

Supporting Information

Mechanism and the Origin of the Regioselectivity of Cobalt-Catalyzed

Annulation of Allenes with Benzamide: A Computational Study

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Section 1. Other possible pathways (Figs. S1-S8 and Schemes S1-S6)

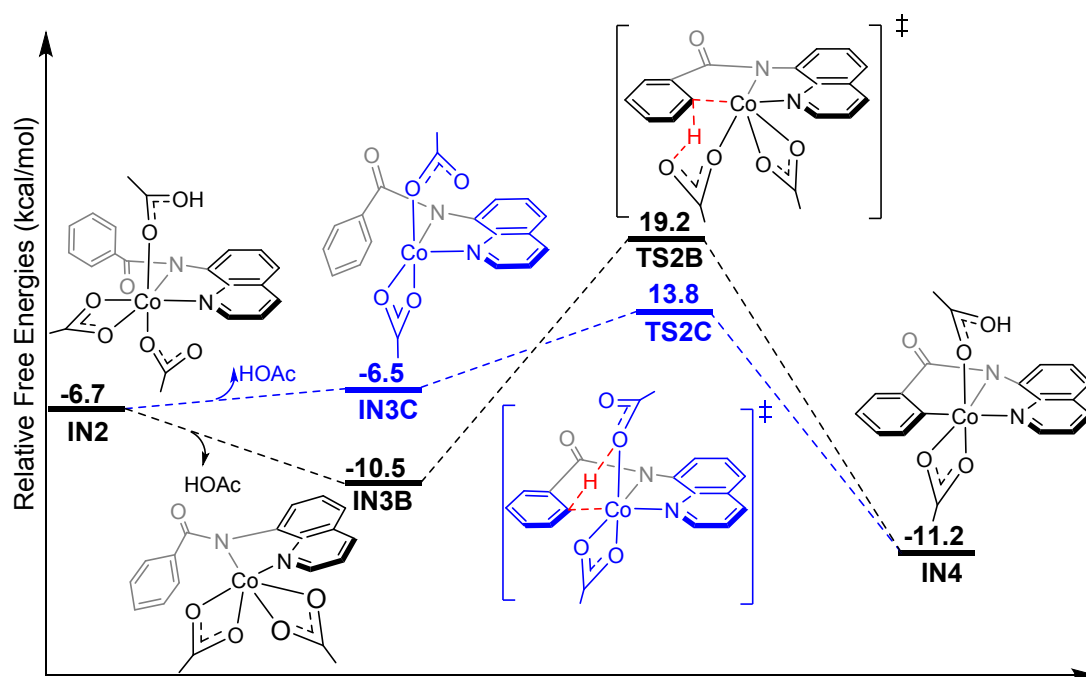
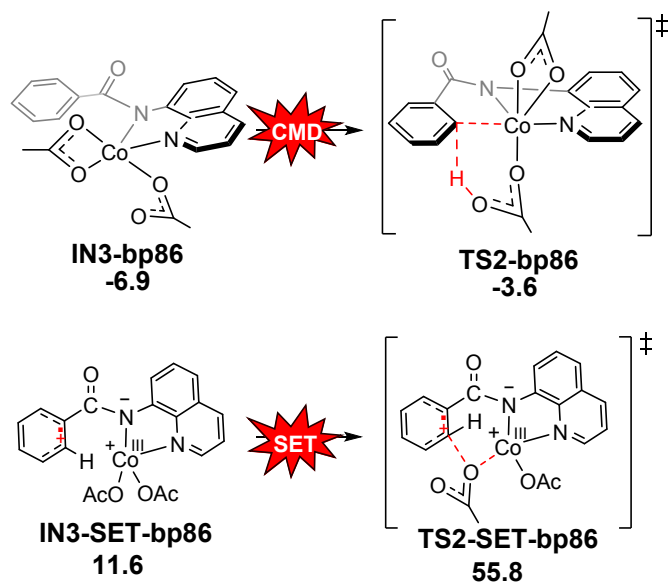
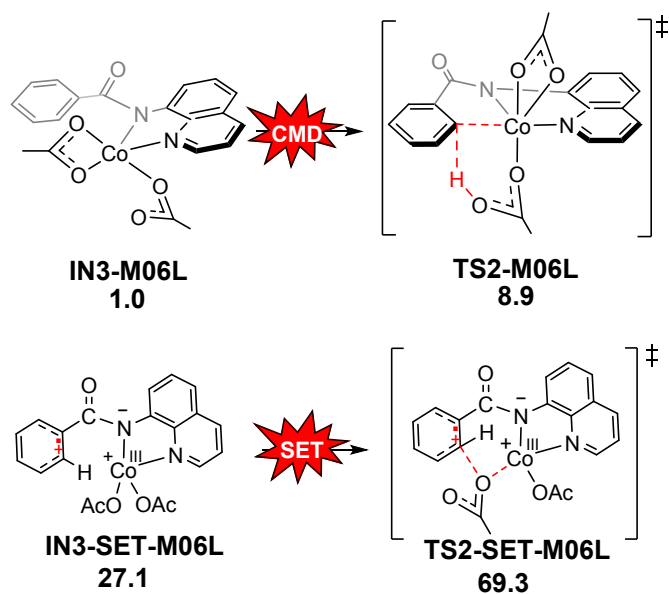


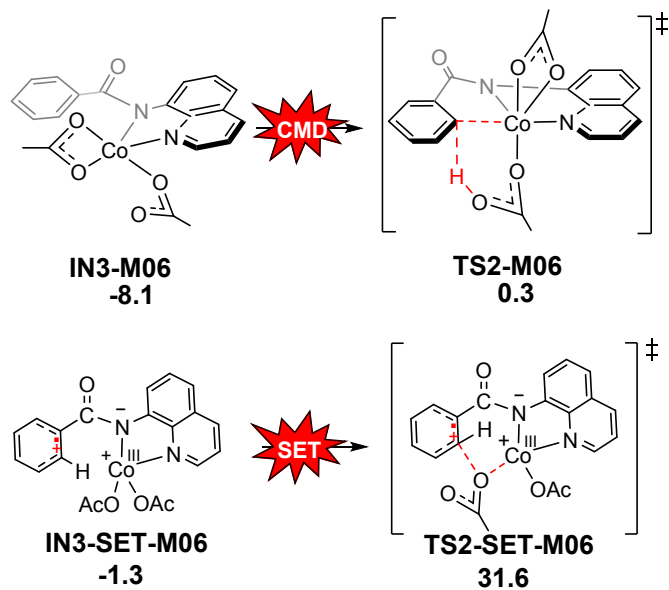
Fig. S1 Calculated free-energy profiles for other possible C–H deprotonation.



