

Supporting Information

Benefit of a hemilabile ligand in deoxygenation of fatty acids to 1-alkenes

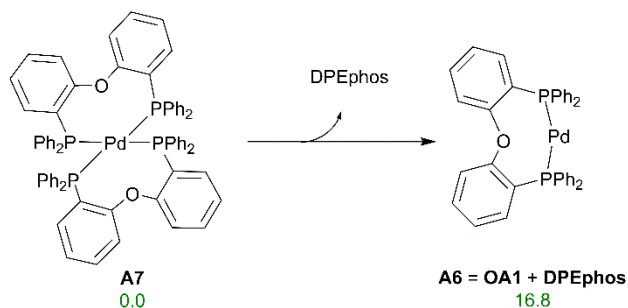
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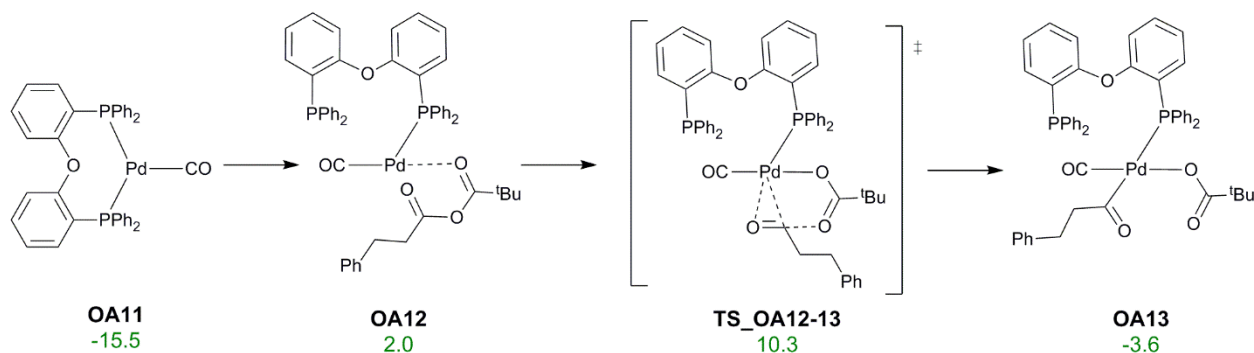
Alternative Pathways

Activation



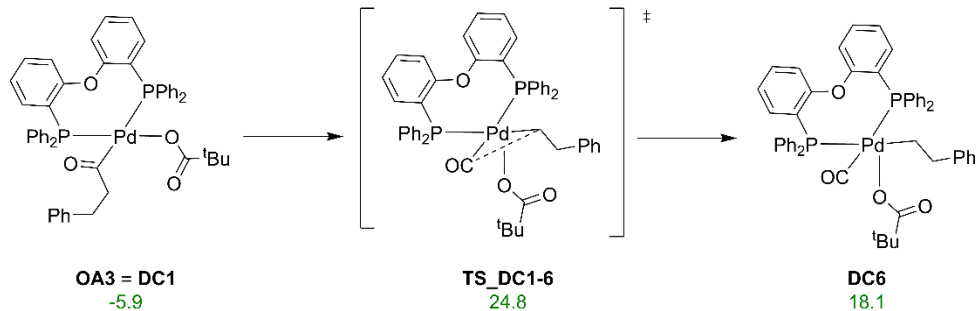
Scheme S1. Alternative activation typically observed in *in-situ* formation of catalyst with excess of ligand. Free energies (kcal/mol) calculated at 100°C using DMA as a solvent.

