Supporting Information

Part I. Energies in Gas Phase

Note 1:
The entries correspond to (use Ni as example)
1. Ni(PH3)2(1) + CH2=CH-Cl(2) → Cl → TS1 → Ni(PH3)2(CH=CH2)Cl(3) oxidative addition
2. Ni(PH3)2(CH=CH2)Cl(3) → Ni(PH3)(CH=CH2)Cl(4) + PH3(5) dissociation
3. Ni(PH3)(CH=CH2)Cl(4) + CH2=CH2(6) → Ni(PH3)(CH=CH2)Cl(6)Cl(7) association
4. Ni(PH3)(CH=CH2)Cl(6)Cl(7) → TS2 → Ni(PH3)(CH2CH2-CH=CH2)Cl(8) insertion
5. Ni(PH3)(CH2CH2-CH=CH2)Cl(8) → TS3 → Ni(PH3)(CH2CH2-CH=CH2)Cl(9) rotation
6. Ni(PH3)(CH2CH2-CH=CH2)Cl(9) → TS4 → Ni(PH3)(CH2=CH-CH=CH2)(H)Cl(10) elimination
7. Ni(PH3)(H)Cl(11) + PH3(5) → Ni(PH3)2(H)Cl(13) association
8. Ni(PH3)2(H)Cl(13) → Ni(PH3)2(1) + HCl(14) regeneration

Note 2:
All of the energies were obtained from the sums of the B3LYP/LANL2DZ+p single-point energies and B3LYP/LANL2DZ thermal correction to free energies.
Table 1. Free energies: (HF)

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a. Tight SCF was used for this B3LYP/LANL2DZ+p single-point calculation.
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Table 6. Free energy changes in the coupling of CH$_2$=CHCl with RCH=CH$_2$.\(^a\)

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\(^a\): Unit for Table 6 is kcal/mol. In each row of the table we used the metal complex to show the stage in the catalytic cycle. The free energy was calculated for all the species at each particular stage. For example, in the first row the free energy was calculated for 1 + RCl + CH$_2$=CH$_2$. In the last row, the free energy was calculated for 1 + R-CH=CH$_2$ + HCl. \(^b\): Tight SCF was used for this single-point energy calculation.
**Table 7.** Gas-phase and solution-phase (THF or DMF) free energy changes in the coupling of CH$_2$=CHCl with CH$_2$=CH$_2$. (kcal/mol)$^a$

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$^a$: In each row of the table we used the metal complex to show the stage in the catalytic cycle. The free energy was calculated for all the species at each particular stage. For example, in the first row the free energy was calculated for 1 + RCl + CH$_2$=CH$_2$. In the last row, the free energy was calculated for 1 + R-CH=CH$_2$ + HCl.
Part II. Solvation Energies in THF Solution: PCM

Note: The values used here are the electrostatic items.

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Part III. B3LYP/LANL2DZ Optimized Geometries

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H    -1.173785    -1.075794     2.740414
H    -1.173785     1.075794     2.740414

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C     1.697812     0.000000     0.092105
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H     2.640894     0.000000    -0.450439

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f. CH2=CH-CH3 + CH2=CH-Cl (C1 selectivity)

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