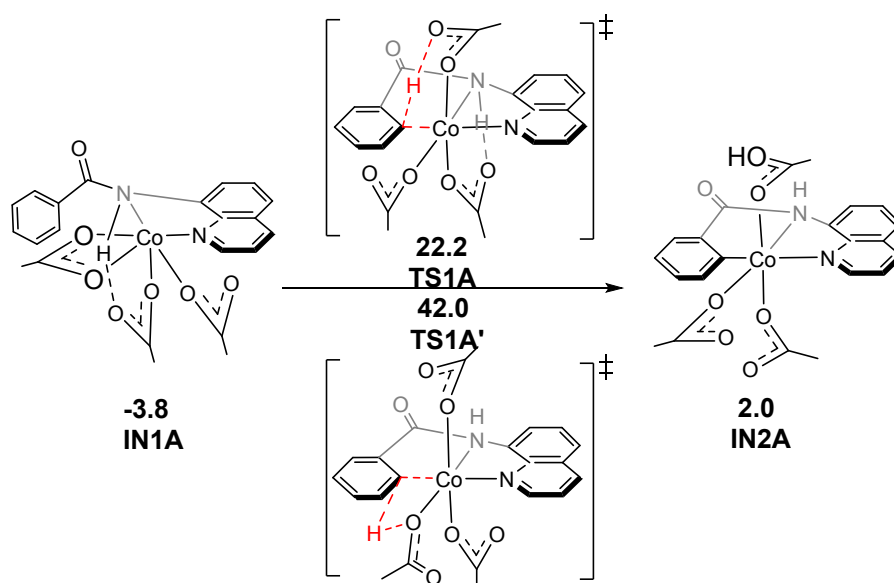
Scheme S1. CMD and SET mechanisms for the C–H activation at the BP86 level of theory.



Scheme S2. CMD and SET mechanisms for the C–H activation at the M06-L level of theory.



Scheme S3. CMD and SET mechanisms for the C–H activation at the M06 level of theory.



Scheme S4. Mechanism for initial C–H deprotonation.

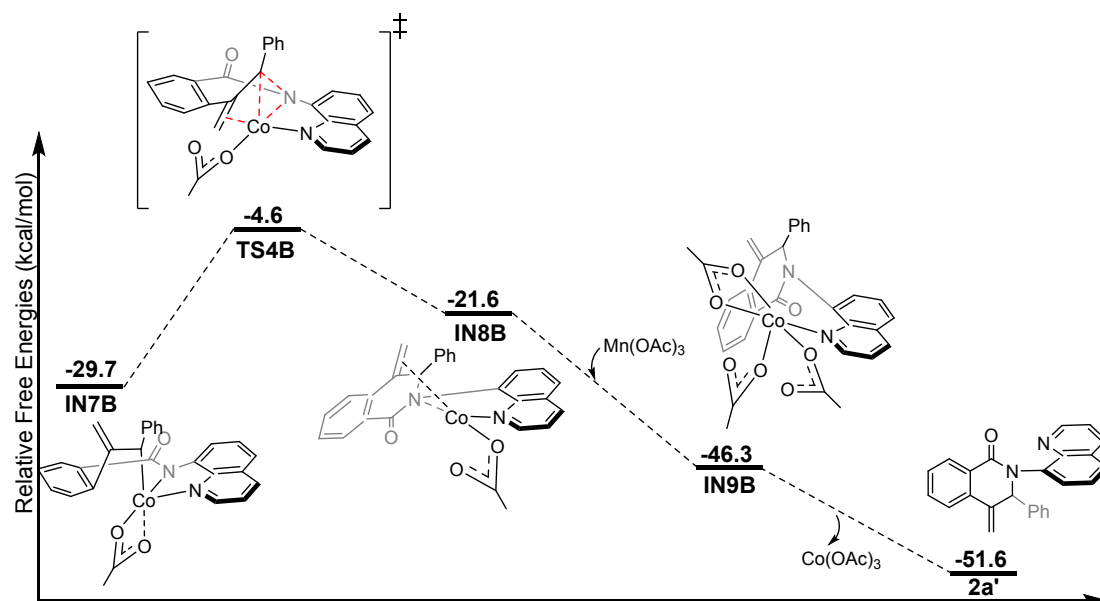
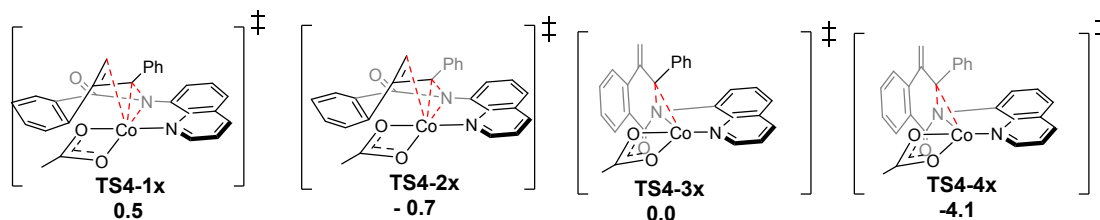


Fig. S2 Calculated free-energy profiles for the other possible reductive elimination of the aryllallene.



Scheme S5. Other conformations of the transition state TS4.

