

Supporting Information

Enantioselective Cu-Catalyzed 1,4-Additions of Organozinc and Grignard Reagents to Enones: Exceptional Performance of the Hydrido-Phosphite-Ligand BIFOP-H

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Experimental

General procedure for the synthesis of (*R*)-3-ethyl-1,3-diphenylpropan-1-one, (*R*)-1,3-diphenylpentan-1-one (15a) or (*R*)-3-methyl-1,3-diphenylpropan-1-one, (*R*)-1,3-diphenylbutan-1-one (15b)

CuCl (0.01 mmol, 1.0 mg, 1 mol%) and **L** (0.02 mmol, s.b., 2 mol%) are dissolved in dry and absolute Et₂O (3.0 mL) and the mixture is stirred at room temperature for 10 min. The mixture is cooled to -78°C and subsequently 1.5 eq. of the corresponding Grignard reagent (EtMgBr or MeMgBr) in solvent are added dropwise. The reaction mixture is stirred at -78°C for another 10 min. Then the chalcone (1.0 mmol, 208 mg, 1.0 eq.) is added portionwise over 1 h. The reaction mixture is stirred for 6 h (full conversion is determined) and quenched with saturated aqueous NH₄Cl solution (3 mL). The mixture is separated and the water layer is extracted with DCM (2×5 mL). The combined organic layers are dried over Na₂SO₄, filtered and the solvent is evaporated under *vacuo*. Purification by flash chromatography over silica gel, using Et₂O:*n*-hexane 1:20 (R_f = 0.1) afforded the desired product.

L = PPh₃, 5.3 mg, racemic product is formed.

L = BIFOP-H, 9.8 mg, enantioselective (*R*)-product is formed.

General procedure for the synthesis of (*R*)-3-ethylcyclohexanone (16a)

CuCl (0.01 mmol, 1.0 mg, 1 mol%) and **L** (0.02 mmol, s.b., 2 mol%) are dissolved in dry and absolute Et₂O (3.0 mL) and the mixture is stirred at room temperature for 10 min. The mixture is cooled to -78°C and subsequently 1.5 eq. of the Grignard reagent (EtMgBr) in solvent is added dropwise. The reaction mixture is stirred at -78°C for another 10 min. Then the cyclohexenone (1.0 mmol, 0.1 mL, 1.0 eq.) is added dropwise over 1 h. The reaction mixture is stirred for 6 h (full conversion is determined) and quenched with saturated aqueous NH₄Cl solution (3 mL). The mixture is separated and the water layer is extracted with DCM (2×5 mL). The combined organic layers are dried over Na₂SO₄, filtered and the solvent is evaporated under *vacuo*. Purification by flash chromatography over silica gel, using EtOAc:*n*-hexane 1:2 (R_f = 0.35) afforded the desired product (with MeMgBr no product is observed).

L = PPh₃, 5.3 mg, racemic product is formed.

L = BIFOP-H, 9.8 mg, enantioselective (*R*)-product is formed.

General procedure for the synthesis of 2-ethylchroman-4-one (17a) or 2-methylchroman-4-one (17b)

CuCl (0.01 mmol, 1.0 mg, 1 mol%) and **L** (0.02 mmol, s.b., 2 mol%) are dissolved in dry and absolute Et₂O (3.0 mL) and the mixture is stirred at room temperature for 10 min. The mixture is cooled to -78°C and subsequently 1.5 eq. of the corresponding Grignard reagent (EtMgBr or MeMgBr) in solvent are added dropwise. The reaction mixture is stirred at -78°C for another 10 min. Then the chromone (1.0 mmol, 146 mg, 1.0 eq.) is added portionwise over 1 h. The reaction mixture is stirred for 6 h (full conversion is determined) and quenched with saturated aqueous NH₄Cl solution (3 mL). The mixture is separated and the water layer is extracted with DCM (2×5 mL). The combined organic layers are dried over Na₂SO₄, filtered and the solvent is evaporated under *vacuo*. Purification by flash chromatography over silica gel, using Et₂O:*n*-hexane 1:10 (R_f = 0.25) afforded the desired product.

L = PPh₃, 5.3 mg, or BIFOP-H, 9.8 mg, racemic product is formed.

X-ray crystal structure

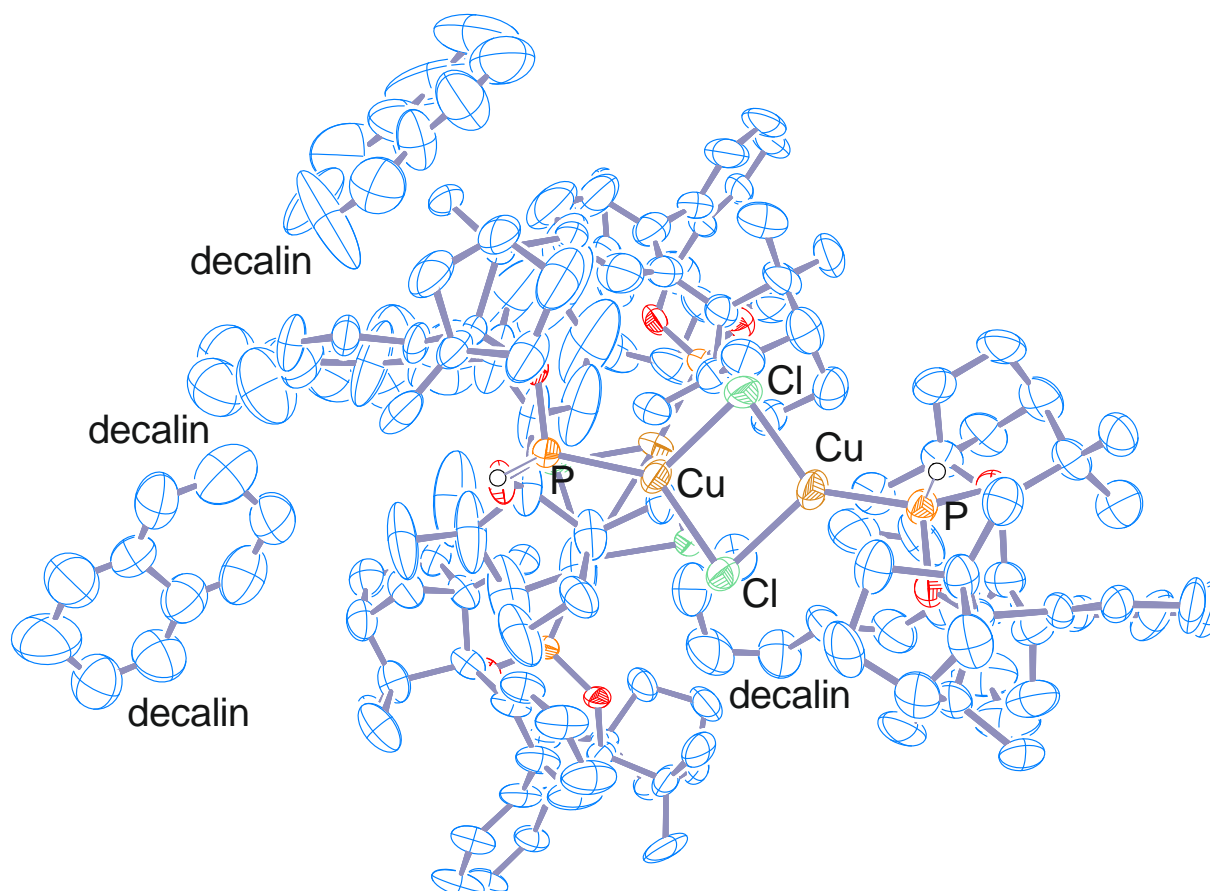


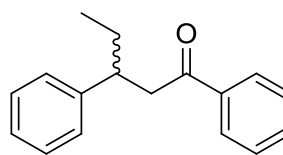
Figure 1: Full X-ray crystal structure (CCDC 1862862) of BIFOP-H • CuCl building up dimers in decalin. The hydrogen atoms at the phosphorus moiety are located from difference in electron maps and refined freely by the crystallographer. The C-H-hydrogens are omitted for clarity. The ellipsoids are shown with 50% probability. Two dimer structures are shown together with four (highly disordered) decalin molecules.

Table 1. Crystal data and structure refinement for eb214_neu3_sq (Figure 1).

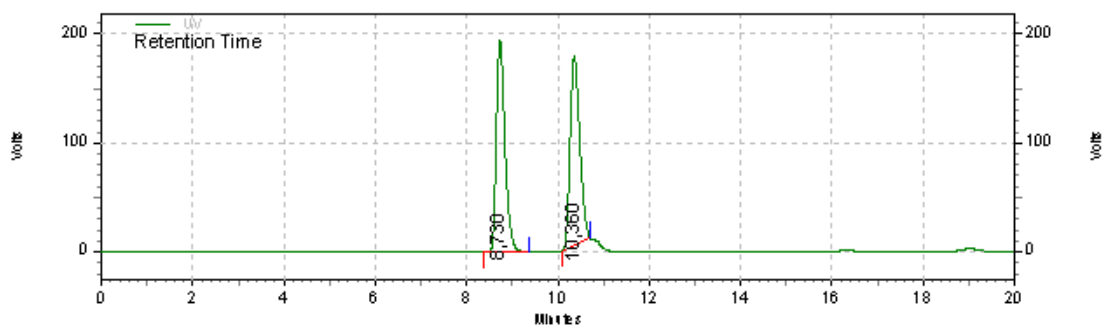
Identification code	eb214_neu3_sq	
Empirical formula	C ₈₄ H ₁₁₈ Cl ₂ Cu ₂ O ₄ P ₂	
Moiety formula	C ₆₄ H ₈₂ Cl ₂ Cu ₂ O ₄ P ₂ , C ₁₀ H ₁₈ [+ C ₁₀ H ₁₈]	
Formula weight	1451.70	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P2 ₁	
Unit cell dimensions	a = 15.1193(16) Å	a = 90°.

	$b = 31.626(4) \text{ \AA}$	$b = 90.221(5)^\circ$.
	$c = 15.4815(17) \text{ \AA}$	$g = 90^\circ$.
Volume	$7402.6(15) \text{ \AA}^3$	
Z	4	
Density (calculated)	1.303 Mg/m^3	
Absorption coefficient	2.163 mm^{-1}	
F(000)	3104	
Crystal size	$0.200 \times 0.200 \times 0.020 \text{ mm}^3$	
Theta range for data collection	$2.854 \text{ to } 75.926^\circ$.	
Index ranges	$-18 \leq h \leq 14, -38 \leq k \leq 38, -19 \leq l \leq 18$	
Reflections collected	80865	
Independent reflections	27388 [R(int) = 0.0564]	
Completeness to theta = 67.679°	96.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.3239 and 0.1972	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	27388 / 1 / 1553	
Goodness-of-fit on F^2	1.048	
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0698, wR2 = 0.1781$	
R indices (all data)	$R1 = 0.0867, wR2 = 0.1878$	
Absolute structure parameter	0.095(5)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.662 and $-0.412 \text{ e.\AA}^{-3}$	

HPLC-spectra



rac-Standard of 1,3-diphenylpentan-1-one (**15a**)

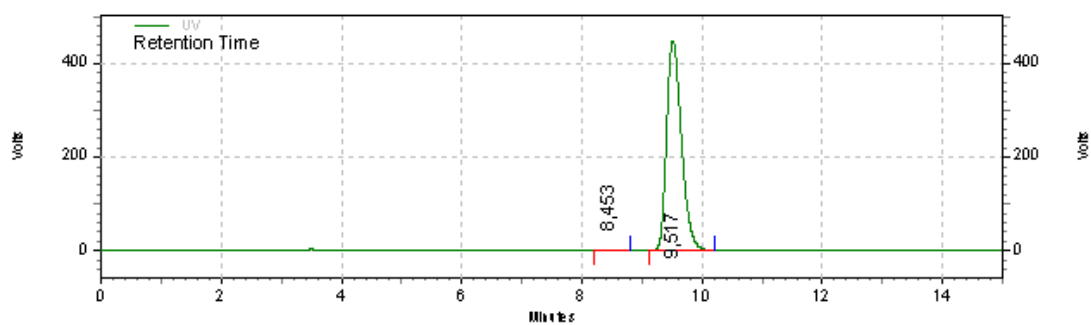
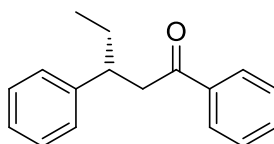


UV Results

Retention Time	Area	Area %	Height	Height %
8,730	10147971	49,98	778986	52,89
10,360	10155275	50,02	693806	47,11

Totals	Area	Area %	Height	Height %
	20303246	100,00	1472792	100,00

(*R*)-1,3-diphenylpentan-1-one ((*R*)-**15a**) after Enantioselective Cu-Catalyzed 1,4-Addition

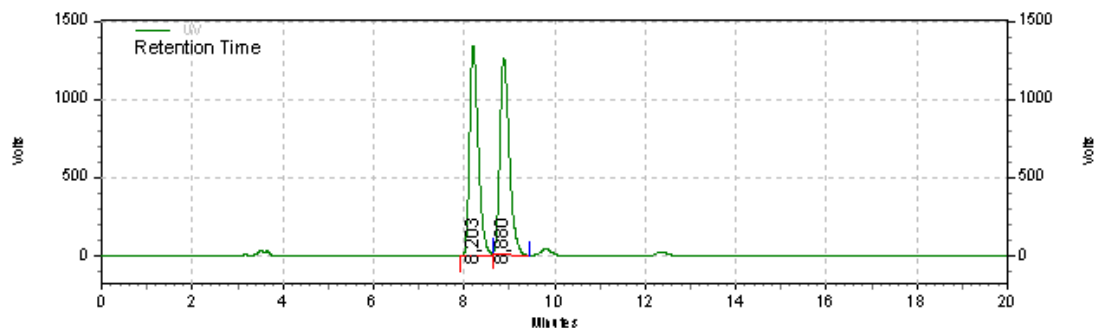
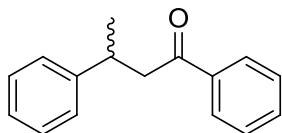


UV Results

Retention Time	Area	Area %	Height	Height %
8,453	113763	0,37	7829	0,44
9,517	30678407	99,63	1790349	99,56

Totals	Area	Area %	Height	Height %
	30792170	100,00	1798178	100,00

rac-Standard of 1,3-diphenylbutan-1-one (**15b**)

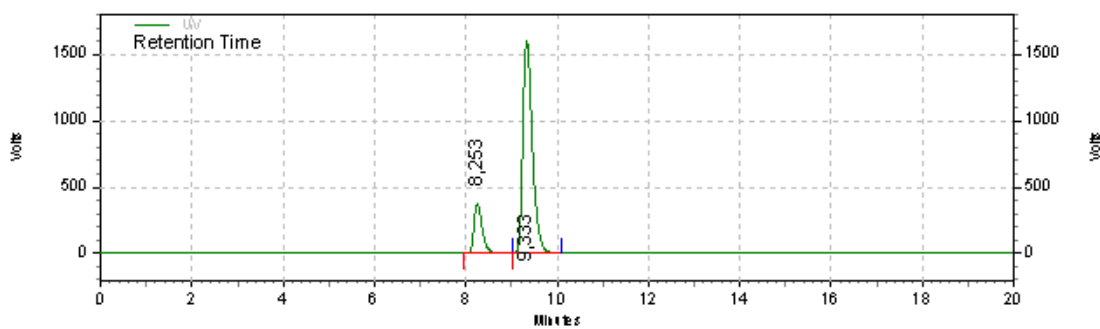
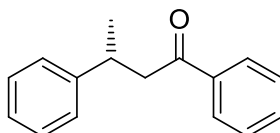


UV Results

Retention Time	Area	Area %	Height	Height %
8,203	72650902	50,12	5389063	51,81
8,880	72307876	49,88	5011559	48,19

Totals	144958778	100,00	10400622	100,00
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(*R*)-1,3-diphenylbutan-1-one ((*R*)-**15b**) after Enantioselective Cu-Catalyzed 1,4-Addition



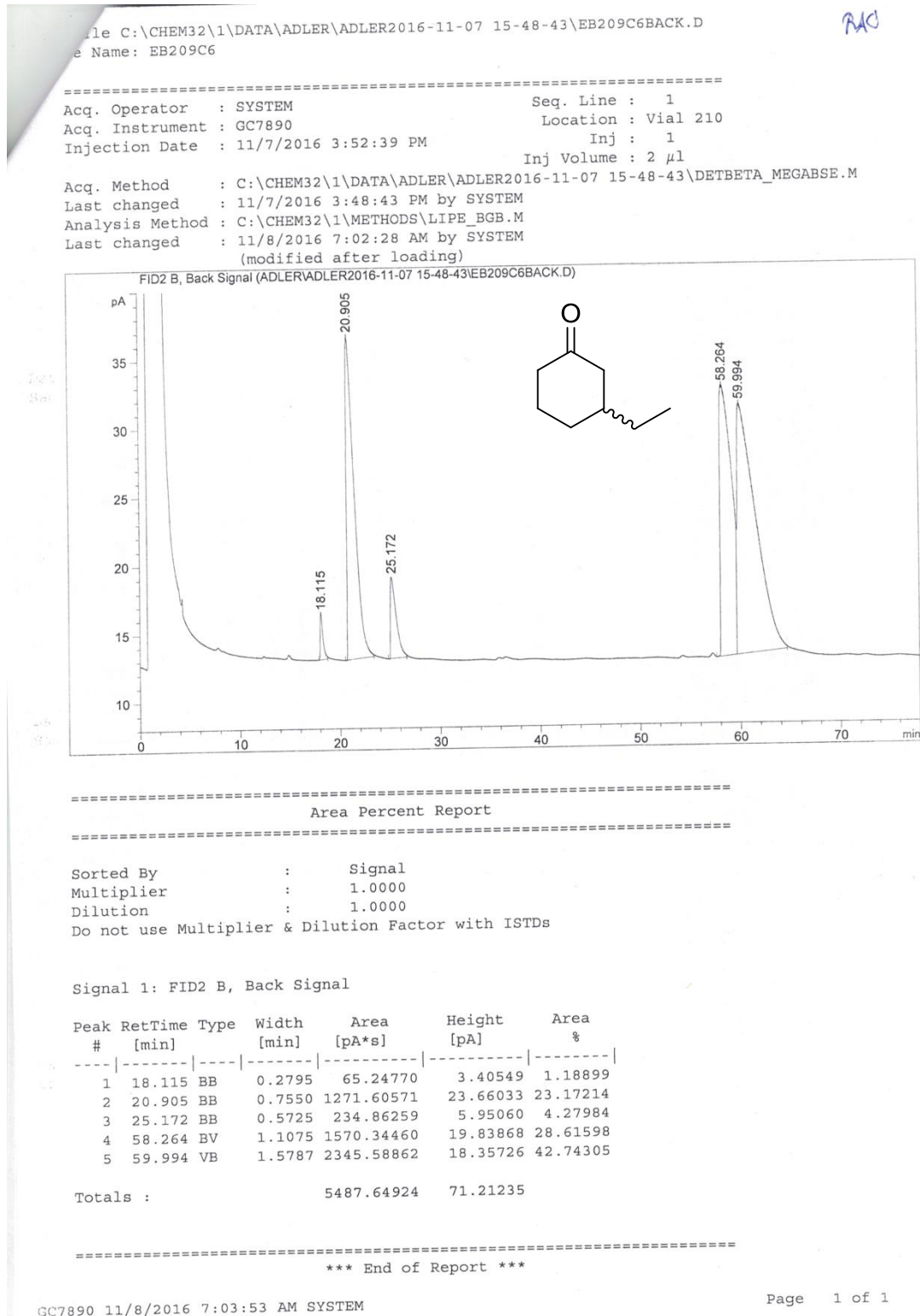
UV Results

Retention Time	Area	Area %	Height	Height %
8,253	18496971	16,56	1488155	18,79
9,333	93183652	83,44	6430569	81,21

Totals	111680623	100,00	7918724	100,00
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GC-spectra

rac-Standard of 3-ethylcyclohexan-1-one (16a)



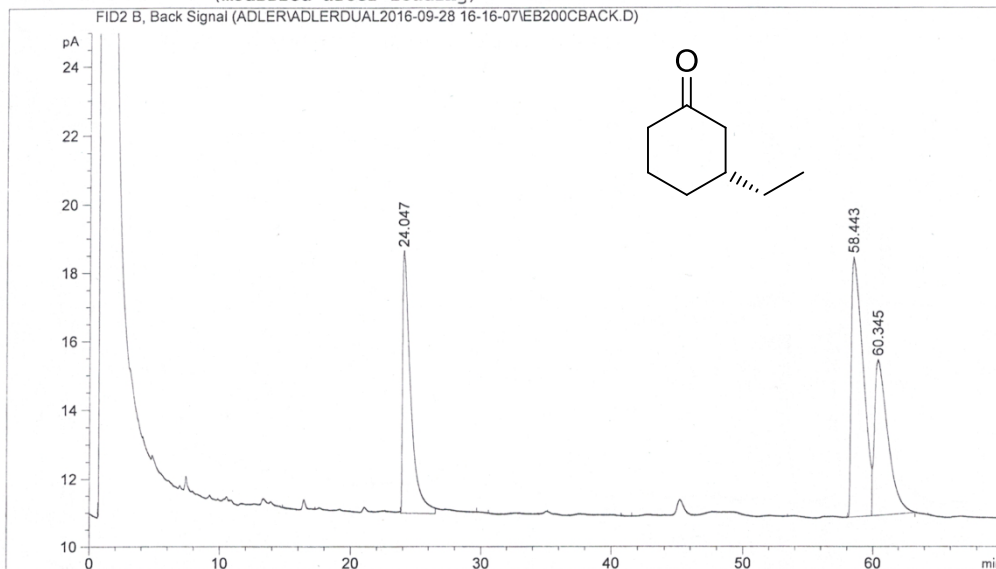
(R)-3-ethylcyclohexan-1-one ((R)-16a)

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Name: eb200c *Int2*

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Acq. Method	: DETBETA_MEGABSE.M		
Analysis Method	: C:\CHEM32\1\METHODS\LIPE_BGB_WS3.M		
Last changed	: 9/29/2016 9:39:45 AM by SYSTEM		

(modified after loading)



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Area Percent Report
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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: FID2 B, Back Signal

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	24.047	VV	0.5550	335.85663	7.63744	29.37475
2	58.443	VV	0.7462	481.12796	7.56334	42.08049
3	60.345	VB	0.8506	326.36691	4.51874	28.54476

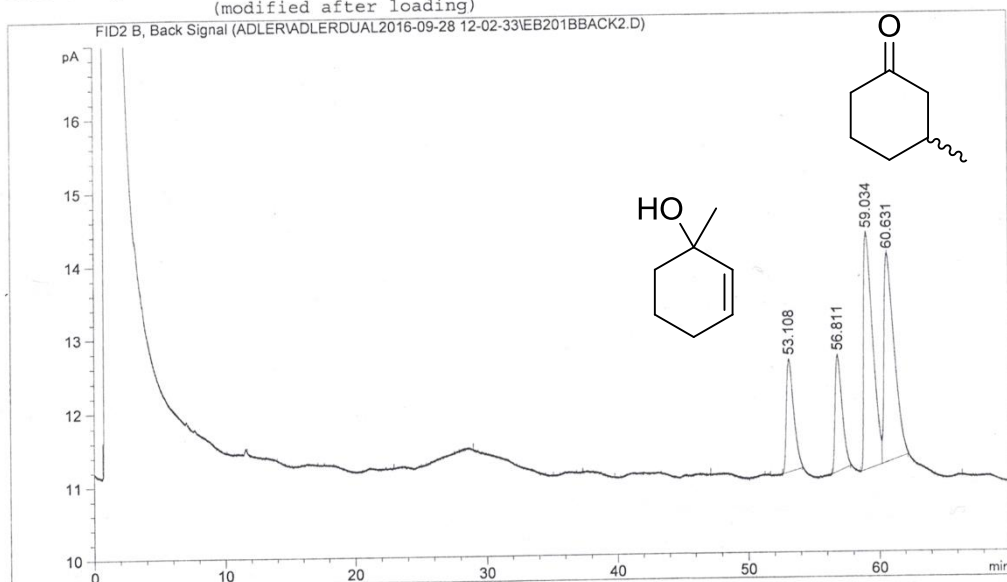
Totals : 1143.35150 19.71952

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*** End of Report ***

rac-Standard of 3-methylcyclohexan-1-one (16b), 1-methylcyclohexen-1-ol is also present

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Name: eb201b *Methyl*

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                                           Inj       :    1
Injection Date  : 9/28/2016 12:03:54 PM
Acq. Method    : DETBETA_MEGABSE.M
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                        Area Percent Report
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Sorted By      : Signal
Multiplier     : 1.0000
Dilution      : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs
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Signal 1: FID2 B, Back Signal

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	53.108	BB	0.4692	60.03876	1.51881	14.00889
2	56.811	BB	0.4416	58.43823	1.57236	13.63543
3	59.034	BV	0.5697	154.78496	3.21507	36.11608
4	60.631	VB	0.6474	155.31432	2.83406	36.23960

Totals : 428.57626 9.14030

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Computational structures

Table 2. Computed transition structures of the reductive elimination (TS-B) of the chalcone **1**• MeCu • BIFOP-H^[a].

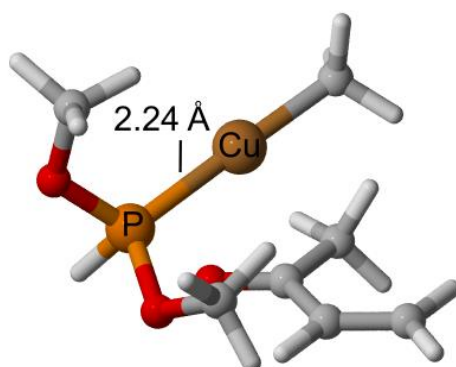
TS-B _{pro(R/S)} ^[b]	Imag. freq. [cm ⁻¹]	Hartree	ΔG [kcal/mol]
TS-1 (R)	-377.22	-4070.170920	0.0
TS-1.1 (R)	-376.75	-4070.170295	0.4
TS-1.2 (R)	-365.02	-4070.168599	1.5
TS-1.3 (R)	-361.41	-4070.166708	2.6
TS-2 (S)	-368.08	-4070.165928	3.1
TS-2.1 (R)	-390.64	-4070.164430	4.1
TS-2.2 (R)	-388.90	-4070.164400	4.1
TS-3 (R)	-398.95	-4070.162638	4.9
TS-3.1 (R)	-384.51	-4070.162732	5.1
TS-4 (S)	-378.86	-4070.162638	5.2
TS-4.1 (S)	-399.72	-4070.161513	5.9
TS-5 (R)	-402.55	-4070.161423	6.0
TS-6 (R)	-382.66	-4070.161142	6.1
TS-7 (S)	-370.94	-4070.160540	6.6
TS-7.1 (R)	-402.44	-4070.158427	7.8
TS-7.2 (R)	-465.11	-4070.152474	11.6
TS-8 (S)	-405.75	-4070.152390	11.6
TS-8.1 (S)	-393.41	-4070.152372	11.6
TS-8.2 (R)	-404.21	-4070.150382	12.9
TS-8.3 (R)	-436.41	-4070.149969	13.1
TS-8.4 (S)	-420.86	-4070.148164	14.3

[a] M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP, solvent = diethylether, T = 293.15 K, p = 1 bar, ZPE scaled by 0.9754 for M06-2X/def2-TZVP and 0.9912 for B3LYP/def2-SVP [1].

Important: The optimized structures are computed in gas phase while the single points are computed in diethylether (scrf=diethylether).

All computations are performed with GAUSSIAN 16 Revision A.03 [1a]. The transitions states are computed by using the B3LYP functional [1b-e] with the def2-SVP basis set [1f]. The energies are refined by using either the M06-2X functional [1g] with the def2-TZVP basis set [1f] or TPSS functional [1h] with def2-TZVP basis set [1f]. Grimme's dispersion (D3) with Becke-Johnson damping (BJ) [1i] is added, too. The ZPE scale factor is for B3LYP/def2-SVP 0.9912, M06-2X/def2-TZVP 0.9871 and TPSS/def2-TZVP 1.0194 [1j]. Everything is implemented in the program package of GAUSSIAN 16.

Optimized separated structure of the hydrido phosphite ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Energy: -2483.313947

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2483.847339

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2484.331000

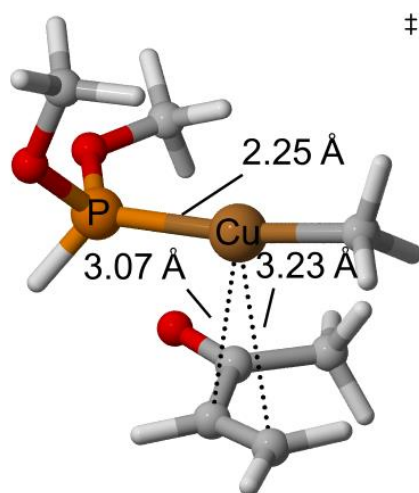
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2484.281236

0 1

O	-2.9768	0.03724	-0.84225
O	-1.39335	-1.87388	0.04519
P	-1.40065	-0.4163	-0.72751
Cu	-0.03559	1.08204	0.23715

C	1.11382	2.33935	1.16408
H	0.55417	3.02444	1.82585
H	1.85119	1.81182	1.79795
H	1.67965	2.97165	0.45451
C	2.04099	-1.35992	0.29229
H	1.19847	-2.05206	0.20635
C	2.81393	-1.33682	1.3854
H	3.65062	-0.64154	1.48978
H	2.62178	-2.00427	2.22964
C	3.39592	0.44607	-0.97581
H	3.30795	1.21036	-0.18788
H	4.34292	-0.09455	-0.82394
H	3.399	0.93951	-1.95547
C	2.21271	-0.48854	-0.90162
O	1.38551	-0.54735	-1.80109
C	-1.40815	-1.89535	1.46724
H	-0.93879	-2.83334	1.79658
H	-0.84553	-1.04317	1.89009
H	-2.44355	-1.86458	1.84646
C	-3.52693	0.94318	0.10631
H	-4.24009	1.59722	-0.41588
H	-4.06202	0.39462	0.89958
H	-2.74009	1.56596	0.56987
H	-1.27042	-0.93286	-2.03034

Optimized oxidative addition transition structure of the hydrido phosphite ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Imaginary frequency: -27.55 cm^{-1}

Energy: -2483.313194

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2483.847266

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2484.330196

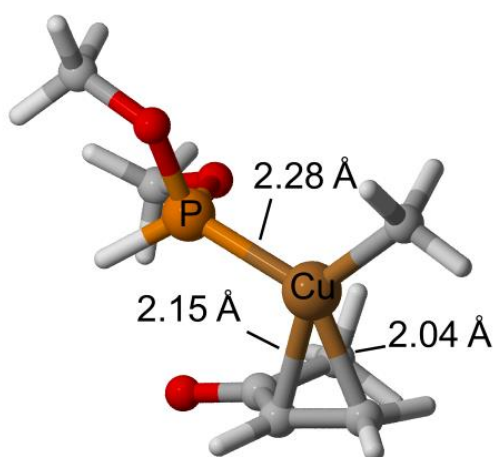
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2484.280794

0 1

O	1.74144	-1.7219	0.343
P	1.29412	-0.48536	-0.62861
Cu	-0.03565	1.0496	0.3319
C	-0.96564	2.46149	1.29564
H	-0.32126	2.93746	2.05663
H	-1.29427	3.2633	0.60788
H	-1.87012	2.11042	1.82862
C	-2.16154	-0.24044	-1.4626
H	-1.62849	-0.58928	-2.35255
C	-2.09651	-1.17971	-0.3108
O	-1.30275	-2.10849	-0.34533
C	-2.74058	0.9676	-1.43256
H	-3.24385	1.34893	-0.54151

H	-2.69983	1.63637	-2.29616
C	-2.97366	-0.93191	0.89347
H	-2.60472	-0.0346	1.41766
H	-4.01941	-0.74649	0.60655
H	-2.91254	-1.79459	1.56856
O	2.71687	0.14628	-1.14504
C	3.42233	1.02314	-0.27372
H	4.10721	1.62437	-0.88742
H	2.7292	1.6963	0.26348
H	4.0078	0.45047	0.4647
C	1.17961	-1.87501	1.64455
H	1.92514	-2.39083	2.26617
H	0.94325	-0.8964	2.09902
H	0.25868	-2.47356	1.58774
H	1.01676	-1.17818	-1.83018

Optimized cuprate structure of the hydrido phosphite ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Energy: -2483.322770

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2483.844563

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2484.348023

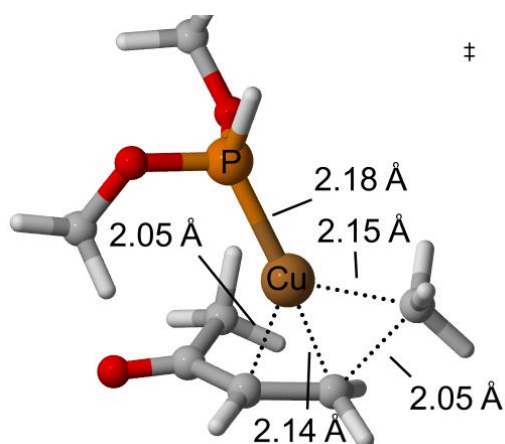
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2484.286904

0 1

O	-1.44617	0.83294	0.94444
O	-2.39688	-1.26266	-0.32241
P	-1.15764	-0.20112	-0.29508
H	-1.51285	0.64644	-1.39781
Cu	0.94704	-1.05119	-0.0328
C	1.18106	-2.73673	0.95047
H	0.56293	-3.51455	0.4695
H	2.22222	-3.09259	0.99719
H	0.81201	-2.60477	1.98269
C	1.95854	0.5675	-1.01245
H	1.73608	0.49645	-2.08229
C	1.37627	1.75883	-0.36666
O	0.6054	2.48717	-0.98553
C	2.8248	-0.34946	-0.41274
H	3.25089	-0.17206	0.57748
H	3.34649	-1.09164	-1.02125
C	1.69169	2.02227	1.09407
H	2.76965	1.95865	1.30403
H	1.3175	3.01741	1.3655
H	1.18142	1.27099	1.72055
C	-2.08359	2.10234	0.78361
H	-1.4344	2.77848	0.20731
H	-3.05962	2.00286	0.27934
H	-2.24573	2.51006	1.79119
C	-3.75025	-0.84908	-0.44688

H	-3.87521	-0.13449	-1.28133
H	-4.35491	-1.74405	-0.64837
H	-4.10607	-0.37954	0.48504

Optimized reductive elimination transition structure of the hydrido phosphite ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Imaginary frequency: -417.83 cm^{-1}

