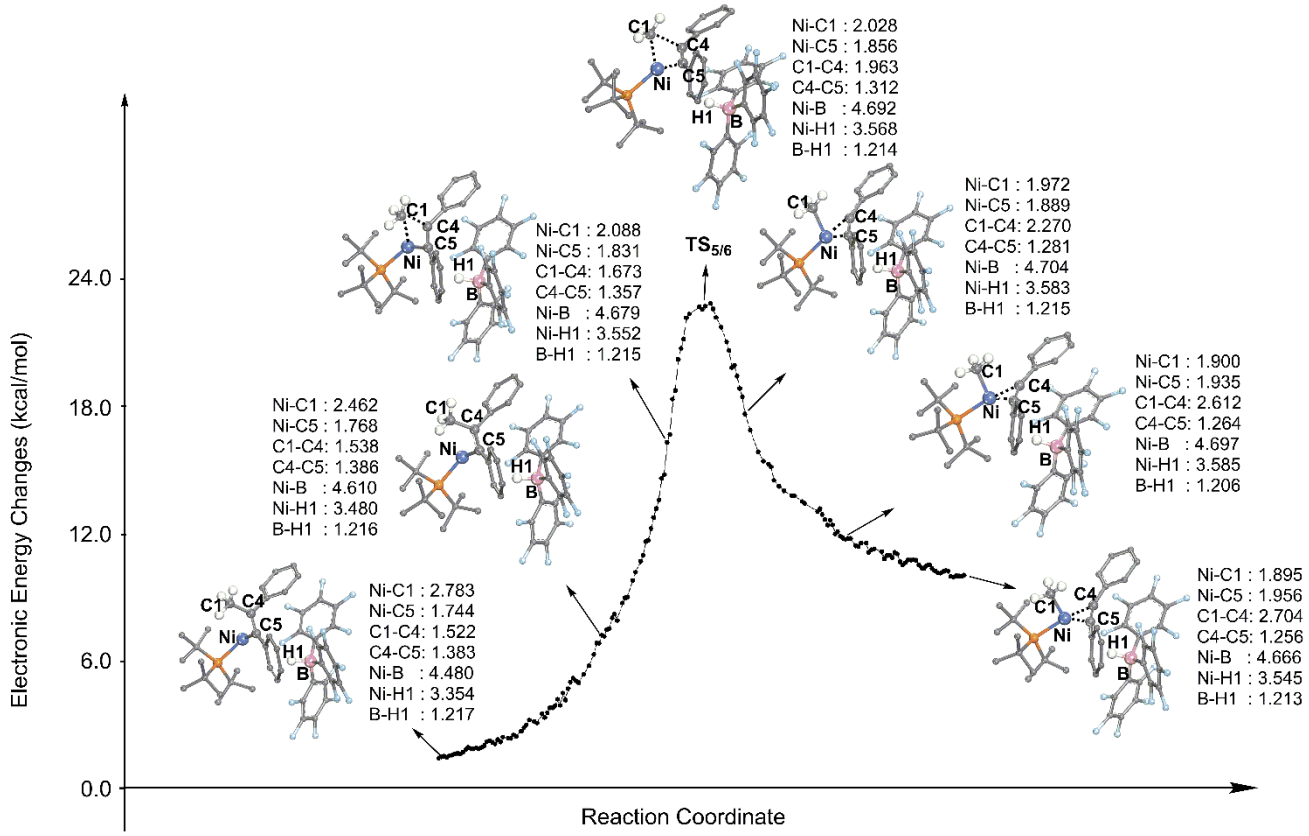

Figure S5. The intrinsic reaction coordinate of **$TS_{5/6}$**.

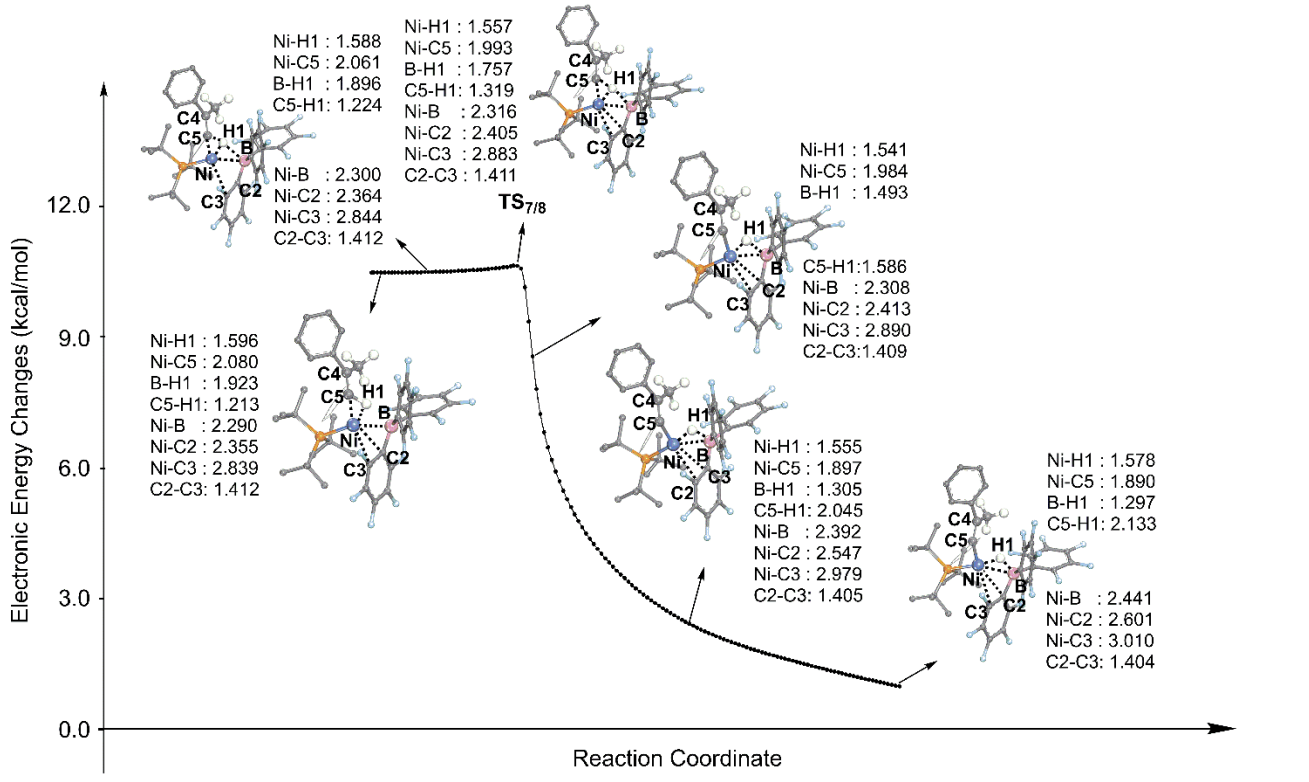

Figure S6. The intrinsic reaction coordinate of **$TS_{7/8}$**.