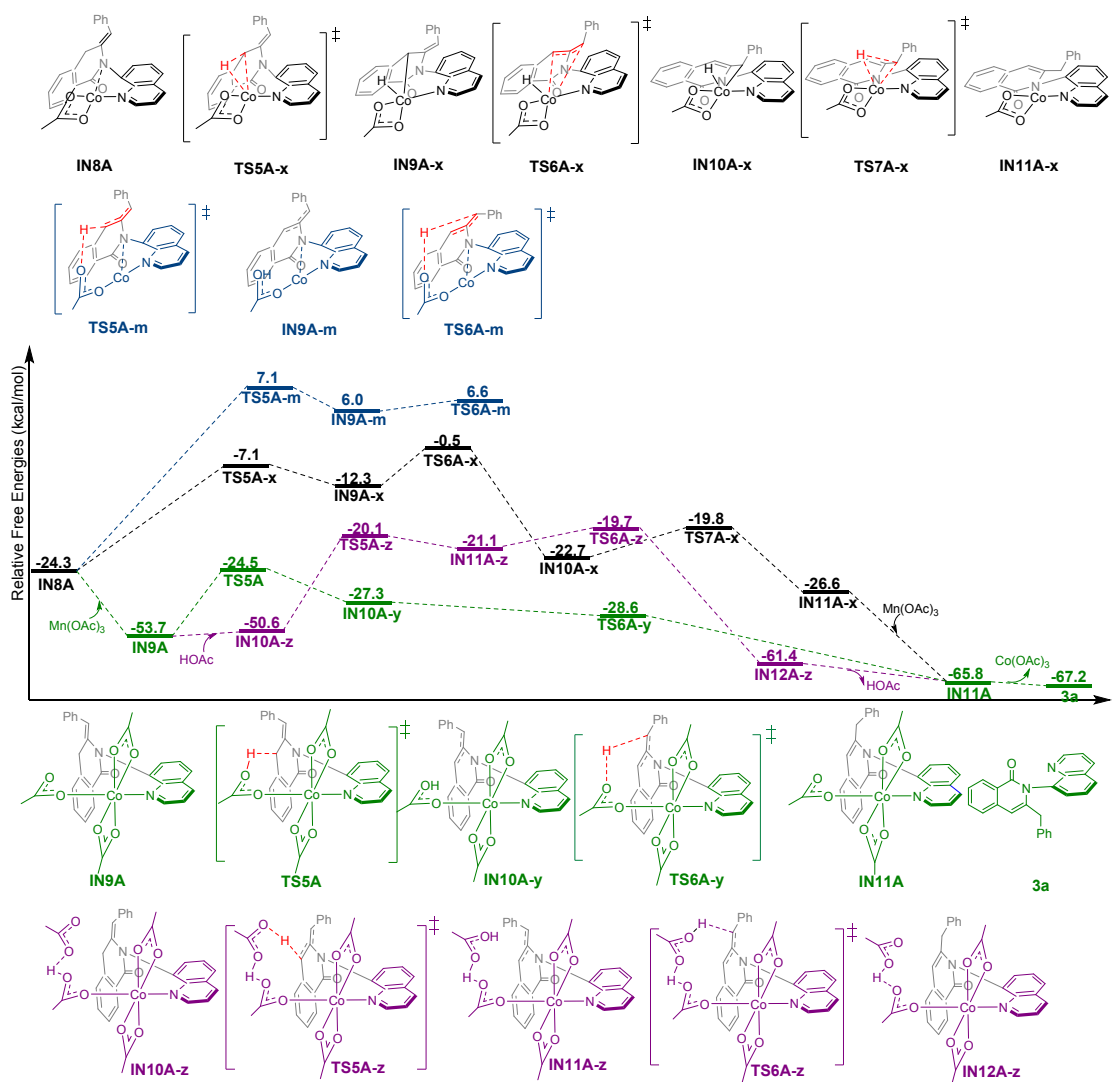


Fig. S3 Calculated free-energy profiles for other possible hydroarylation pathways of the allenylphosphonate starting from **2IN8A**.

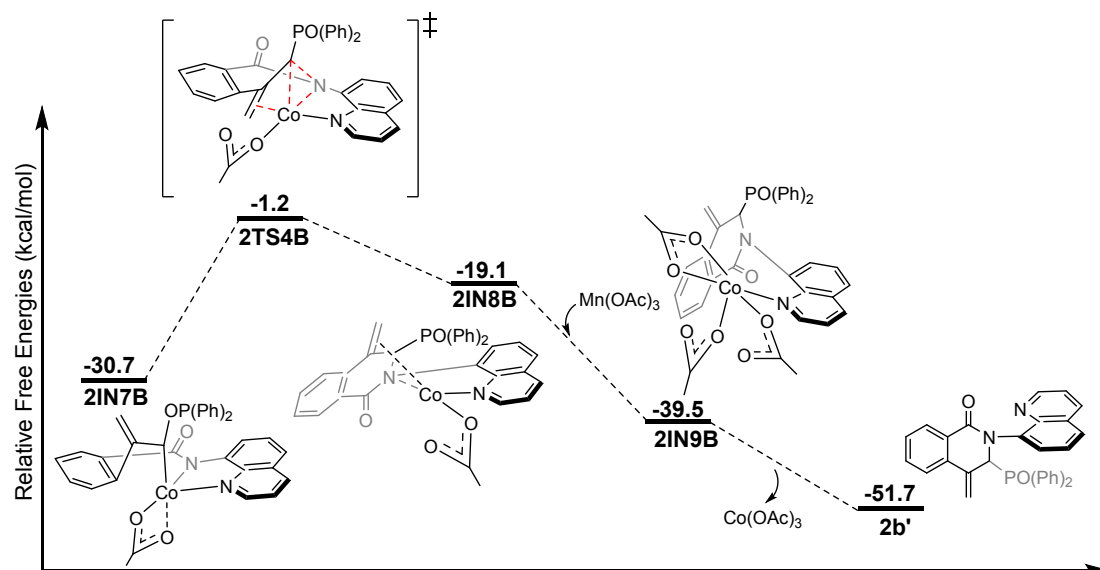
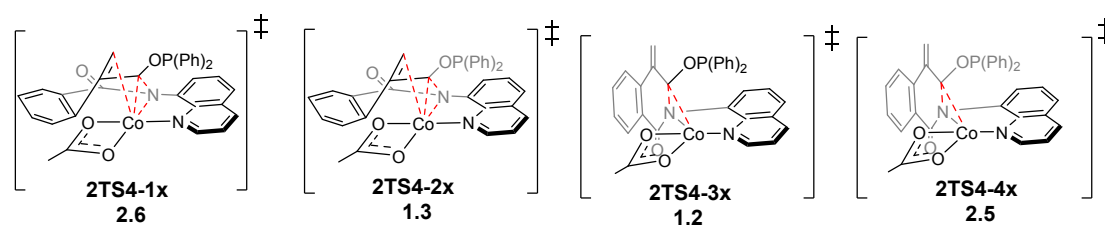


Fig. S5 Calculated free-energy profiles for the other possible reductive elimination of the allenylphosphonate.



Scheme S6. Other conformations of the transition state **2TTS4**.

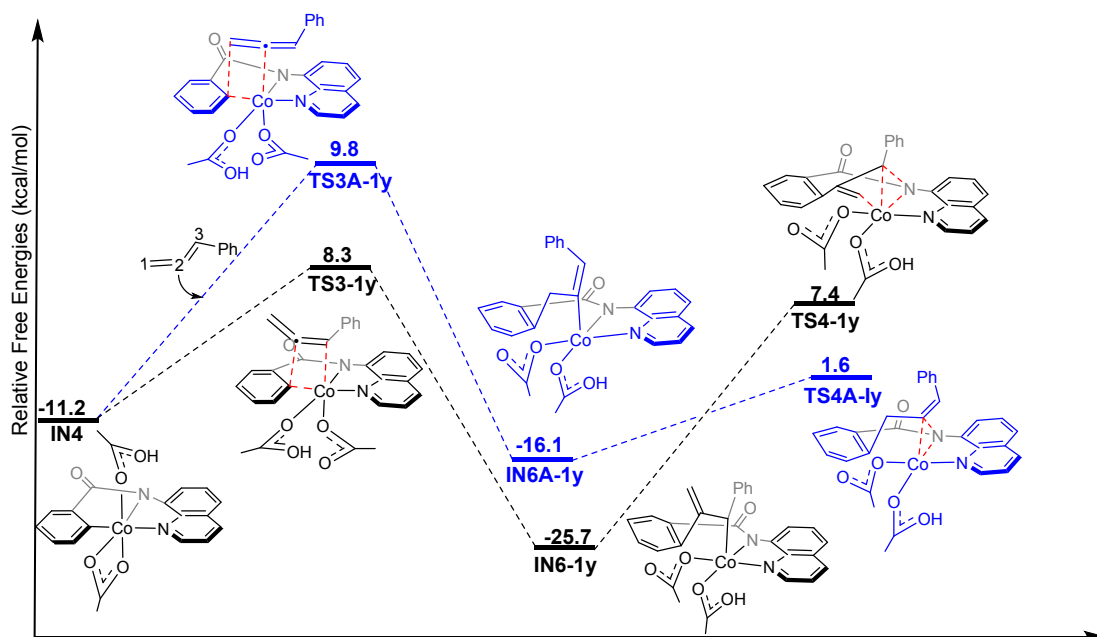


Fig. S5 Calculated free-energy profiles for the other possible C=C bond insertion of the aryllallene.