Energy: -2483.287612

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2483.823009

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2484.315083

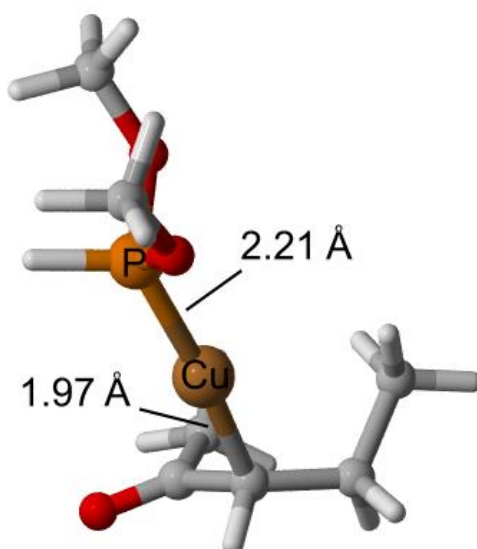
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2484.254244

0 1

O	-2.21336	0.50099	-1.2434
O	-1.98689	-0.58819	1.12991
P	-1.51363	-0.73144	-0.43257
Cu	0.6692	-0.76771	-0.41189
C	1.95054	-2.40807	0.12531
H	1.29479	-2.6675	0.97283
H	1.6138	-2.93226	-0.78714
H	2.95981	-2.76097	0.35689

C	2.09974	0.703	-0.43585
H	2.27966	1.03555	-1.46347
C	1.48055	1.69622	0.41828
O	1.07428	2.78069	-0.00939
C	2.75012	-0.5265	0.01135
H	3.05737	-0.56469	1.06101
H	3.542	-0.87806	-0.65567
C	1.25967	1.35864	1.8974
H	2.10248	0.82082	2.35819
H	1.08114	2.29612	2.44071
H	0.36106	0.72497	2.00707
C	-1.55189	1.78062	-1.27558
H	-0.51036	1.68717	-1.61421
H	-2.12223	2.40903	-1.97141
H	-1.53595	2.24624	-0.2799
C	-3.36248	-0.4173	1.46278
H	-3.95906	-1.28174	1.12058
H	-3.42657	-0.34382	2.55649
H	-3.76952	0.49874	1.00703
H	-2.42056	-1.72195	-0.91454

Optimized product structure of the hydrido phosphite ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Energy: -2483.339758

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2483.885040

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2484.361946

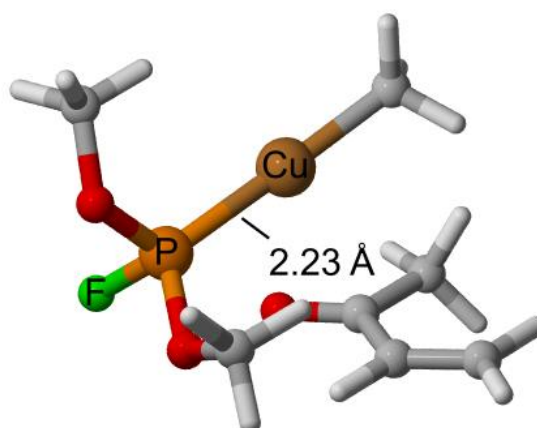
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2484.313376

0 1

O	-2.246	0.78723	1.21591
O	-2.76591	-1.06218	-0.61365
P	-1.80207	0.19916	-0.23892
H	-2.38063	1.20373	-1.08907
Cu	0.35782	-0.26683	-0.3587
C	2.35333	-1.5423	1.81541
H	2.45651	-0.56598	2.31343
H	1.27535	-1.78197	1.78978
H	2.85107	-2.29248	2.45315
C	2.29999	-0.53442	-0.5857
H	2.33507	-0.90842	-1.62311
C	2.93272	-1.52793	0.39724
H	2.8099	-2.53882	-0.02693

C	2.75882	0.87392	-0.62652
O	2.61674	1.58841	-1.61455
H	4.0286	-1.37616	0.46329
C	3.39778	1.4702	0.62902
H	4.25105	0.86682	0.97802
H	3.73253	2.49101	0.40272
H	2.66856	1.50265	1.45438
C	-3.46821	1.46673	1.47281
H	-3.79085	2.05881	0.59749
H	-4.26469	0.75317	1.73934
H	-3.3023	2.14633	2.32029
C	-4.15541	-0.95553	-0.89529
H	-4.74866	-1.0068	0.0321
H	-4.38771	-0.01215	-1.42166
H	-4.43232	-1.80067	-1.54076

Optimized separated structure of the fluoro phosphite ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Energy: -2582.516139

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2583.847339

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2583.671423

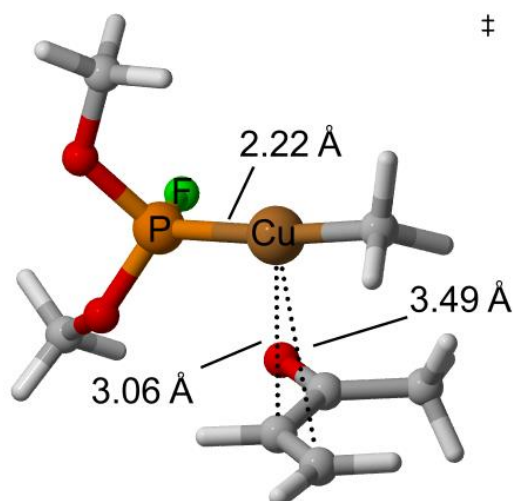
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2583.617013

0 1

O	-2.92716	0.02472	0.08224
O	-1.30583	-1.85271	0.16877
P	-1.40998	-0.33293	-0.39155
Cu	0.13294	1.1371	0.24862
C	1.3286	2.4067	1.09559
H	0.79723	3.14055	1.72692
H	2.0585	1.89114	1.74734
H	1.90265	2.98192	0.34555
C	2.14877	-1.37753	0.33202
H	1.26957	-2.02678	0.29157
C	2.99846	-1.41644	1.36612
H	3.87383	-0.76429	1.42214
H	2.83751	-2.09563	2.2076
C	3.49895	0.38494	-1.00307
H	3.52451	1.13228	-0.1946
H	4.4207	-0.21419	-0.94491
H	3.44867	0.90476	-1.96763
C	2.27123	-0.47993	-0.84867
O	1.36393	-0.45701	-1.6691
C	-1.35099	-2.07689	1.57716
H	-1.1153	-3.13654	1.74056
H	-0.60844	-1.45486	2.1067
H	-2.35501	-1.85729	1.97168
C	-3.35182	1.38358	0.18759
H	-3.82539	1.70863	-0.75205
H	-4.08559	1.44256	1.00294

H	-2.50212	2.05089	0.41636
F	-1.62819	-0.70576	-1.92807

Optimized oxidative addition transition structure of the fluoro phosphite ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Imaginary frequency: -43.54 cm^{-1}

Energy: -2582.519812

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2583.156799

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2583.671910

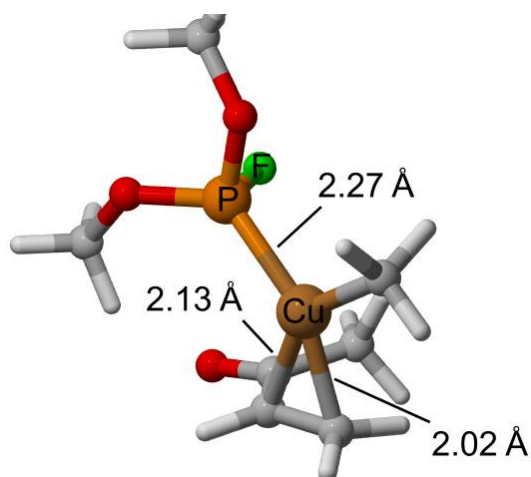
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2583.618313

0 1

P	1.33185	-0.14825	0.00917
Cu	-0.32836	1.33106	-0.01378
C	-1.65104	2.74895	0.0287
H	-1.21656	3.72961	0.29215
H	-2.13557	2.86155	-0.9588
H	-2.45473	2.55183	0.76291
C	-2.0195	-1.01007	-1.01093
H	-1.17993	-1.47009	-1.53887

C	-2.01302	-1.24773	0.45885
O	-1.0799	-1.85012	0.96791
C	-2.93595	-0.28557	-1.66676
H	-3.76395	0.20878	-1.1532
H	-2.86946	-0.13436	-2.74727
C	-3.1527	-0.71542	1.29754
H	-3.13636	0.38592	1.27267
H	-4.12835	-1.04692	0.91034
H	-3.02317	-1.05695	2.33186
O	2.81237	0.41514	-0.36284
C	3.20175	1.71947	0.06868
H	3.95018	2.09482	-0.64193
H	2.33854	2.40808	0.08368
H	3.64419	1.675	1.07661
O	1.26955	-1.44055	-0.93949
C	1.75838	-2.73569	-0.56881
H	2.79517	-2.67768	-0.20547
H	1.10493	-3.16304	0.20433
H	1.72254	-3.35265	-1.47578
F	1.63926	-0.80334	1.45341

Optimized cuprate structure of the fluoro phosphite ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Energy: -2582.531898

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2583.156583

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2583.693446

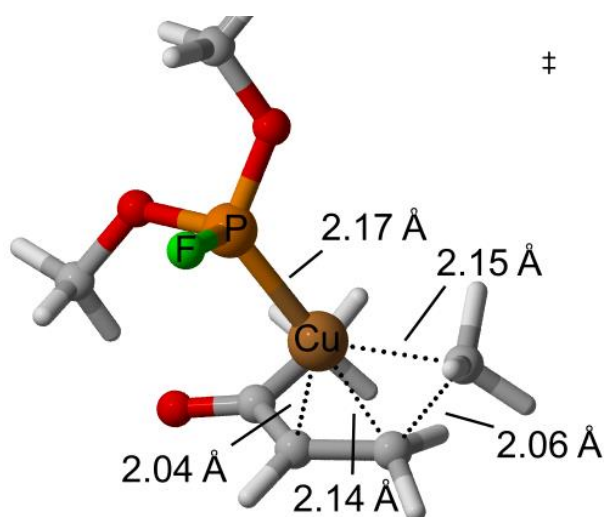
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2583.635487

0 1

O	-2.44381	-0.96742	0.25728
O	-1.90065	1.10577	-0.96964
P	-1.20072	0.01168	0.00188
Cu	0.74592	-1.10833	-0.31409
C	0.47937	-3.03142	0.01573
H	1.37206	-3.64818	-0.17118
H	0.16661	-3.17999	1.06405
H	-0.3414	-3.38861	-0.62991
C	2.18331	0.40519	-0.74627
H	2.01221	0.78256	-1.76001
C	2.00714	1.42633	0.30859
O	1.63246	2.55565	0.02409
C	2.7401	-0.86409	-0.56548
H	3.17008	-1.17047	0.3912

H	3.05112	-1.45669	-1.42908
C	2.26877	1.03059	1.75031
H	1.61558	0.19242	2.04553
H	3.31013	0.70029	1.89049
H	2.06331	1.89226	2.39697
C	-1.29748	2.37672	-1.25651
H	-1.50034	3.07917	-0.43434
H	-0.20744	2.29828	-1.37812
H	-1.7575	2.74504	-2.18255
C	-3.76717	-0.50529	0.55475
H	-3.75077	0.19218	1.40608
H	-4.20473	-0.00572	-0.32132
H	-4.35773	-1.3922	0.81656
F	-1.13892	0.86064	1.3906

Optimized reductive elimination transition structure of the fluoro phosphite ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Imaginary frequency: -411.35 cm^{-1}

Energy: -2582.495134

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2583.135441

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2583.660161

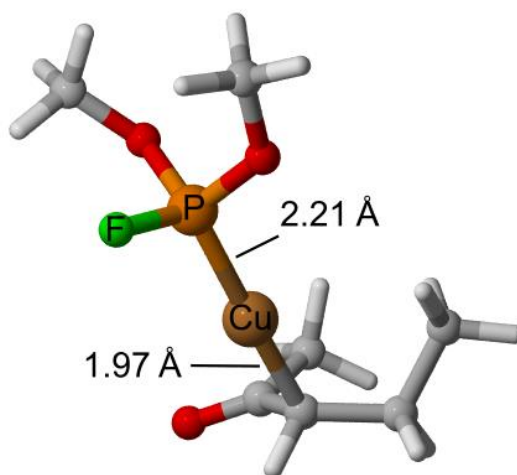
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2583.594440

0 1

O	-1.78303	1.42699	0.04487
O	-2.44316	-0.75788	0.99628
P	-1.48598	-0.14727	-0.13765
Cu	0.58775	-0.77186	-0.2492
C	1.42423	-2.70933	0.13601
H	0.88711	-2.73511	1.09952
H	0.79351	-3.14702	-0.65679
H	2.32132	-3.3272	0.23466
C	2.3247	0.21053	-0.68798
H	2.29028	0.49343	-1.74482
C	2.28905	1.31335	0.24779
O	2.06075	2.47873	-0.09342
C	2.68862	-1.15974	-0.33745
H	3.24394	-1.29192	0.59536
H	3.12681	-1.73777	-1.15586
C	2.53539	1.00972	1.73008
H	3.57624	0.68668	1.89952
H	2.34872	1.92529	2.30554
H	1.88238	0.20432	2.10841
C	-1.11469	2.41899	-0.76241
H	-0.01944	2.36766	-0.64918
H	-1.40265	2.29753	-1.81819
H	-1.46893	3.3928	-0.40224
C	-3.77459	-0.28183	1.24267
H	-4.36493	-0.29022	0.3139

H	-4.22346	-0.96834	1.97152
H	-3.74631	0.73812	1.65131
F	-2.32361	-0.44534	-1.495

Optimized product structure of the fluoro phosphite ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Energy: -2582.546812

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2583.195206

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2583.704234

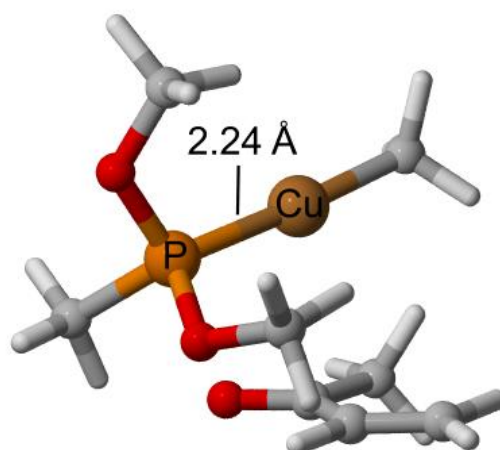
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2583.650430

0 1

O	2.17435	-1.07164	0.89524
O	2.30388	1.41492	0.1779
P	1.66645	-0.01208	-0.21047
Cu	-0.51666	0.07591	-0.50919
C	-2.39246	2.23444	0.85222
H	-2.42686	1.64781	1.78317
H	-1.32736	2.42001	0.62364
H	-2.86747	3.2086	1.05819

C	-2.47558	0.14583	-0.7041
H	-2.59922	-0.05787	-1.78115
C	-3.07257	1.50506	-0.31127
H	-3.0187	2.16009	-1.19716
C	-2.89279	-1.08581	0.01032
O	-2.81927	-2.19991	-0.49609
H	-4.15406	1.4124	-0.08845
C	-3.3973	-0.95897	1.44884
H	-4.23661	-0.24929	1.52514
H	-3.71599	-1.94952	1.79875
H	-2.59726	-0.58266	2.10648
C	3.38213	-1.83954	0.89032
H	3.58812	-2.23843	-0.11293
H	4.23589	-1.22926	1.22382
H	3.23339	-2.66843	1.59403
C	3.67979	1.63261	0.50294
H	3.90312	1.23583	1.50557
H	4.33779	1.16173	-0.24356
H	3.84435	2.71752	0.49864
F	2.61424	-0.43971	-1.45807

Optimized separated structure of the methylphosphite ligand of the reaction pathway
(B3LYP-D3(BJ)/def2-SVP)



Energy: -2522.624479

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2523.173884

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2523.686367

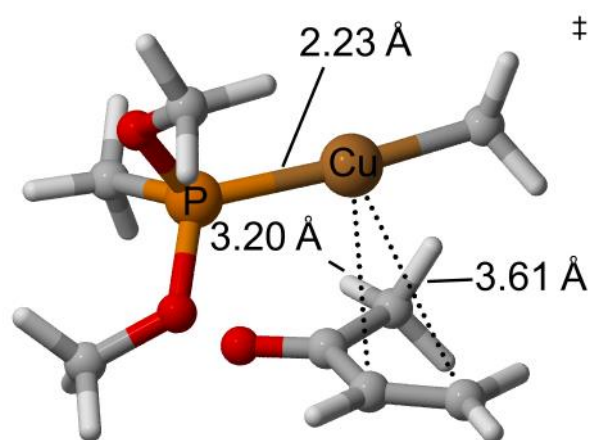
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2523.634713

0 1

O	-2.94352	0.05989	-0.52854
O	-1.40759	-1.55596	0.8551
P	-1.39073	-0.47282	-0.39482
Cu	0.09588	1.18402	-0.1172
C	1.2819	2.69676	0.15963
H	0.72871	3.62515	0.39167
H	1.97673	2.52348	1.00322
H	1.89716	2.91149	-0.73381
C	1.96275	-1.17749	0.81662
H	1.14195	-1.89938	0.85172
C	2.4787	-0.66435	1.94078
H	3.28316	0.07494	1.92585
H	2.09363	-0.95148	2.92286
C	3.60303	0.06294	-0.75562

H	3.37499	1.06444	-0.36066
H	4.48366	-0.32419	-0.21945
H	3.82298	0.13883	-1.8276
C	2.41045	-0.84422	-0.56497
O	1.80984	-1.31813	-1.51655
C	-1.34983	-1.06988	2.1889
H	-0.93434	-1.86695	2.82216
H	-0.70426	-0.17672	2.2653
H	-2.35833	-0.81509	2.55631
C	-3.34382	1.28208	0.07871
H	-4.08553	1.76329	-0.5752
H	-3.80638	1.09367	1.06222
H	-2.48541	1.96482	0.21154
C	-1.3675	-1.65616	-1.75831
H	-0.37081	-2.11582	-1.79208
H	-2.15493	-2.40702	-1.6008
H	-1.5465	-1.11232	-2.69682

Optimized oxidative addition transition structure of the methylphosphite ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Imaginary frequency: -35.29 cm⁻¹

Energy: -2522.623812

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2523.173483

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2523.684588

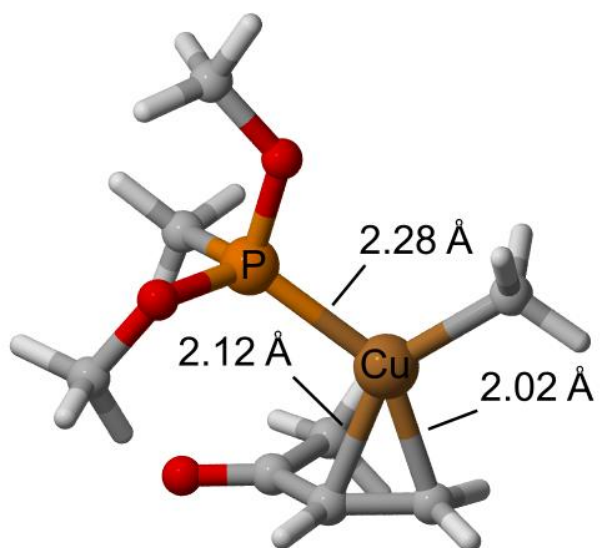
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2523.633900

0 1

P	-1.33538	-0.08284	-0.28105
Cu	0.35171	1.36966	-0.14903
C	1.77026	2.69656	-0.17894
H	1.37651	3.72549	-0.08845
H	2.48093	2.55023	0.6556
H	2.3585	2.66985	-1.11565
C	1.95051	-1.05581	1.18786
H	1.07702	-1.48347	1.68569
C	2.02444	-1.36611	-0.26384
O	1.16709	-2.07576	-0.77123
C	2.83566	-0.30594	1.85718
H	3.69537	0.15767	1.36787
H	2.71373	-0.10596	2.92488
C	3.14605	-0.7774	-1.08867
H	3.0488	0.32003	-1.10105
H	4.13042	-1.02362	-0.66147
H	3.07879	-1.16434	-2.11305
O	-2.85203	0.5635	-0.18374
C	-3.09519	1.57329	0.78885
H	-3.17179	1.13976	1.80029
H	-2.2903	2.32956	0.78677
H	-4.0473	2.05857	0.53283

O	-1.29252	-1.20094	0.92072
C	-1.97501	-2.44715	0.8607
H	-3.02393	-2.32135	0.54474
H	-1.45439	-3.13454	0.17555
H	-1.96121	-2.87415	1.87337
C	-1.57528	-1.00239	-1.83173
H	-0.70364	-1.65124	-1.99116
H	-2.50444	-1.58924	-1.80821
H	-1.64089	-0.2655	-2.64555

Optimized cuprate structure of the methylphosphite ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Energy: -2522.628583

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP):

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP):

Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP):

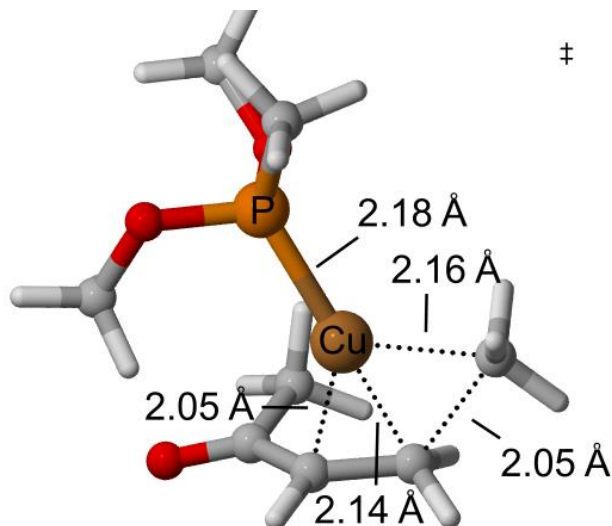
0 1

O	2.42419	1.00057	0.35207
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O	1.85654	-0.93091	-1.13968
P	1.21209	-0.05581	0.10127
Cu	-0.73236	1.06922	-0.25986
C	-0.50921	2.99812	0.07509
H	-1.37609	3.61805	-0.20029
H	-0.29624	3.14783	1.14814
H	0.37381	3.33838	-0.49177
C	-2.12767	-0.42028	-0.8235
H	-1.82569	-0.83259	-1.79133
C	-2.04809	-1.36921	0.29515
O	-1.52926	-2.47592	0.16204
C	-2.68203	0.86715	-0.75337
H	-3.23846	1.20437	0.12401
H	-2.87872	1.42698	-1.67069
C	-2.57882	-0.93178	1.65049
H	-2.03585	-0.04143	2.01221
H	-3.64302	-0.6548	1.59168
H	-2.45108	-1.75307	2.36663
C	1.30957	-2.18885	-1.53681
H	1.8392	-3.01104	-1.02632
H	0.2363	-2.27549	-1.30484
H	1.46229	-2.289	-2.62094
C	3.77927	0.60296	0.53513
H	3.93414	0.16073	1.53405
H	4.08712	-0.11895	-0.2365
H	4.39337	1.50983	0.45184
C	1.29022	-1.22229	1.51331
H	1.06654	-0.67053	2.43931
H	0.51988	-1.99619	1.36887

H 2.27862 -1.69836 1.59427

Optimized reductive elimination transition structure of the methylphosphite ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Imaginary frequency: -416.02 cm^{-1}

Energy: -2522.594701

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2523.147852

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2523.668818

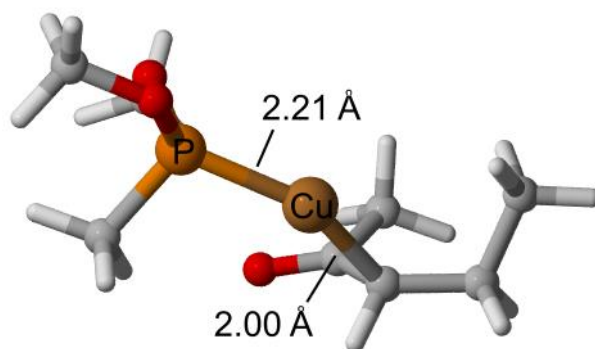
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2523.605425

0 1

O	-1.96975	0.93451	-1.11677
O	-1.81111	0.02995	1.32533
P	-1.48403	-0.35948	-0.23877
Cu	0.65109	-0.81555	-0.30498
C	1.58408	-2.62573	0.40055
H	0.96369	-2.61753	1.31176
H	1.06059	-3.16883	-0.40678
H	2.50728	-3.16984	0.62171
C	2.36565	0.27928	-0.58965

H	2.53604	0.44074	-1.65906
C	2.03956	1.47566	0.15794
O	1.84366	2.56873	-0.38231
C	2.76163	-1.004	-0.01459
H	3.13594	-0.98473	1.01371
H	3.40227	-1.6037	-0.66709
C	1.86589	1.36368	1.67771
H	2.63845	0.74677	2.16259
H	1.88603	2.37667	2.10106
H	0.88521	0.91219	1.91391
C	-1.08265	2.0596	-1.2534
H	-0.92095	2.55855	-0.28668
H	-0.09919	1.75619	-1.6389
H	-1.56487	2.75574	-1.95174
C	-3.06385	0.57618	1.72944
H	-3.82819	-0.21356	1.82453
H	-2.91286	1.04425	2.71159
H	-3.41597	1.33725	1.01522
C	-2.82545	-1.49272	-0.73015
H	-2.81196	-2.37519	-0.07339
H	-3.80417	-0.99386	-0.67634
H	-2.64999	-1.81529	-1.76715

Optimized product structure of the methylphosphite ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Energy: -2522.652875

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2523.206372

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2523.710646

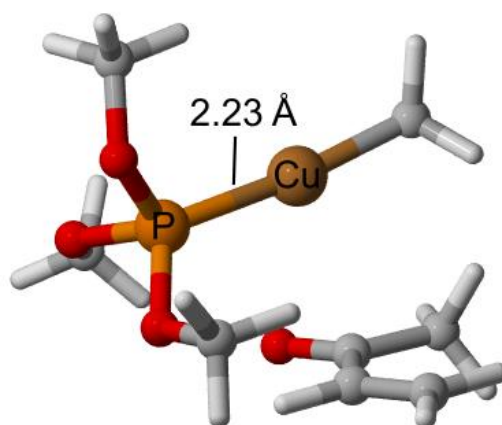
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2523.658571

0 1

O	2.08519	-0.94768	1.03714
O	2.82259	1.3456	0.32118
P	1.69176	0.23396	-0.0367
Cu	-0.44546	0.76652	-0.15002
C	-3.46302	1.5437	1.1499
H	-3.33538	0.71576	1.86497
H	-2.60121	2.22075	1.27885
H	-4.37662	2.09098	1.43708
C	-2.28983	0.30062	-0.78244
H	-2.05937	0.46771	-1.84803
C	-3.52867	1.04169	-0.29555
H	-3.68007	1.91261	-0.95471
C	-2.02893	-1.09625	-0.45298
O	-1.10877	-1.74987	-0.98913
H	-4.43999	0.42333	-0.42025
C	-2.8338	-1.77838	0.64762

H	-3.89291	-1.48194	0.65426
H	-2.74637	-2.86576	0.51977
H	-2.41143	-1.51393	1.63119
C	1.47969	-2.24251	0.96141
H	0.48835	-2.2142	0.47722
H	2.127	-2.92746	0.38862
H	1.38207	-2.6215	1.98859
C	4.21468	1.03676	0.36888
H	4.40123	0.16336	1.01158
H	4.61382	0.84086	-0.64066
H	4.72347	1.91546	0.78733
C	2.16308	-0.49493	-1.64672
H	1.3552	-1.19561	-1.91291
H	2.19308	0.30152	-2.40628
H	3.12963	-1.01917	-1.60971

Optimized separated structure of the phosphite ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Energy: -2597.792775

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2598.417123

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2598.962211

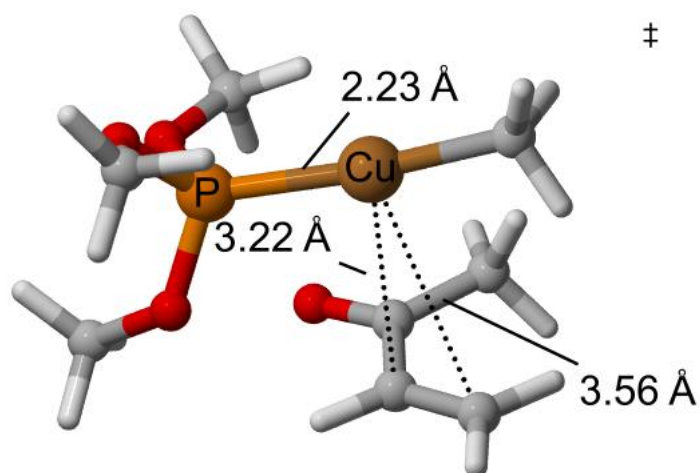
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2598.901964

0 1

O	-2.87882	0.02827	0.5724
O	-1.32519	-1.86651	0.24
P	-1.45241	-0.28889	-0.15772
Cu	0.18661	1.1078	0.42925
C	1.43281	2.4449	1.0814
H	0.91046	3.30332	1.54141
H	2.10623	2.03182	1.85602
H	2.0678	2.85405	0.27459
C	2.05335	-1.38812	0.29937
H	1.19907	-1.98499	-0.03251
C	2.52951	-1.49471	1.5468
H	3.37169	-0.89469	1.90022
H	2.07705	-2.17877	2.26957
C	3.84715	0.31655	-0.46214
H	3.64193	1.03651	0.34405
H	4.67522	-0.33387	-0.13939
H	4.13505	0.86366	-1.36817
C	2.60625	-0.49283	-0.75551
O	2.0561	-0.44316	-1.84398
C	-1.22315	-2.22276	1.61607
H	-0.90015	-3.27184	1.65772
H	-0.48105	-1.59607	2.14097
H	-2.19839	-2.11635	2.11534
C	-3.37255	1.36414	0.57165
H	-3.8277	1.60867	-0.40202
H	-4.13725	1.43485	1.35687

H	-2.56724	2.08938	0.78547
O	-1.90218	-0.41643	-1.7055
C	-1.01877	-0.05447	-2.77877
H	-1.42116	-0.52518	-3.68545
H	-1.01048	1.03912	-2.91473
H	0.00638	-0.40604	-2.59879

Optimized oxidative addition transition structure of the phosphite ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Imaginary frequency: -38.09 cm^{-1}

Energy: -2597.795967

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2598.419116

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2598.962248

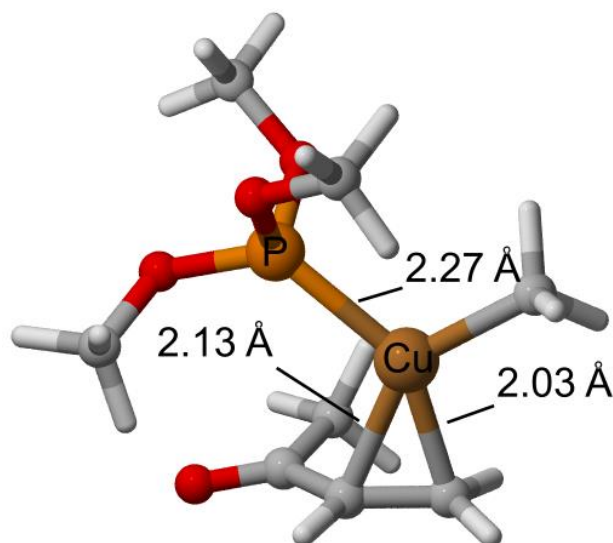
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2598.902589

0 1

P	1.30977	0.01745	0.10198
Cu	-0.43203	1.40314	0.20301
C	-1.89581	2.65496	0.45178
H	-1.54597	3.70332	0.43391

H	-2.66066	2.55887	-0.34087
H	-2.41194	2.5151	1.42026
C	-1.91924	-0.92605	-1.45707
H	-1.04912	-1.30667	-1.99667
C	-2.01299	-1.40648	-0.05336
O	-1.15527	-2.16041	0.38335
C	-2.77856	-0.07661	-2.035
H	-3.63313	0.34334	-1.49956
H	-2.63976	0.25135	-3.06852
C	-3.15423	-0.92781	0.81546
H	-3.05467	0.1576	0.97805
H	-4.12857	-1.10703	0.33569
H	-3.11514	-1.44867	1.78027
O	2.80494	0.68296	-0.00407
C	3.04571	1.61144	-1.05476
H	3.10132	1.1014	-2.03109
H	2.25417	2.38105	-1.10069
H	4.00658	2.10126	-0.84699
O	1.2892	-1.02087	-1.15096
C	1.92778	-2.29928	-1.10167
H	2.94097	-2.22417	-0.67797
H	1.31954	-2.98815	-0.49835
H	1.98948	-2.66535	-2.13561
O	1.60779	-0.91588	1.39033
C	0.72484	-0.97271	2.51295
H	0.07962	-1.85708	2.42969
H	1.34429	-1.02597	3.41907
H	0.08701	-0.07403	2.56334

Optimized cuprate structure of the phosphite ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Energy: -2597.806321

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2598.417429

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2598.983828

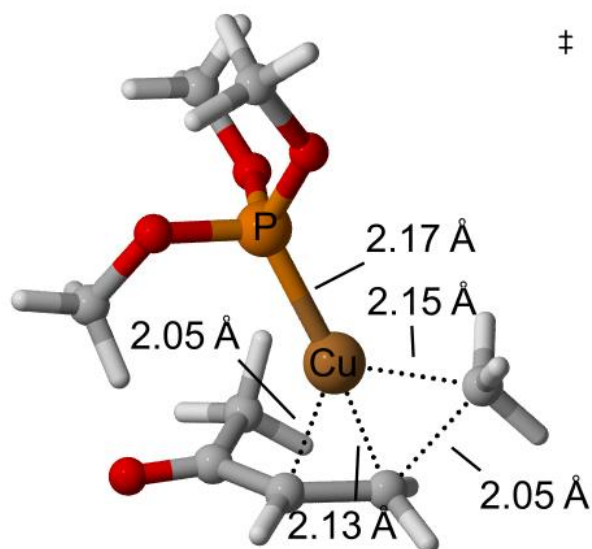
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2598.910221

0 1

O	1.15914	1.82318	0.34571
P	1.09098	0.23353	0.01114
Cu	-0.71694	-1.14057	0.08651
C	-0.2581	-2.96368	-0.53168
H	0.64765	-2.95415	-1.1616
H	-0.05998	-3.61367	0.34022
H	-1.07235	-3.42923	-1.11056
C	-2.34373	0.0574	0.76849
H	-2.23018	0.25228	1.84003
C	-2.28825	1.27702	-0.06498
O	-2.10712	2.37257	0.44623

