SUPPORTING INFORMATION

Theoretical Investigations toward the [3+2]-Dipolar Cycloaddition of Nitrones with Vinyldiazoacetates Catalyzed by Rh$_2$(R-TPCP)$_4$: Mechanism and Enantioselectivity

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1. Computational Details

All calculations were performed with Gaussian’09 software package. The geometries optimization of all the equilibriums and transition states involving rhodium system were performed by ONIOM methodology, the substrates and dirhodium(II) carboxylates were in the high level layer using DFT/B3LYP method of theory that including the LANL2DZ basis set (aliased as [Rh-LA2] in following) on Rh and 6-31G(d) basis set on smaller atoms. The ligands including adamantly variants and pathalimidos were in the low level layer and performed by semiempirical PM6. Heavy-atom basis set definitions and corresponding pseudopotential parameters were obtained from the EMSL basis set exchange library. At the ONIOM-optimized geometries, vibrational frequencies were calculated to identify whether the optimized geometries is equilibrium or transition state, and to evaluate the zero-point vibration energy (ZPE), as well as to obtain the thermal corrections to the Gibbs free energy (298.15K and 1 atm). The solvent energies for certain important structures were calculated by single point calculations on the optimized structures with ONIOM(B3LYP/6-311+G (d,p)[Rh-LA2]:PM6). All of the relative energies discussed in main text are Gibbs free energies in n-pentane with thermal corrections, unless otherwise stated.
2. Coordinates of all Stationary Points and Computed Energies

2.1. Catalysis configuration

Catalyst Rh$_4$(R-TPCP)$_4$ with $C_4$ symmetry

Sum of electronic and zero-point Energies = -973.821306
Sum of electronic and thermal Energies = -973.734976
Sum of electronic and thermal Enthalpies = -973.734032
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S-34
### 2.3. C≡C=N2 \textit{s-trans} vinylcarbenoid 2-II and aryl nitrene 3a

\textit{s-trans} vinyldiazoacetate 2-II and aryl nitrene 3a with an approach over Si-face

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**Standard orientation:**

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s-trans vinyl diazoacetate 2-II and aryl nitrone 3a with an approach over Re-face

Standard orientation:

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2.4. C=C=N$_2$ s-trans vinylcarbenoid 2-II and styryl nitrone 3b

$s$-trans vinyldiazoacetate 2-II and styryl nitrone 3b with an approach over Si-face

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S-127
### 3. Computed Energies

Sum of electronic and zero-point energies ($E_0$, in Hartree), sum of electronic and thermal enthalpies ($H$, in Hartree), sum of electronic and thermal free energies ($G$, in Hartree), thermal correction to Gibbs free energy ($TCGFE$, in Hartree), total free energy in solution ($E_{sol}$, in Hartree, solvent = n-pentane), and thermo corrected Gibbs free energy in solvent ($G_{sol}$, which equals to $E_{sol} + TCGFE$, in Hartree). Reactive energies at 298.15K and 1atm are reported in kcal/mol.

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4. Functional Effects and Basis Set effects

In consideration of the inadequacy of B3LYP to describe the vdW dispersion corrections, we compared the computed energy profiles of M06L, M062X and B3LYP-D3 with the BJ-damping (-D3(BJ)) methods. The initial step of metal catalyzed reaction is especially important for the dispersion force, thus the carbenoid formation of vinyldiazoacetate \(2a-I\) (the same below) can be adopted as example reaction to efficiently estimate the discrepancies induced by theoretical methods. The M06L, M062X calculations of geometries optimization and single-point energies in solvent (\(n\)-pentane) were performed using the same basis sets as original level using Gaussian’09. The B3LYP-D3 calculations were performed on the optimized geometries using the same level. In addition, a higher basis set was tested on the example reaction to evaluate the basis set effects, and the results were shown in Table S1.

**Table S1. Test of M06L, M062X and B3LYP-D3 methods.**

<table>
<thead>
<tr>
<th>Structure</th>
<th>(E_s)</th>
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<th>(G)</th>
<th>(TCGFE)</th>
<th>(E_{cal})</th>
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</table>

\(a\) solvent = \(n\)-pentane
\(b\) ONIOM(B3LYP/6-311+G(d,p)[Rh-LA2]:PM6)//B3LYP/6-31G(d,p)[Rh-LA2]:PM6
\(c\) ONIOM(M06L/6-311+G(d,p)[Rh-LA2]:PM6)//M06L/6-31G(d)[Rh-LA2]:PM6
\(d\) ONIOM(M062X/6-311+G(d,p)[Rh-LA2]:PM6)//M062X/6-31G(d)[Rh-LA2]:PM6
\(e\) ONIOM(B3LYP-D3//6-31G(d)[Rh-LA2]:PM6)//B3LYP/6-31G(d,p)[Rh-LA2]:PM6
\(f\) ONIOM(B3LYP/6-311+G(2d,p)[Rh-LA2]:PM6)//B3LYP/6-31G(d,p)[Rh-LA2]:PM6