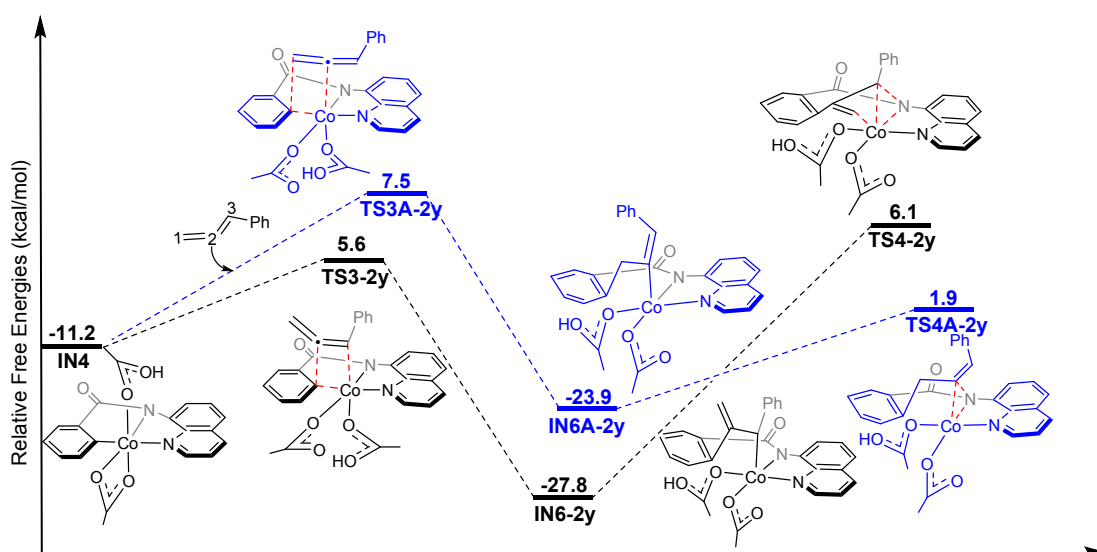


Fig. S6 Calculated free-energy profiles for the other possible C=C bond insertion of the aryllallene.

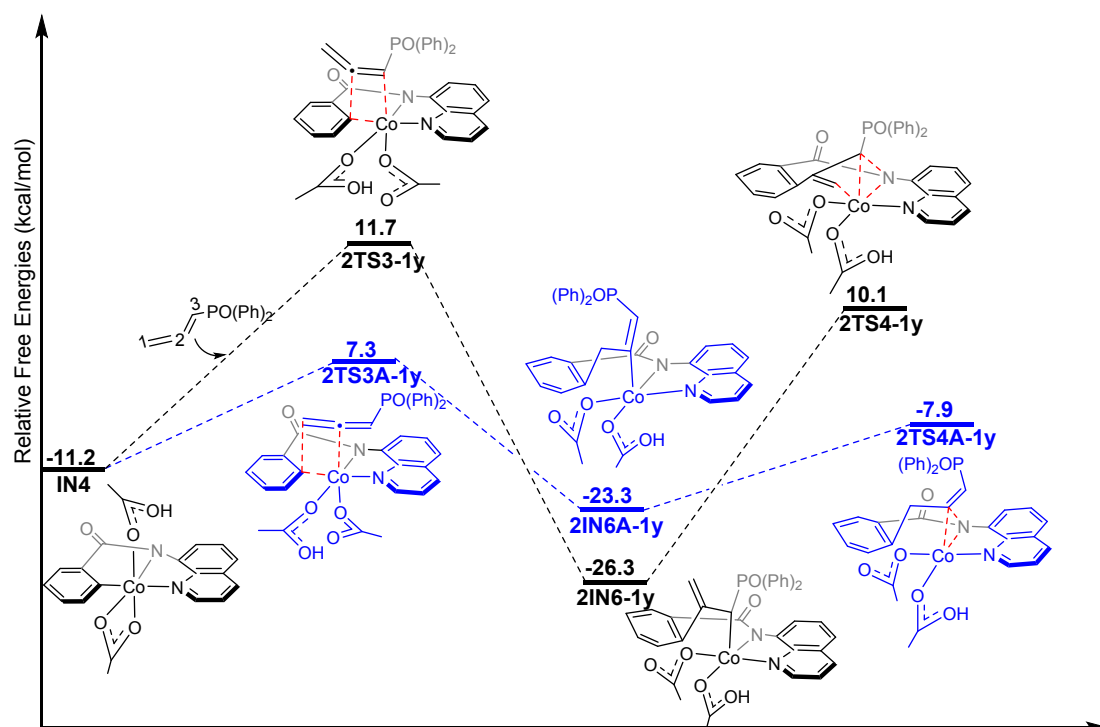


Fig. S7 Calculated free-energy profiles for the other possible C=C bond insertion of the allenylphosphonate.