C	-2.73183	-1.21159	0.33404
H	-3.11019	-1.37931	-0.67731
H	-2.97146	-1.993	1.05912
C	-2.42972	1.13178	-1.57113
H	-3.38958	0.66345	-1.84042
H	-2.36365	2.12609	-2.02979
H	-1.62811	0.4906	-1.97663
C	0.83471	2.32776	1.64328
H	-0.2456	2.23973	1.83177
H	1.41859	1.80788	2.41965
H	1.10572	3.3918	1.64301
C	2.70483	1.06706	-1.94993
H	3.56207	0.93333	-1.27199
H	2.97534	0.7273	-2.95838
H	2.42639	2.13066	-1.9743
O	2.3963	-0.24133	0.89051
C	2.65125	-1.62748	1.11016
H	3.01016	-2.1139	0.18893
H	3.42882	-1.69506	1.88312
H	1.74647	-2.1554	1.45075
O	1.59435	0.26989	-1.5276

Optimized reductive elimination transition structure of the phosphite ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Imaginary frequency: -410.70 cm^{-1}

Energy: -2597.767682

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2598.393127

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2598.946784

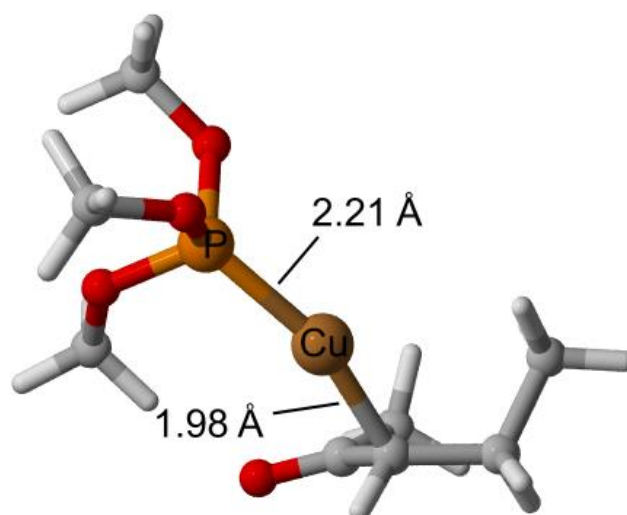
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2598.874274

0 1

O	-1.7728	1.01461	-0.98374
O	-1.45938	0.34811	1.47795
P	-1.27539	-0.22418	-0.04112
Cu	0.79311	-0.86381	-0.23291
C	1.68185	-2.67484	0.49737
H	1.15782	-2.57286	1.46174
H	1.0487	-3.22974	-0.21783
H	2.59123	-3.26004	0.66205
C	2.52112	0.11329	-0.74907
H	2.58655	0.19983	-1.83858
C	2.34526	1.37006	-0.05171
O	2.1486	2.43848	-0.63958

C	2.90328	-1.15665	-0.13424
H	3.38095	-1.09999	0.84877
H	3.43956	-1.83189	-0.80663
C	2.3422	1.36077	1.48153
H	3.14859	0.74884	1.91498
H	2.43978	2.39699	1.83122
H	1.38362	0.95957	1.85733
C	-0.87616	2.1097	-1.24406
H	0.08578	1.76199	-1.64612
H	-1.37858	2.75974	-1.97169
H	-0.66713	2.67526	-0.32387
C	-2.63155	1.01693	1.93822
H	-3.40847	0.28495	2.21279
H	-2.35246	1.59415	2.82998
H	-3.02646	1.70162	1.17131
O	-2.50632	-1.2479	-0.30608
C	-3.8081	-0.906	-0.78456
H	-4.31192	-1.85045	-1.03051
H	-4.39166	-0.37862	-0.01311
H	-3.74336	-0.27221	-1.68004

Optimized product structure of the phosphite ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Energy: -2597.830158

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2598.457656

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2598.995989

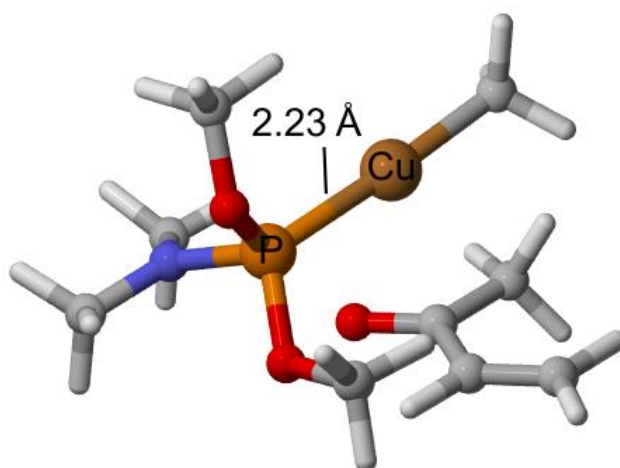
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2598.935123

0 1

O	-1.98777	-0.28465	1.60749
O	-2.64703	-1.20853	-0.71418
P	-1.57725	-0.24534	0.03352
Cu	0.58848	-0.5102	-0.3148
C	3.25211	-2.09118	0.74226
H	3.25719	-1.48158	1.6592
H	2.26443	-2.5814	0.68301
H	4.01551	-2.87798	0.86458
C	2.47755	-0.14219	-0.78357
H	2.33131	0.04061	-1.86199
C	3.50192	-1.24465	-0.50963
H	3.50489	-1.92087	-1.38096
C	2.57164	1.16972	-0.12383

O	1.95867	2.16454	-0.52931
H	4.52935	-0.83221	-0.4624
C	3.41788	1.30604	1.13884
H	4.43802	0.91701	0.99383
H	3.45751	2.36531	1.42429
H	2.96825	0.72995	1.96336
C	-3.31473	-0.03515	2.06848
H	-3.73378	0.86843	1.59767
H	-3.96564	-0.89806	1.85397
H	-3.26149	0.11327	3.1552
C	-3.86407	-0.80418	-1.34236
H	-4.63289	-0.54999	-0.59521
H	-3.70079	0.06474	-1.99517
H	-4.2105	-1.65927	-1.93812
C	-1.25351	2.36412	-0.39166
H	-0.22159	2.14864	-0.71793
H	-1.69328	3.13393	-1.03879
H	-1.23032	2.73143	0.64648
O	-2.10587	1.20723	-0.49099

Optimized separated structure of the phosphoramidite ligand of the reaction pathway
(B3LYP-D3(BJ)/def2-SVP)



Energy: -2617.230859

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2617.839795

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2618.411076

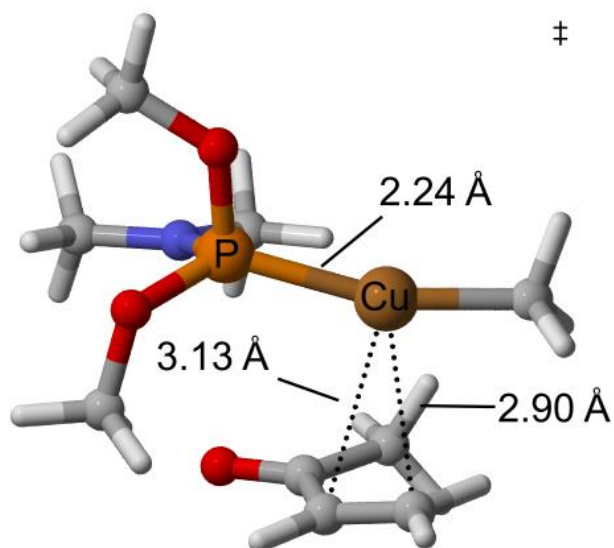
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2618.347803

0 1

O	-2.53605	0.98723	0.55196
O	-1.17653	-0.74276	1.63223
P	-1.24412	0.01867	0.17314
Cu	0.54119	1.16063	-0.52635
C	1.98823	2.32516	-1.09135
H	1.63599	3.34812	-1.31723
H	2.75947	2.42216	-0.30389
H	2.49277	1.95454	-2.00265
C	2.16326	-0.88962	1.26207
H	1.23107	-1.32891	1.62711
C	2.93602	-0.13246	2.05116
H	3.85841	0.3295	1.69018
H	2.65885	0.07072	3.08913
C	3.7522	-0.77522	-0.78011

H	3.79962	0.32376	-0.80287
H	4.61071	-1.14344	-0.19659
H	3.80735	-1.15882	-1.80638
C	2.44762	-1.22059	-0.16193
O	1.62268	-1.85941	-0.79568
C	-0.96708	0.03294	2.80696
H	-0.76141	-0.66766	3.62837
H	-0.10344	0.71183	2.6907
H	-1.85985	0.63103	3.04509
C	-2.93624	1.95796	-0.4037
H	-3.40836	1.48217	-1.2809
H	-3.66647	2.62065	0.08119
H	-2.07738	2.56022	-0.75041
N	-1.88885	-1.15014	-0.81739
C	-3.05988	-1.91343	-0.41736
H	-2.78768	-2.93968	-0.11154
H	-3.55955	-1.41855	0.42574
H	-3.77473	-1.97981	-1.25593
C	-1.16492	-1.63541	-1.982
H	-0.29406	-0.99624	-2.17737
H	-0.78434	-2.65835	-1.82542
H	-1.8238	-1.6268	-2.86802

Optimized oxidative addition transition structure of the phosphoramidite ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Imaginary frequency: -47.62 cm^{-1}

Energy: -2617.227931

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2617.837450

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2618.410181

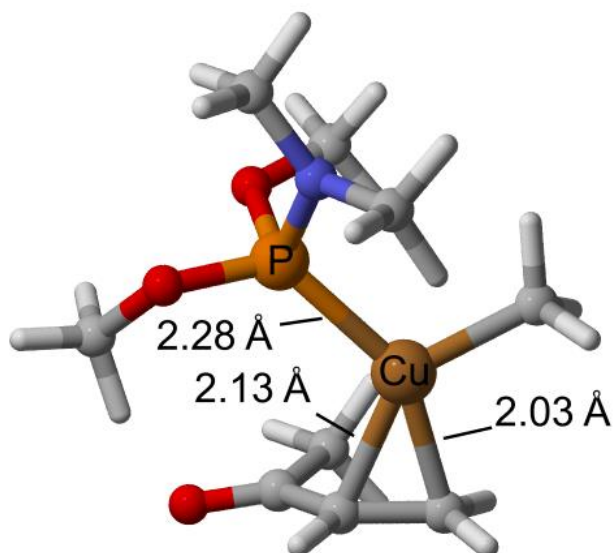
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2618.345324

0 1

O	-2.33253	1.51484	0.00562
O	-1.7653	-0.33682	1.51666
P	-1.16765	0.37747	0.15584
Cu	0.79151	1.45248	-0.05084
C	2.21369	2.6902	-0.55465
H	2.73323	3.10646	0.32795
H	2.98876	2.24143	-1.2043
H	1.7893	3.5446	-1.11184
C	2.25126	-0.99522	1.25017
H	1.71412	-1.40594	2.10754

C	2.04433	-1.73227	-0.01855
O	1.21426	-2.62856	-0.0786
C	2.95917	0.14183	1.36323
H	3.51089	0.57756	0.53079
H	3.02162	0.67574	2.31502
C	2.83748	-1.30451	-1.23313
H	2.57191	-0.26596	-1.49515
H	3.9188	-1.31787	-1.02734
H	2.60994	-1.97063	-2.07411
C	-1.11096	-1.43338	2.14611
H	-1.88618	-2.05445	2.61862
H	-0.5406	-2.04596	1.43011
H	-0.42962	-1.06639	2.93118
C	-3.72441	1.22699	0.02322
H	-4.00825	0.58538	-0.8284
H	-4.01556	0.73249	0.96283
H	-4.25527	2.18485	-0.06452
N	-1.40279	-0.8347	-0.98778
C	-2.41584	-1.87212	-0.91401
H	-3.11917	-1.80773	-1.76496
H	-1.943	-2.87022	-0.93366
H	-2.98931	-1.78054	0.01664
C	-0.58027	-0.85871	-2.18483
H	0.16785	-0.05246	-2.13798
H	-0.04902	-1.82142	-2.26714
H	-1.18827	-0.70249	-3.09474

Optimized cuprate structure of the phosphoramidite ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Energy: -2617.239665

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2617.834993

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2618.430015

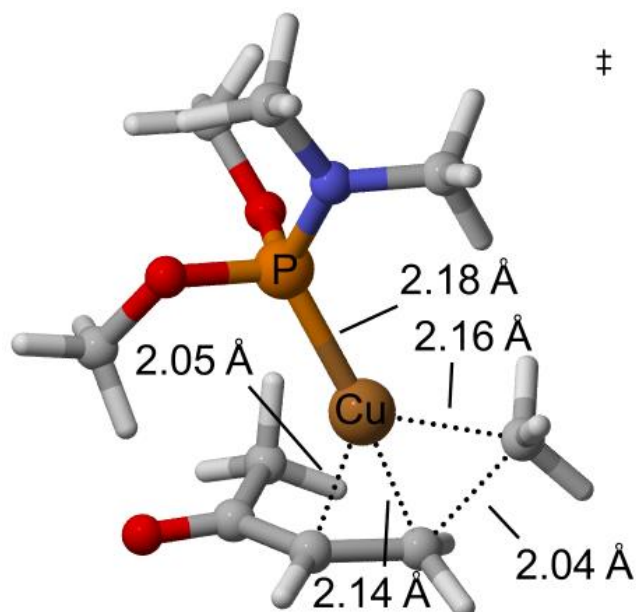
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2618.325897

0 1

O	-1.25669	1.80743	-0.89394
P	-1.05897	0.41207	-0.06626
Cu	0.65625	-1.08591	-0.23076
C	0.12545	-2.82269	0.57518
H	0.15743	-3.63952	-0.16673
H	0.82428	-3.09354	1.38593
H	-0.89192	-2.78747	1.00013
C	2.38135	-0.13991	-1.0535
H	2.15406	0.21805	-2.06229
C	2.75035	0.92681	-0.10001
O	2.74307	2.10362	-0.43091
C	2.55252	-1.50569	-0.80655
H	3.06187	-1.86733	0.08898

H	2.49125	-2.22394	-1.62841
C	3.12989	0.52482	1.31686
H	2.35474	-0.11513	1.77059
H	4.06741	-0.0543	1.3211
H	3.26195	1.43242	1.91871
C	-0.34337	2.90187	-0.77164
H	-0.28229	3.23983	0.27441
H	0.66453	2.63105	-1.11825
H	-0.7422	3.71547	-1.39286
C	-3.77497	0.4252	-0.07867
H	-3.58303	1.25812	0.61042
H	-4.18741	0.83706	-1.01806
H	-4.53393	-0.23543	0.37445
O	-1.17716	1.0509	1.45345
C	-1.06582	0.18499	2.57484
H	-1.11041	0.81095	3.47664
H	-1.89148	-0.54594	2.59587
H	-0.11399	-0.3726	2.5671
N	-2.546	-0.31909	-0.30642
C	-2.66049	-1.48609	-1.16325
H	-3.02873	-1.22288	-2.173
H	-1.68085	-1.97489	-1.26009
H	-3.35915	-2.21735	-0.7221

Optimized reductive elimination transition structure of the phosphoramidite ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Imaginary frequency: -419.32 cm^{-1}

Energy: -2617.201998

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2617.812609

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2618.393766

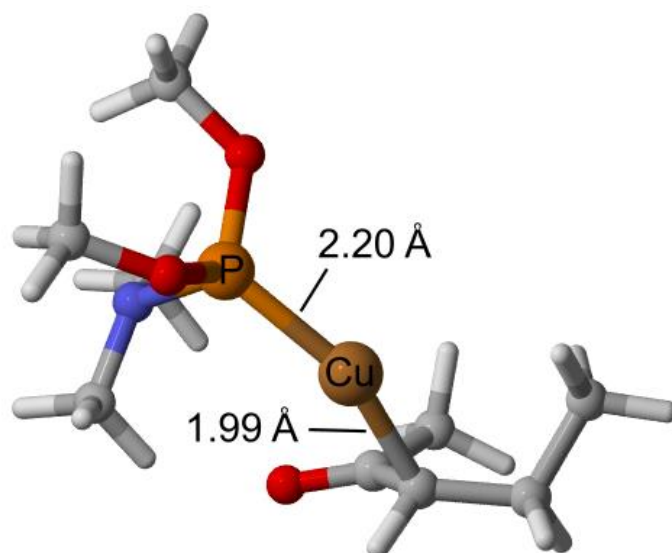
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2618.318555

0 1

O	1.45422	-1.36694	-1.05227
O	1.1768	-0.78892	1.43258
P	1.14659	-0.09699	-0.06749
Cu	-0.81313	0.84474	-0.22349
C	-1.45031	2.79129	0.46126
H	-0.87864	2.64359	1.3929
H	-0.8113	3.26231	-0.30665
H	-2.27109	3.48129	0.67922
C	-2.66984	0.13489	-0.73961
H	-2.74727	0.06112	-1.82938
C	-2.67275	-1.13881	-0.05097

O	-2.63826	-2.21875	-0.64997
C	-2.86762	1.44484	-0.12491
H	-3.33746	1.45444	0.86346
H	-3.31646	2.18516	-0.79319
C	-2.64686	-1.15251	1.48121
H	-3.23412	-0.34606	1.94613
H	-3.02384	-2.12613	1.82237
H	-1.6036	-1.05272	1.83075
C	0.43613	-2.36862	-1.21534
H	-0.50695	-1.93887	-1.58231
H	0.82676	-3.09534	-1.93924
H	0.22378	-2.87546	-0.26158
C	2.27102	-1.57876	1.8814
H	3.17379	-0.95966	2.01814
H	1.98743	-2.0146	2.849
H	2.49962	-2.39065	1.17218
C	3.84373	0.16481	-0.70761
H	4.26936	0.7132	-1.56674
H	4.57918	0.20553	0.11805
H	3.69838	-0.87894	-1.00833
N	2.57117	0.75223	-0.32193
C	2.60452	2.15894	0.0345
H	3.22178	2.34571	0.93343
H	3.01881	2.76059	-0.79408
H	1.58558	2.51787	0.24071

Optimized product structure of the phosphoramidite ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Energy: -2617.259480

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2617.872684

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2618.438126

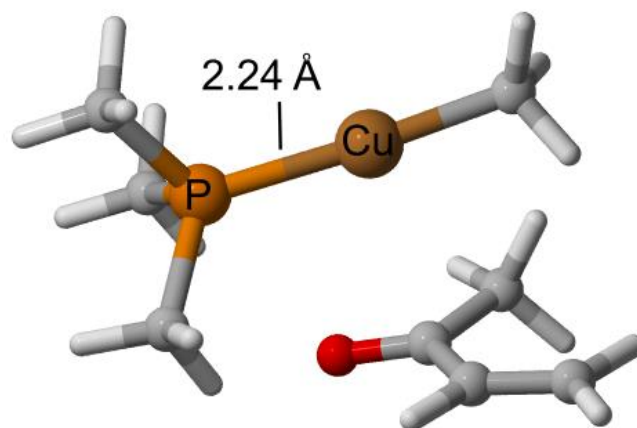
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2618.374040

0 1

O	-1.94545	-0.84501	1.52928
O	-2.40568	-1.14334	-1.05504
P	-1.40858	-0.45848	0.03911
Cu	0.74673	-0.70229	-0.34696
C	3.61378	-1.90436	0.69665
H	3.48992	-1.33081	1.62844
H	2.72231	-2.5467	0.58906
H	4.49248	-2.55875	0.82557
C	2.57529	-0.06305	-0.80159
H	2.40927	0.11479	-1.87731
C	3.75865	-0.9891	-0.52304
H	3.89929	-1.62684	-1.41171
C	2.4107	1.2102	-0.09498

O	1.65522	2.11025	-0.49596
H	4.70175	-0.41456	-0.42909
C	3.13824	1.42623	1.22989
H	4.18949	1.10263	1.19148
H	3.08255	2.49111	1.49175
H	2.64722	0.84262	2.0258
C	-3.25685	-0.57667	2.02292
H	-3.65467	0.36896	1.62467
H	-3.93754	-1.40165	1.75911
H	-3.18899	-0.50875	3.11765
C	-3.77959	-0.81535	-1.26026
H	-4.41989	-1.53261	-0.72302
H	-4.00373	0.20674	-0.92094
H	-3.98416	-0.89405	-2.33757
C	-1.5526	1.78163	-1.40734
H	-2.12249	2.71948	-1.50786
H	-0.47672	1.99978	-1.53577
H	-1.88227	1.09823	-2.20199
N	-1.8213	1.19797	-0.08382
C	-1.32992	2.07025	0.99084
H	-0.27638	2.36052	0.82512
H	-1.94564	2.98436	1.01964
H	-1.41774	1.56945	1.96402

Optimized separated structure of the phosphine ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Energy: -2372.288687

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2372.694697

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2373.138726

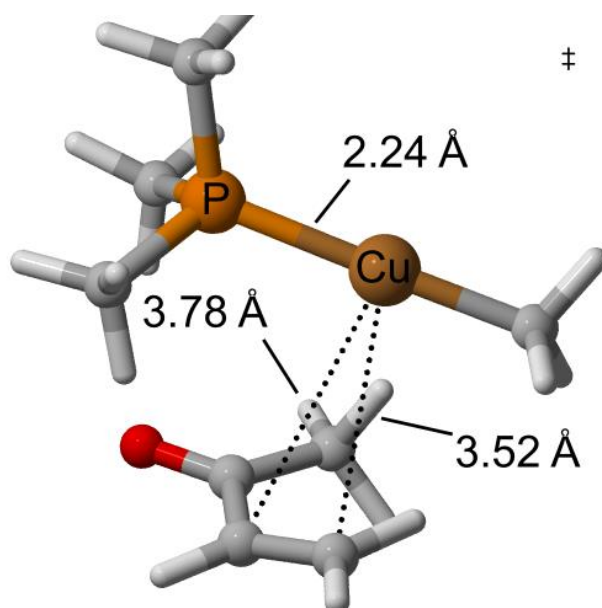
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2373.106402

0 1

P	-1.82606	-0.1801	0.08419
Cu	-0.08429	1.2249	-0.06718
C	1.36474	2.50126	-0.2664
H	1.04729	3.53262	-0.0261
H	2.20826	2.25793	0.40529
H	1.76151	2.53063	-1.29919
C	2.19321	-0.91776	1.07865
H	1.50374	-1.30166	1.83644
C	3.28711	-0.23174	1.43303
H	3.98468	0.16998	0.69454
H	3.51274	-0.02787	2.48282
C	2.65215	-0.73618	-1.45783
H	2.66388	0.3638	-1.44345
H	3.69147	-1.0904	-1.36722

H	2.22664	-1.089	-2.40539
C	1.80925	-1.2547	-0.31641
O	0.8298	-1.96102	-0.51614
C	-1.76005	-1.48521	1.37776
H	-0.89379	-2.1228	1.15263
H	-1.62295	-1.02176	2.36613
H	-2.68037	-2.09053	1.38346
C	-3.44196	0.64417	0.41141
H	-3.39526	1.17095	1.37634
H	-3.63662	1.38985	-0.37385
H	-4.27004	-0.08218	0.43515
C	-2.15296	-1.14174	-1.44776
H	-2.33244	-0.44846	-2.28291
H	-1.25565	-1.73789	-1.66542
H	-3.02525	-1.80409	-1.32947

Optimized oxidative addition transition structure of the phosphine ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Imaginary frequency: -17.96 cm⁻¹

Energy: -2372.286371

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2372.693127

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2373.138630

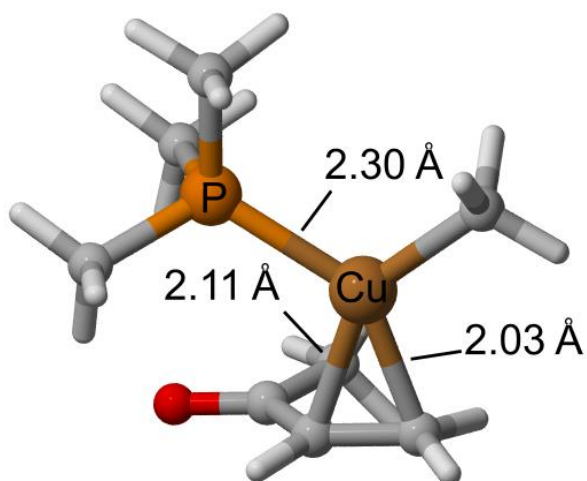
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2373.106056

0 1

P	-1.6225	-0.36891	0.07637
Cu	-0.28068	1.41906	-0.11502
C	0.8411	3.00107	-0.24689
H	1.25435	3.29143	0.73722
H	1.69965	2.88398	-0.93478
H	0.26195	3.86804	-0.61466
C	2.41193	-0.97766	1.03609
H	2.39599	-1.78258	1.78002
C	1.97657	-1.40726	-0.3185
O	1.39335	-2.47412	-0.44475
C	2.70138	0.28709	1.37289
H	2.67578	1.10449	0.6489
H	2.94269	0.55556	2.4051
C	2.20953	-0.48566	-1.49074
H	1.57081	0.41087	-1.37895
H	3.25084	-0.13257	-1.52966
H	1.9482	-1.00473	-2.42139
C	-1.63004	-1.58557	-1.30232
H	-1.85411	-1.06585	-2.24575
H	-0.63831	-2.05518	-1.37479
H	-2.38784	-2.3659	-1.12809
C	-1.25903	-1.39346	1.56244

H	-1.74393	-2.38014	1.51679
H	-0.17016	-1.50939	1.62719
H	-1.60074	-0.85448	2.45887
C	-3.41023	0.03268	0.26833
H	-3.76587	0.55029	-0.63506
H	-4.01186	-0.87687	0.42435
H	-3.54426	0.70956	1.12505

Optimized cuprate structure of the phosphine ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Energy: -2372.300354

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2372.691822

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2373.159857

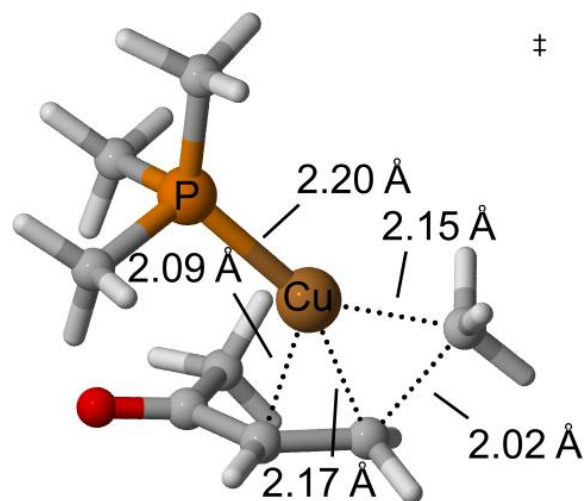
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2373.113326

0 1

P	1.49749	-0.34279	-0.01245
Cu	-0.3124	1.06757	-0.11921
C	0.09429	2.88484	0.53273
H	0.89635	3.31746	-0.09261

H	-0.76051	3.5793	0.52078
H	0.47683	2.83114	1.56825
C	-1.77659	-0.20681	-0.95718
H	-1.46712	-0.44735	-1.97938
C	-1.74552	-1.35218	-0.03528
O	-1.26147	-2.43062	-0.36941
C	-2.27448	1.0671	-0.65431
H	-2.82454	1.26255	0.26906
H	-2.42908	1.798	-1.45144
C	-2.28482	-1.15544	1.37286
H	-3.33314	-0.8188	1.35479
H	-2.21279	-2.10407	1.91943
H	-1.70782	-0.3804	1.90597
C	3.10778	0.52645	0.15507
H	3.0805	1.15749	1.05576
H	3.95133	-0.17858	0.22315
H	3.25277	1.18692	-0.7128
C	1.73141	-1.45931	-1.45255
H	0.82867	-2.08444	-1.53146
H	1.83629	-0.8609	-2.36993
H	2.62003	-2.09918	-1.33253
C	1.48945	-1.516	1.40362
H	0.64343	-2.20646	1.27172
H	2.42576	-2.09468	1.44469
H	1.36283	-0.96274	2.34591

Optimized reductive elimination transition structure of the phosphine ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Imaginary frequency: -433.24 cm^{-1}

Energy: -2372.259962

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2372.668643

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2373.117698

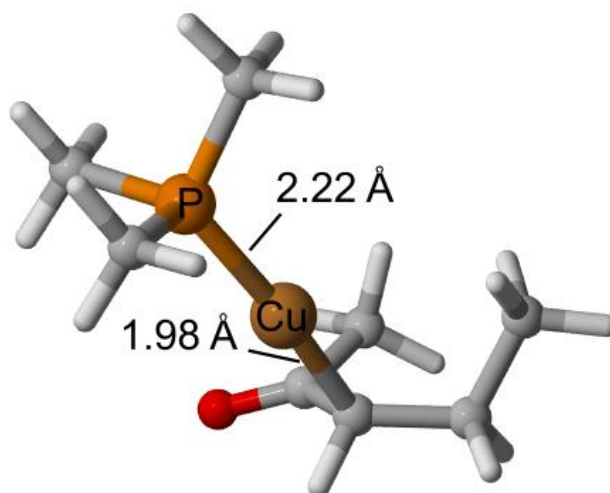
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2373.074243

0 1

P	1.69876	0.17836	0.05362
Cu	-0.39372	0.86216	-0.04542
C	-1.87315	2.35781	0.3812
H	-1.45531	2.39496	1.40284
H	-1.34149	3.07434	-0.26859
H	-2.91817	2.67483	0.4454
C	-1.72007	-0.48712	-0.93245
H	-1.4317	-0.50242	-1.98851
C	-1.31926	-1.62841	-0.16051
O	-0.56681	-2.52363	-0.58791
C	-2.51831	0.63123	-0.43705
H	-3.1707	0.41092	0.4138

H	-3.05597	1.17465	-1.21981
C	-1.81201	-1.72469	1.2899
H	-2.90407	-1.60352	1.37028
H	-1.52692	-2.70731	1.68759
H	-1.35405	-0.94259	1.92261
C	2.03206	-0.69903	-1.52436
H	3.02565	-1.1747	-1.51827
H	1.24561	-1.46719	-1.62259
H	1.96653	0.00262	-2.36886
C	1.89652	-1.17328	1.28265
H	1.67168	-0.81236	2.29666
H	1.18478	-1.96697	1.0055
H	2.92152	-1.57587	1.25598
C	3.17847	1.24346	0.31582
H	4.10786	0.65403	0.26082
H	3.20515	2.03097	-0.45213
H	3.11479	1.72695	1.3022

Optimized product structure of the phosphine ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)



Energy: -2372.318055

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2372.733496

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2373.172783

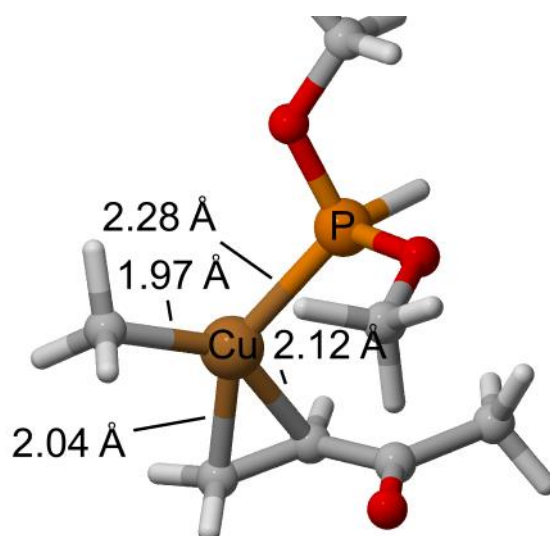
Energy (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2373.139523

0 1

P	2.16724	0.02117	0.08935
Cu	0.00242	0.17362	-0.39187
C	-2.32875	2.20713	0.59909
H	-2.39099	1.66731	1.55677
H	-1.28111	2.53494	0.47779
H	-2.9593	3.10841	0.68676
C	-1.92767	0.05664	-0.8092
H	-1.87492	-0.21455	-1.87754
C	-2.7522	1.32802	-0.58222
H	-2.68137	1.93886	-1.49819
C	-2.22996	-1.18343	-0.06418
O	-1.8696	-2.2948	-0.44824
H	-3.83035	1.09218	-0.47839
C	-2.98185	-1.07458	1.26436
H	-3.93005	-0.52445	1.1538
H	-3.18047	-2.08693	1.64005
H	-2.37804	-0.52641	2.00537
C	2.78104	1.08566	1.45835
H	3.85114	0.91347	1.65475
H	2.62463	2.14279	1.19703
H	2.20498	0.87074	2.37055
C	2.64786	-1.67208	0.62035
H	2.39289	-2.38494	-0.17758

H	3.72428	-1.73763	0.84479
H	2.06899	-1.94805	1.51404
C	3.34198	0.38305	-1.27918
H	4.38696	0.23996	-0.96158
H	3.12528	-0.28335	-2.12719
H	3.20288	1.42118	-1.6156

Optimized cuprate structure of the hydrido phosphine ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP) with the *syn*-methyl-vinyl ketone



Energy: -2483.325979

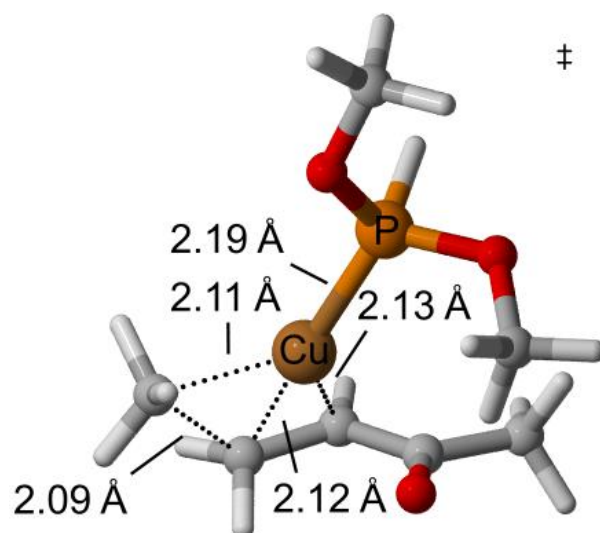
Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2484.350866

0 1

O	-1.38714	1.44642	0.69929
O	-2.63505	-0.50305	-0.52349
P	-1.22282	0.31704	-0.48072
H	-1.42724	1.2334	-1.55877
Cu	0.54641	-1.07478	-0.14301
C	0.02839	-2.70124	0.83913
H	-1.03223	-2.92915	0.64348

H	0.64192	-3.57376	0.56434
H	0.15586	-2.5232	1.92128
C	2.19692	0.0031	-0.92228
H	2.11935	0.06669	-2.01149
C	2.03019	1.24007	-0.13493
O	2.16763	1.25626	1.08429
C	2.57271	-1.1919	-0.30271
H	2.89728	-1.16791	0.74076
H	2.85481	-2.06576	-0.89366
C	1.63057	2.50658	-0.87374
H	1.51294	2.36201	-1.95699
H	0.6865	2.88119	-0.4478
H	2.39433	3.27912	-0.6927
C	-0.95961	1.13247	2.03682
H	-1.16937	0.08037	2.28787
H	0.11706	1.32836	2.14219
H	-1.53002	1.78367	2.71316
C	-3.87683	0.17998	-0.65731
H	-3.90631	0.76653	-1.59342
H	-4.66912	-0.58019	-0.683
H	-4.04702	0.86027	0.19225