Oxidative Addition



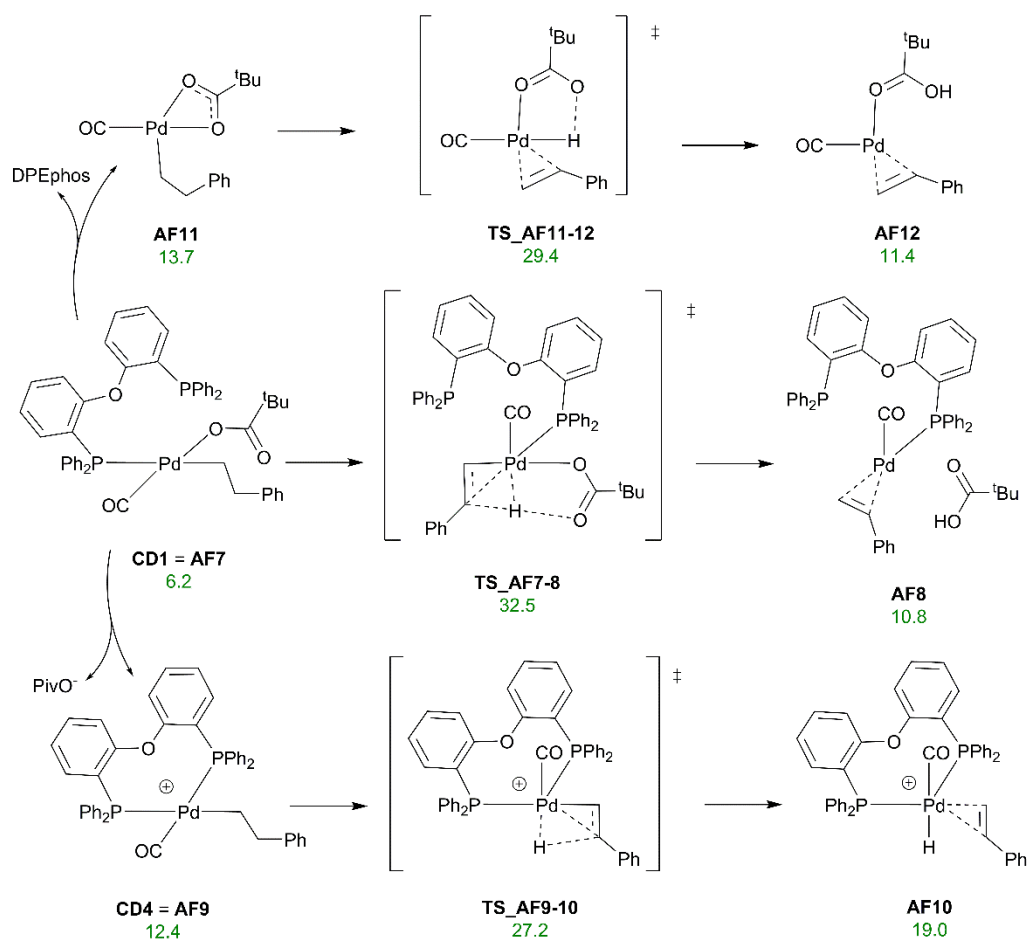
Scheme S2. Alternative oxidative addition with CO still attached to the catalyst. Free energies (kcal/mol) calculated at 100°C using DMA as solvent.

Decarbonylation



Scheme S3. Alternative pathway for decarbonylation where nothing dissociates from the metal. Free energies (kcal/mol) calculated at 100°C using DMA as solvent.

Alkene formation



Scheme S4. Alternative pathways with CO still attached to the catalyst for alkene formation. Free energies (kcal/mol) calculated at 100° using DMA as solvent.

Energies of intermediates and TSs

Compound	E(QZ)	G(QZ)	G(DMA)
1	-499.598657	-499.472086	-499.487594
1a	-538.922817	-538.770619	-538.787456
2	-617.805762	-617.593463	-617.607642
3	-770.265210	-770.032771	-770.052443
3a	-809.593989	-809.335547	-809.349385
4	-309.730137	-309.634375	-309.641031
4a	-349.048512	-348.927936	-348.935397
4b	-349.060329	-348.939854	-348.947966