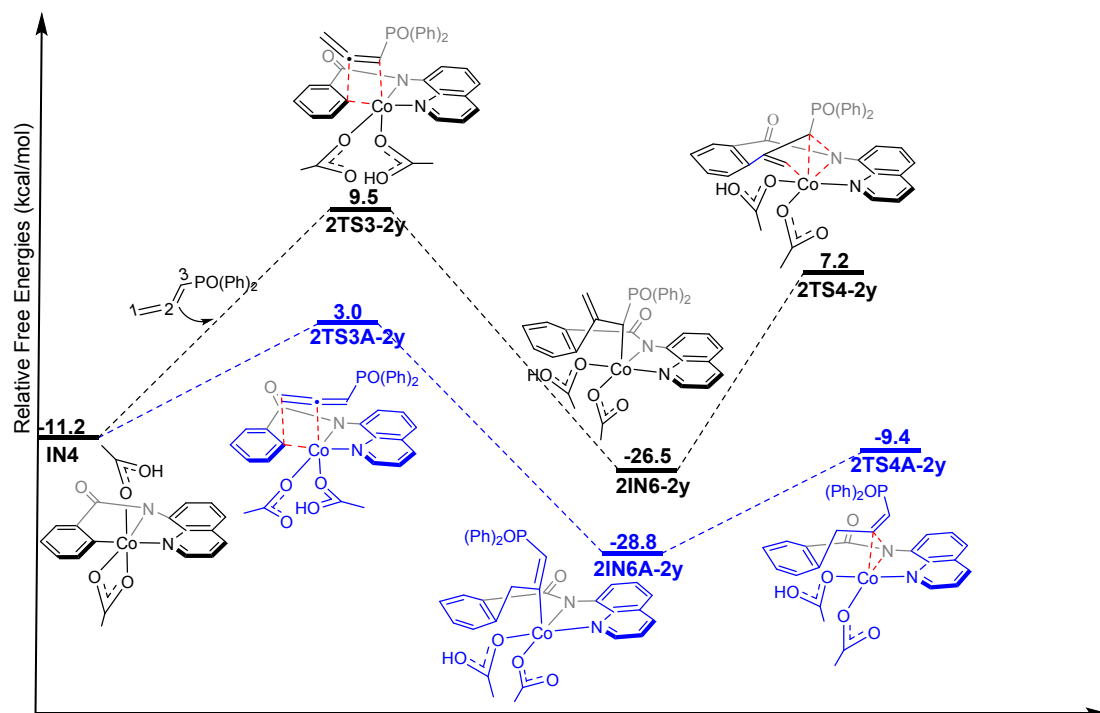


Fig. S8 Calculated free-energy profiles for the other possible C=C bond insertion of the allenylphosphonate.

Section 2. Energies (in Hartree) for all TSs and intermediates.

Species	E ₀	E	H ₂₉₈	G ₂₉₈	E (M06)
1	-801.641863	-801.627554	-801.626610	-801.684985	-801.1313996
1-m	-840.936911	-840.920954	-840.920010	-840.981880	-840.3987999
Co(acac) ₂	-835.540786	-835.523870	-835.522926	-835.586056	-836.011961

Mn(OAc) ₃	-789.474476	-789.459168	-789.458224	-789.517416	-789.5689292
R ₁	-347.662626	-347.654902	-347.653958	-347.695255	-347.4232293
R ₂	-995.921816	-995.906302	-995.905357	-995.966384	-995.4688142
R ₃	-578.683443	-578.671115	-578.670170	-578.723424	-578.2794291
HOAc	-229.092096	-229.087602	-229.086658	-229.119034	-229.0129585
Co(acac) ₂ (OAc)	-1064.038876	-1064.017214	-1064.016270	-1064.089132	-1064.319855
Co(acac)(OAc) ₂	-947.343034	-947.324736	-947.323792	-947.389822	-947.7127501
Co(OAc) ₃	-830.644148	-830.629088	-830.628144	-830.687358	-831.1037995
Mn(OAc) ₂	-560.977911	-560.966785	-560.965841	-561.016824	-561.1785757
Mn(acac)(OAc)	-677.691403	-677.677153	-677.676208	-677.733767	-677.7209506
Mn(acac) ₂	-794.361612	-794.344066	-794.343122	-794.408369	-794.3785437
IN1-a	-1865.657070	-1865.619349	-1865.618404	-1865.728124	-1865.434969
TS1-a	-1865.648689	-1865.611814	-1865.610869	-1865.717138	-1865.428988
IN2-a	-1865.645842	-1865.608706	-1865.607762	-1865.713911	-1865.425729
IN1-b	-1748.964102	-1748.929952	-1748.929008	-1749.030956	-1749.030956
TS1-b	-1748.957258	-1748.923773	-1748.922829	-1749.021651	-1748.820827
IN2-b	-1748.956589	-1748.922132	-1748.921188	-1749.024002	-1748.823587
IN1	-1632.303541	-1632.273167	-1632.272223	-1632.366354	-1632.24788
TS1	-1632.297885	-1632.267828	-1632.266884	-1632.359313	-1632.246586
IN2	-1632.296103	-1632.265789	-1632.264845	-1632.357652	-1632.245813
IN3	-1403.186556	-1403.161490	-1403.160546	-1403.241973	-1403.231291
TS2	-1403.170773	-1403.146251	-1403.145307	-1403.225106	-1403.219167
IN4	-1403.190198	-1403.165485	-1403.164541	-1403.243917	-1403.240131

IN5	-1174.072702	-1174.053294	-1174.052350	-1174.120436	-1174.216966
IN1A	-1632.293981	-1632.263380	-1632.262436	-1632.356359	-1632.241192
TS1A	-1632.251541	-1632.221501	-1632.220557	-1632.312373	-1632.199809
IN2A	-1632.280838	-1632.250281	-1632.249337	-1632.342618	-1632.231958
TS1A'	-1632.214963	-1632.184701	-1632.183757	-1632.275667	-1632.168335
IN3B	-1403.195152	-1403.170343	-1403.169398	-1403.249822	-1403.239002
TS2B	-1403.138126	-1403.113863	-1403.112919	-1403.191053	-1403.191613
IN3C	-1403.186376	-1403.160898	-1403.159954	-1403.243215	-1403.232618
TS2C	-1403.148902	-1403.124315	-1403.123370	-1403.203015	-1403.200201
IN6	-1521.736342	-1521.706983	-1521.706039	-1521.800412	-1521.642276
TS3	-1521.721764	-1521.694119	-1521.693175	-1521.779346	-1521.64314
IN7	-1521.770544	-1521.742610	-1521.741666	-1521.829253	-1521.683591
TS4	-1521.715001	-1521.687457	-1521.686512	-1521.773421	-1521.641853
IN8	-1521.742737	-1521.715226	-1521.714282	-1521.800587	-1521.668571
IN9	-1978.781976	-1978.744797	-1978.743853	-1978.850969	-1978.491574
2a	-1148.136879	-1148.115967	-1148.115023	-1148.187671	-1147.390983
IN6A	-1521.735421	-1521.707039	-1521.706095	-1521.794823	-1521.6391
TS3A	-1521.729808	-1521.702598	-1521.701654	-1521.786836	-1521.63977
IN7A	-1521.771204	-1521.743647	-1521.742703	-1521.829780	-1521.673415
TS4A	-1521.735837	-1521.709034	-1521.708090	-1521.792365	-1521.644471
IN8A	-1521.757980	-1521.730396	-1521.729452	-1521.817088	-1521.671306
IN9A	-1978.797712	-1978.760463	-1978.759518	-1978.867861	-1978.498612
TS5A	-1978.747854	-1978.711480	-1978.710536	-1978.815377	-1978.452008
IN10A	-1978.813677	-1978.776516	-1978.775572	-1978.882912	-1978.522064