Optimized reductive elimination transition structure of the hydrido phosphine ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP) with the *syn*-methyl-vinyl ketone



Imaginary frequency: -371.26 cm^{-1}

Energy: -2483.295708

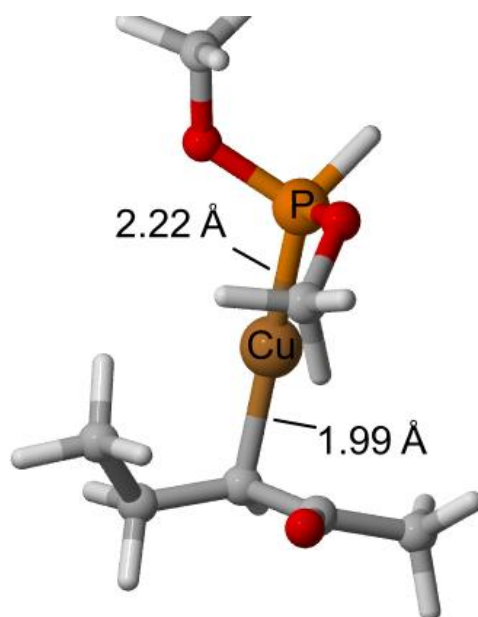
Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2484.320923

0 1

O	-1.78579	1.52289	-0.01308
O	-2.6863	-0.93128	-0.00197
P	-1.44503	0.00417	-0.52297
Cu	0.55638	-0.73468	-0.04316
C	1.18537	-2.62571	0.65911
H	0.41453	-2.47292	1.43488
H	0.78394	-3.24425	-0.1577
H	2.02475	-3.14363	1.13173
C	2.42815	-0.02727	-0.77237
H	2.64462	-0.00971	-1.84212
C	2.03903	1.15424	-0.07824
O	1.6682	1.10081	1.13088
C	2.61144	-1.25559	-0.00363
H	2.99404	-1.09815	1.00926

H	3.11525	-2.05899	-0.54496
C	2.00481	2.48825	-0.79781
H	0.96366	2.84746	-0.84683
H	2.57215	3.22515	-0.20792
H	2.41615	2.44066	-1.81626
C	-1.40168	1.91827	1.31748
H	-1.69124	2.97244	1.42171
H	-1.94699	1.32224	2.06794
H	-0.31442	1.8061	1.46031
C	-4.0332	-0.58539	-0.30882
H	-4.19221	-0.55099	-1.40188
H	-4.67968	-1.36072	0.12417
H	-4.2987	0.39517	0.11734
H	-1.83755	0.23298	-1.87455

Optimized product structure of the hydrido phosphine ligand of the reaction pathway (B3LYP-D3(BJ)/def2-SVP) with the *syn*-methyl-vinyl ketone



Energy: -2483.355115

Energy (TPSS-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -2484.369206

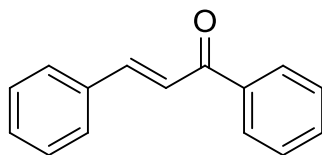
0 1

O	-1.8822	1.40317	0.76888
O	-2.75739	-0.81325	-0.32306
P	-1.781	0.47272	-0.56864
Cu	0.30532	-0.18346	-0.92395
C	1.12106	-2.10729	1.27123
H	1.11336	-1.2772	1.99082
H	0.14154	-2.12638	0.75604
H	1.21823	-3.0542	1.82822
C	2.2103	-0.62916	-0.55233
H	2.7533	-0.69086	-1.50705
C	2.45736	0.62977	0.14807
O	2.29743	0.79419	1.36498
C	2.26737	-1.91885	0.27103
H	3.2213	-1.95758	0.83203
H	2.28494	-2.77612	-0.42321
C	2.91629	1.82291	-0.69189
H	2.37344	2.72723	-0.37743
H	3.9847	2.00054	-0.48279
H	2.7943	1.66894	-1.77416
C	-1.00266	1.14888	1.88125
H	-1.22647	1.9166	2.63284
H	-1.19786	0.15377	2.31092
H	0.06083	1.21545	1.59613
C	-4.11879	-0.63658	0.0645
H	-4.67394	-0.06786	-0.70261
H	-4.56205	-1.63609	0.16494

H	-4.18969	-0.1028	1.02502
H	-2.60366	1.30515	-1.38297

Optimized “syn”-structure of trans-chalcone of rotational analysis (B3LYP-D3(BJ)/def2-TZVP)

Energy: -654.338973



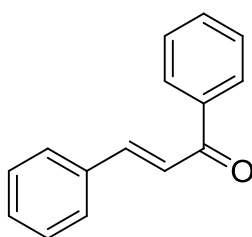
0 1

C	-4.09365300	1.64503600	-0.23444700
C	-2.80882900	1.13307400	-0.18933600
C	-2.58951400	-0.23736300	0.01324500
C	-3.70522400	-1.07007500	0.16659600
C	-4.99375100	-0.55742100	0.12211500
C	-5.19238500	0.80250500	-0.07836300
H	-4.24442000	2.70511100	-0.39256900
H	-1.96738900	1.80098100	-0.31479900
H	-3.55010900	-2.13049000	0.32226900
H	-5.84177100	-1.21872800	0.24331700
H	-6.19554200	1.20690200	-0.11436700
C	-1.26219500	-0.83292400	0.07045500
C	-0.07983200	-0.20936200	-0.02807000
C	1.18202400	-0.97869700	0.03154100
C	2.47742400	-0.22834000	0.01549000
C	2.57250900	1.13830200	0.28819400
C	3.64539100	-0.94511500	-0.26061200
C	3.80774800	1.77351500	0.28556000
H	1.68917900	1.71243700	0.52882600
C	4.87555500	-0.30915300	-0.27736200
H	3.55989800	-2.00445000	-0.45871500

C	4.95993000	1.05325000	-0.00311400
H	3.86996900	2.83054300	0.50940700
H	5.77203900	-0.87276900	-0.50131100
H	5.92152400	1.55026300	-0.01213700
O	1.18364800	-2.19918700	0.07775500
H	-0.02514100	0.85947300	-0.17282700
H	-1.22861100	-1.90917300	0.20951700

Optimized "anti"-structure of trans-chalcone of rotational analysis

Energy: -654.337405

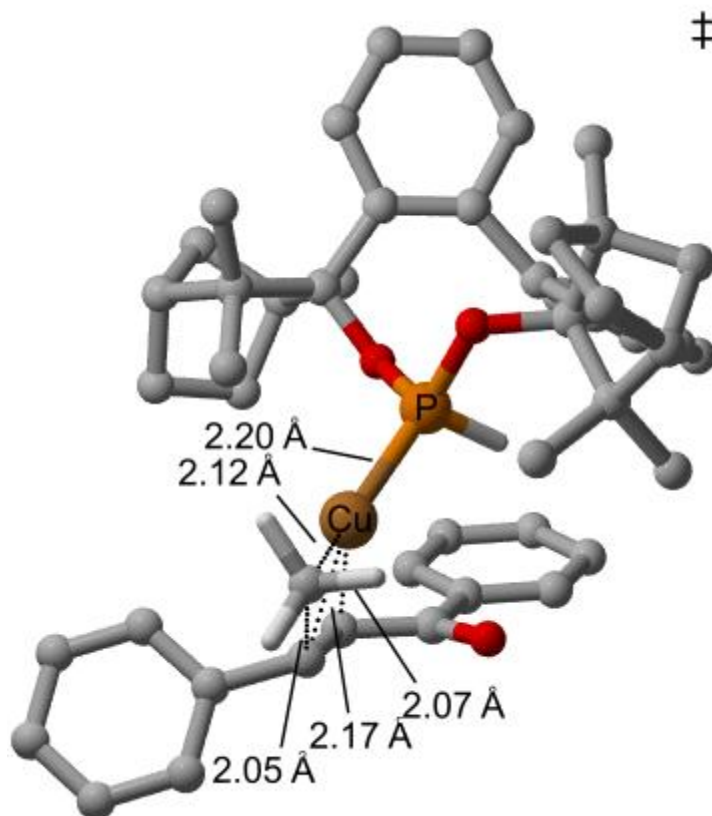


0 1

C	-4.49283500	0.63336900	0.30921900
C	-3.13850200	0.91891300	0.30880200
C	-2.20401800	-0.04698200	-0.09004500
C	-2.67789600	-1.30348200	-0.48630500
C	-4.03552700	-1.59003100	-0.48665100
C	-4.94811600	-0.62174300	-0.08851300
H	-5.20055000	1.39096700	0.61994600
H	-2.80274200	1.89857200	0.62014200
H	-1.96689100	-2.05916600	-0.79751800
H	-4.38045600	-2.56754000	-0.79756700
H	-6.00802500	-0.84007500	-0.08718800
C	-0.76491600	0.19326800	-0.10649400
C	-0.13085900	1.33215300	0.20748400
C	1.31994400	1.55794500	0.07268400
C	2.27230700	0.40306300	0.06907200
C	2.09728200	-0.71589500	0.88514600

C	3.41065900	0.48910100	-0.73488000
C	3.04155000	-1.73492100	0.88983400
H	1.23761200	-0.77648300	1.53799800
C	4.34089700	-0.53838000	-0.74616200
H	3.54976300	1.37256200	-1.34295100
C	4.15836000	-1.65296100	0.06734400
H	2.90663500	-2.59072700	1.53857300
H	5.21298200	-0.46999400	-1.38353700
H	4.88932100	-2.45132200	0.06507400
O	1.73987000	2.69732400	-0.05582400
H	-0.67840100	2.22587600	0.48148900
H	-0.16818100	-0.65175800	-0.43107700

Optimized reductive elimination transition structure of the active catalyst system (MeCu • BIFOP-H • chalcone) of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)**TS-3 (R)**



Imaginary frequency: -398.95 cm⁻¹

Energy: -4068.823932

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -4070.162638

0 1

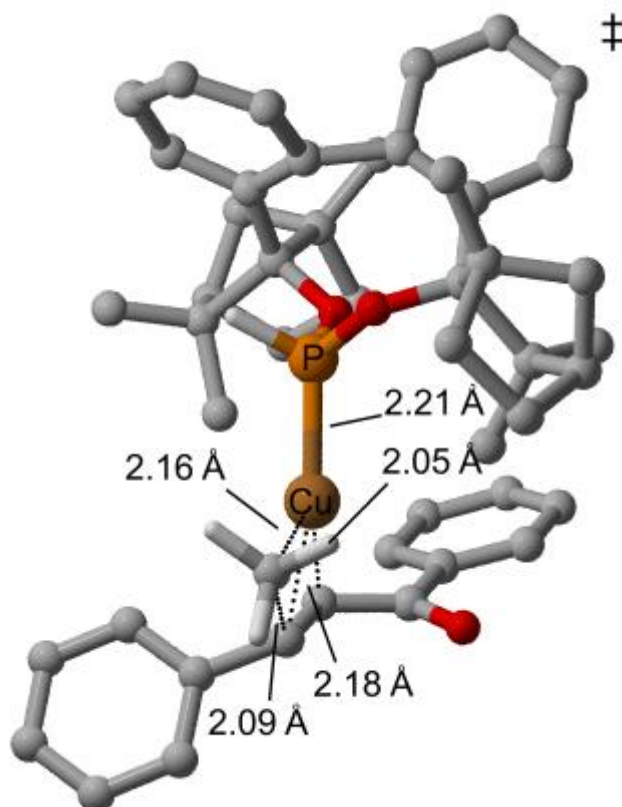
Cu	2.01238	-0.85958	-0.65155
C	3.26802	-1.85625	-2.03859
C	3.24542	-1.03378	1.00045
C	3.99662	-1.57739	-0.14302
H	2.99038	-1.038	-2.72842
H	4.27566	-2.17598	-2.313
H	2.57813	-2.70748	-2.13081
C	-3.69123	-1.63392	2.83638
C	-3.42393	-1.9742	1.51125
C	-3.45684	-0.33235	3.26221
C	-2.92719	-1.06963	0.55908
C	-3.09674	0.61861	2.31176
C	-2.88085	0.30894	0.95689
O	-1.39697	-0.62958	-1.22372
O	-0.2829	1.16059	0.32244
C	-3.04599	1.52786	0.0626
C	-4.42467	1.83809	-0.00906
P	-0.09201	-0.36161	-0.24203
C	-2.12519	2.43207	-0.53375
C	-4.93823	2.93197	-0.69039
C	-2.67989	3.52797	-1.22739
C	-4.04265	3.78255	-1.32893
H	-2.02422	4.24282	-1.69999
H	-4.38924	4.65612	-1.88578

H	-6.01523	3.11128	-0.71655
H	-5.11693	1.16817	0.50134
H	-3.0435	1.6662	2.60589
H	-3.60518	-0.04017	4.30382
H	-4.05683	-2.39729	3.52672
H	-3.59926	-3.00002	1.21968
H	-0.49935	-1.0331	0.9338
C	-2.41668	-1.57653	-0.81763
C	-3.53562	-1.65506	-1.92681
C	-1.78285	-3.10691	-0.92477
C	-2.85112	-1.83484	-3.313
C	-4.08626	-3.07135	-1.66237
C	-2.76442	-3.79187	-1.92955
C	-2.48546	-3.33851	-3.37122
H	-1.98123	-1.17295	-3.40753
H	-3.56041	-1.55801	-4.10696
H	-4.48545	-3.20029	-0.64719
H	-4.88075	-3.34048	-2.3761
H	-2.76927	-4.88459	-1.80363
H	-1.45866	-3.52823	-3.7067
H	-3.15173	-3.88158	-4.05952
C	-4.58236	-0.56033	-1.95018
H	-5.10682	-0.47803	-0.99033
H	-4.14663	0.41693	-2.1929
H	-5.33211	-0.79618	-2.7224
C	-1.67945	-3.96448	0.35263
H	-2.63101	-4.41662	0.65956
H	-0.99394	-4.79929	0.14412
H	-1.25614	-3.41055	1.20028

C	-0.34797	-3.1039	-1.48582
H	-0.18757	-2.4001	-2.3086
H	0.3892	-2.90541	-0.69398
H	-0.11914	-4.11592	-1.85379
C	-0.59976	2.40896	-0.29012
C	0.38868	2.82438	-1.5275
C	1.08503	4.11617	-0.97802
H	1.47181	4.74033	-1.79748
C	-0.28459	3.11155	-2.88575
H	0.48259	3.06542	-3.67379
H	-1.05618	2.36565	-3.12386
H	-0.73357	4.10879	-2.95862
C	1.4485	1.76344	-1.85156
H	1.01915	0.92799	-2.42106
H	2.22866	2.21938	-2.48078
H	1.94315	1.36464	-0.95655
C	0.02067	4.75727	-0.07872
H	0.42174	5.59392	0.51467
H	-0.8748	5.12045	-0.59124
C	-0.19661	3.50677	0.79214
C	-1.14333	3.62918	1.97237
H	-1.14789	2.69511	2.55259
H	-0.8035	4.43709	2.6395
H	-2.17324	3.85569	1.66195
C	1.26643	3.21629	1.24077
H	1.46443	3.74803	2.18336
H	1.41481	2.14894	1.43292
C	2.14192	3.76163	0.0837
H	2.67449	4.67694	0.3838

H	2.90692	3.0527	-0.25623
C	2.26194	-1.84977	1.64619
C	5.24364	-0.82748	-0.4789
C	5.20396	0.53567	-0.81449
C	6.48793	-1.47133	-0.44243
C	6.37558	1.23816	-1.09499
H	4.23947	1.04495	-0.86736
C	7.66433	-0.76954	-0.72176
H	6.53326	-2.53223	-0.18338
C	7.61323	0.58758	-1.04784
H	6.3231	2.29812	-1.35622
H	8.62584	-1.28751	-0.68318
H	8.53204	1.13602	-1.26846
H	4.12786	-2.66094	-0.06951
O	1.94297	-2.97786	1.2023
C	1.47999	-1.29254	2.81322
C	1.62048	0.01728	3.29819
C	0.48877	-2.11264	3.37607
C	0.78238	0.49877	4.3054
H	2.3792	0.67832	2.87983
C	-0.34669	-1.63618	4.38561
H	0.39374	-3.12562	2.98238
C	-0.20738	-0.32499	4.84999
H	0.89772	1.52605	4.66004
H	-1.12093	-2.28432	4.80248
H	-0.86998	0.056	5.63094
H	3.55631	-0.07672	1.41528

Optimized reductive elimination transition structure of the active catalyst system (MeCu • BIFOP-H • chalcone) of the reaction pathway (B3LYP-D3(BJ)/def2-SVP) **TS-3.1 (R)**



Imaginary frequency: -384.51 cm^{-1}

Energy: -4068.821521

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -4070.162732

0 1

Cu	1.92381	-0.81074	-0.53159
C	2.92383	-2.06382	-1.97736
C	3.52621	-0.49632	0.71081
C	4.05673	-1.25753	-0.42151
H	2.63244	-1.40747	-2.81233
H	3.84301	-2.58217	-2.26133
H	2.15196	-2.82778	-1.78445
C	-2.88354	2.99224	-3.58096

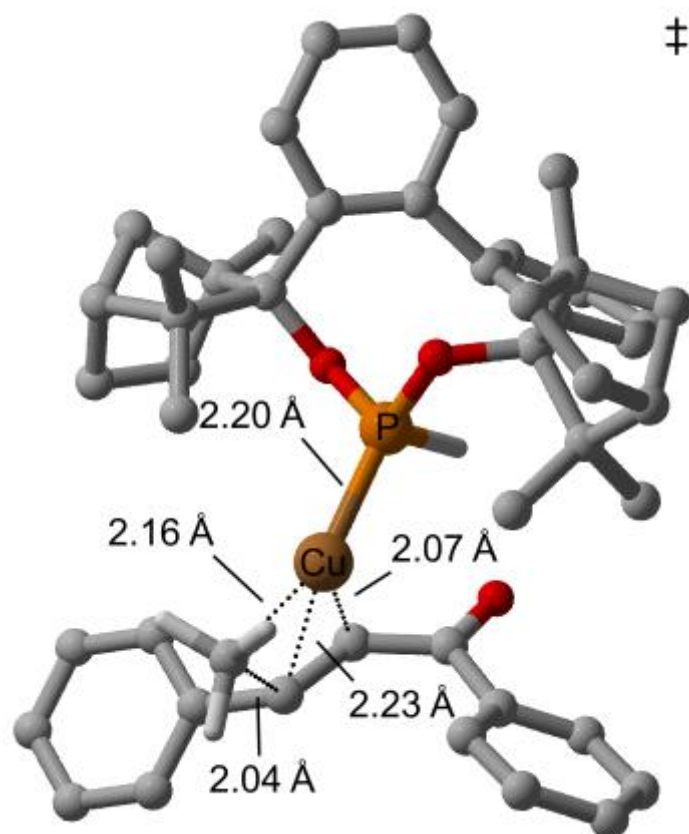
C	-2.22436	3.16131	-2.36333
C	-3.50172	1.77727	-3.8543
C	-2.14546	2.16758	-1.37451
C	-3.56999	0.82937	-2.83579
C	-2.97124	1.01101	-1.57599
O	-0.77589	0.96289	0.17396
O	-1.29348	-1.2144	-1.14411
C	-3.64827	0.18202	-0.49959
C	-4.90854	0.76794	-0.22891
P	-0.13257	-0.09492	-0.91559
C	-3.33245	-1.05256	0.12388
C	-5.82662	0.24393	0.66821
C	-4.28325	-1.55268	1.03934
C	-5.49273	-0.93347	1.32931
H	-4.09101	-2.48624	1.54431
H	-6.17277	-1.38949	2.05236
H	-6.7798	0.74762	0.84261
H	-5.1586	1.68924	-0.75626
H	-4.17849	-0.06351	-2.98071
H	-3.98532	1.58994	-4.81564
H	-2.88796	3.80509	-4.31051
H	-1.74104	4.11269	-2.19143
H	-0.33781	0.6143	-2.13151
C	-1.15909	2.31332	-0.18362
C	-1.76026	3.02975	1.08604
C	0.21735	3.20975	-0.40097
C	-0.78803	2.82274	2.28637
C	-1.49585	4.50317	0.71428
C	0.02549	4.36087	0.63979

C	0.33113	3.86782	2.06142
H	-0.41122	1.79359	2.32766
H	-1.32855	3.0036	3.2266
H	-1.97953	4.80909	-0.22382
H	-1.82731	5.19139	1.50729
H	0.5872	5.26202	0.35236
H	1.33854	3.45629	2.18465
H	0.24012	4.70804	2.76733
C	-3.19336	2.7113	1.4583
H	-3.88752	2.93591	0.63968
H	-3.31737	1.65781	1.73972
H	-3.48502	3.32791	2.32338
C	0.51564	3.82323	-1.78414
H	-0.06016	4.73103	-2.00163
H	1.57412	4.12612	-1.79516
H	0.36824	3.11126	-2.60832
C	1.47287	2.3866	-0.07561
H	1.38775	1.75978	0.81478
H	1.74424	1.73246	-0.91889
H	2.32429	3.06998	0.06419
C	-2.15734	-1.96799	-0.27682
C	-1.37945	-2.77643	0.90679
C	-1.64271	-4.26909	0.51598
H	-1.51958	-4.93524	1.38229
C	-1.84508	-2.51028	2.35451
H	-1.057	-2.85942	3.0376
H	-1.99506	-1.43855	2.54605
H	-2.75803	-3.04698	2.63858
C	0.12017	-2.49321	0.94655

H	0.3246	-1.50405	1.37849
H	0.63095	-3.21748	1.59397
H	0.60186	-2.57039	-0.03395
C	-3.03392	-4.24031	-0.1289
H	-3.29735	-5.19722	-0.60655
H	-3.85841	-3.97215	0.53808
C	-2.67758	-3.1728	-1.18064
C	-3.74896	-2.80321	-2.19142
H	-3.35626	-2.07561	-2.91693
H	-4.06074	-3.6991	-2.75098
H	-4.64124	-2.37167	-1.71591
C	-1.43839	-3.8446	-1.8426
H	-1.78353	-4.48818	-2.66552
H	-0.75932	-3.1009	-2.27464
C	-0.79502	-4.67745	-0.70244
H	-0.91436	-5.75645	-0.88373
H	0.27948	-4.49628	-0.57815
C	3.05506	-1.20994	1.86578
C	5.05573	-0.56192	-1.28224
C	4.79669	0.70366	-1.83425
C	6.29596	-1.16186	-1.54298
C	5.75208	1.35309	-2.61532
H	3.83046	1.17994	-1.65448
C	7.25668	-0.5123	-2.3231
H	6.511	-2.14677	-1.12053
C	6.98911	0.7479	-2.8623
H	5.53005	2.33653	-3.03742
H	8.21944	-0.99471	-2.50942
H	7.73804	1.25584	-3.47452

H	4.34088	-2.2693	-0.12196
O	2.9991	-2.45192	1.91691
C	2.50546	-0.41063	3.0273
C	2.72068	0.96475	3.21104
C	1.7065	-1.09275	3.95844
C	2.13759	1.64045	4.28512
H	3.35993	1.51553	2.51995
C	1.10751	-0.41692	5.02182
H	1.57503	-2.16626	3.81642
C	1.31833	0.95552	5.18752
H	2.32246	2.70897	4.41873
H	0.47711	-0.96247	5.72889
H	0.85416	1.48843	6.02106
H	3.70173	0.57698	0.75145

Optimized reductive elimination transition structure of the active catalyst system (MeCu • BIFOP-H • chalcone) of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)**TS-8.3 (R)**



Imaginary frequency: -436.41 cm^{-1}

Energy: -4068.809011

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -4070.149969

0 1

Cu	-1.91554	0.00861	-0.71445
C	-3.58999	-0.41478	-2.01389
C	-3.06103	0.17875	0.99714
C	-4.03562	-0.18895	-0.0376
H	-3.38259	-1.46759	-2.24455
H	-4.62288	-0.18053	-2.28536
H	-2.9432	0.24483	-2.63068
C	2.71966	2.16512	3.48755
C	2.52971	2.4845	2.14439

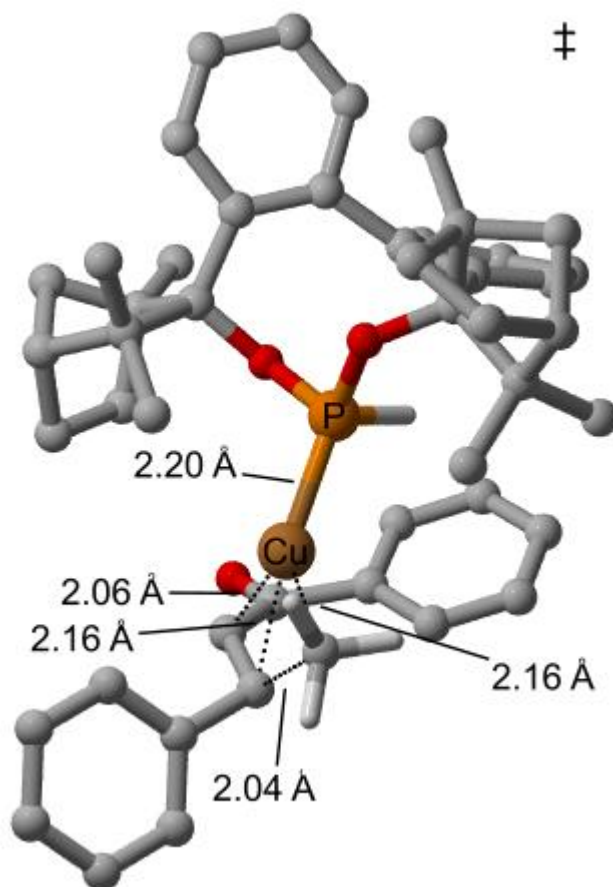
C	2.91434	0.83741	3.84723
C	2.51761	1.53453	1.1115
C	3.02847	-0.11241	2.83552
C	2.8808	0.1926	1.47015
O	1.48125	0.75133	-0.89194
O	0.74784	-1.3797	0.47505
C	3.51615	-0.8617	0.57578
C	4.92193	-0.7538	0.68733
P	0.20138	0.04818	-0.11378
C	2.98832	-1.94548	-0.18263
C	5.81898	-1.58309	0.02886
C	3.9256	-2.75282	-0.85929
C	5.30415	-2.586	-0.78408
H	3.57694	-3.57778	-1.46073
H	5.96104	-3.25887	-1.34005
H	6.89498	-1.43965	0.14896
H	5.31482	0.04015	1.32266
H	3.30678	-1.13197	3.09915
H	3.02878	0.5439	4.89304
H	2.69197	2.95606	4.24001
H	2.36476	3.52454	1.9027
H	0.19738	0.74569	1.11906
C	2.08157	1.94329	-0.32041
C	3.27289	2.44007	-1.22693
C	1.01932	3.20017	-0.5186
C	2.78671	2.51165	-2.70441
C	3.305	3.93124	-0.83171
C	1.88452	4.23718	-1.30764
C	2.00191	3.84415	-2.78895

H	2.17988	1.63291	-2.95785
H	3.65808	2.50933	-3.37565
H	3.47806	4.09243	0.24059
H	4.07797	4.48475	-1.38771
H	1.52553	5.26445	-1.1487
H	1.03904	3.75681	-3.30709
H	2.58264	4.6116	-3.32408
C	4.60226	1.72454	-1.1057
H	4.97487	1.72976	-0.07424
H	4.53906	0.68433	-1.44837
H	5.34622	2.24138	-1.73307
C	0.40262	3.87426	0.72488
H	1.08192	4.5751	1.22611
H	-0.45723	4.4739	0.38979
H	0.01374	3.15615	1.4607
C	-0.19963	2.77671	-1.35827
H	0.03909	2.1476	-2.22098
H	-0.93464	2.24734	-0.73657
H	-0.72007	3.67889	-1.71102
C	1.51942	-2.42652	-0.11421
C	0.83893	-3.08143	-1.45229
C	0.59109	-4.5652	-1.00906
H	0.52482	-5.23623	-1.87849
C	1.67239	-3.0329	-2.74991
H	0.99808	-3.18517	-3.60656
H	2.16612	-2.0592	-2.88003
H	2.43292	-3.81931	-2.82141
C	-0.49883	-2.43543	-1.84068
H	-0.34865	-1.48377	-2.36643

H	-1.02818	-3.1108	-2.53072
H	-1.16223	-2.25677	-0.98729
C	1.71865	-4.85097	-0.011
H	1.57781	-5.8054	0.52019
H	2.73065	-4.85338	-0.42596
C	1.40504	-3.65105	0.90024
C	2.21996	-3.52269	2.17398
H	1.86891	-2.66751	2.76831
H	2.09672	-4.43023	2.78574
H	3.29256	-3.39211	1.97263
C	-0.10703	-3.89504	1.18792
H	-0.20661	-4.50095	2.10036
H	-0.63177	-2.94936	1.3706
C	-0.6195	-4.65628	-0.06222
H	-0.8167	-5.71385	0.17116
H	-1.54914	-4.24883	-0.47656
C	-2.6541	1.48297	1.44548
C	-4.68607	-1.52699	0.12425
C	-3.94743	-2.6645	0.49057
C	-6.06105	-1.67154	-0.10528
C	-4.56536	-3.90712	0.62305
H	-2.87583	-2.57843	0.67611
C	-6.68554	-2.91444	0.03317
H	-6.65072	-0.79623	-0.39102
C	-5.93972	-4.0381	0.39528
H	-3.96957	-4.77805	0.90698
H	-7.76035	-3.00325	-0.14298
H	-6.42522	-5.01108	0.50099
H	-4.76251	0.59588	-0.25497

O	-1.83074	1.61856	2.37164
C	-3.19527	2.7559	0.82176
C	-3.592	2.9005	-0.51735
C	-3.2147	3.89548	1.64462
C	-3.99806	4.14189	-1.01735
H	-3.54551	2.05821	-1.20506
C	-3.63724	5.12974	1.15549
H	-2.86812	3.78053	2.67256
C	-4.03038	5.2596	-0.1819
H	-4.28453	4.23322	-2.06817
H	-3.65239	6.00052	1.81605
H	-4.35297	6.22859	-0.57082
H	-2.6841	-0.61462	1.64758

Optimized reductive elimination transition structure of the active catalyst system (MeCu • BIFOP-H • chalcone) of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)**TS-8.2 (R)**



Imaginary frequency: -404.21 cm^{-1}

Energy: -4068.813337

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -4070.150382

0 1

Cu	2.04841	-0.61298	-0.15817
C	3.2211	-2.01725	-1.30448
C	3.53286	-0.04423	1.15632
C	4.13708	-1.02526	0.23073
H	2.7796	-1.49253	-2.17058
H	4.20939	-2.36749	-1.61159
H	2.60371	-2.88061	-1.02182
C	-3.81088	-2.18047	2.51791
C	-3.49715	-2.29328	1.16275

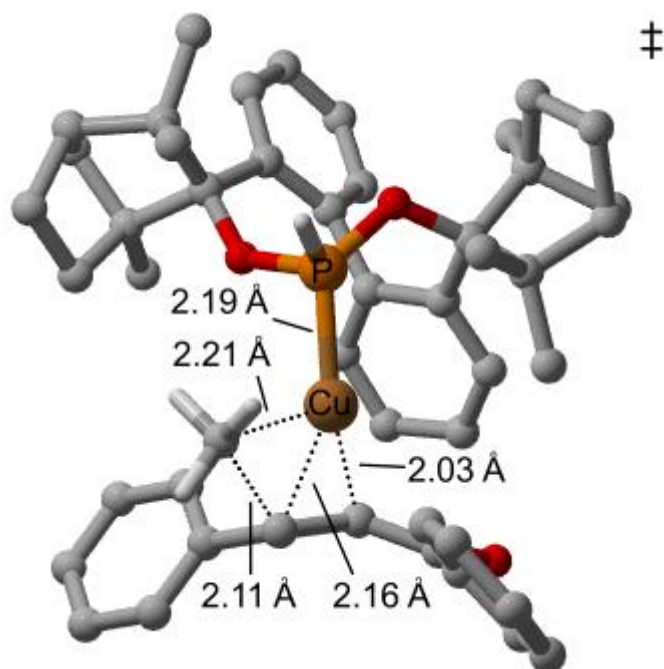
C	-3.60474	-0.96693	3.16425
C	-2.98667	-1.23677	0.39311
C	-3.24702	0.13768	2.39411
C	-3.00778	0.05974	1.01107
O	-1.28218	-0.51633	-1.11808
O	-0.46519	1.14987	0.65778
C	-3.22426	1.39245	0.31969
C	-4.61825	1.64409	0.28966
P	-0.12681	-0.32265	0.05628
C	-2.34585	2.40726	-0.13559
C	-5.18144	2.8011	-0.22491
C	-2.9522	3.57135	-0.65655
C	-4.32403	3.77713	-0.72385
H	-2.33037	4.38137	-1.00545
H	-4.71015	4.70973	-1.14161
H	-6.26532	2.93485	-0.23032
H	-5.2775	0.87176	0.68811
H	-3.21912	1.12621	2.85525
H	-3.783	-0.85723	4.23636
H	-4.18688	-3.05149	3.05919
H	-3.64632	-3.25784	0.69895
H	-0.65924	-1.10369	1.10764
C	-2.34428	-1.49401	-0.99966
C	-3.33414	-1.33635	-2.22046
C	-1.6971	-2.98503	-1.33247
C	-2.49875	-1.22727	-3.52836
C	-3.88243	-2.77445	-2.31587
C	-2.52633	-3.43001	-2.57728
C	-2.08078	-2.68447	-3.84398

H	-1.64643	-0.54983	-3.3946
H	-3.12919	-0.80583	-4.32512
H	-4.38136	-3.10792	-1.39428
H	-4.59245	-2.88857	-3.14987
H	-2.52713	-4.52436	-2.68876
H	-1.01301	-2.79697	-4.07035
H	-2.63323	-3.07644	-4.71206
C	-4.39702	-0.25968	-2.14016
H	-5.02167	-0.36779	-1.2454
H	-3.96227	0.74759	-2.13912
H	-5.05509	-0.34119	-3.02011
C	-1.77173	-4.10413	-0.27553
H	-2.76691	-4.5577	-0.18407
H	-1.09789	-4.91276	-0.59893
H	-1.43426	-3.77548	0.71487
C	-0.20028	-2.88356	-1.66438
H	0.05931	-2.0551	-2.32957
H	0.39545	-2.77843	-0.74633
H	0.12223	-3.82086	-2.14267
C	-0.81803	2.41406	0.08478
C	0.11811	2.89064	-1.16594
C	0.88708	4.10539	-0.5515
H	1.30209	4.75135	-1.34012
C	-0.63366	3.33028	-2.43987
H	0.08884	3.38864	-3.26796
H	-1.41263	2.60858	-2.72347
H	-1.09382	4.32166	-2.36618
C	1.10423	1.82803	-1.66085
H	0.59059	1.01157	-2.18856