As shown in Table S1, the energy barriers of the example reaction computed by M06L and B3LYP-D3 theoretical methods in the high level of ONIOM methodology are 12.6 and 12.0 kcal/mol, respectively. The discrepancies induced by these two functionals are subtle compared with the original data 12.1 kcal/mol computed by that of B3LYP basis sets. The energy barrier obtained by M062X method is lower 1.4 kcal/mol than the original result, the slight difference can be attributed the insufficiency of M062X to describe the ubiquitous long-rang dispersion corrections. Thus we believe that B3LYP method is suitable for studying the present system.

In addition, we used the bigger basis set of ONIOM(B3LYP/6-311+G(2d,p)[Rh-LA2]:PM6)//B3LYP/6-31G(d,p)[Rh-LA2]:PM6 and the discrepancy induced by this higher basis set compared with the original result is not more than 0.1 kcal/mol, this result suggested this present system is not sensitive to the basis sets used in calculations.
5. Solvent Effects

Except for the effect of solvent polarity illustrated in main text, we also supplement the theoretical tests of solvent model and the optimization in solvent of the structures of the example reactions above. The calculated results are shown in Table S2.

**Table S2.** The effect of solvent.

<table>
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<tr>
<th>Structure</th>
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<th>$H$</th>
<th>$G$</th>
<th>TCGFE</th>
<th>$E_{sol}$</th>
<th>$G_{sol}$</th>
<th>$\Delta H_{gas}$</th>
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$^a$ SMD$^3$-ONIOM(B3LYP/6-311+G(d,p)\[Rh-LA2\]:PM6)//B3LYP/6-31G(d)\[Rh-LA2\]:PM6, optimized in solvent

$^b$ CPCM-ONIOM(B3LYP/6-311+G(d,p)\[Rh-LA2\]:PM6)//B3LYP/6-31G(d)\[Rh-LA2\]:PM6, optimized in solvent

As shown in Table 2S, the energy barrier of example reactions with solvent method SMD in n-pentane which is also popular displays a barrier of 12.3 kcal/mol, this result suggests the chosen solvent method in this rhodium has a negligible influence on the single point energies of the structures. Besides, the geometries of the example reaction are optimized in the solvent n-pentane and obtained an energy barrier of 12.1 kcal/mol. This value is not more 0.1 kcal/mol than the computed energy barrier which geometries optimized in gas-phase, thus the geometries of this system optimized in gas-phase is reasonable.

Polar solvent has been reported to dramatically enhance the vinylogous reactivity. With an attempt to determine the influence of solvent polarity on vinylcarbenoid we conduct an array of tests on solvent polarity using hexane, dichloromethane (DCM), acetone. We adopt the initial step of carbenoid formation of vinyldiazoacetate 1 catalyzed by Rh$_2$(S-TPCP)$_4$ and the vinylogous reaction with aryl nitrone 3a as example reactions. The calculated results are shown in Table 1.

**Table S3.** Effects of solvent polarity.

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<th>$\Delta G_{sol\text{b}}$</th>
<th>$G_{sol\text{c}}$</th>
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<th>$G_{sol\text{e}}$</th>
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<th>$G_{sol\text{g}}$</th>
<th>$\Delta G_{sol\text{h}}$</th>
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$^a$ Gibbs free energies in solvent with thermal corrections of stationary points, in Hartree. $^b$ Relative energies, in kcal/mol.

As can be seen in the first column of Table. S3, along with the dielectric coefficient $\varepsilon$ rising, the relative Gibbs free energies with thermal corrections gradually increase. That is to say, the decomposition of certain vinyldiazoacetate within polar solvent should overcome distinctly high energy barrier. As the competing pathway shown in column 2 and 3, this vinylogous reaction of
aryl nitrone all has a preference of the approach from the $Si$-face rather than that from the $Re$-face.
The differences between competitive pathways with the opposite faces in vinylogous reaction also become large with the dielectric coefficient $\varepsilon$ rising, are 2.52, 2.52, 2.71 and 3.30 kcal/mol, respectively. These comparative tests illuminate that weak polar solvent is favor of decomposition of vinyldiazoacetate to form rhodium vinylcarbenoid, while relatively the polar solvents support vinylogous reaction. This theoretical result of solvent polarity can provide a reliable guide for other analogous catalytic reactions.