TS6A	-1978.756452	-1978.719587	-1978.718643	-1978.825517	-1978.46049
IN11A	-1978.813363	-1978.776268	-1978.775324	-1978.883782	-1978.517813
3a	-1148.168820	-1148.147785	-1148.146841	-1148.220910	-1147.41633
IN7B	-1521.768502	-1521.740832	-1521.739888	-1521.826645	-1521.679915
TS4B	-1521.713908	-1521.686622	-1521.685678	-1521.771999	-1521.639901
IN8B	-1521.740248	-1521.712704	-1521.711760	-1521.798174	-1521.666993
IN9B	-1978.777212	-1978.740928	-1978.739984	-1978.844131	-1978.486822
2a'	-1148.139160	-1148.118230	-1148.117286	-1148.189676	-1147.391338
TS4-1x	-1521.716806	-1521.689448	-1521.688504	-1521.774807	-1521.631709
TS4-2x	-1521.720700	-1521.693513	-1521.692569	-1521.777775	-1521.63366
TS4-3x	-1521.713331	-1521.685887	-1521.684943	-1521.771040	-1521.632507
TS4-4x	-1521.720329	-1521.692747	-1521.691803	-1521.778775	-1521.639031
TS5A-x	-1521.723918	-1521.696796	-1521.695852	-1521.781616	-1521.643832
IN9A-x	-1521.741069	-1521.713927	-1521.712982	-1521.798847	-1521.652107
TS6A-x	-1521.723452	-1521.696723	-1521.695779	-1521.780703	-1521.633357
IN10A-x	-1521.758886	-1521.731683	-1521.730739	-1521.816841	-1521.668758
TS7A-x	-1521.747150	-1521.720000	-1521.719056	-1521.805435	-1521.664125
IN11A-x	-1521.757840	-1521.730301	-1521.729357	-1521.816292	-1521.67491
IN10A-y	-1978.752316	-1978.714174	-1978.713230	-1978.824541	-1978.456483
TS6A-y	-1978.751580	-1978.715028	-1978.714084	-1978.819619	-1978.458544
IN10A-z	-2207.901253	-2207.858081	-2207.857137	-2207.980088	-2207.506542
TS5A-z	-2207.848670	-2207.806398	-2207.805454	-2207.924879	-2207.45799
IN11A-z	-2207.851316	-2207.807399	-2207.806455	-2207.930890	-2207.459596

TS6A-z	-2207.847549	-2207.805583	-2207.804639	-2207.922752	-2207.457352
IN12A-z	-2207.917995	-2207.874992	-2207.874048	-2207.996779	-2207.523849
TS5A-m	-1521.705226	-1521.677893	-1521.676949	-1521.763298	-1521.621225
IN9A-m	-1521.703452	-1521.675391	-1521.674447	-1521.764341	-1521.622955
TS6A-m	-1521.704033	-1521.676842	-1521.675898	-1521.761987	-1521.622069
TS3-1y	-1750.806547	-1750.773216	-1750.772272	-1750.870637	-1750.632224
IN6-1y	-1750.858384	-1750.825004	-1750.824060	-1750.923141	-1750.677273
TS4-1y	-1750.813161	-1750.779976	-1750.779032	-1750.878543	-1750.633615
TS3A-1y	-1750.815276	-1750.782060	-1750.781115	-1750.879830	-1750.62992
IN6A-1y	-1750.860628	-1750.827377	-1750.826433	-1750.925995	-1750.67338
TS4A-1y	-1750.822280	-1750.789405	-1750.788460	-1750.887595	-1750.642922
TS3-2y	-1750.810553	-1750.776970	-1750.776026	-1750.875017	-1750.636544
IN6-2y	-1750.865237	-1750.831572	-1750.830628	-1750.931244	-1750.685468
TS4-2y	-1750.815687	-1750.782640	-1750.781696	-1750.880196	-1750.635686
TS3A-2y	-1750.819283	-1750.786009	-1750.785065	-1750.883683	-1750.633542
IN6A-2y	-1750.868083	-1750.834434	-1750.833490	-1750.935236	-1750.67842
TS4A-2y	-1750.826328	-1750.793412	-1750.792468	-1750.891228	-1750.642385
2IN6	-2169.995902	-2169.959003	-2169.958059	-2170.068303	-2169.68452
2TS3	-2169.973156	-2169.938030	-2169.937086	-2170.039923	-2169.682373
2IN7	-2170.022407	-2169.986881	-2169.985937	-2170.091143	-2169.726566
2TS4	-2169.959298	-2169.924103	-2169.923159	-2170.027937	-2169.680409
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2TS3A	-2169.988711	-2169.953430	-2169.952486	-2170.057869	-2169.689584
2IN7A	-2170.034053	-2169.998722	-2169.997777	-2170.103459	-2169.724798
2TS4A	-2170.005908	-2169.970927	-2169.969983	-2170.074540	-2169.705134
2IN8A	-2170.020125	-2169.984709	-2169.983765	-2170.089903	-2169.721805
2IN9A	-2627.061058	-2627.016275	-2627.015331	-2627.140070	-2626.549734
2TS5A	-2627.017833	-2626.973518	-2626.972574	-2627.096897	-2626.515223
2IN10A	-2627.063978	-2627.018963	-2627.018018	-2627.143684	-2626.565802
2TS6A	-2627.023031	-2626.978572	-2626.977628	-2627.101004	-2626.522356
2IN11A	-2627.079053	-2627.034343	-2627.033398	-2627.158540	-2626.568388
3b	-1796.429937	-1796.401232	-1796.400288	-1796.492301	-1795.464761
2IN7B	-2170.028924	-2169.993955	-2169.993010	-2170.095302	-2169.727001
2TS4B	-2169.964886	-2169.929749	-2169.928805	-2170.032987	-2169.680059
2IN8B	-2169.992084	-2169.957024	-2169.956080	-2170.059340	-2169.708515
2IN9B	-2627.021597	-2626.977049	-2626.976105	-2627.097904	-2626.521581
2b'	-1796.392979	-1796.364390	-1796.363446	-1796.452915	-1795.437191
2TS4-1x	-2169.970088	-2169.935134	-2169.934189	-2170.038251	-2169.673963
2TS4-2x	-2169.974081	-2169.939265	-2169.938321	-2170.041691	-2169.675971
2TS4-3x	-2169.967873	-2169.932837	-2169.931893	-2170.035303	-2169.676165
2TS4-4x	-2169.967527	-2169.932203	-2169.931258	-2170.035748	-2169.674152
2TS5A-d	-2169.987705	-2169.952567	-2169.951622	-2170.057185	-2169.69368
2IN9A-d	-2170.006232	-2169.971087	-2169.970143	-2170.075887	-2169.70563
2TS6A-d	-2169.988419	-2169.953909	-2169.952965	-2170.055815	-2169.687115