H	1.79888	2.29415	-2.37687
H	1.71595	1.4128	-0.85037
C	-0.14999	4.75321	0.37526
H	0.2865	5.54605	1.00251
H	-1.02251	5.1824	-0.12638
C	-0.41364	3.47797	1.20083
C	-1.38613	3.56875	2.36474
H	-1.45502	2.59612	2.87555
H	-1.02546	4.30541	3.09925
H	-2.39636	3.86617	2.04938
C	1.03688	3.16046	1.66182
H	1.24471	3.73451	2.57645
H	1.1885	2.10962	1.91964
C	1.92701	3.64419	0.48747
H	2.54954	4.50175	0.78446
H	2.61571	2.8721	0.12452
C	2.77862	-0.2073	2.38069
C	5.25863	-0.43583	-0.57011
C	5.0533	0.68604	-1.3888
C	6.54373	-0.98866	-0.50035
C	6.10715	1.24418	-2.11143
H	4.05401	1.12001	-1.46203
C	7.60265	-0.42958	-1.22219
H	6.71901	-1.86154	0.13415
C	7.38877	0.68896	-2.03011
H	5.92758	2.11687	-2.74425
H	8.59978	-0.87076	-1.14956
H	8.21491	1.126	-2.59583
H	4.42252	-1.98279	0.67436

O	2.68614	0.72134	3.19344
C	1.8945	-1.42624	2.62248
C	2.03575	-2.6899	2.02186
C	0.79218	-1.21626	3.47116
C	1.08513	-3.69396	2.23559
H	2.89219	-2.91615	1.39193
C	-0.16263	-2.2101	3.6737
H	0.70981	-0.23575	3.94173
C	-0.02346	-3.45532	3.05099
H	1.21431	-4.66858	1.75834
H	-1.02876	-2.0116	4.30808
H	-0.77391	-4.23433	3.20393
H	3.92538	0.97154	1.06971

Optimized reductive elimination transition structure of the active catalyst system (MeCu • BIFOP-H • chalcone) of the reaction pathway (B3LYP-D3(BJ)/def2-SVP) **TS-6 (R)**



Imaginary frequency: -382.66 cm^{-1}

Energy: -4068.822935

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -4070.161142

0 1

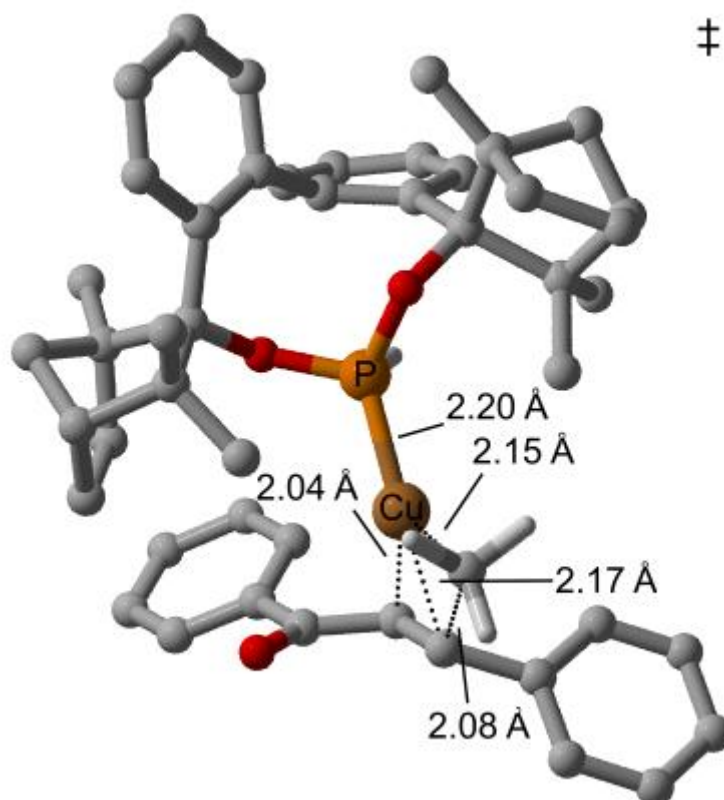
Cu	-1.44772	-0.60202	-0.46436
C	-1.71624	-2.32271	-1.82928
H	-2.32463	-3.20348	-2.05613
H	-1.87098	-1.58625	-2.63759
H	-0.66234	-2.63097	-1.78374
C	-2.78837	-1.14828	0.96257
H	-2.20103	-1.23191	1.87825
C	-2.71044	-2.28284	0.03098
C	-3.888	-0.21865	1.09544
O	-4.06348	0.44531	2.12483
H	-3.64602	-2.50561	-0.48513
C	-4.87032	-0.00963	-0.03979
C	-6.18175	0.36027	0.29827
C	-4.52484	-0.07849	-1.39669
C	-7.12839	0.62039	-0.69189
H	-6.42814	0.45098	1.35752
C	-5.46448	0.19889	-2.39317
H	-3.5032	-0.32501	-1.68926
C	-6.77305	0.54016	-2.04334
H	-8.14819	0.89657	-0.41162
H	-5.17071	0.15201	-3.44493
H	-7.51202	0.75153	-2.8203
C	-2.0158	-3.49253	0.56437
C	-0.71246	-3.40421	1.08442
C	-2.65523	-4.73868	0.5656

C	-0.07353	-4.53031	1.59946
H	-0.18985	-2.44449	1.06379
C	-2.0167	-5.86924	1.0854
H	-3.66753	-4.82234	0.16145
C	-0.7248	-5.76945	1.60513
H	0.9418	-4.44259	1.99231
H	-2.53346	-6.83219	1.08255
H	-0.22369	-6.65253	2.00862
C	-1.20691	0.90484	3.30791
C	-0.94505	1.81269	2.28317
C	-0.33682	-0.15912	3.50605
C	0.15217	1.70958	1.41736
C	0.82921	-0.21946	2.74579
C	1.13282	0.70289	1.72869
O	1.0112	1.82002	-0.7929
O	1.52023	-0.77266	-0.72901
C	2.62311	0.75754	1.41144
C	3.28591	1.35553	2.50799
P	0.4095	0.33234	-1.16502
C	3.42527	0.25801	0.3423
C	4.65563	1.57557	2.56367
C	4.80554	0.53409	0.41117
C	5.42347	1.18726	1.47284
H	5.45186	0.19569	-0.38358
H	6.50225	1.35728	1.44846
H	5.10314	2.05288	3.43806
H	2.67131	1.67893	3.34824
H	1.57746	-0.97284	2.98889
H	-0.53468	-0.91624	4.26793

H	-2.12481	1.00605	3.88567
H	-1.66412	2.60631	2.14025
H	0.59607	0.4515	-2.55624
C	0.26544	2.6148	0.16529
C	1.00951	3.98209	0.42319
C	-1.10626	3.16043	-0.58818
C	1.40319	4.60188	-0.9488
C	-0.18504	4.86572	0.83833
C	-0.94653	4.70915	-0.47728
C	0.09404	5.23983	-1.4753
H	1.81602	3.83769	-1.61967
H	2.18833	5.35652	-0.79376
H	-0.71685	4.48784	1.72238
H	0.12567	5.90218	1.04276
H	-1.92006	5.21664	-0.54123
H	-0.12633	4.99377	-2.52175
H	0.13503	6.3382	-1.4098
C	2.1681	3.99128	1.39921
H	1.88449	3.57604	2.37431
H	3.02854	3.42942	1.01675
H	2.49175	5.03236	1.55906
C	-2.47203	2.75428	-0.01128
H	-2.51846	1.68539	0.22314
H	-2.76202	3.31398	0.88545
H	-3.24583	2.95927	-0.76614
C	-1.16104	2.72616	-2.06614
H	-1.51246	1.68589	-2.15846
H	-1.90913	3.34394	-2.58502
H	-0.21041	2.82207	-2.60036

C	2.95331	-0.78327	-0.69871
C	3.35597	-2.23939	-0.17813
C	3.60025	-0.80599	-2.20116
C	2.5641	-3.28918	-1.00999
C	4.76518	-2.40542	-0.77515
C	4.32627	-2.19477	-2.22699
C	3.31238	-3.34558	-2.3665
H	1.50748	-3.01564	-1.10182
H	2.59565	-4.25708	-0.48908
H	5.504	-1.69173	-0.3974
H	5.15917	-3.41784	-0.5946
H	5.12267	-2.21278	-2.98603
H	2.64954	-3.25941	-3.23576
H	3.85747	-4.29525	-2.47888
C	3.22198	-2.47037	1.31621
H	3.83	-1.77335	1.90865
H	2.17465	-2.36863	1.62866
H	3.54473	-3.49495	1.5588
C	2.55403	-0.75783	-3.32967
H	1.66407	-1.36764	-3.14163
H	2.23875	0.27298	-3.53867
H	3.02673	-1.13581	-4.24946
C	4.59317	0.32212	-2.54897
H	5.60608	0.1567	-2.16229
H	4.69354	0.3763	-3.64382
H	4.24075	1.30163	-2.19473

Optimized reductive elimination transition structure of the active catalyst system (MeCu • BIFOP-H • chalcone) of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)**TS-4 (S)**



Imaginary frequency: -378.86 cm^{-1}

Energy: -4068.823932

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -4070.162638

0 1

Cu	-2.01044	-0.0561	-0.63227
C	-3.17872	0.71172	-2.27062
C	-3.50775	-1.04389	0.34522
H	-3.65645	-0.64771	1.34971
C	-4.15369	-0.38333	-0.79291
C	-2.96953	-2.36356	0.16348
O	-2.96519	-2.95027	-0.93797
C	-2.34536	-3.05288	1.35021
C	-1.77322	-2.35091	2.42271
C	-2.25703	-4.45241	1.33346

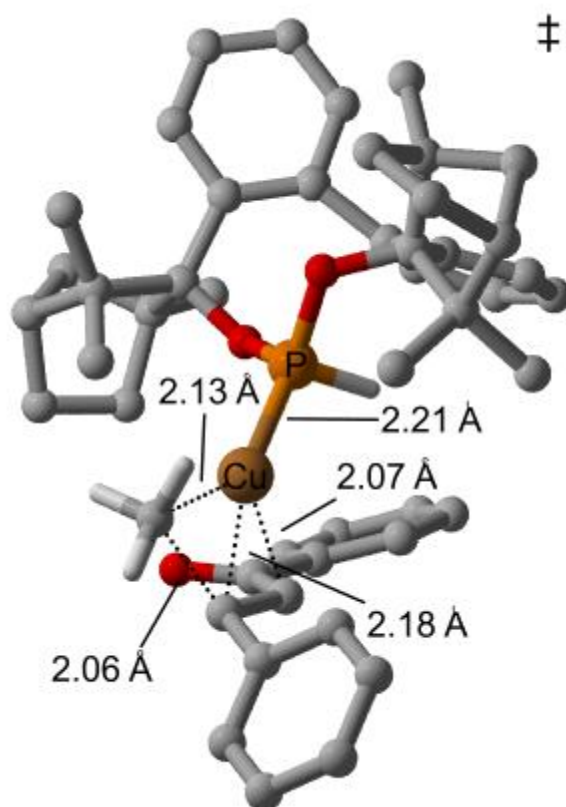
C	-1.12338	-3.03313	3.45304
H	-1.80443	-1.25998	2.43076
C	-1.62332	-5.13707	2.37017
H	-2.68195	-4.98075	0.47842
C	-1.04882	-4.42919	3.43122
H	-0.66358	-2.47237	4.27076
H	-1.56481	-6.22832	2.3471
H	-0.53802	-4.96367	4.23609
H	-2.39172	0.28487	-2.91448
H	-4.12101	0.65637	-2.82063
H	-2.97693	1.76715	-2.03718
H	-4.46927	-1.10955	-1.54658
C	-5.1734	0.65612	-0.47283
C	-4.90334	1.69752	0.43055
C	-6.43997	0.60557	-1.07222
C	-5.87232	2.65459	0.73028
H	-3.91788	1.76208	0.89673
C	-7.41444	1.56118	-0.77158
H	-6.66396	-0.19887	-1.7776
C	-7.13465	2.59002	0.1305
H	-5.64184	3.4576	1.43502
H	-8.39747	1.49993	-1.24502
H	-7.89446	3.33934	0.36479
C	2.67512	1.9421	3.87578
C	2.19459	2.56542	2.72474
C	3.1649	0.64392	3.78827
C	2.17298	1.95621	1.4596
C	3.28725	0.06797	2.52612
C	2.86401	0.70372	1.34458

O	0.97849	1.50418	-0.55949
O	1.04541	-1.04023	0.07378
C	3.58399	0.16246	0.11918
C	4.91406	0.64508	0.14749
P	0.06573	0.25607	0.03803
C	3.23929	-0.7975	-0.87078
C	5.88583	0.29107	-0.77681
C	4.25	-1.13448	-1.79548
C	5.53586	-0.60759	-1.77858
H	4.04329	-1.8685	-2.5584
H	6.25913	-0.92439	-2.53345
H	6.89357	0.70607	-0.70639
H	5.181	1.33731	0.94644
H	3.79979	-0.88829	2.42839
H	3.51013	0.10662	4.67443
H	2.64472	2.47165	4.83059
H	1.80985	3.57004	2.83151
H	0.12881	0.53881	1.42889
C	1.38968	2.60308	0.28653
C	2.23078	3.63463	-0.56201
C	0.05461	3.52678	0.6316
C	1.46022	3.94174	-1.87925
C	1.98955	4.92315	0.25054
C	0.47079	4.92528	0.07162
C	0.36991	4.95935	-1.46163
H	1.05205	3.02237	-2.31726
H	2.15567	4.3719	-2.61464
H	2.33237	4.85199	1.2917
H	2.48117	5.79455	-0.20933

H	-0.07902	5.7382	0.56864
H	-0.62771	4.72018	-1.85006
H	0.61495	5.97156	-1.81861
C	3.68706	3.30868	-0.8208
H	4.2432	3.16025	0.11279
H	3.80048	2.40951	-1.439
H	4.15351	4.14956	-1.35856
C	-0.3954	3.68165	2.09819
H	0.2072	4.39424	2.67417
H	-1.42084	4.08275	2.09656
H	-0.41544	2.72577	2.64009
C	-1.19855	3.01044	-0.09428
H	-1.02267	2.7047	-1.12866
H	-1.64489	2.15691	0.44074
H	-1.96591	3.79913	-0.09425
C	1.94962	-1.6453	-0.86478
C	1.25287	-2.02798	-2.29331
C	1.30847	-3.59032	-2.2787
H	1.2163	-3.9981	-3.29651
C	1.93729	-1.48508	-3.56589
H	1.22309	-1.55938	-4.39963
H	2.22264	-0.42834	-3.46309
H	2.82199	-2.0545	-3.87458
C	-0.19729	-1.55345	-2.41494
H	-0.24254	-0.46889	-2.59027
H	-0.66117	-2.04233	-3.28485
H	-0.82173	-1.8175	-1.55637
C	2.6203	-3.89083	-1.54464
H	2.74053	-4.9618	-1.31808

H	3.53251	-3.55929	-2.05178
C	2.25373	-3.09661	-0.27641
C	3.23763	-3.14399	0.87925
H	2.82067	-2.62799	1.75602
H	3.41566	-4.19196	1.16703
H	4.20799	-2.69024	0.63184
C	0.89679	-3.7598	0.08396
H	1.08734	-4.63272	0.72462
H	0.25533	-3.08445	0.65529
C	0.29058	-4.17543	-1.28086
H	0.27449	-5.27134	-1.38616
H	-0.74201	-3.83185	-1.41678

Optimized reductive elimination transition structure of the active catalyst system (MeCu • BIFOP-H • chalcone) of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)**TS-4.1 (S)**



Imaginary frequency: -399.72 cm⁻¹

Energy: -4068.823399

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -4070.161513

0 1

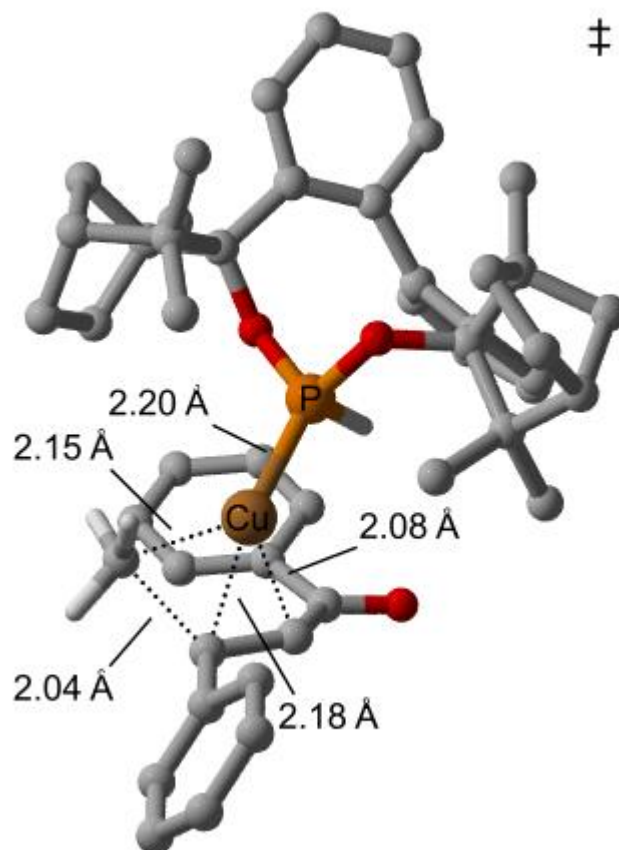
Cu	-2.0985	-0.41352	-0.74468
C	-3.45193	-0.76899	-2.34701
C	-3.32969	-1.06584	0.78953
H	-3.5852	-0.28603	1.50558
C	-4.12221	-1.17132	-0.44253
C	-2.38341	-2.08768	1.1212
O	-2.15087	-3.06201	0.36816
C	-1.55649	-1.93506	2.37686
C	-1.39689	-0.71208	3.05107
C	-0.83419	-3.04853	2.83105
C	-0.51739	-0.59912	4.12874
H	-1.93833	0.17173	2.71068
C	0.03621	-2.94206	3.91637
H	-0.9629	-3.98965	2.29544
C	0.20616	-1.71375	4.56276
H	-0.38105	0.36746	4.61887
H	0.59408	-3.81921	4.25427
H	0.90271	-1.62308	5.39991
H	-2.8275	-1.56569	-2.77507
H	-4.48456	-0.90564	-2.67479
H	-3.12877	0.227	-2.70284
H	-4.28049	-2.21121	-0.74359
C	-5.35589	-0.33027	-0.46394
C	-5.29024	1.06323	-0.30336

C	-6.61366	-0.92738	-0.62495
C	-6.45067	1.83686	-0.29487
H	-4.31556	1.54428	-0.19634
C	-7.77841	-0.15446	-0.61477
H	-6.67843	-2.01111	-0.75134
C	-7.70183	1.23018	-0.4491
H	-6.37956	2.92054	-0.1717
H	-8.75058	-0.63856	-0.73654
H	-8.61137	1.83548	-0.44378
C	2.1591	2.18497	3.64204
C	1.69689	2.70307	2.43255
C	2.77906	0.94132	3.65251
C	1.82019	2.03811	1.20211
C	3.04048	0.32267	2.4329
C	2.63456	0.85543	1.19671
O	0.80302	1.37678	-0.86049
O	1.0542	-1.11655	-0.05163
C	3.46305	0.32448	0.03778
C	4.74377	0.92127	0.10305
P	-0.01988	0.09388	-0.20505
C	3.24351	-0.69052	-0.93457
C	5.7747	0.63908	-0.78182
C	4.3036	-0.93618	-1.83164
C	5.53521	-0.29244	-1.78559
H	4.1839	-1.68616	-2.5978
H	6.30409	-0.54515	-2.51929
H	6.73964	1.14142	-0.68534
H	4.91845	1.65203	0.89327
H	3.64246	-0.58457	2.41849

H	3.11052	0.47966	4.58501
H	2.01127	2.751	4.56447
H	1.20674	3.66613	2.46363
H	-0.0143	0.47125	1.15793
C	1.05585	2.54867	-0.05101
C	1.85107	3.61855	-0.89415
C	-0.38155	3.35182	0.16172
C	1.14169	3.80059	-2.26773
C	1.44207	4.9095	-0.15548
C	-0.05605	4.76334	-0.42656
C	-0.05725	4.7326	-1.96349
H	0.84388	2.83049	-2.68499
H	1.84182	4.26025	-2.98048
H	1.72255	4.91125	0.90629
H	1.88068	5.8047	-0.62319
H	-0.70862	5.53903	0.00101
H	-1.00246	4.39309	-2.40464
H	0.12394	5.74886	-2.34624
C	3.34426	3.41913	-1.05088
H	3.85112	3.3571	-0.08026
H	3.5763	2.51156	-1.62196
H	3.76673	4.27855	-1.59572
C	-0.94868	3.5062	1.58723
H	-0.46501	4.29658	2.17347
H	-2.00801	3.79453	1.50334
H	-0.90534	2.57094	2.16287
C	-1.53101	2.69752	-0.62889
H	-1.25278	2.35298	-1.62905
H	-1.95089	1.84134	-0.07471

H	-2.35101	3.42464	-0.72909
C	2.04665	-1.66849	-0.92464
C	1.45297	-2.19655	-2.3501
C	1.77532	-3.73071	-2.29868
H	1.82899	-4.16022	-3.31047
C	2.04424	-1.55838	-3.62434
H	1.35359	-1.74501	-4.46075
H	2.15895	-0.46947	-3.52125
H	3.00924	-1.98011	-3.92972
C	-0.06133	-1.98949	-2.48375
H	-0.29784	-0.94509	-2.73136
H	-0.4232	-2.60566	-3.32179
H	-0.63124	-2.28147	-1.59522
C	3.05475	-3.81477	-1.45534
H	3.30595	-4.85111	-1.1803
H	3.94974	-3.36919	-1.89987
C	2.47597	-3.04605	-0.25321
C	3.34722	-2.92537	0.98406
H	2.78701	-2.43809	1.79521
H	3.63118	-3.93031	1.33395
H	4.27053	-2.35782	0.79838
C	1.18322	-3.86992	0.01887
H	1.41016	-4.65786	0.75252
H	0.38299	-3.25707	0.44157
C	0.79918	-4.46109	-1.35932
H	0.99834	-5.54309	-1.40365
H	-0.2618	-4.32061	-1.59431

Optimized reductive elimination transition structure of the active catalyst system (MeCu • BIFOP-H • chalcone) of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)**TS-8.4 (S)**



Imaginary frequency: -420.86 cm^{-1}

Energy: -4068.812788

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -4070.148164

0 1

Cu	-2.13825	-0.37671	-0.232
C	-3.37955	-1.86615	-1.15883
C	-3.5018	0.18885	1.22879
H	-3.83186	1.22602	1.13696
C	-4.20022	-0.77957	0.35872
C	-2.55826	0.02612	2.30802
O	-2.18713	1.00633	2.97838

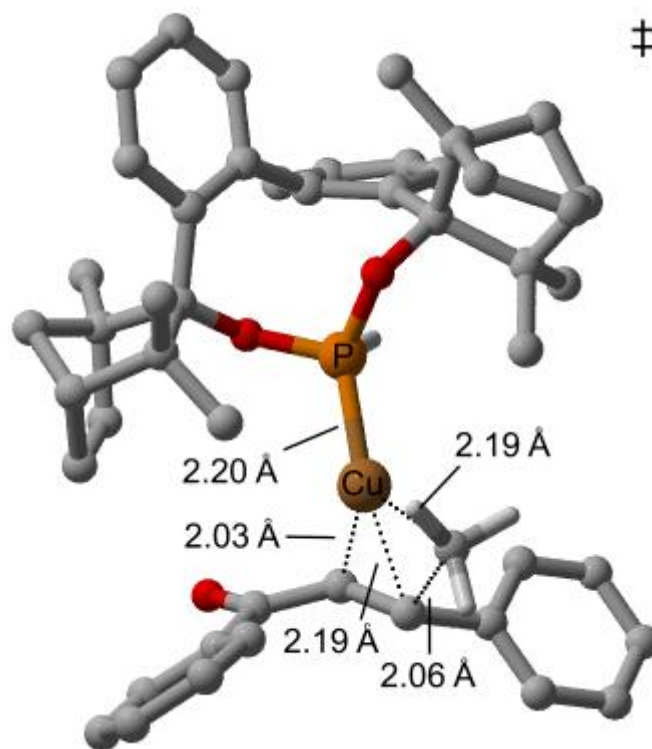
C	-1.83478	-1.29005	2.56931
C	-2.2581	-2.56895	2.16518
C	-0.60984	-1.19036	3.25675
C	-1.47555	-3.69868	2.42002
H	-3.21197	-2.70797	1.66422
C	0.18253	-2.31196	3.49026
H	-0.30484	-0.20005	3.59538
C	-0.24655	-3.57479	3.07083
H	-1.82835	-4.68181	2.09889
H	1.14095	-2.199	4.00224
H	0.37354	-4.45668	3.24848
H	-2.6469	-2.64263	-0.88875
H	-4.35693	-2.33293	-1.30281
H	-3.10718	-1.3805	-2.11223
H	-4.51349	-1.70889	0.83768
C	-5.32573	-0.16682	-0.41821
C	-5.11603	0.95202	-1.24051
C	-6.6178	-0.70151	-0.33264
C	-6.17108	1.5244	-1.95019
H	-4.11237	1.37651	-1.32524
C	-7.67819	-0.12845	-1.0409
H	-6.79679	-1.57244	0.30365
C	-7.45898	0.9866	-1.85221
H	-5.98769	2.39419	-2.58582
H	-8.68025	-0.55591	-0.95558
H	-8.28601	1.43453	-2.40804
C	2.03716	1.96613	3.74387
C	1.71056	2.54669	2.51745
C	2.57689	0.68591	3.76761

C	1.90121	1.9114	1.28216
C	2.91083	0.08761	2.55419
C	2.65347	0.68624	1.30881
O	0.83663	1.25229	-0.74871
O	1.07155	-1.2075	-0.05017
C	3.54164	0.1066	0.22207
C	4.85603	0.5987	0.42149
P	0.01425	0.02257	-0.00994
C	3.34244	-0.89512	-0.76182
C	5.95243	0.19884	-0.32501
C	4.484	-1.29111	-1.49382
C	5.75504	-0.76473	-1.31027
H	4.39148	-2.07267	-2.23304
H	6.58442	-1.12818	-1.92129
H	6.93981	0.62268	-0.12959
H	5.00063	1.33604	1.21201
H	3.44741	-0.86295	2.5548
H	2.78825	0.17745	4.71099
H	1.83085	2.50904	4.66843
H	1.25501	3.52581	2.53927
H	0.15637	0.3729	1.34765
C	1.20129	2.4446	-0.00285
C	2.11319	3.37833	-0.88631
C	-0.15738	3.38788	0.12037
C	1.45354	3.56045	-2.2845
C	1.81793	4.73495	-0.21271
C	0.32159	4.72885	-0.52563
C	0.35532	4.62789	-2.05808
H	1.06102	2.60668	-2.66005

H	2.21219	3.90324	-3.00333
H	2.06154	4.74468	0.8593
H	2.36296	5.56107	-0.69568
H	-0.25852	5.58486	-0.1517
H	-0.61044	4.36974	-2.50978
H	0.6555	5.59919	-2.48137
C	3.58524	3.039	-1.00159
H	4.06954	2.98395	-0.01968
H	3.74899	2.0872	-1.52259
H	4.08961	3.83011	-1.57925
C	-0.76545	3.68217	1.50587
H	-0.20304	4.42994	2.08002
H	-1.7615	4.12141	1.34017
H	-0.9244	2.78323	2.11809
C	-1.32673	2.78444	-0.68199
H	-1.04618	2.39046	-1.66387
H	-1.81275	1.97936	-0.10964
H	-2.09284	3.56128	-0.82575
C	2.0377	-1.69051	-0.98661
C	1.50243	-1.8021	-2.52399
C	1.4014	-3.34913	-2.7192
H	1.36353	-3.61359	-3.78658
C	2.43656	-1.20288	-3.59463
H	1.89125	-1.16821	-4.54997
H	2.73655	-0.17663	-3.34069
H	3.3442	-1.78821	-3.77645
C	0.15032	-1.12709	-2.77683
H	0.23945	-0.03213	-2.74217
H	-0.1979	-1.39927	-3.78547

H	-0.62747	-1.43164	-2.0743
C	2.60419	-3.88819	-1.93375
H	2.59471	-4.98651	-1.85097
H	3.5822	-3.60564	-2.33399
C	2.20512	-3.22785	-0.59794
C	3.07494	-3.47065	0.62424
H	2.65134	-2.94722	1.49527
H	3.10686	-4.54596	0.86053
H	4.10699	-3.12143	0.4809
C	0.77843	-3.82807	-0.44022
H	0.87107	-4.81833	0.03049
H	0.14689	-3.22166	0.21339
C	0.24578	-3.94417	-1.89254
H	0.09251	-4.99564	-2.17964
H	-0.71382	-3.43473	-2.04569

Optimized reductive elimination transition structure of the active catalyst system (MeCu • BIFOP-H • chalcone) of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)**TS-8 (S)**



Imaginary frequency: -405.75 cm^{-1}

Energy: -4068.810051

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -4070.152390

0 1

Cu	-1.78352	0.59823	-0.21084
C	-2.87854	1.73685	-1.72867
C	-3.33424	0.42611	1.09561
H	-2.96735	0.86343	2.02785
C	-3.82577	1.35343	0.06516
C	-3.68936	-0.967	1.26527
O	-3.43066	-1.57128	2.31338
C	-4.396	-1.7508	0.17197
C	-4.31213	-1.48115	-1.20278
C	-5.12631	-2.87888	0.58421
C	-4.9404	-2.31061	-2.13708

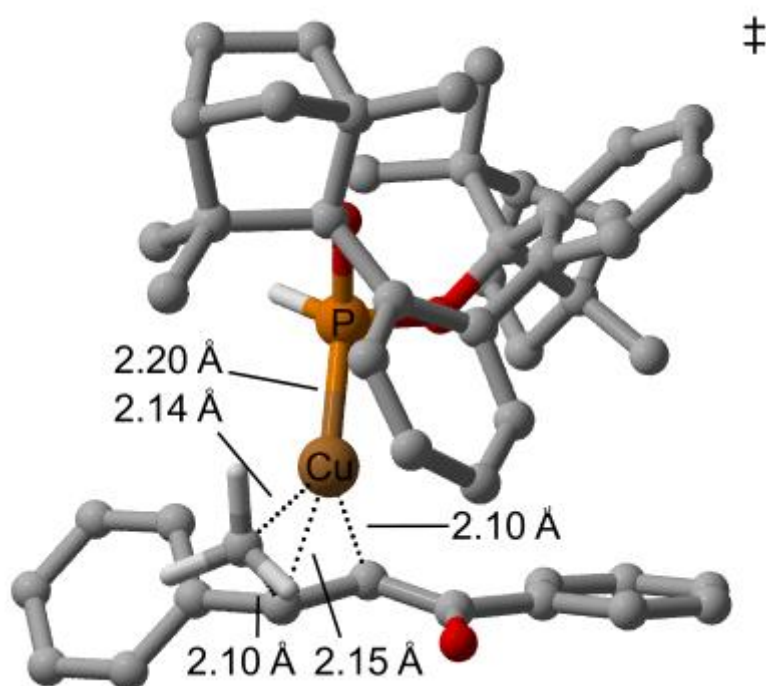
H	-3.7235	-0.64265	-1.56748
C	-5.76811	-3.6978	-0.34232
H	-5.15167	-3.09727	1.65275
C	-5.67638	-3.4176	-1.71072
H	-4.84848	-2.08972	-3.20364
H	-6.33653	-4.56636	0.00016
H	-6.1714	-4.06338	-2.44032
H	-2.30793	1.02623	-2.35867
H	-3.85395	1.87338	-2.20497
H	-2.35807	2.70026	-1.68447
H	-4.70338	0.98945	-0.47026
C	-3.96247	2.7847	0.47358
C	-2.94969	3.44151	1.19372
C	-5.11074	3.50967	0.12786
C	-3.08345	4.78014	1.55807
H	-2.04503	2.89473	1.46954
C	-5.25065	4.85102	0.49619
H	-5.90722	3.01391	-0.43336
C	-4.2371	5.49238	1.2109
H	-2.28333	5.27165	2.11724
H	-6.15735	5.39609	0.22236
H	-4.34353	6.54128	1.49739
C	3.84483	2.02488	3.19132
C	3.54574	2.31119	1.85947
C	3.72841	0.71615	3.64599
C	3.131	1.34472	0.92913
C	3.45983	-0.28452	2.71508
C	3.22148	-0.02381	1.35358
O	1.59449	0.73767	-0.79908

O	0.72796	-1.15675	0.7521
C	3.51421	-1.23313	0.48226
C	4.91848	-1.40343	0.42901
P	0.35318	0.33317	0.22417
C	2.69308	-2.22685	-0.11358
C	5.54567	-2.44446	-0.23879
C	3.36287	-3.26527	-0.79506
C	4.74487	-3.38271	-0.88124
H	2.78683	-4.04583	-1.2669
H	5.18225	-4.22099	-1.42833
H	6.6353	-2.51678	-0.25233
H	5.53479	-0.66274	0.93975
H	3.50334	-1.32769	3.02835
H	3.90587	0.46128	4.69314
H	4.14435	2.83182	3.86371
H	3.62945	3.34217	1.54513
H	0.73699	1.04149	1.39346
C	2.54626	1.76949	-0.44617
C	3.62561	1.91133	-1.58812
C	1.78717	3.23792	-0.57596
C	2.89513	2.01222	-2.95913
C	4.07086	3.37047	-1.35933
C	2.69221	3.98338	-1.61017
C	2.42188	3.48467	-3.03842
H	2.07304	1.2878	-3.01799
H	3.60147	1.76882	-3.76618
H	4.47948	3.54717	-0.35506
H	4.82694	3.68814	-2.09414
H	2.61522	5.07531	-1.50133

H	1.37954	3.59591	-3.36145
H	3.03734	4.06077	-3.74659
C	4.7524	0.89971	-1.62219
H	5.31257	0.88159	-0.67975
H	4.38566	-0.11399	-1.82685
H	5.45591	1.17284	-2.42491
C	1.61992	4.11601	0.68083
H	2.52976	4.65682	0.96854
H	0.86473	4.88551	0.45762
H	1.26334	3.54842	1.55186
C	0.3565	3.08903	-1.12065
H	0.25613	2.36867	-1.93709
H	-0.34481	2.79394	-0.32685
H	0.01024	4.06979	-1.47989
C	1.17193	-2.36193	0.11525
C	0.24644	-2.84359	-1.14112
C	-0.34734	-4.1945	-0.61618
H	-0.67513	-4.83354	-1.44986
C	0.96953	-3.06051	-2.48692
H	0.21436	-3.08352	-3.28728
H	1.6722	-2.24509	-2.71103
H	1.51058	-4.01131	-2.55421
C	-0.88862	-1.87087	-1.47693
H	-0.51322	-0.98677	-2.01327
H	-1.60785	-2.37456	-2.13915
H	-1.45287	-1.55584	-0.59055
C	0.76386	-4.75982	0.27735
H	0.42911	-5.63565	0.85468
H	1.68912	-5.04201	-0.23401