5	-808.676600	-808.567827	-808.580548
6	-694.984736	-694.752632	-694.766994
PivOH	-347.138638	-347.031347	-347.041054
PivO⁻	-346.572321	-346.479101	-346.565834
DPEphos	-2147.053352	-2146.609445	-2146.636435
Cl⁻	-460.283572	-460.298988	-460.404989
CO (10⁻⁵ atm)	-113.348331	-113.381825	-113.377195
CO (1 atm)		-113,368226	-113,363596
water	-76.452147	-76.450522	-76.457740
A1	-3083.444807	-3082.868215	-3082.914334
A2	-2623.015324	-2622.434771	-2622.513478
A3	-2969.736097	-2969.036336	-2969.075479
A4	-3083.422642	-3082.845919	-3082.880482
A5	-2969.714217	-2969.012195	-2969.051875
A6=OA1	-2274.698392	-2274.258319	-2274.284368
A7	-4421.810294	-4420.889916	-4420.938682
OA2	-3044.995116	-3044.290389	-3044.328669
TS_OA2-3	-3044.984666	-3044.281469	-3044.322620
OA3 = DC1	-3045.010378	-3044.306161	-3044.346244
OA4	-3044.995786	-3044.291242	-3044.330369
TS_OA4-5	-3044.980216	-3044.277549	-3044.315772
OA5	-3045.003356	-3044.301663	-3044.343784
OA6	-2774.317464	-2773.724705	-2773.763136
TS_OA6-7	-2774.278384	-2773.686111	-2773.726555
OA7	-2774.286043	-2773.694797	-2773.737529
OA8	-3197.456944	-3044.270889	-3044.310959
TS_OA8-9	-3197.444550	-3044.258607	-3044.302030
OA9	-3197.469914	-3044.287054	-3044.330781
OA10	-2388.094229	-2387.652527	-2387.679377
OA11	-3158.360046	-3157.656398	-3157.697247
TS_OA11-12	-3158.347483	-3157.642719	-3157.683947
OA12	-3158.370087	-3157.665240	-3157.706157
TS_DC1-2	-3044.993697	-3044.290783	-3044.329486
DC2	-3044.997146	-3044.297415	-3044.337933
TS_DC2-3	-3044.969827	-3044.271983	-3044.310425
DC3 = CD1 = AF7	-3044.987156	-3044.290446	-3044.326922
DC4	-2698.254809	-2697.674591	-2697.761117
TS_DC4-5	-2698.230909	-2697.651370	-2697.732969
DC5 = CD4 = AF9	-2698.256633	-2697.673563	-2697.751202
TS_DC1-6	-3044.956219	-3044.257410	-3044.297210
DC6	-3044.966964	-3044.268975	-3044.307935
TS_CD1-2	-3044.976790	-3044.278307	-3044.316149
CD2	-3044.977639	-3044.281171	-3044.319474

TS_CD2-3	-3044.971707	-3044.275103	-3044.312941
CD3 = AF1	-2931.623341	-2930.927948	-2930.969284
TS_CD4-5	-2698.235001	-2697.658184	-2697.737838
CD5 = AF4	-2584.881048	-2584.306361	-2584.385924
TS_AF1-2	-2931.584365	-2930.894634	-2930.930713
AF2	-2931.631068	-2930.939360	-2930.974451
AF3	-2584.475016	-2583.911884	-2583.943686
TS_AF3-A6	-2584.448560	-2583.888261	-2583.920064
TS_AF4-5	-2584.866460	-2584.294308	-2584.370854
AF5	-2584.872214	-2584.298784	-2584.374273
TS_AF5-6	-2584.849513	-2584.278630	-2584.355819
AF6 = IS8	-2275.100797	-2274.652313	-2274.732516
TS_AF6-A6 =	-2621.842518	-2621.275925	-2621.308239
TS_IS9-A6			
TS_AF7-8	-3044.939016	-3044.247914	-3044.285092
AF8	-3044.978379	-3044.283794	-3044.319657
AF9	-2698.220999	-2697.648809	-2697.727693
AF10	-2698.236175	-2697.663887	-2697.740628
AF11	-897.891372	-897.665009	-897.678561
TS_AF11-12	-897.859825	-897.639311	-897.653503
AF12	-897.892326	-897.669652	-897.682231
IS1	-2970.946940	-2970.223736	-2970.265598
TS_IS1-2	-2970.910062	-2970.192823	-2970.231328
IS2	-2623.791487	-2623.201758	-2623.820478
IS3	-2624.205743	-2623.605005	-2624.284155
TS_IS3-4	-2624.190102	-2623.592117	-2624.266042
IS4	-2624.195965	-2623.595384	-2624.269556
TS_IS4-5	-2624.181379	-2623.582298	-2624.257216
IS5	-2624.193446	-2623.593785	-2624.266460
TS_IS5-6	-2624.191294	-2623.592616	-2624.264595
IS6	-2624.214325	-2623.613190	-2624.289227
TS_IS6-7	-2624.191384	-2623.594180	-2624.265547
IS7	-2624.196694	-2623.599230	-2624.270065
TS_IS7-8	-2624.187339	-2623.589520	-2624.260250
IS8 = AF6	-2275.100797	-2274.652313	-2275.177983
IS9	-2621.860789	-2621.291329	-2621.892500
TS_IS9-A6 =	-2621.842518	-2621.275925	-2621.871814
TS_AF6-A6			
IS10	-2970.956266	-2970.231047	-2970.990122
TS_IS7-11	-2624.186050	-2623.586084	-2623.664083
IS11	-2970.956266	-2970.231047	-2970.267917
TS_IS11-12	2970.925276	-2970.206997	-2970,243789
IS12	-2623.797819	-2623.208280	-2623.826983

TS_IS12-A6	-2623.779755	-2623.193495	-2623.809222
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