2IN10A-d	-2170.021206	-2169.986330	-2169.985386	-2170.089994	-2169.724336
2TS7A-d	-2170.004623	-2169.969796	-2169.968852	-2170.073324	-2169.714358
2IN11A-d	-2170.013166	-2169.977694	-2169.976750	-2170.083052	-2169.721014
2TS3-1y	-2399.059450	-2399.018168	-2399.017224	-2399.134594	-2398.672357
2IN6-1y	-2399.114255	-2399.073120	-2399.072176	-2399.189149	-2398.724555
2TS4-1y	-2399.067027	-2399.026300	-2399.025356	-2399.141694	-2398.674978
2TS3A-1y	-2399.074007	-2399.032896	-2399.031951	-2399.150117	-2398.679464
2IN6A-1y	-2399.123038	-2399.081990	-2399.081046	-2399.199572	-2398.727607
2TS4A-1y	-2399.093456	-2399.052640	-2399.051696	-2399.171096	-2398.703642
2TS3-2y	-2399.061465	-2399.020170	-2399.019226	-2399.135943	-2398.675984
2IN6-2y	-2399.118235	-2399.076930	-2399.075986	-2399.194296	-2398.731203
2TS4-2y	-2399.070221	-2399.029409	-2399.028464	-2399.145462	-2398.679569
2TS3A-2y	-2399.078665	-2399.037156	-2399.036212	-2399.156798	-2398.686305
2IN6A-2y	-2399.131011	-2399.089604	-2399.088660	-2399.208810	-2398.731957
2TS4A-2y	-2399.098274	-2399.057201	-2399.056257	-2399.176026	-2398.705975
3IN5	-1213.368405	-1213.347402	-1213.346458	-1213.417979	-1213.484449
3IN6	-1792.040783	-1792.006291	-1792.005347	-1792.106973	-1791.765157
3TS3	-1792.022244	-1791.988454	-1791.987510	-1792.086846	-1791.756039
3IN7	-1792.063833	-1792.029836	-1792.028892	-1792.127727	-1791.797838
3IN6A	-1792.053373	-1792.018268	-1792.017324	-1792.122789	-1791.762274
2TS3A	-1792.032667	-1791.998904	-1791.997960	-1792.097933	-1791.761119
3IN7A	-1792.081352	-1792.046871	-1792.045927	-1792.149282	-1791.805376
2IN8A-a	-2399.143236	-2399.102025	-2399.101081	-2399.221421	-2398.744165
2TS4A-a	-2399.129972	-2399.089703	-2399.088759	-2399.206006	-2398.727976

2IN9A-a	-2399.127259	-2399.086820	-2399.085875	-2399.203715	-2398.723886
2IN10A-a	-2628.219003	-2628.172737	-2628.171793	-2628.300729	-2627.720039
2TS5A-a	-2628.194525	-2628.148693	-2628.147749	-2628.277695	-2627.691687
2IN11A-a	-2628.223500	-2628.176766	-2628.175821	-2628.308765	-2627.715686
2IN8A-b	-2399.145024	-2399.104501	-2399.103556	-2399.220685	-2398.743687
2TS4A-b	-2399.108536	-2399.068658	-2399.067714	-2399.182922	-2398.705147
2IN9A-b	-2399.129165	-2399.088111	-2399.087167	-2399.208192	-2398.722333
2IN10A-b	-2628.249716	-2628.203566	-2628.202621	-2628.332571	-2627.734273
2TS5A-b	-2628.232934	-2628.186780	-2628.185836	-2628.318110	-2627.72668
2IN11A-b	-2628.236215	-2628.189781	-2628.188836	-2628.320410	-2627.725908
3ah	-1797.587422	-1797.556929	-1797.555985	-1797.656119	-1796.621526
2TS4A-c	-2170.003285	-2169.968387	-2169.967443	-2170.072493	-2169.698714
2IN8A-c	-2170.019984	-2169.984504	-2169.983560	-2170.090411	-2169.718493
2TS5A-c	-2170.003523	-2169.968153	-2169.967209	-2170.073569	-2169.702832
2IN9A-c	-2170.003107	-2169.967342	-2169.966398	-2170.073846	-2169.700728
2IN10A-c	-2627.039387	-2626.993260	-2626.992316	-2627.123500	-2626.525396
3ch	-1796.382271	-1796.352168	-1796.351224	-1796.448242	-1795.41172
Co(OAc) ₂	-602.147815	-602.137002	-602.136058	-602.187640	-602.7170681
HO ₂ Piv	-346.975621	-346.967368	-346.966424	-347.007724	-346.8107943
OAc ⁻	-228.632210	-228.627813	-228.626869	-228.659787	-228.5657467
OPiv ⁻	-346.516618	-346.508791	-346.507846	-346.548151	-346.3610403
IN1-SET	-801.157625	-801.143515	-801.142571	-801.200521	-800.6528141
IN2-SET	-800.989705	-800.975441	-800.974497	-801.033565	-800.4776597

IN3-SET	-1403.001979	-1402.977019	-1402.976075	-1403.058377	-1403.041703
TS2-SET	-1402.957067	-1402.931812	-1402.930868	-1403.013797	-1402.998513
IN4-SET	-1402.976615	-1402.951848	-1402.950904	-1403.031790	-1403.020874
IN5-SET	-1631.623612	-1631.594077	-1631.593132	-1631.683749	-1631.571702
Mn(OAc) ₃ -SET	-789.661493	-789.644420	-789.643476	-789.710551	-789.7440682
IN6-SET	-1521.541150	-1521.511792	-1521.510848	-1521.605085	-1521.440697
TS3-SET	-1521.526377	-1521.498725	-1521.497781	-1521.584376	-1521.442112
IN6A-SET	-1521.541026	-1521.512591	-1521.511647	-1521.600999	-1521.439531
TS3A-SET	-1521.532742	-1521.505388	-1521.504444	-1521.591091	-1521.437628
2IN6-SET	-2169.801757	-2169.764667	-2169.763723	-2169.874603	-2169.472189
2TS3-SET	-2169.778628	-2169.743190	-2169.742246	-2169.846854	-2169.475776
2IN6A-SET	-2169.798995	-2169.762756	-2169.761812	-2169.870276	-2169.474603
2TS3A-SET	-2169.790611	-2169.755353	-2169.754409	-2169.860242	-2169.474929

E_0 = Sum of electronic and zero-point Energies by B3LYP in solvent

E = Sum of electronic and thermal Energies by B3LYP in solvent

H_{298} = Sum of electronic and thermal Enthalpies by B3LYP in solvent

G_{298} = Sum of electronic and thermal Free Energies by B3LYP in solvent

$E_{(M06)}$ = Single point energies calculated by M06 in solvent

Species	E_0	E	H_{298}	G_{298}	E (M06L)
1-M06L	-801.528393	-801.514233	-801.513289	-801.570243	-801.6099343