C	0.86751	-3.51175	1.1745
C	1.83051	-3.57321	2.34705
H	1.76984	-2.64818	2.93904
H	1.55772	-4.40985	3.00896
H	2.8733	-3.71667	2.02889
C	-0.6168	-3.37136	1.62635
H	-0.76593	-3.96549	2.53959
H	-0.89204	-2.3418	1.87603
C	-1.43594	-3.94537	0.44233
H	-1.90706	-4.90304	0.71045
H	-2.24778	-3.28758	0.11911

Optimized reductive elimination transition structure of the active catalyst system (MeCu • BIFOP-H • chalcone) of the reaction pathway (B3LYP-D3(BJ)/def2-SVP) **TS-2.1 (R)**



Imaginary frequency: -390.64 cm^{-1}

Energy: -4068.829003

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -4070.164430

0 1

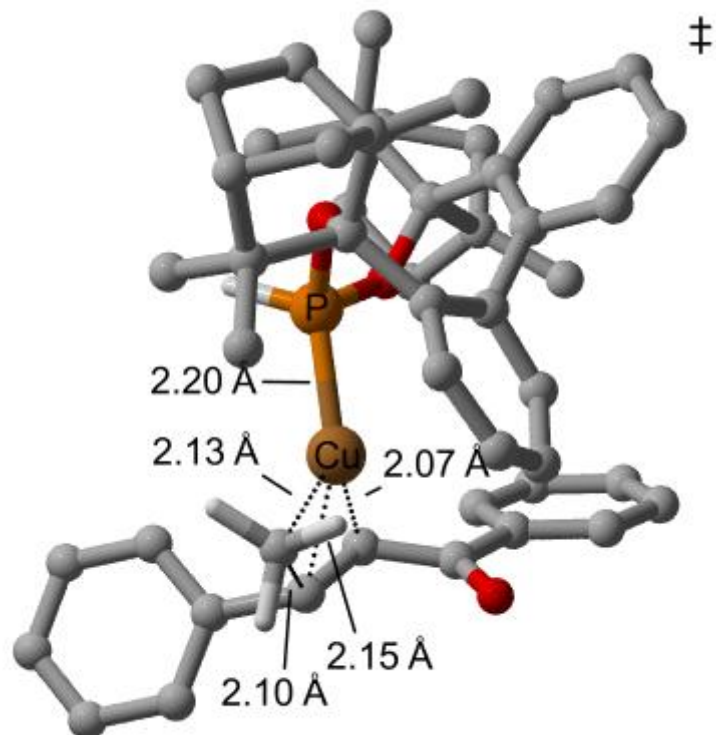
Cu	1.70066	0.8773	-0.41554
C	2.72664	2.42134	-1.47668
H	1.70327	2.82308	-1.39497
H	3.42781	3.19881	-1.16067
H	2.90438	2.08196	-2.5013
C	3.33889	-0.42485	-0.30997
H	3.34475	-0.86153	0.687
C	3.84412	0.93404	-0.49899
C	3.17173	-1.23748	-1.47997
O	3.24232	-0.76176	-2.63011
H	4.46837	1.02639	-1.38937
C	2.87926	-2.70945	-1.3236
C	2.42701	-3.4095	-2.45359
C	3.07594	-3.42017	-0.12955
C	2.1661	-4.77826	-2.39218
H	2.30496	-2.84739	-3.3807
C	2.83146	-4.79357	-0.06933
H	3.44261	-2.9049	0.75886
C	2.37216	-5.47728	-1.19854
H	1.80846	-5.30607	-3.27998
H	3.00228	-5.33369	0.86532
H	2.1774	-6.55151	-1.14882
C	4.38069	1.64833	0.69432
C	3.71236	1.63589	1.93129
C	5.58545	2.36133	0.59903
C	4.23129	2.31268	3.03457
H	2.7698	1.09189	2.02643

C	6.11069	3.03672	1.70346
H	6.11724	2.3809	-0.35566
C	5.43511	3.01685	2.926
H	3.69323	2.2915	3.98562
H	7.05322	3.58142	1.60747
H	5.84276	3.547	3.78995
C	0.1984	1.61835	-3.63979
C	-0.69954	2.19963	-2.73897
C	0.57057	0.28857	-3.47798
C	-1.27768	1.49046	-1.67977
C	-0.13053	-0.48427	-2.54851
C	-1.1155	0.05773	-1.70773
O	-1.61334	1.31853	0.65504
O	-0.39772	-0.90454	0.96047
C	-2.17809	-0.93558	-1.27193
C	-2.96555	-1.23294	-2.41197
P	-0.09305	0.68405	0.84561
C	-2.49717	-1.57878	-0.04644
C	-4.09091	-2.04237	-2.38229
C	-3.67603	-2.35503	-0.04206
C	-4.47232	-2.5815	-1.15813
H	-3.98	-2.84728	0.86882
H	-5.36646	-3.20225	-1.06624
H	-4.66415	-2.22715	-3.2932
H	-2.68138	-0.76383	-3.35498
H	0.04059	-1.56158	-2.51063
H	1.36289	-0.16337	-4.07291
H	0.64721	2.23272	-4.4229
H	-0.91506	3.25373	-2.85266

H	0.09006	1.05439	2.20129
C	-1.92504	2.19022	-0.45902
C	-3.49953	2.3764	-0.52603
C	-1.43988	3.71014	-0.02413
C	-4.03661	2.51789	0.92196
C	-3.60483	3.83134	-1.02116
C	-2.80732	4.43851	0.13336
C	-3.59925	3.9399	1.35425
H	-3.65131	1.72544	1.57258
H	-5.13302	2.42513	0.90071
H	-3.15674	3.985	-2.01408
H	-4.65203	4.16953	-1.06156
H	-2.68072	5.53087	0.1147
H	-3.01383	3.95233	2.28286
H	-4.47074	4.59175	1.52014
C	-4.3059	1.38358	-1.34147
H	-3.8995	1.25464	-2.35295
H	-4.35682	0.40037	-0.86042
H	-5.33725	1.75937	-1.43825
C	-0.60234	4.55995	-0.99965
H	0.34445	4.08757	-1.28375
H	-1.14276	4.84283	-1.91169
H	-0.35042	5.49968	-0.48468
C	-0.62796	3.70051	1.28055
H	0.3851	3.30104	1.10801
H	-0.50266	4.73605	1.63254
H	-1.09499	3.12758	2.08714
C	-1.55854	-1.71507	1.17184
C	-0.97463	-3.20387	1.22204

C	-2.18189	-1.55583	2.66348
C	0.27403	-3.19468	2.14824
C	-1.97182	-3.92391	2.15218
C	-1.82263	-2.93257	3.31339
C	-0.30944	-3.05211	3.57907
H	0.97951	-2.40428	1.87457
H	0.79879	-4.15215	2.02322
H	-2.98693	-4.03265	1.7593
H	-1.6141	-4.93322	2.41006
H	-2.44323	-3.12767	4.20103
H	0.10911	-2.2066	4.13926
H	-0.1146	-3.95387	4.17967
C	-0.68754	-3.81989	-0.13639
H	-1.59071	-3.91701	-0.7538
H	0.04617	-3.21409	-0.68761
H	-0.24865	-4.82	-0.01111
C	-1.56933	-0.3975	3.46087
H	-0.47607	-0.39373	3.45026
H	-1.92907	0.57152	3.08802
H	-1.88655	-0.48713	4.51164
C	-3.70479	-1.32515	2.74239
H	-4.30029	-2.23036	2.57517
H	-3.95413	-0.97665	3.75624
H	-4.03959	-0.55712	2.03161

Optimized reductive elimination transition structure of the active catalyst system (MeCu • BIFOP-H • chalcone) of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)**TS-1.3 (R)**



Imaginary frequency: -361.41 cm^{-1}

Energy: -4068.830081

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -4070.166708

0 1

Cu	-1.67921	-0.89025	-0.36087
C	-2.71354	-2.61683	-1.06044
H	-2.3781	-3.27707	-0.2486
H	-3.6603	-3.00056	-1.44708
H	-1.99052	-2.5833	-1.89192
C	-3.27598	0.43382	-0.35033
H	-3.33206	0.88378	0.63947
C	-3.82286	-0.90814	-0.55328
C	-3.05054	1.23896	-1.51926
O	-3.08042	0.7618	-2.66884

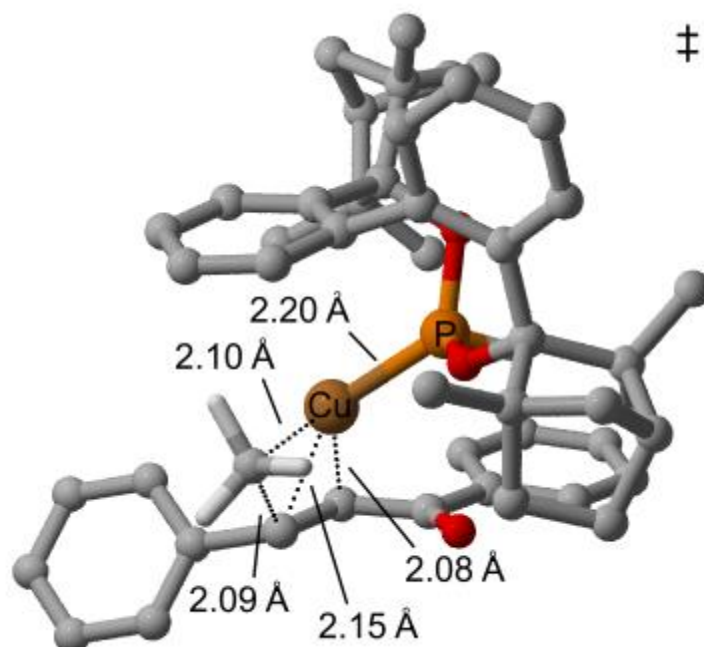
H	-4.30702	-0.99098	-1.52797
C	-2.76606	2.71279	-1.35977
C	-2.30683	3.41204	-2.48762
C	-2.97689	3.42577	-0.16967
C	-2.05525	4.78246	-2.42865
H	-2.1721	2.84683	-3.41102
C	-2.74016	4.80073	-0.11154
H	-3.34732	2.91193	0.71782
C	-2.27562	5.48376	-1.23891
H	-1.69297	5.30958	-3.31495
H	-2.9216	5.34248	0.82011
H	-2.08763	6.55927	-1.19069
C	-4.58296	-1.50636	0.58013
C	-5.88341	-1.98997	0.38079
C	-4.02835	-1.59045	1.86884
C	-6.61626	-2.53208	1.4406
H	-6.32646	-1.93261	-0.61677
C	-4.75593	-2.13163	2.92758
H	-3.00759	-1.23498	2.03463
C	-6.05631	-2.60449	2.71785
H	-7.63056	-2.89943	1.26574
H	-4.30627	-2.18962	3.92206
H	-6.62717	-3.03014	3.54649
C	-0.13658	-1.72811	-3.6126
C	0.73287	-2.29565	-2.67536
C	-0.49307	-0.38883	-3.49646
C	1.29755	-1.56401	-1.62433
C	0.19903	0.39993	-2.5743
C	1.15892	-0.13097	-1.69835

O	1.63139	-1.31844	0.70502
O	0.44665	0.92633	0.94211
C	2.23645	0.85592	-1.28264
C	3.03791	1.10095	-2.42571
P	0.11931	-0.66026	0.87838
C	2.56312	1.52858	-0.07501
C	4.18056	1.88617	-2.41365
C	3.75822	2.27951	-0.08747
C	4.56593	2.4549	-1.2044
H	4.06863	2.79139	0.81016
H	5.4728	3.05872	-1.12531
H	4.76326	2.02964	-3.32601
H	2.74989	0.60917	-3.35586
H	0.04362	1.48021	-2.57132
H	-1.26246	0.05851	-4.12354
H	-0.57313	-2.35685	-4.39155
H	0.93805	-3.35517	-2.75542
H	-0.06948	-0.98375	2.24457
C	1.91894	-2.237	-0.37612
C	3.48274	-2.4772	-0.44137
C	1.38861	-3.72713	0.1003
C	4.01471	-2.64408	1.00747
C	3.52731	-3.93187	-0.9485
C	2.72573	-4.51834	0.21389
C	3.56518	-4.06811	1.42052
H	3.63001	-1.85711	1.66604
H	5.11151	-2.55651	0.99537
H	3.05783	-4.06037	-1.93508
H	4.55977	-4.31014	-1.00822

H	2.55083	-5.60388	0.18516
H	3.01322	-4.09507	2.36901
H	4.42985	-4.73946	1.53767
C	4.32223	-1.5077	-1.25106
H	3.9331	-1.37782	-2.26897
H	4.38574	-0.52174	-0.77624
H	5.3468	-1.90547	-1.33031
C	0.4618	-4.53285	-0.82836
H	-0.43571	-3.97921	-1.1217
H	0.96391	-4.9013	-1.7321
H	0.12971	-5.42498	-0.27522
C	0.63981	-3.66003	1.44104
H	-0.36636	-3.23184	1.30299
H	0.49794	-4.68246	1.82351
H	1.15966	-3.0815	2.2107
C	1.62507	1.71705	1.13711
C	1.07387	3.21818	1.14945
C	2.245	1.58309	2.63307
C	-0.17092	3.26086	2.0805
C	2.08986	3.9422	2.05585
C	1.92393	2.98696	3.24463
C	0.41554	3.15112	3.51303
H	-0.8919	2.4756	1.83388
H	-0.6787	4.22332	1.92791
H	3.10527	4.01977	1.65692
H	1.75397	4.96536	2.28719
H	2.55371	3.19157	4.12364
H	-0.02072	2.33511	4.10258
H	0.24561	4.07674	4.0842

C	0.79464	3.80119	-0.22491
H	1.69857	3.86552	-0.84557
H	0.05075	3.19149	-0.75765
H	0.37231	4.81153	-0.1276
C	1.60205	0.46658	3.46555
H	0.50907	0.48926	3.45222
H	1.93921	-0.52236	3.12558
H	1.91943	0.58265	4.51369
C	3.76064	1.31029	2.71688
H	4.38268	2.19185	2.52268
H	4.00178	0.9839	3.74004
H	4.07005	0.51213	2.02794

Optimized reductive elimination transition structure of the active catalyst system (MeCu • BIFOP-H • chalcone) of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)**TS-1.2 (R)**



Imaginary frequency: -365.02 cm^{-1}

Energy: -4068.831997

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -4070.168599

0 1

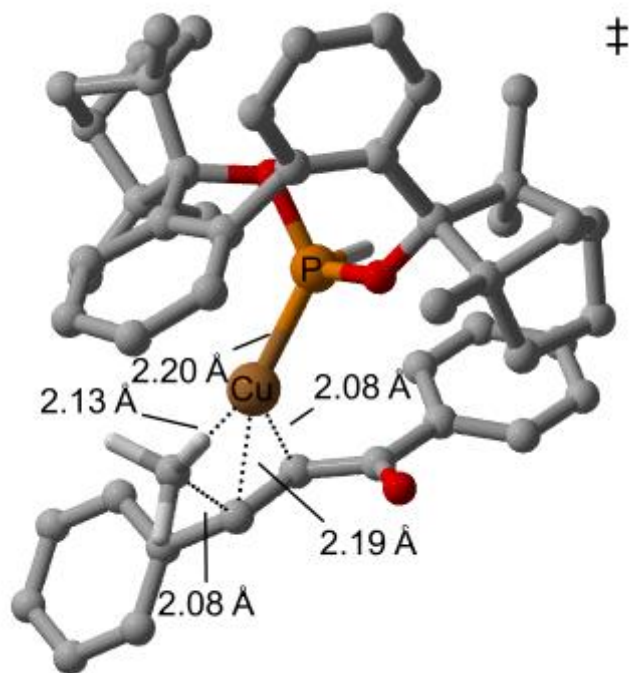
Cu	-1.66164	0.02651	-0.46859
C	-1.8765	0.16011	-2.55132
H	-1.64284	-0.91835	-2.55569
H	-2.55536	0.36068	-3.38251
H	-0.96267	0.763	-2.65004
C	-3.31687	1.13937	0.12348
H	-4.06383	0.60631	0.70891
C	-3.35889	1.0078	-1.34272
C	-2.46509	2.12098	0.71663
O	-1.63767	2.78443	0.04011
H	-3.15663	1.95601	-1.8486
C	-2.47981	2.31258	2.21341
C	-1.68223	3.33814	2.74649
C	-3.20222	1.4976	3.10126
C	-1.60184	3.54189	4.12448
H	-1.1302	3.96456	2.04518
C	-3.12152	1.69746	4.48018
H	-3.8223	0.68624	2.71869
C	-2.31933	2.71945	4.99821
H	-0.97622	4.34611	4.52035
H	-3.68607	1.04961	5.15563
H	-2.2554	2.87339	6.07829
C	-4.5295	0.25763	-1.88211
C	-5.37783	0.85336	-2.826
C	-4.81613	-1.04979	-1.45578
C	-6.48922	0.16712	-3.32371

H	-5.16569	1.86978	-3.16748
C	-5.92344	-1.7374	-1.95149
H	-4.15436	-1.53431	-0.73364
C	-6.76703	-1.13049	-2.8883
H	-7.14132	0.65068	-4.05535
H	-6.1281	-2.75498	-1.60912
H	-7.63392	-1.66893	-3.27857
C	-0.38447	-3.44087	-2.45327
C	-0.16428	-3.32062	-1.08217
C	0.31498	-2.61495	-3.32536
C	0.73294	-2.40117	-0.51474
C	1.28728	-1.76698	-2.80186
C	1.55905	-1.65546	-1.42527
O	1.24617	-0.85484	1.20821
O	1.18568	1.05572	-0.62055
C	2.9472	-1.07453	-1.16072
C	3.90608	-2.04704	-1.52578
P	0.29368	0.31324	0.50779
C	3.42144	0.21874	-0.78358
C	5.2791	-1.85107	-1.45544
C	4.81895	0.37661	-0.70362
C	5.74099	-0.61913	-1.00941
H	5.22331	1.33495	-0.41601
H	6.80996	-0.41163	-0.92236
H	5.9657	-2.65036	-1.74264
H	3.53709	-3.01192	-1.87323
H	1.91735	-1.20403	-3.48841
H	0.1449	-2.65546	-4.40328
H	-1.11014	-4.16806	-2.82386

H	-0.72726	-3.97558	-0.43152
H	0.30525	1.18955	1.60222
C	0.80311	-2.21204	1.02292
C	1.78923	-3.21922	1.73346
C	-0.55833	-2.44053	1.9416
C	2.04128	-2.72288	3.18707
C	0.8414	-4.41365	1.96731
C	-0.14516	-3.64608	2.84728
C	0.79224	-3.1878	3.97607
H	2.18766	-1.63539	3.2065
H	2.96197	-3.18242	3.5754
H	0.4164	-4.82112	1.04038
H	1.34555	-5.23637	2.49783
H	-1.02342	-4.20596	3.20181
H	0.36674	-2.41248	4.62442
H	1.02975	-4.04786	4.62121
C	3.08043	-3.5679	1.02239
H	2.89815	-3.96296	0.01504
H	3.74772	-2.70147	0.94161
H	3.60698	-4.34668	1.59705
C	-1.88086	-2.76937	1.22402
H	-2.0534	-2.12064	0.34958
H	-1.9646	-3.81283	0.89653
H	-2.71076	-2.594	1.92512
C	-0.8806	-1.20619	2.80784
H	-1.4086	-0.4365	2.22885
H	-1.57236	-1.50759	3.60865
H	-0.00575	-0.74339	3.27369
C	2.54278	1.48782	-0.70626

C	2.63669	2.2857	-2.08332
C	2.90045	2.67731	0.35985
C	1.47621	3.32561	-2.11279
C	3.84638	3.20248	-1.83065
C	3.25019	3.87506	-0.59008
C	1.97272	4.47744	-1.2031
H	0.52893	2.89383	-1.76843
H	1.32858	3.66388	-3.1494
H	4.79184	2.67292	-1.67252
H	3.99671	3.9079	-2.66303
H	3.88845	4.61227	-0.0799
H	1.22413	4.79508	-0.46858
H	2.24069	5.36711	-1.794
C	2.67195	1.43639	-3.34087
H	3.49963	0.71291	-3.34109
H	1.72601	0.88959	-3.46055
H	2.79106	2.08838	-4.22049
C	1.72013	3.07959	1.26434
H	0.7483	3.10594	0.75938
H	1.64614	2.42283	2.14166
H	1.92254	4.09003	1.65325
C	4.06782	2.40908	1.33081
H	5.06059	2.55518	0.88725
H	3.99987	3.12582	2.16342
H	4.02293	1.3958	1.75623

Optimized reductive elimination transition structure of the active catalyst system (MeCu • BIFOP-H • chalcone) of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)**TS-1 (R)**



Imaginary frequency: -377.22 cm^{-1}

Energy: -4068.831603

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -4070.170920

0 1

Cu	1.71091	0.27022	0.49538
C	2.73361	-0.4421	2.21911
H	3.02766	-1.42704	1.83309
H	3.39897	-0.17165	3.04133
H	1.70417	-0.46948	2.61562
C	3.01649	1.81944	0.02076
H	3.50546	1.72495	-0.94786
C	3.59092	1.14369	1.18885
C	1.9805	2.783	0.23671
O	1.47613	2.98886	1.36416
H	3.49887	1.76023	2.08659

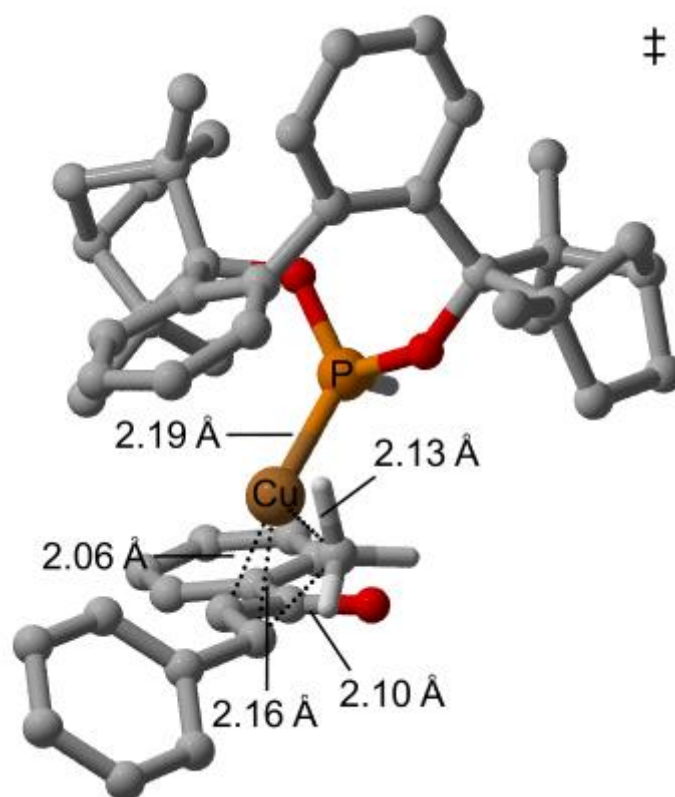
C	1.42936	3.54285	-0.94373
C	0.73222	4.73382	-0.68956
C	1.5187	3.0822	-2.26734
C	0.15175	5.45655	-1.73206
H	0.65097	5.06076	0.34821
C	0.92424	3.79573	-3.31033
H	2.03491	2.14484	-2.48158
C	0.24062	4.98681	-3.04661
H	-0.38312	6.38566	-1.51913
H	0.98946	3.41763	-4.33377
H	-0.22465	5.54458	-3.8631
C	4.93035	0.51575	1.00914
C	5.21174	-0.30753	-0.09379
C	5.94609	0.74061	1.94928
C	6.47153	-0.88351	-0.25427
H	4.4287	-0.50451	-0.82842
C	7.21078	0.16787	1.78982
H	5.7413	1.37935	2.81245
C	7.47865	-0.64737	0.68777
H	6.66975	-1.52247	-1.11863
H	7.99058	0.36112	2.53068
H	8.46611	-1.09801	0.56276
C	0.86982	-3.38321	2.61264
C	0.66453	-3.37206	1.23403
C	0.08407	-2.57118	3.42227
C	-0.31152	-2.58598	0.60207
C	-0.96822	-1.87042	2.8382
C	-1.23746	-1.89579	1.45716
O	-0.96499	-1.18299	-1.19582

O	-1.30278	0.82	0.49069
C	-2.69389	-1.56411	1.1481
C	-3.48212	-2.65741	1.57865
P	-0.23799	0.14743	-0.52078
C	-3.36739	-0.40369	0.66612
C	-4.86575	-2.70479	1.48142
C	-4.77004	-0.49611	0.55835
C	-5.51766	-1.60697	0.93332
H	-5.3253	0.35175	0.18962
H	-6.60385	-1.59101	0.81814
H	-5.41384	-3.58512	1.82394
H	-2.9612	-3.51771	1.99931
H	-1.66719	-1.33465	3.47949
H	0.24877	-2.51811	4.50051
H	1.66031	-4.00582	3.03673
H	1.30685	-4.00024	0.63165
H	-0.32366	0.94142	-1.67659
C	-0.3611	-2.4652	-0.94222
C	-1.1986	-3.60384	-1.64632
C	1.04563	-2.55126	-1.81452
C	-1.48524	-3.17083	-3.11337
C	-0.10446	-4.67282	-1.84285
C	0.79585	-3.80068	-2.71821
C	-0.16713	-3.47041	-3.86959
H	-1.78235	-2.11548	-3.15754
H	-2.32354	-3.76239	-3.50962
H	0.35156	-5.00807	-0.90148
H	-0.49069	-5.56076	-2.3671
H	1.74195	-4.25365	-3.04991

H	0.17012	-2.64677	-4.51098
H	-0.27443	-4.35388	-4.51778
C	-2.44876	-4.09633	-0.94678
H	-2.23823	-4.43724	0.07465
H	-3.22237	-3.32036	-0.90145
H	-2.86075	-4.95061	-1.50757
C	2.371	-2.7374	-1.05579
H	2.46397	-2.04901	-0.20507
H	2.53705	-3.75907	-0.69398
H	3.1988	-2.51935	-1.74771
C	1.26395	-1.29336	-2.67982
H	1.67345	-0.46374	-2.08084
H	2.01995	-1.52121	-3.44651
H	0.36193	-0.93843	-3.18723
C	-2.72532	0.99226	0.49627
C	-3.01939	1.87631	1.78929
C	-3.25837	1.98626	-0.68663
C	-2.07855	3.11812	1.75447
C	-4.36506	2.52944	1.42494
C	-3.85394	3.18141	0.13495
C	-2.72977	4.0614	0.71011
H	-1.03886	2.85837	1.52146
H	-2.07184	3.57581	2.75502
H	-5.1983	1.8296	1.3055
H	-4.66476	3.27242	2.18061
H	-4.59549	3.73823	-0.45775
H	-2.02173	4.42998	-0.03986
H	-3.17394	4.94637	1.19201
C	-2.94231	1.13835	3.11383

H	-3.6324	0.28398	3.16419
H	-1.91865	0.77655	3.2876
H	-3.19381	1.82747	3.93507
C	-2.14412	2.50396	-1.61095
H	-1.22248	2.78146	-1.09357
H	-1.90534	1.77508	-2.39711
H	-2.51021	3.40708	-2.12176
C	-4.32245	1.41691	-1.64805
H	-5.34185	1.42452	-1.24336
H	-4.3503	2.04968	-2.54824
H	-4.08235	0.39186	-1.96608

Optimized reductive elimination transition structure of the active catalyst system (MeCu • BIFOP-H • chalcone) of the reaction pathway (B3LYP-D3(BJ)/def2-SVP) **TS-1.1 (R)**



Imaginary frequency: -376.75 cm^{-1}

Energy: -4068.832571

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -4070.170295

0 1

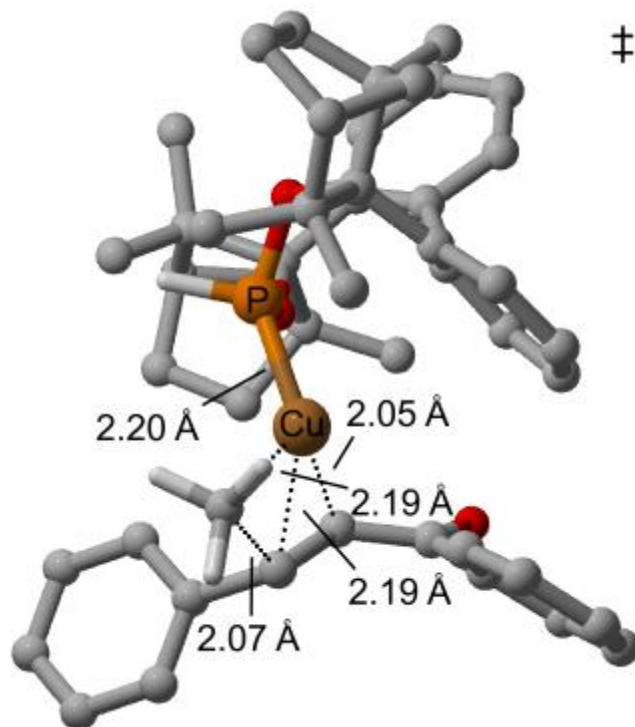
Cu	1.47115	-0.71389	0.48655
C	1.28005	-2.78985	0.92122
H	0.53878	-2.73653	0.10677
H	1.80102	-3.74657	0.84046
H	0.79691	-2.69073	1.90153
C	3.44934	-0.46545	1.02198
H	4.09666	-0.06423	0.24515
C	3.17989	-1.9101	1.0378
C	3.04257	0.32669	2.14536
O	2.30594	-0.13417	3.0475
H	3.21093	-2.33205	2.04588
C	3.41909	1.78758	2.18974
C	2.74896	2.59972	3.11789
C	4.3549	2.38226	1.32863
C	2.98282	3.97394	3.16645
H	2.03666	2.11324	3.78653
C	4.59502	3.75678	1.37821
H	4.90527	1.77049	0.61283
C	3.90391	4.55949	2.29171
H	2.44567	4.59394	3.889
H	5.3274	4.20454	0.70156
H	4.08919	5.63602	2.32641
C	3.89755	-2.71682	0.0108
C	4.56838	-3.89387	0.37415
C	3.92109	-2.32442	-1.33744

C	5.24963	-4.65467	-0.57987
H	4.55878	-4.21196	1.41992
C	4.59757	-3.08284	-2.29213
H	3.38798	-1.42192	-1.63973
C	5.26679	-4.25301	-1.91773
H	5.7706	-5.56571	-0.27499
H	4.60204	-2.76086	-3.33693
H	5.79721	-4.84784	-2.66512
C	1.10621	-1.61752	-3.23974
C	0.78829	-0.29081	-2.94597
C	0.32512	-2.63896	-2.7132
C	-0.29856	0.08453	-2.1417
C	-0.83194	-2.2959	-2.01763
C	-1.20554	-0.96447	-1.75723
O	-1.11336	1.41972	-0.36342
O	-1.53633	-0.66985	1.11209
C	-2.69667	-0.81588	-1.49434
C	-3.37938	-1.08511	-2.7045
P	-0.38998	0.41937	0.73993
C	-3.47484	-0.553	-0.33062
C	-4.75684	-1.00601	-2.852
C	-4.86596	-0.43314	-0.52754
C	-5.50886	-0.63293	-1.74454
H	-5.49947	-0.20479	0.31499
H	-6.59407	-0.52432	-1.80602
H	-5.22255	-1.21442	-3.8175
H	-2.77599	-1.33985	-3.57636
H	-1.51832	-3.08363	-1.70573
H	0.58194	-3.6874	-2.87642

H	1.97814	-1.84126	-3.85691
H	1.42872	0.4781	-3.35551
H	-0.40232	1.30238	1.83504
C	-0.47273	1.5479	-1.65349
C	-1.35087	2.44512	-2.61047
C	0.85168	2.52481	-1.4651
C	-1.76829	3.73084	-1.83891
C	-0.25608	2.98277	-3.55488
C	0.54622	3.68739	-2.46136
C	-0.51661	4.6406	-1.89522
H	-2.08298	3.48735	-0.81617
H	-2.62967	4.19285	-2.3434
H	0.28861	2.18704	-4.08313
H	-0.66837	3.67165	-4.30857
H	1.4678	4.195	-2.78165
H	-0.24652	5.07907	-0.92671
H	-0.66688	5.47768	-2.59471
C	-2.53038	1.80568	-3.31427
H	-2.23648	0.91458	-3.88264
H	-3.32381	1.52557	-2.61098
H	-2.95539	2.53131	-4.02629
C	2.24961	1.96226	-1.77951
H	2.42341	0.99244	-1.29421
H	2.46115	1.8764	-2.8531
H	2.99344	2.66097	-1.36914
C	0.95811	3.04456	-0.0205
H	1.38141	2.27809	0.64093
H	1.67041	3.88201	0.00894
H	0.00915	3.38638	0.40331

C	-2.96587	-0.67053	1.12499
C	-3.35874	-2.11227	1.68921
C	-3.58927	0.29888	2.27734
C	-2.53619	-2.36224	2.98704
C	-4.75154	-1.85078	2.29082
C	-4.28655	-0.73121	3.23119
C	-3.24673	-1.50251	4.0646
H	-1.47983	-2.10649	2.84992
H	-2.58269	-3.43355	3.23268
H	-5.51938	-1.56903	1.56413
H	-5.12334	-2.73167	2.83754
H	-5.06796	-0.24779	3.83653
H	-2.5622	-0.86183	4.63297
H	-3.76847	-2.13662	4.79772
C	-3.22262	-3.25384	0.69617
H	-3.85201	-3.11825	-0.19422
H	-2.17567	-3.35264	0.37283
H	-3.51272	-4.2011	1.17716
C	-2.52133	1.09179	3.04861
H	-1.64134	0.5029	3.32532
H	-2.1928	1.97083	2.47711
H	-2.97497	1.46669	3.97936
C	-4.60088	1.36752	1.81368
H	-5.61521	0.98208	1.65391
H	-4.68883	2.13132	2.6013
H	-4.27005	1.87082	0.89374

Optimized reductive elimination transition structure of the active catalyst system (MeCu • BIFOP-H • chalcone) of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)**TS-7.1 (R)**



Imaginary frequency: -402.44 cm^{-1}

Energy: -4068.819540

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -4070.158427

0 1

Cu	-1.51404	-0.33461	0.75003
C	-3.04882	-0.57087	2.28841
H	-2.62799	-1.59157	2.34368
H	-2.58535	0.07308	3.04877
H	-4.11841	-0.65251	2.50368
C	-2.70424	0.58183	-0.64478
H	-2.2363	1.55425	-0.81069
C	-3.5476	0.44069	0.55256
C	-2.80331	-0.18245	-1.86033
O	-2.32134	0.22087	-2.92987
H	-4.41143	-0.21068	0.40732

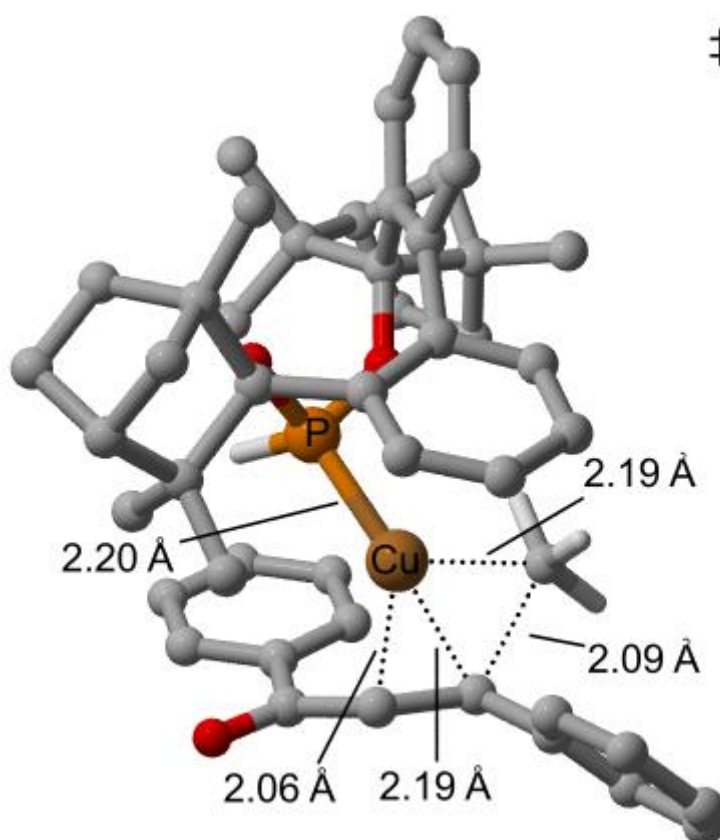
C	-3.5034	-1.52535	-1.87673
C	-4.11559	-1.92436	-3.07539
C	-3.49427	-2.4254	-0.80234
C	-4.72076	-3.1757	-3.18799
H	-4.08338	-1.23112	-3.91776
C	-4.08587	-3.68609	-0.91299
H	-2.98599	-2.16504	0.1266
C	-4.70815	-4.06326	-2.10546
H	-5.1994	-3.46714	-4.1265
H	-4.05161	-4.37768	-0.0673
H	-5.17547	-5.04716	-2.19464
C	-3.89349	1.72399	1.23712
C	-5.22355	2.02081	1.56093
C	-2.9013	2.66624	1.55905
C	-5.55807	3.23067	2.17751
H	-6.00761	1.29851	1.31859
C	-3.23027	3.87159	2.17559
H	-1.85833	2.44672	1.32203
C	-4.56394	4.1609	2.48679
H	-6.60272	3.44611	2.41528
H	-2.44221	4.59038	2.41416
H	-4.82429	5.10619	2.96868
C	-0.38907	-3.31865	-1.81311
C	0.3947	-3.22839	-0.66277
C	-0.43778	-2.24071	-2.68773
C	1.16432	-2.09972	-0.33978
C	0.40526	-1.15809	-2.45713
C	1.25848	-1.07441	-1.34417
O	1.92975	-0.53206	1.27191

O	0.72543	1.44413	-0.00387
C	2.45667	-0.16476	-1.59656
C	3.31961	-0.83345	-2.49642
P	0.53315	0.34361	1.16679
C	2.78437	1.17312	-1.23062
C	4.50794	-0.30104	-2.97633
C	4.01057	1.67333	-1.71451
C	4.8712	0.9709	-2.55079
H	4.30826	2.67777	-1.45741
H	5.80172	1.43676	-2.88309
H	5.13257	-0.87533	-3.6639
H	3.02883	-1.83337	-2.81892
H	0.44082	-0.35957	-3.1948
H	-1.101	-2.23407	-3.55195
H	-0.98866	-4.21301	-1.99209
H	0.38773	-4.07475	0.011
H	0.74791	1.09518	2.34246
C	1.83298	-1.95839	1.04946
C	3.26484	-2.61244	1.15152
C	1.10182	-2.63348	2.37231
C	3.96056	-2.08999	2.44185
C	2.88052	-4.04879	1.56215
C	2.18439	-3.64717	2.86311
C	3.33333	-2.92575	3.58527
H	3.80811	-1.00952	2.55813
H	5.04457	-2.25904	2.36396
H	2.23514	-4.55193	0.82949
H	3.76887	-4.67946	1.72199
H	1.73679	-4.46276	3.4503

H	3.01297	-2.32557	4.44593
H	4.04699	-3.67206	3.96725
C	4.17043	-2.51897	-0.05913
H	3.69216	-2.9269	-0.95811
H	4.47023	-1.48425	-0.26501
H	5.0849	-3.10367	0.13061
C	-0.23099	-3.37769	2.17127
H	-0.92619	-2.8153	1.53403
H	-0.11586	-4.38268	1.74826
H	-0.70989	-3.50532	3.15417
C	0.80528	-1.58631	3.46431
H	-0.10982	-1.02115	3.23144
H	0.61113	-2.11145	4.41179
H	1.61909	-0.8742	3.63173
C	1.81042	2.178	-0.57761
C	1.14271	3.08239	-1.71188
C	2.38361	3.31999	0.43806
C	-0.07716	3.82097	-1.08876
C	2.14981	4.24407	-1.8095
C	2.04894	4.64352	-0.33185
C	0.5455	4.96423	-0.24815
H	-0.70173	3.13719	-0.50596
H	-0.70701	4.21058	-1.90124
H	3.14807	3.95605	-2.15344
H	1.78375	5.03333	-2.48456
H	2.69708	5.4702	-0.00375
H	0.1531	5.02039	0.77493
H	0.35796	5.94536	-0.71059
C	0.76625	2.36886	-2.99958

H	1.6135	1.83022	-3.44657
H	-0.06554	1.66692	-2.83612
H	0.41738	3.11191	-3.73413
C	1.68371	3.31665	1.80799
H	0.5976	3.18936	1.75359
H	2.09676	2.53639	2.46178
H	1.87959	4.28223	2.29961
C	3.88759	3.26669	0.77737
H	4.53306	3.69845	0.00316
H	4.06348	3.86403	1.68527
H	4.22642	2.24025	0.97926

Optimized reductive elimination transition structure of the active catalyst system (MeCu • BIFOP-H • chalcone) of the reaction pathway (B3LYP-D3(BJ)/def2-SVP) **TS-2.2 (R)**



Imaginary frequency: -388.90 cm^{-1}

Energy: -4068.827153

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -4070.164400

0 1

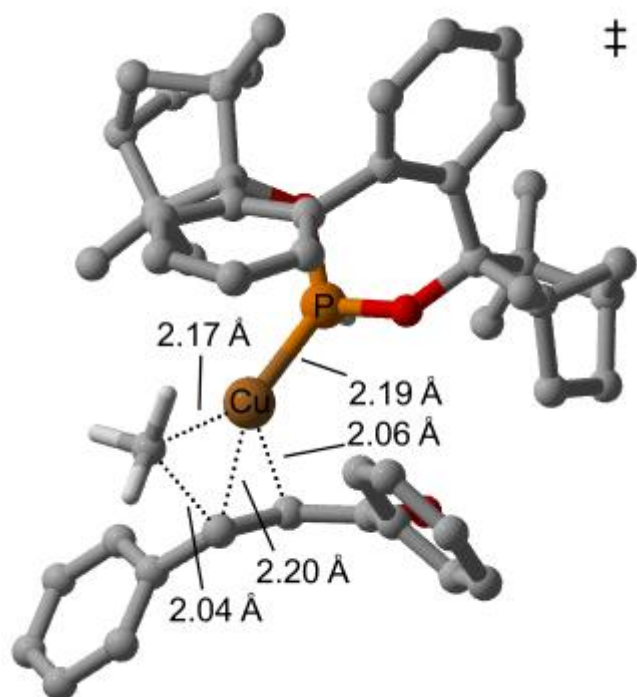
Cu	-1.70657	0.32967	0.10443
C	-2.16799	1.43923	-1.72245
H	-1.12317	1.76658	-1.59427
H	-2.21951	0.57575	-2.39531
H	-2.74448	2.267	-2.14514
C	-3.54563	0.52726	1.0041
H	-4.12688	-0.39112	1.10767
C	-3.67114	1.22955	-0.27966
C	-3.03003	0.97565	2.27752
O	-3.25316	0.32475	3.30984
H	-3.77304	2.31374	-0.21176
C	-2.06018	2.15306	2.40474
C	-1.41767	2.27382	3.65077
C	-1.69099	3.05748	1.39015
C	-0.43015	3.23248	3.87109
H	-1.72187	1.57196	4.42821
C	-0.70191	4.02252	1.6094
H	-2.15649	3.02812	0.41072
C	-0.06241	4.1123	2.84699
H	0.05859	3.29476	4.84682
H	-0.43317	4.70753	0.80183
H	0.71412	4.86282	3.01328
C	-4.66585	0.64489	-1.22811
C	-5.55832	1.47842	-1.91613
C	-4.72525	-0.73823	-1.46475

C	-6.49317	0.94733	-2.80927
H	-5.52348	2.55768	-1.7442
C	-5.65306	-1.27058	-2.35843
H	-4.0267	-1.3994	-0.95039
C	-6.54371	-0.42974	-3.0352
H	-7.18523	1.61408	-3.32951
H	-5.68263	-2.34983	-2.52958
H	-7.27208	-0.84711	-3.73445
C	-1.82781	-2.7313	-2.0623
C	-1.14204	-2.90351	-0.85879
C	-1.3382	-1.83417	-3.00457
C	0.04678	-2.22727	-0.54318
C	-0.10198	-1.23576	-2.77106
C	0.64374	-1.44992	-1.5977
O	1.31088	-0.99955	1.03882
O	1.24664	1.1446	-0.40627
C	2.12972	-1.19101	-1.80548
C	2.62254	-2.20618	-2.66199
P	0.4029	0.34701	0.73049
C	3.02302	-0.15424	-1.4147
C	3.94277	-2.30092	-3.07577
C	4.3635	-0.29838	-1.83082
C	4.8365	-1.33718	-2.62353
H	5.0842	0.4541	-1.55259
H	5.89261	-1.36744	-2.90093
H	4.26051	-3.11675	-3.72843
H	1.91809	-2.96966	-2.99305
H	0.3489	-0.62167	-3.55177
H	-1.88238	-1.63556	-3.93009

H	-2.75394	-3.28125	-2.24018
H	-1.56504	-3.5867	-0.13499
H	0.68318	1.06349	1.90672
C	0.64707	-2.27706	0.88739
C	1.67749	-3.4508	1.11062
C	-0.34593	-2.49245	2.19591
C	2.48929	-3.15573	2.4048
C	0.72093	-4.56418	1.5845
C	0.21787	-3.81007	2.81514
C	1.53855	-3.55967	3.55845
H	2.79637	-2.10288	2.44264
H	3.4065	-3.76311	2.40255
H	-0.05753	-4.80939	0.84779
H	1.2626	-5.49128	1.82912
H	-0.54087	-4.32139	3.42502
H	1.46301	-2.80509	4.35091
H	1.87196	-4.49367	4.03706
C	2.57919	-3.84188	-0.04303
H	2.00827	-4.07685	-0.95013
H	3.30403	-3.05422	-0.28201
H	3.14599	-4.74399	0.23805
C	-1.85824	-2.66311	1.96544
H	-2.26119	-1.90253	1.28471
H	-2.13658	-3.66133	1.60166
H	-2.37284	-2.51546	2.92525
C	-0.23076	-1.32104	3.18829
H	-0.8339	-0.46322	2.86381
H	-0.66816	-1.63166	4.14825
H	0.7963	-0.98884	3.36943

C	2.6177	1.20866	-0.80705
C	2.63198	2.32616	-1.94838
C	3.57964	1.88733	0.31977
C	1.84184	3.55987	-1.42298
C	4.06834	2.87489	-1.85588
C	3.98205	3.23521	-0.36673
C	2.79785	4.22015	-0.39531
H	0.87534	3.27418	-0.99486
H	1.64071	4.23108	-2.27138
H	4.85453	2.16183	-2.1214
H	4.19977	3.76076	-2.49718
H	4.89342	3.65525	0.08449
H	2.33336	4.38362	0.58463
H	3.14731	5.20182	-0.75009
C	2.13399	1.85791	-3.30564
H	2.73666	1.03492	-3.71414
H	1.0894	1.51832	-3.23226
H	2.16395	2.69191	-4.02431
C	2.86388	2.15601	1.65061
H	1.88452	2.62768	1.54281
H	2.74735	1.22957	2.23063
H	3.48884	2.83613	2.25055
C	4.84563	1.09994	0.71733
H	5.66826	1.1812	-0.00319
H	5.22833	1.51275	1.66303
H	4.62951	0.03452	0.88013

Optimized reductive elimination transition structure of the active catalyst system (MeCu • BIFOP-H • chalcone) of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)**TS-5 (R)**



Imaginary frequency: -402.55 cm^{-1}

Energy: -4068.823835

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -4070.161423

0 1

Cu	-1.78138	0.31402	-0.02893
C	-3.19624	0.92483	1.4931
H	-2.23348	0.96937	2.03456
H	-3.49691	1.9273	1.16551
H	-3.93877	0.54009	2.19707
C	-3.04614	-1.00505	-0.98341
H	-3.23479	-0.60696	-1.98429
C	-3.83006	-0.46832	0.13773
C	-2.3109	-2.2397	-0.9808
O	-1.83916	-2.74783	-2.01155
H	-3.99623	-1.20677	0.92495

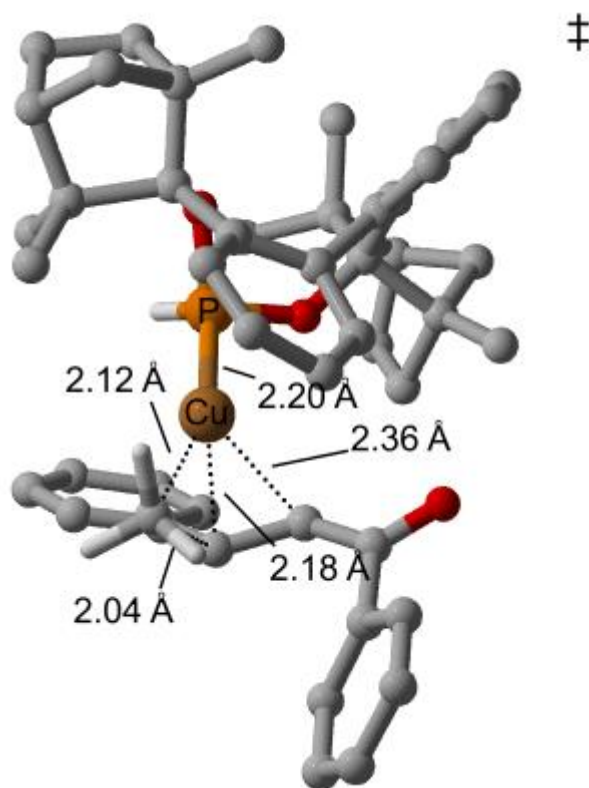
C	-2.08618	-2.97937	0.3246
C	-2.25948	-4.37186	0.3304
C	-1.60694	-2.36046	1.48663
C	-1.99252	-5.11904	1.47728
H	-2.58666	-4.8565	-0.5914
C	-1.31714	-3.10672	2.63145
H	-1.39708	-1.28759	1.50139
C	-1.51873	-4.48864	2.63388
H	-2.14204	-6.20175	1.46864
H	-0.92491	-2.6039	3.51866
H	-1.29817	-5.07497	3.52928
C	-5.08056	0.2581	-0.24114
C	-6.30893	-0.11866	0.31691
C	-5.05988	1.3147	-1.16612
C	-7.49111	0.53263	-0.04833
H	-6.33964	-0.93816	1.03985
C	-6.23611	1.96796	-1.53032
H	-4.10691	1.63255	-1.59698
C	-7.45941	1.57776	-0.97329
H	-8.44059	0.21973	0.39304
H	-6.2003	2.78822	-2.2516
H	-8.38168	2.08924	-1.25864
C	-0.29012	1.8532	3.55996
C	0.14309	2.52953	2.41872
C	0.08559	0.52743	3.74969
C	0.94908	1.94015	1.43372
C	1.00101	-0.03716	2.86327
C	1.49848	0.64631	1.74066
O	1.39913	1.5434	-0.85814

O	0.921	-1.01909	-0.50247
C	2.83393	0.11632	1.24404
C	3.82476	0.45062	2.19386
P	0.21571	0.37787	-0.93128
C	3.22431	-0.64305	0.10238
C	5.17869	0.19375	2.01834
C	4.60971	-0.81792	-0.0814
C	5.57826	-0.40526	0.83012
H	4.9643	-1.33578	-0.95936
H	6.63345	-0.58901	0.61536
H	5.9009	0.48579	2.78365
H	3.50366	0.97285	3.09609
H	1.40394	-1.02746	3.07229
H	-0.27601	-0.04489	4.60691
H	-0.93955	2.36224	4.2751
H	-0.18519	3.55234	2.29123
H	0.17165	0.31968	-2.33358
C	1.19794	2.63062	0.06675
C	2.44689	3.59725	0.04541
C	0.03963	3.631	-0.57038
C	2.81231	3.89831	-1.43679
C	1.78068	4.91829	0.48051
C	0.80624	4.98499	-0.69512
C	1.78394	4.96785	-1.87996
H	2.77731	2.98334	-2.04134
H	3.84207	4.28166	-1.48518
H	1.30407	4.85913	1.46926
H	2.49966	5.752	0.49896
H	0.11319	5.83924	-0.70732

H	1.30919	4.74962	-2.84476
H	2.25731	5.95728	-1.97578
C	3.66585	3.20805	0.85613
H	3.41573	3.00772	1.90544
H	4.16525	2.32462	0.44142
H	4.38737	4.04067	0.83615
C	-1.25189	3.86865	0.22928
H	-1.69136	2.9315	0.5886
H	-1.12545	4.54808	1.08117
H	-1.98715	4.34533	-0.43747
C	-0.43962	3.14531	-1.95208
H	-1.17578	2.33095	-1.8529
H	-0.96274	3.97303	-2.45462
H	0.36484	2.80188	-2.60936
C	2.25259	-1.51446	-0.72775
C	2.28736	-2.99027	-0.12324
C	2.55274	-1.82452	-2.30057
C	1.10534	-3.79444	-0.73622
C	3.47744	-3.60058	-0.88694
C	2.88251	-3.3606	-2.27941
C	1.59297	-4.19091	-2.14932
H	0.1853	-3.21062	-0.77742
H	0.89826	-4.67129	-0.10616
H	4.44256	-3.12444	-0.69064
H	3.58588	-4.67214	-0.65765
H	3.51322	-3.64212	-3.13632
H	0.83777	-4.00032	-2.91965
H	1.84811	-5.26084	-2.20419
C	2.32191	-3.09058	1.3917

H	3.18547	-2.57702	1.83644
H	1.39842	-2.67936	1.82112
H	2.36881	-4.15122	1.68352
C	1.34239	-1.58674	-3.22804
H	0.37395	-1.88783	-2.81015
H	1.28857	-0.53771	-3.54881
H	1.50265	-2.17617	-4.14395
C	3.70719	-1.02642	-2.93924
H	4.70362	-1.42975	-2.72019
H	3.59995	-1.06589	-4.03393
H	3.6863	0.03138	-2.63672

Optimized reductive elimination transition structure of the active catalyst system (MeCu • BIFOP-H • chalcone) of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)**TS-7.2 (R)**



Imaginary frequency: -465.11 cm^{-1}

Energy: -4068.813130

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -4070.152474

0 1

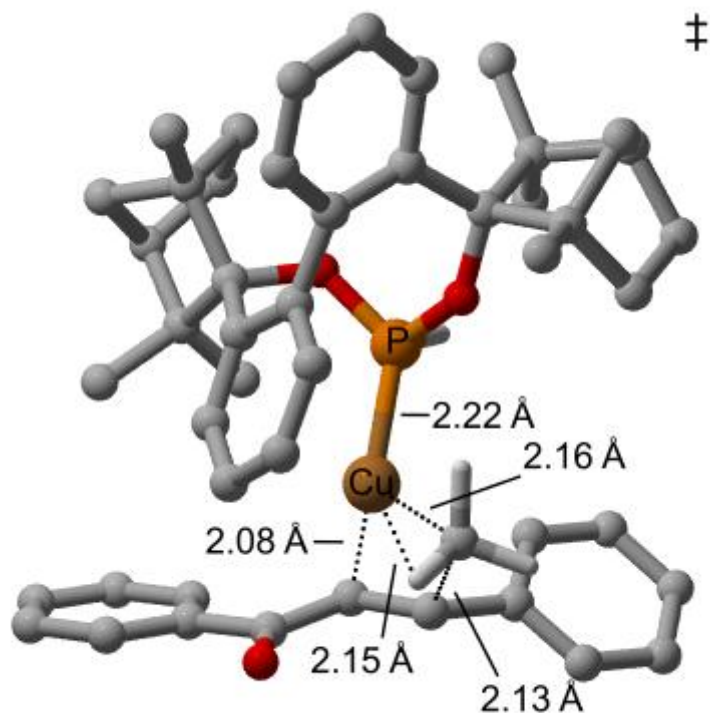
Cu	-1.30965	-0.90626	0.5831
C	-3.07884	-2.03909	0.83436
H	-3.86158	-1.9455	0.07425
H	-2.26995	-2.67131	0.39375
H	-3.45501	-2.56482	1.71925
C	-2.8537	0.86346	0.30906
H	-1.91456	1.41917	0.36421
C	-3.15399	-0.07008	1.38109
C	-3.51111	1.00506	-0.94693
O	-2.99342	1.59278	-1.92053
H	-4.20581	-0.30081	1.55477
C	-4.88004	0.39873	-1.16373
C	-5.16653	-0.16177	-2.4182
C	-5.89632	0.43192	-0.19681
C	-6.41305	-0.73071	-2.68079
H	-4.39265	-0.11683	-3.18675
C	-7.15243	-0.12048	-0.46163
H	-5.71203	0.92728	0.75851
C	-7.40962	-0.71816	-1.69875
H	-6.61542	-1.17526	-3.65883
H	-7.93719	-0.07609	0.29808
H	-8.38929	-1.15723	-1.90357
C	-2.4037	0.16169	2.68286
C	-2.15273	-0.86638	3.61124
C	-1.91149	1.44523	2.98498

C	-1.41065	-0.63035	4.76919
H	-2.51516	-1.87383	3.40919
C	-1.16599	1.68336	4.14322
H	-2.12014	2.26311	2.29701
C	-0.90221	0.64515	5.0382
H	-1.22198	-1.45263	5.46382
H	-0.7906	2.69059	4.34063
H	-0.31112	0.82591	5.939
C	-1.08796	-2.90771	-2.26679
C	0.12872	-3.04345	-1.59128
C	-1.58398	-1.63398	-2.52628
C	0.90474	-1.94609	-1.19372
C	-0.75944	-0.5304	-2.29321
C	0.52247	-0.66433	-1.72897
O	2.09149	-0.77427	0.50478
O	0.66878	1.36695	0.40614
C	1.50833	0.41031	-2.1613
C	1.82319	0.14792	-3.5177
P	0.68496	-0.10963	1.06878
C	2.10669	1.53899	-1.53808
C	2.74844	0.87469	-4.25159
C	3.07155	2.22953	-2.30177
C	3.40972	1.91757	-3.61295
H	3.57093	3.08323	-1.87099
H	4.16605	2.51139	-4.13118
H	2.95348	0.61756	-5.29286
H	1.32342	-0.69541	-3.99635
H	-1.10754	0.46022	-2.59218
H	-2.57789	-1.48748	-2.94998

H	-1.66098	-3.79868	-2.53175
H	0.4557	-4.04437	-1.33886
H	1.07152	0.15142	2.40075
C	2.03272	-2.06998	-0.13686
C	3.44727	-2.4271	-0.73233
C	1.89333	-3.20904	1.04879
C	4.52815	-2.13618	0.34697
C	3.37593	-3.96756	-0.69344
C	3.17749	-4.06693	0.82078
C	4.43381	-3.33672	1.3222
H	4.35035	-1.16751	0.83048
H	5.51516	-2.08373	-0.13576
H	2.55156	-4.37975	-1.29223
H	4.31282	-4.42961	-1.04159
H	3.06393	-5.08096	1.23182
H	4.38306	-3.04289	2.37814
H	5.30639	-4.00008	1.21881
C	3.80729	-1.83254	-2.07979
H	3.05607	-2.06666	-2.84454
H	3.91679	-0.74177	-2.02875
H	4.7701	-2.25211	-2.41287
C	0.66457	-4.13572	1.04343
H	-0.2733	-3.57317	0.94692
H	0.69498	-4.90941	0.26727
H	0.63414	-4.66609	2.00769
C	1.88566	-2.57071	2.45063
H	0.89511	-2.15141	2.68934
H	2.07633	-3.35715	3.19693
H	2.63477	-1.78497	2.58797

C	1.63422	2.21172	-0.23074
C	0.8233	3.54407	-0.58188
C	2.74692	2.7667	0.81563
C	0.01531	3.95566	0.68128
C	1.92922	4.61903	-0.5359
C	2.39292	4.28884	0.88878
C	1.07882	4.52165	1.65863
H	-0.54769	3.11387	1.09134
H	-0.71428	4.72487	0.38918
H	2.69773	4.5354	-1.30984
H	1.49896	5.62972	-0.61505
H	3.24001	4.87679	1.27349
H	1.05554	4.04939	2.64899
H	0.93765	5.6013	1.82039
C	-0.04945	3.46885	-1.82481
H	0.5267	3.21912	-2.72665
H	-0.86365	2.73518	-1.7117
H	-0.52568	4.44781	-1.99419
C	2.64822	2.11573	2.20263
H	1.63085	2.08663	2.60345
H	3.05152	1.09306	2.18542
H	3.26305	2.69723	2.9074
C	4.22244	2.58699	0.40533
H	4.56611	3.30574	-0.34779
H	4.85435	2.74709	1.29234
H	4.41956	1.57248	0.03049

Optimized reductive elimination transition structure of the active catalyst system (MeCu • BIFOP-H • chalcone) of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)**TS-2 (S)**



Imaginary frequency: -368.08 cm^{-1}

Energy: -4068.831421

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -4070.165928

0 1

Cu	1.38017	1.05005	0.56085
C	0.95796	2.58669	2.01743
H	-0.02842	2.09881	1.93159
H	1.44998	2.29561	2.95094
H	0.81149	3.66845	1.95657
C	3.34226	1.6056	0.15903
C	2.67081	2.75397	0.76859
C	1.60122	-0.85438	2.71726
C	1.36788	-1.53053	1.51728
C	0.51845	-0.39255	3.4598
C	0.07991	-1.7942	0.99811

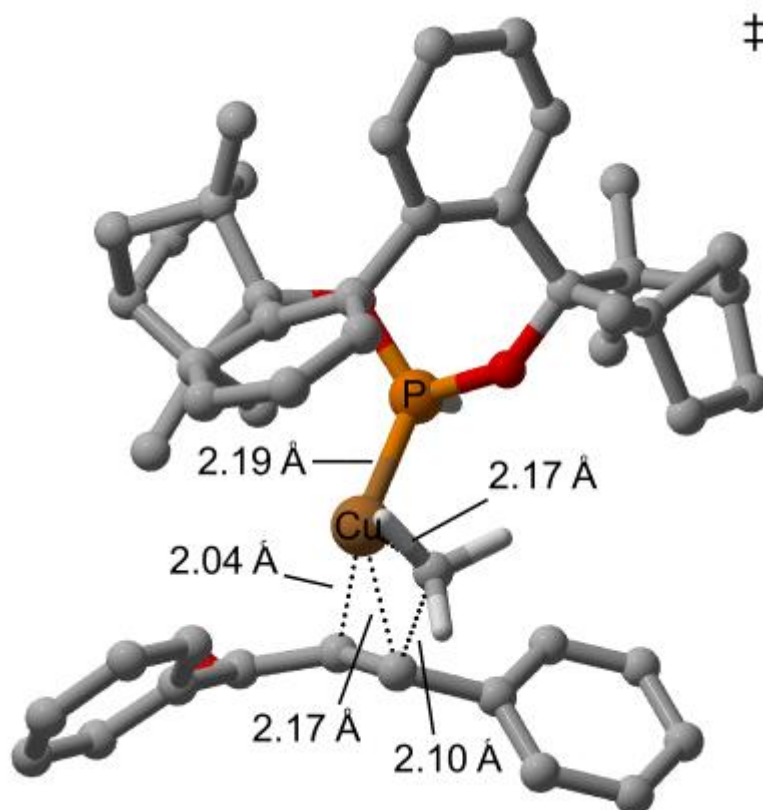
C	-0.7608	-0.59439	2.96244
C	-1.01812	-1.25079	1.74007
O	-0.65908	-1.15671	-1.14321
O	-1.72925	0.90558	-0.02943
C	-2.49611	-1.43587	1.50237
C	-3.02251	-2.36892	2.42591
P	-0.3324	0.38576	-0.6844
C	-3.39313	-0.7605	0.62631
C	-4.35285	-2.75725	2.45245
C	-4.72591	-1.22755	0.64094
C	-5.20882	-2.20332	1.5056
H	-5.44894	-0.78446	-0.02516
H	-6.25977	-2.49653	1.45288
H	-4.70312	-3.49189	3.18045
H	-2.32415	-2.82804	3.12705
H	-1.61785	-0.22357	3.52523
H	0.66901	0.14427	4.39821
H	2.62629	-0.6545	3.02929
H	2.24084	-1.84781	0.96874
H	-0.35467	0.91716	-1.99416
C	-0.05498	-2.3051	-0.4622
C	-0.98111	-3.58233	-0.80448
C	1.28329	-2.65833	-1.31751
C	-1.65869	-3.28034	-2.16313
C	0.02697	-4.6484	-1.28973
C	0.7233	-3.73471	-2.29123
C	-0.46453	-3.24285	-3.15209
H	-2.24803	-2.35927	-2.14778
H	-2.34138	-4.11356	-2.39173

H	0.67321	-5.05271	-0.50188
H	-0.50862	-5.49121	-1.75285
H	1.53387	-4.17833	-2.88697
H	-0.2971	-2.24012	-3.56717
H	-0.61903	-3.9241	-4.0027
C	-1.94274	-4.14544	0.22586
H	-1.50015	-4.18615	1.22995
H	-2.88001	-3.58588	0.27575
H	-2.19693	-5.17747	-0.06528
C	2.44999	-3.34913	-0.55266
H	3.24244	-2.6443	-0.27754
H	2.14157	-3.88169	0.35458
H	2.9222	-4.08471	-1.22113
C	1.87851	-1.45901	-2.05857
H	2.19984	-0.67284	-1.35986
H	2.77467	-1.78437	-2.6074
H	1.18287	-1.01817	-2.78337
C	-3.12691	0.59044	-0.09232
C	-3.81152	1.76486	0.75558
C	-3.77761	0.84331	-1.5655
C	-3.21174	3.11907	0.27763
C	-5.21132	1.85954	0.1201
C	-4.69934	2.08246	-1.30892
C	-3.87389	3.3663	-1.10332
H	-2.11763	3.09493	0.24187
H	-3.49713	3.89772	1.00059
H	-5.84389	0.97801	0.25973
H	-5.76789	2.7269	0.50872
H	-5.46802	2.17377	-2.09093

H	-3.15104	3.56457	-1.90416
H	-4.55163	4.233	-1.06976
C	-3.72697	1.60122	2.26393
H	-4.21848	0.68481	2.6185
H	-2.67539	1.57725	2.58718
H	-4.20822	2.45906	2.75927
C	-2.73389	1.1598	-2.64429
H	-2.01957	1.93266	-2.34795
H	-2.17949	0.25649	-2.93548
H	-3.2587	1.52702	-3.54005
C	-4.61531	-0.30656	-2.16548
H	-5.63519	-0.36721	-1.76689
H	-4.72312	-0.1317	-3.24657
H	-4.13314	-1.28453	-2.03314
C	4.10555	0.73167	1.00165
O	4.11092	0.83549	2.24329
H	3.46094	1.58091	-0.9227
C	4.86662	-0.41119	0.36967
C	5.35255	-1.41612	1.22184
C	5.10018	-0.53349	-1.00952
C	6.02711	-2.52555	0.71138
H	5.18418	-1.29303	2.2928
C	5.78439	-1.6371	-1.52261
H	4.75026	0.2389	-1.69482
C	6.24393	-2.64162	-0.66534
H	6.38934	-3.30281	1.38911
H	5.95926	-1.71407	-2.59874
H	6.77328	-3.50832	-1.06882
H	3.14949	3.07946	1.69386

C	2.24982	3.86419	-0.13188
C	2.43501	5.19813	0.26281
C	1.65128	3.61945	-1.38071
C	2.03328	6.25418	-0.55878
H	2.90155	5.40636	1.22904
C	1.24351	4.67118	-2.20075
H	1.49896	2.58956	-1.70943
C	1.43176	5.99595	-1.79292
H	2.19072	7.28493	-0.23157
H	0.77725	4.45631	-3.16573
H	1.113	6.82073	-2.43459

Optimized reductive elimination transition structure of the active catalyst system (MeCu • BIFOP-H • chalcone) of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)**TS-7 (S)**