Co(OAc) ₃ -M06L	-830.607292	-830.593773	-830.592829	-830.648340	-831.4726752
Co(OAc) ₂ -M06L	-602.128641	-602.118762	-602.117818	-602.166017	-602.953112
HOAc-M06L	-229.057241	-229.052727	-229.051782	-229.084237	-229.1100238
HOPiv-M06L	-346.919863	-346.911641	-346.910697	-346.952172	-346.9850619
OPiv-M06L	-346.459748	-346.452086	-346.451142	-346.491039	-346.5299208
OAc ⁻ -M06L	-228.596293	-228.592761	-228.591817	-228.622150	-228.6561087
IN3-M06L	-1403.075239	-1403.050244	-1403.049299	-1403.129832	-1403.970921
TS2-M06L	-1403.063564	-1403.039035	-1403.038091	-1403.118394	-1403.958343
IN3-SET-M06L	-1402.896984	-1402.871972	-1402.871027	-1402.952787	-1403.791597
TS2-SET-M06L	-1402.845397	-1402.820713	-1402.819769	-1402.900509	-1403.723839

E_0 = Sum of electronic and zero-point Energies by M06-L in solvent

E = Sum of electronic and thermal Energies by M06-L in solvent

H_{298} = Sum of electronic and thermal Enthalpies by M06-L in solvent

G_{298} = Sum of electronic and thermal Free Energies by M06-L in solvent

$E_{(M06)}$ = Single point energies calculated by M06-L in solvent

Species	E_0	E	H_{298}	G_{298}	E (BP86)
1-bp86	-801.645603	-801.630869	-801.629925	-801.688615	-801.7525497
Co(OAc) ₃ -bp86	-830.763539	-830.748109	-830.747165	-830.807167	-831.6520701
Co(OAc) ₂ -bp86	-602.240762	-602.229993	-602.229049	-602.279165	-603.0979917
HOAc-bp86	-229.095248	-229.090670	-229.089726	-229.122301	-229.1526189

HOPIV-bp86	-346.972966	-346.964511	-346.963567	-347.005257	-347.0519928
OPIV-bp86	-346.516177	-346.508131	-346.507187	-346.547885	-346.6020384
OAc-bp86	-228.636930	-228.632431	-228.631487	-228.664990	-228.7056271
IN3-bp86	-1403.307734	-1403.281782	-1403.280838	-1403.364741	-1404.262949
TS2-bp86	-1403.304861	-1403.279923	-1403.278979	-1403.358489	-1404.257799
IN3-SET-bp86	-1403.125356	-1403.099358	-1403.098414	-1403.183951	-1404.079075
TS2-SET-bp86	-1403.071646	-1403.046501	-1403.045556	-1403.126545	-1404.008516

E_0 = Sum of electronic and zero-point Energies by BP86 in solvent

E = Sum of electronic and thermal Energies by BP86 in solvent

H_{298} = Sum of electronic and thermal Enthalpies by BP86 in solvent

G_{298} = Sum of electronic and thermal Free Energies by BP86 in solvent

$E_{(M06)}$ = Single point energies calculated by BP86 in solvent

Species	E_0	E	H_{298}	G_{298}	$E (M06)$
1-M06	-801.050393	-801.036147	-801.035203	-801.092450	-801.1317806
Co(OAc) ₃ -M06	-830.236090	-830.222840	-830.221896	-830.276416	-831.1022953
Co(OAc) ₂ -M06	-601.868829	-601.858736	-601.857792	-601.908724	-602.7181947
HOAc-M06	-228.960401	-228.955798	-228.954853	-228.987934	-229.0139037
HOPIV-M06	-346.748473	-346.740336	-346.739392	-346.780628	-346.8114897
OPIV-M06	-346.292069	-346.284296	-346.283351	-346.323580	-346.3616685
OAc-M06	-228.502414	-228.498911	-228.497967	-228.528244	-228.5639338

IN3-M06	-1402.334148	-1402.309237	-1402.308293	-1402.388846	-1403.23315
TS2-M06	-1402.324185	-1402.300024	-1402.299080	-1402.377059	-1403.219773
IN3-SET-M06	-1402.147139	-1402.123121	-1402.122177	-1402.201742	-1403.042589
TS2-SET-M06	-1402.107654	-1402.082978	-1402.082034	-1402.162808	-1402.990101

E_0 = Sum of electronic and zero-point Energies by M06 in solvent

E = Sum of electronic and thermal Energies by M06 in solvent

H_{298} = Sum of electronic and thermal Enthalpies by M06 in solvent

G_{298} = Sum of electronic and thermal Free Energies by M06 in solvent

$E_{(M06)}$ = Single point energies calculated by M06 in solvent

Section 3. Calculated imaginary frequencies of all transition states species

Species	Frequency
TS1-a	-819.98
TS1-b	-1133.82
TS1	-1156.31
TS2	-1247.50
TS1A	-1171.06
TS1A'	-1653.84
TS2B	-1525.41

TS2C	-1499.78
TS3	-249.06
TS4	-387.50
TS3A	-166.31
TS4A	-353.91
TS5A	-885.63
TS6A	-1497.62
TS4B	-317.67
TS4-1x	-469.70
TS4-2x	-497.33
TS4-3x	-291.96
TS4-4x	-248.20
TS5A-x	-856.65
TS6A-x	-202.25
TS7A-x	-813.06
TS6A-y	-454.37
TS5A-z	-1153.36
TS6A-z	-346.25
TS5A-m	-1074.62
TS6A-m	-853.59
TS3-1y	-297.24
TS4-1y	-480.34
TS3A-1y	-218.02
TS4A-1y	-350.28

TS3-2y	-249.26
TS4-2y	-483.96
TS3A-2y	-139.32
TS4A-2y	-353.77
2TS3	-256.11
2TS4	-420.94
2TS3A	-156.90
2TS4A	-329.97
2TS5A	-1059.95
2TS6A	-1546.20
2TS4B	-417.92
2TS4-1x	-491.11
2TS4-2x	-519.88
2TS4-3x	-277.94
2TS4-4x	-224.72
2TS5A-d	-831.30
2TS6A-d	-210.42
2TS7A-d	-854.96
2TS3-1y	-310.06
2TS4-1y	-499.83
2TS3A-1y	-216.17
2TS4A-1y	-321.36
2TS3-2y	-266.84

2TS4-2y	-502.93
2TS3A-2y	-126.79
2TS4A-2y	-312.56
3TS3	-256.21
3TS3A	-95.04
2TS4A-a	-988.61
2TS5A-a	-1255.74
2TS4A-b	-1082.12
2TS5A-b	-1246.81
2TS4A-c	-1484.25
2TS5A-c	-1232.87
TS2-SET	-110.87
TS3-SET	-280.89
TS3A-SET	-199.17
2TS3-SET	-297.14
2TS3A-SET	-196.07
TS2-bp86	-887.92
TS2-SET-bp86	-264.52
TS2-M06L	-1390.02
TS2-SET-M06L	-214.72
TS2-M06	-1596.48
TS2-SET-M06	-18.58