Imaginary frequency: -370.94 cm^{-1}

Energy: -4068.820674

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -4070.160540

0 1

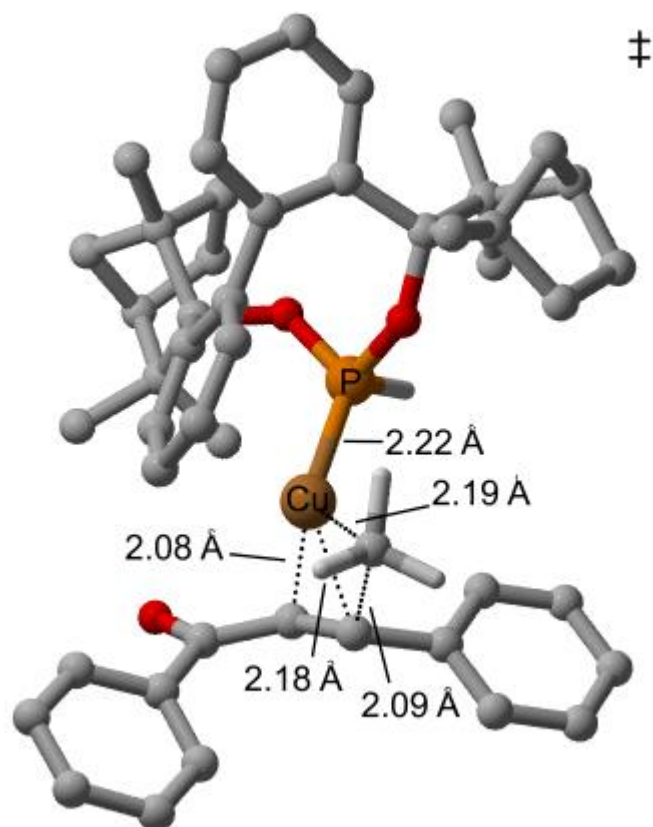
Cu	1.43609	0.62923	-0.1934
C	1.34259	1.8995	1.56111
H	1.19723	0.91797	2.04577
H	1.92324	2.52994	2.24051
H	0.36999	2.36442	1.36001
C	3.0847	1.45365	-1.06848
C	2.75784	2.3256	0.07017
C	1.45384	-2.03872	2.83251
C	1.12476	-2.49683	1.55703
C	0.58607	-1.17323	3.48752
C	-0.04746	-2.12936	0.87771
C	-0.63629	-0.87726	2.88778
C	-1.01071	-1.3583	1.61981
O	-1.0997	-1.47206	-1.14114
O	-1.61026	0.89776	-0.09199
C	-2.52366	-1.33572	1.4201
C	-3.0874	-2.32707	2.25661
P	-0.52929	0.0677	-0.97562
C	-3.41627	-0.48512	0.70122
C	-4.44823	-2.58481	2.35053
C	-4.78795	-0.7946	0.79576
C	-5.3117	-1.81886	1.57751
H	-5.50196	-0.19009	0.25861
H	-6.39074	-1.98774	1.59508
H	-4.81621	-3.37438	3.00909

H	-2.40213	-2.93399	2.84826
H	-1.36857	-0.29466	3.44505
H	0.82701	-0.76602	4.4718
H	2.39539	-2.35031	3.28795
H	1.82824	-3.15895	1.07235
H	-0.81258	0.47711	-2.29271
C	-0.25873	-2.52416	-0.60705
C	-0.95673	-3.92522	-0.80348
C	1.05216	-2.69956	-1.61109
C	-1.46318	-4.02212	-2.27181
C	0.2802	-4.84638	-0.83506
C	0.92028	-4.18961	-2.0573
C	-0.19807	-4.36717	-3.09534
H	-1.94248	-3.0853	-2.58289
H	-2.22237	-4.81512	-2.3412
H	0.88354	-4.79593	0.08214
H	0.00011	-5.89849	-1.0001
H	1.89	-4.59576	-2.37925
H	-0.0736	-3.74704	-3.99147
H	-0.21956	-5.4149	-3.4332
C	-2.02363	-4.33741	0.19004
H	-1.65809	-4.29803	1.22407
H	-2.91919	-3.7096	0.11181
H	-2.3234	-5.37684	-0.01888
C	2.45885	-2.47932	-1.02922
H	2.5154	-1.5815	-0.40184
H	2.83323	-3.33045	-0.44573
H	3.16897	-2.31504	-1.85115
C	0.978	-1.75785	-2.8293

H	1.32128	-0.74574	-2.56609
H	1.68302	-2.12057	-3.59146
H	-0.01557	-1.69372	-3.28511
C	-3.03051	0.86954	0.06271
C	-3.357	2.04636	1.08988
C	-3.81567	1.3992	-1.26941
C	-2.63864	3.33666	0.59354
C	-4.81677	2.37844	0.73201
C	-4.52941	2.69164	-0.74086
C	-3.5243	3.84568	-0.57197
H	-1.60329	3.1384	0.29457
H	-2.60054	4.06301	1.41852
H	-5.52543	1.56407	0.91206
H	-5.17618	3.25856	1.2879
H	-5.39891	2.94917	-1.36398
H	-2.95555	4.08644	-1.47813
H	-4.06749	4.76018	-0.28877
C	-3.05204	1.74988	2.5473
H	-3.58622	0.86433	2.91903
H	-1.97285	1.59472	2.68794
H	-3.34758	2.61031	3.16787
C	-2.87397	1.76847	-2.42936
H	-1.97264	2.3063	-2.11697
H	-2.57548	0.87832	-2.99885
H	-3.42473	2.42012	-3.12522
C	-4.84541	0.43998	-1.90111
H	-5.81657	0.43171	-1.39158
H	-5.04792	0.77161	-2.931
H	-4.46845	-0.5919	-1.94861

C	4.143	0.4729	-1.15111
O	4.50163	-0.00109	-2.23655
H	2.75479	1.77985	-2.05861
C	4.85134	-0.02732	0.09426
C	6.17575	-0.46917	-0.06087
C	4.25298	-0.14865	1.35721
C	6.89173	-0.98182	1.01974
H	6.61551	-0.40954	-1.05779
C	4.96219	-0.67739	2.43986
H	3.21298	0.13683	1.50764
C	6.28737	-1.08638	2.27811
H	7.92518	-1.31023	0.88183
H	4.47254	-0.76893	3.41274
H	6.84545	-1.49262	3.12549
H	3.53897	2.37955	0.83007
C	2.1698	3.65803	-0.26299
C	2.63508	4.8189	0.36867
C	1.117	3.77954	-1.18731
C	2.0689	6.066	0.08679
H	3.45219	4.74323	1.09094
C	0.54512	5.01937	-1.46527
H	0.73481	2.8853	-1.68486
C	1.01933	6.17173	-0.82782
H	2.45032	6.95904	0.58807
H	-0.27683	5.08824	-2.18244
H	0.57217	7.14466	-1.0445

Optimized reductive elimination transition structure of the active catalyst system (MeCu • BIFOP-H • chalcone) of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)**TS-8.1 (S)**



Imaginary frequency: -393.41 cm^{-1}

Energy: -4068.816126

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -4070.152372

0 1

Cu	-1.55896	0.37057	-0.01411
C	-2.14403	1.78604	-1.57491
H	-1.05249	1.69446	-1.71774
H	-2.67044	1.21907	-2.35195
H	-2.39716	2.84859	-1.62984
C	-3.3955	0.37158	0.97138
C	-3.3985	1.53088	0.07227
H	-4.18959	1.53243	-0.6734
C	-3.23739	2.86702	0.72464

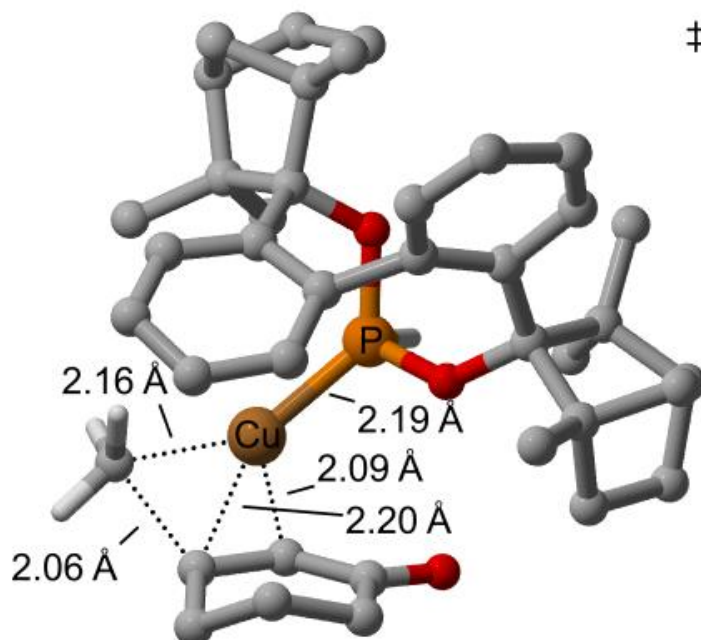
C	-4.09667	3.92113	0.38119
C	-2.23981	3.10981	1.68385
C	-3.96835	5.17834	0.97782
H	-4.8776	3.75199	-0.36512
C	-2.10498	4.36443	2.27721
H	-1.55873	2.30482	1.96519
C	-2.96995	5.40666	1.92722
H	-4.65236	5.98323	0.69747
H	-1.31984	4.5305	3.0192
H	-2.86527	6.38961	2.39238
H	-3.02449	0.51744	1.98902
C	-4.00901	-0.91638	0.76905
O	-3.78817	-1.88251	1.51971
C	-4.96269	-1.15542	-0.38412
C	-5.93042	-0.22341	-0.78824
C	-4.95372	-2.41818	-0.99844
C	-6.83026	-0.52636	-1.81432
H	-6.01026	0.73208	-0.26774
C	-5.83568	-2.71755	-2.03665
H	-4.24768	-3.16487	-0.63028
C	-6.77389	-1.76697	-2.45427
H	-7.58525	0.20724	-2.10836
H	-5.80299	-3.70024	-2.5141
H	-7.4715	-2.00071	-3.26232
C	-1.66819	-1.67245	-1.91182
C	-1.00771	-2.10706	-0.75932
C	-0.94605	-1.05107	-2.92674
C	0.38558	-1.96763	-0.55707
C	0.41435	-0.85468	-2.74238

C	1.10052	-1.2632	-1.57886
O	1.35889	-0.8782	1.28259
O	1.5204	1.22246	-0.18687
C	2.58472	-1.02319	-1.69015
C	3.14715	-1.89661	-2.64971
P	0.5015	0.44323	0.8197
C	3.41501	-0.02923	-1.09799
C	4.49672	-1.92455	-2.96478
C	4.79177	-0.13246	-1.39522
C	5.339	-1.05123	-2.28383
H	5.48304	0.56391	-0.94811
H	6.41695	-1.05211	-2.46058
H	4.88037	-2.62927	-3.70537
H	2.47705	-2.60875	-3.13347
H	0.99195	-0.35157	-3.51812
H	-1.43854	-0.70099	-3.83576
H	-2.74422	-1.81896	-1.99788
H	-1.61875	-2.55356	0.01142
H	0.6391	1.1359	2.04428
C	0.96861	-2.22763	0.85978
C	2.26625	-3.16709	1.04736
C	0.00253	-2.79417	2.04216
C	3.10999	-2.52695	2.17605
C	1.72636	-4.38429	1.83149
C	1.03977	-3.55941	2.91239
C	2.20023	-2.67298	3.42339
H	3.39616	-1.49448	1.95657
H	4.03354	-3.11724	2.28237
H	1.0603	-5.03552	1.2533

H	2.56357	-4.99684	2.20007
H	0.53547	-4.11533	3.7153
H	1.85193	-1.7034	3.80311
H	2.72291	-3.17668	4.25082
C	3.10113	-3.59475	-0.1463
H	2.4825	-3.87636	-1.00884
H	3.81463	-2.82799	-0.458
H	3.68691	-4.48233	0.14249
C	-1.07317	-3.84406	1.63345
H	-2.06586	-3.38621	1.52994
H	-0.83736	-4.39493	0.71439
H	-1.15949	-4.58598	2.44222
C	-0.72179	-1.70136	2.8304
H	-1.43763	-1.15921	2.19974
H	-1.32054	-2.17159	3.62494
H	-0.03503	-0.989	3.30449
C	2.93296	1.28873	-0.43144
C	3.0708	2.47822	-1.49627
C	3.77825	1.89134	0.82582
C	2.22901	3.68371	-0.98663
C	4.488	3.01252	-1.21622
C	4.24193	3.28121	0.27405
C	3.06647	4.27152	0.17957
H	1.21775	3.38382	-0.69297
H	2.1291	4.40794	-1.80886
H	5.29929	2.31356	-1.43937
H	4.68555	3.93536	-1.78409
H	5.09894	3.66859	0.84513
H	2.49962	4.3801	1.11238

H	3.452	5.27125	-0.0724
C	2.72554	2.10163	-2.92733
H	3.37232	1.30661	-3.3232
H	1.68093	1.7614	-2.99108
H	2.83012	2.98218	-3.58046
C	2.93629	2.06704	2.09592
H	1.98838	2.58377	1.92319
H	2.7311	1.09789	2.57201
H	3.51107	2.67186	2.81452
C	5.01105	1.08533	1.2891
H	5.90094	1.23924	0.66684
H	5.28722	1.42165	2.29978
H	4.80703	0.00751	1.3417

Optimized reductive elimination transition structure of the active catalyst system (MeCu • BIFOP-H • cyclohexenone) of the reaction pathway (B3LYP-D3(BJ)/def2-SVP) **TS-9 (R)**



Imaginary frequency: -429.13 cm^{-1}

Energy: -3723.660165

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -3724.807506

0 1

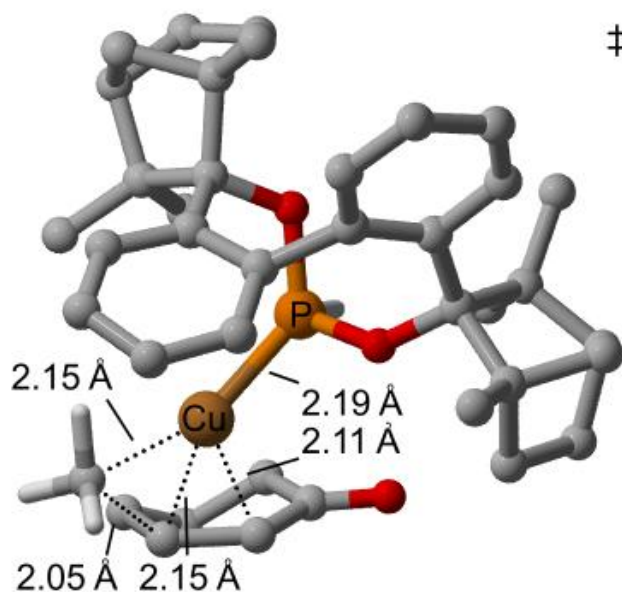
Cu	-2.10664	-0.85074	0.80099
C	-3.59083	-0.49258	2.31407
H	-3.08713	0.48694	2.20416
H	-4.67011	-0.3066	2.27127
H	-3.30757	-0.90658	3.28972
C	-1.37296	2.24463	3.28964
C	-1.25782	2.62811	1.95278
C	-0.53559	1.2517	3.78687
C	-0.32613	2.06598	1.06772
C	0.49663	0.78581	2.97413
C	0.67734	1.21414	1.64731
O	0.15332	1.11818	-1.05259
O	0.76762	-1.15625	0.06266
C	2.11201	1.0677	1.16121
C	2.89346	2.04072	1.8274
P	-0.475	-0.34405	-0.57131
C	2.77357	0.14894	0.29785
C	4.2539	2.21638	1.61614
C	4.14634	0.3814	0.07615
C	4.88167	1.38778	0.69339
H	4.6905	-0.27257	-0.58743
H	5.94525	1.49441	0.468
H	4.80137	2.99343	2.15385
H	2.38384	2.70269	2.52871
H	1.24678	0.11657	3.3959
H	-0.63688	0.88748	4.81144

H	-2.13844	2.70283	3.91929
H	-1.9444	3.38089	1.58859
H	-0.63168	-0.88694	-1.85795
C	-0.41642	2.3033	-0.46288
C	0.3575	3.58267	-0.96694
C	-1.8979	2.55574	-1.15838
C	0.50713	3.49289	-2.51305
C	-0.74811	4.64786	-0.81894
C	-1.7272	3.97684	-1.78314
C	-0.87566	3.92443	-3.06127
H	0.80031	2.48068	-2.81882
H	1.30421	4.17632	-2.84067
H	-1.11604	4.75242	0.21137
H	-0.41052	5.63858	-1.16098
H	-2.69772	4.47655	-1.91971
H	-1.27254	3.2533	-3.8331
H	-0.82839	4.92951	-3.50831
C	1.66905	3.92839	-0.29153
H	1.55727	4.02681	0.79546
H	2.44224	3.17718	-0.49393
H	2.02864	4.89445	-0.68082
C	-3.14975	2.5491	-0.26304
H	-3.17145	1.67855	0.40479
H	-3.27222	3.4596	0.33593
H	-4.03555	2.48856	-0.91429
C	-2.199	1.51046	-2.24998
H	-2.55337	0.56717	-1.80607
H	-3.02271	1.88344	-2.87752
H	-1.3492	1.285	-2.90109

C	2.17892	-1.19498	-0.1797
C	2.71522	-2.36669	0.76051
C	2.5647	-1.77351	-1.65421
C	1.8284	-3.62302	0.51808
C	4.00544	-2.79036	0.03405
C	3.31338	-3.10328	-1.29836
C	2.32247	-4.18805	-0.83693
H	0.75798	-3.39437	0.49015
H	1.99912	-4.33502	1.34001
H	4.78652	-2.02421	-0.00578
H	4.44685	-3.68609	0.4987
H	3.96869	-3.42028	-2.12388
H	1.49544	-4.37918	-1.52928
H	2.86377	-5.13804	-0.7048
C	2.82862	-2.01707	2.23442
H	3.49359	-1.16185	2.42075
H	1.83595	-1.78457	2.64783
H	3.22319	-2.88234	2.78975
C	1.3458	-2.08691	-2.53875
H	0.5305	-2.60868	-2.02514
H	0.95881	-1.17185	-3.01065
H	1.68511	-2.7409	-3.35774
C	3.46389	-0.87384	-2.5266
H	4.52756	-0.91227	-2.26092
H	3.39908	-1.22343	-3.56815
H	3.13762	0.17631	-2.50449
O	-1.15458	-3.792	-0.97093
C	-2.19937	-3.23658	-0.59502
C	-2.50698	-2.92457	0.77173

H	-1.86447	-3.38511	1.52898
C	-3.71228	-2.22225	1.21145
H	-4.1544	-2.63722	2.12161
C	-3.26663	-2.8772	-1.63904
H	-3.16125	-3.60127	-2.4604
H	-3.03013	-1.88439	-2.06901
C	-4.67544	-2.86519	-1.04744
H	-4.93407	-3.88068	-0.70157
H	-5.42243	-2.58691	-1.80954
C	-4.74347	-1.88529	0.12434
H	-5.75071	-1.85706	0.56909
H	-4.5636	-0.87015	-0.26982

Optimized reductive elimination transition structure of the active catalyst system (MeCu • BIFOP-H • cyclohexenone) of the reaction pathway (B3LYP-D3(BJ)/def2-SVP)**TS-10 (S)**



Imaginary frequency: -463.18 cm^{-1}

Energy: -3723.656037

Energy (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP): -3724.802586

0 1			
Cu	0.20455	-2.53549	-0.41386
C	-0.70915	-4.33202	0.35015
H	-1.36935	-4.52884	-0.50773
H	-0.5655	-5.26368	0.90397
H	-1.18422	-3.61897	1.04524
C	-2.03879	-1.98493	2.92006
C	-2.59622	-1.33208	1.81814
C	-0.77661	-1.61112	3.36857
C	-1.94558	-0.30014	1.12845
C	-0.17943	-0.48351	2.80517
C	-0.75784	0.23187	1.74449
O	-1.23737	0.63008	-0.93181
O	1.26415	0.36203	-0.28807
C	-0.318	1.68122	1.6599
C	-0.85123	2.37045	2.773
P	0.04244	-0.43094	-1.00773
C	0.47862	2.41005	0.732
C	-0.75604	3.74545	2.94364
C	0.47209	3.81123	0.88314
C	-0.1327	4.48158	1.94324
H	0.99291	4.42305	0.16283
H	-0.0801	5.57164	1.99124
H	-1.1966	4.22681	3.81924
H	-1.40629	1.78742	3.50934
H	0.74113	-0.09122	3.23904
H	-0.28736	-2.14222	4.18784
H	-2.58499	-2.80253	3.39513

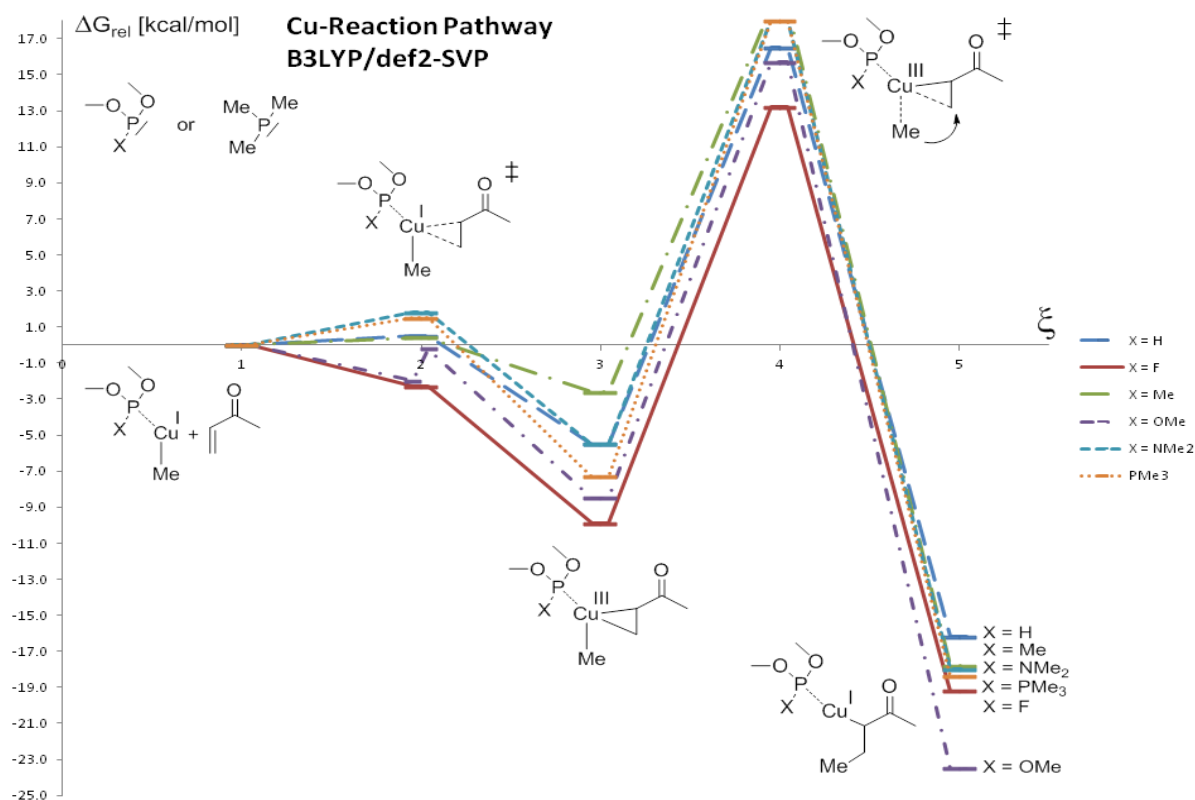
H	-3.56586	-1.66858	1.47604
H	0.2979	-0.26404	-2.37976
C	-2.43735	0.20457	-0.25444
C	-3.46907	1.40062	-0.18732
C	-3.24367	-0.82858	-1.26704
C	-3.53687	2.07038	-1.58936
C	-4.79787	0.61932	-0.14838
C	-4.5951	-0.08256	-1.49041
C	-4.4278	1.12195	-2.42898
H	-2.53205	2.20761	-2.00752
H	-3.98895	3.0683	-1.49076
H	-4.87708	-0.05773	0.71463
H	-5.66797	1.29397	-0.13343
H	-5.38904	-0.77686	-1.80312
H	-3.99859	0.86475	-3.4056
H	-5.41332	1.57257	-2.62392
C	-3.31232	2.42485	0.91817
H	-3.26661	1.95792	1.90992
H	-2.41655	3.04113	0.77968
H	-4.18475	3.0979	0.90419
C	-3.55574	-2.25248	-0.77907
H	-2.67534	-2.74949	-0.3604
H	-4.37059	-2.2967	-0.04545
H	-3.89023	-2.84442	-1.64518
C	-2.49229	-1.02449	-2.59644
H	-1.65901	-1.736	-2.47751
H	-3.18056	-1.47359	-3.3287
H	-2.09618	-0.09904	-3.02501
C	1.54599	1.76894	-0.18732

C	2.95242	1.86954	0.55523
C	1.90443	2.46565	-1.6113
C	3.99098	1.01177	-0.22886
C	3.40734	3.28601	0.1579
C	3.35338	3.02354	-1.3544
C	4.38901	1.88993	-1.44067
H	3.59952	0.04302	-0.55263
H	4.85188	0.81218	0.42699
H	2.77568	4.09633	0.52997
H	4.43284	3.48431	0.50672
H	3.57078	3.88229	-2.00748
H	4.38602	1.33297	-2.38416
H	5.39827	2.31385	-1.32162
C	2.92252	1.53542	2.03725
H	2.27297	2.20974	2.61255
H	2.57144	0.5033	2.18796
H	3.93948	1.60462	2.45366
C	1.94262	1.46882	-2.78757
H	2.38258	0.49423	-2.54377
H	0.93754	1.31544	-3.20278
H	2.54281	1.91735	-3.59403
C	0.95327	3.58859	-2.07262
H	1.15245	4.56288	-1.61012
H	1.08042	3.73704	-3.15584
H	-0.0994	3.32605	-1.88953
O	3.4263	-1.82763	-1.68881
C	1.86046	-3.52961	-1.19982
H	1.66182	-3.65489	-2.26938
C	2.88523	-2.5773	-0.86309

C	3.34804	-2.52814	0.60033
H	3.51065	-1.47621	0.87145
H	4.34266	-3.00873	0.62596
C	2.40303	-3.21232	1.58723
H	1.49552	-2.5922	1.7269
H	2.87002	-3.29021	2.58274
C	1.98364	-4.58849	1.07502
H	1.3718	-5.12024	1.81835
H	2.88677	-5.20213	0.90001
C	1.25538	-4.46272	-0.25198
H	0.97465	-5.42011	-0.70086

Computed reaction pathways of the MeCu-catalyzed 1,4-addition

Full-optimized structures (B3LYP-D3(BJ)/def2-SVP)

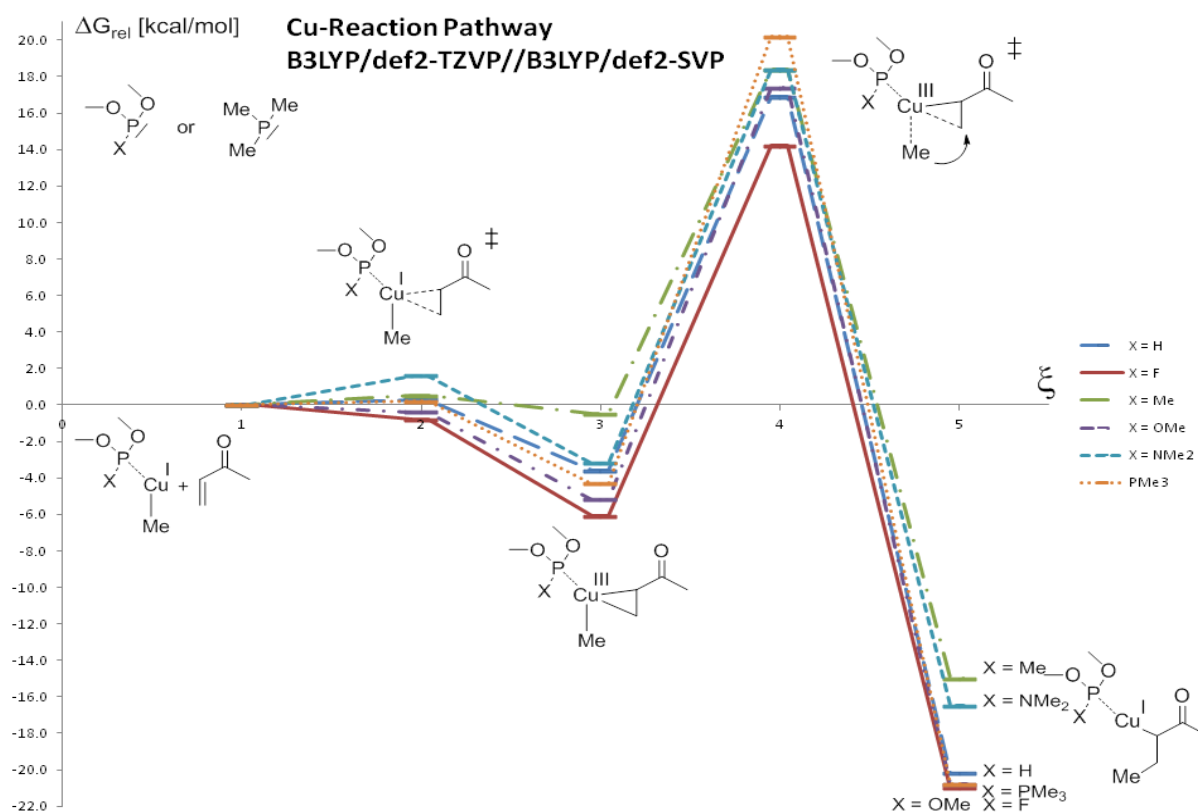


Energy Table 1 of full-optimized structures (B3LYP-D3(BJ)/def2-SVP)

Energy Table 1. Computed reaction pathway of the MeCu-catalyzed 1,4-addition to methyl-vinyl ketone with six different phosphorus ligands (T = 293.15 K, B3LYP-D3(BJ)/def2-SVP, solvent = diethylether, ZPE scaled by 0.9912 for B3LYP-D3(BJ)/def2-SVP [1].

(MeO) ₂ P-X or PMe ₃	E _a [kcal/mol] oxidative addition ‡	E _H [kcal/mol] cuprate	E _a [kcal/mol] reductive elimination ‡	E _H [kcal/mol] product
X = H	0.5	-5.5	22.0	-16.2
X = F	-2.3	-9.9	23.1	-19.2
X = Me	0.4	-2.6	21.3	-17.8
X = OMe	-2.0	-8.5	24.2	-23.5
X = NMe ₂	1.8	-5.5	22.6	-18.0
PMe ₃	1.5	-7.3	25.3	-18.4

Singlepoint structures (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP)

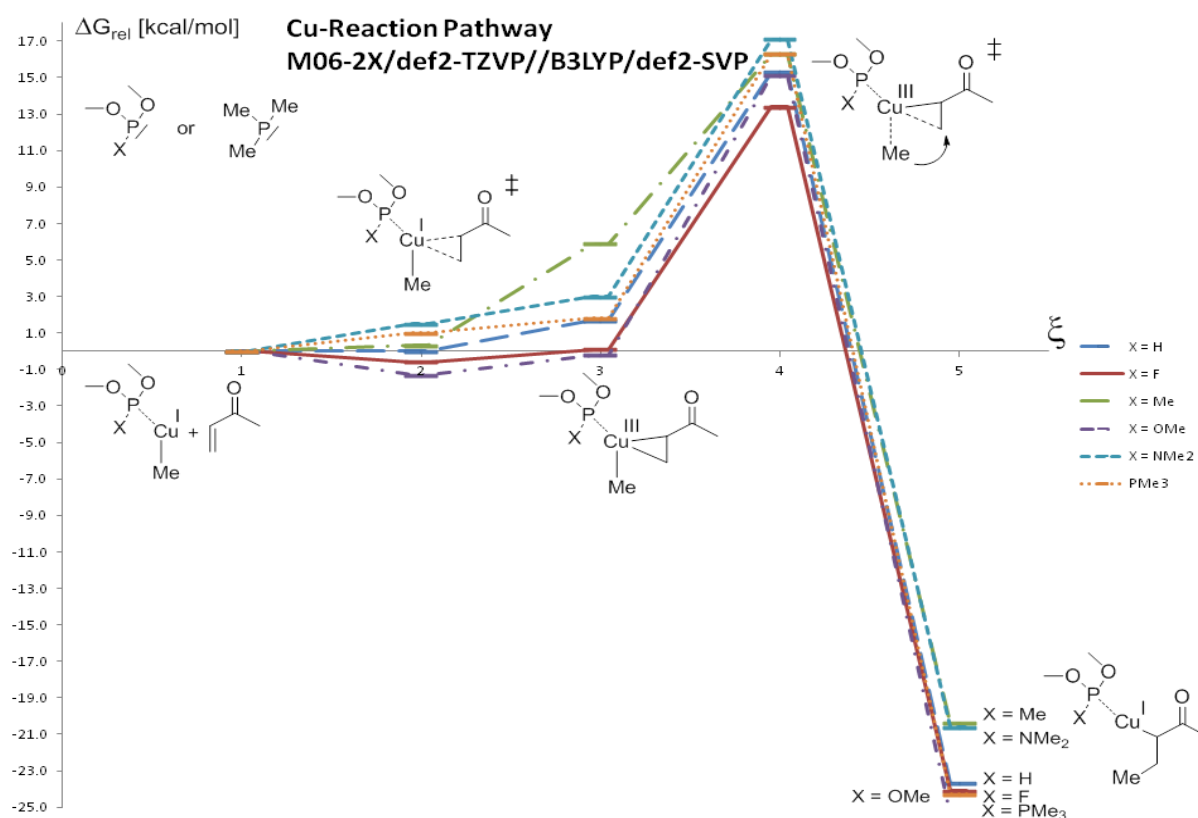


Energy Table 2 of singlepoint structures (B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP)

Energy Table 2. Computed reaction pathway of the MeCu-catalyzed 1,4-addition to methylvinyl ketone with six different phosphorus ligands (T = 293.15 K, B3LYP-D3(BJ)/def2-TZVP//B3LYP-D3(BJ)/def2-SVP, solvent = diethylether, ZPE scaled by 0.9896 for B3LYP-D3(BJ)/def2-TZVP and 0.9912 for B3LYP-D3(BJ)/def2-SVP [1].

(MeO) ₂ P-X) or PMe ₃	E _{a‡} [kcal/mol] oxidative addition	E _H [kcal/mol] cuprate	E _{a‡} [kcal/mol] reductive elimination	E _H [kcal/mol] product
X = H	0.3	-3.6	20.5	-20.2
X = F	-0.8	-6.1	20.3	-21.0
X = Me	0.5	-0.5	18.9	-15.0
X = OMe	-0.4	-5.2	22.6	-20.8
X = NMe ₂	1.6	-3.2	21.6	-16.5
PMe ₃	0.2	-4.3	24.5	-20.8

Singlepoint structures (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP)



Important: The singlepoint structures of the M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP method are not appropriate for the cuprate-intermediate structure and not taken.

Energy Table 3 of singlepoint structures (M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP)

Energy Table 3. Computed reaction pathway of the MeCu-catalyzed 1,4-addition to methyl-vinyl ketone with six different phosphorus ligands (T = 293.15 K, M06-2X-D3/def2-TZVP//B3LYP-D3(BJ)/def2-SVP, solvent = diethylether, ZPE scaled by 0.9754 for M06-2X-D3/def2-TZVP and 0.9912 for B3LYP-D3(BJ)/def2-SVP [1].

(MeO) ₂ P-X) or PMe ₃	E _a [kcal/mol] oxidative addition ‡	E _H [kcal/mol] cuprate	E _a [kcal/mol] reductive elimination ‡	E _H [kcal/mol] product
X = H	0.0	1.7	13.6	-23.7
X = F	-0.36	0.1	13.3	-24.1
X = Me	0.3	5.9	10.4	-20.4
X = OMe	-1.3	-0.2	15.3	-25.4
X = NMe ₂	1.5	3.0	14.1	-20.6
PMe ₃	1.0	1.8	14.5	-24.3

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