

Electronic Supplementary Information for

**On the catalytic performance of $(\text{ZrO})_n$ ($n = 1-4, 12$) clusters for
Suzuki-Miyaura cross-coupling: A DFT study**

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1. Tables

Table S1 Binding energy (E_b , in eV) and energy gap (E_g , in eV) values of $(\text{ZrO})_n$ ($n = 1-4, 12$) and Pd_n ($n = 1-4, 12$) clusters at the PBE0/Def2-TZVP level.

Clusters	E_b	E_g
ZrO	---	3.12
$(\text{ZrO})_2$	1.66	2.29
$(\text{ZrO})_3$	2.58	2.12
$(\text{ZrO})_4$	3.30	1.95
$(\text{ZrO})_{12}$	4.21	1.49
Pd	---	3.03
Pd_2	0.51	3.15
Pd_3	0.86	2.17
Pd_4	1.31	2.15
Pd_{12}	1.97	1.71

Table S2 Fukui function and dual descriptor values of orbital weights for each atom of $(\text{ZrO})_n$ ($n = 1-4$) clusters (in $|e|$).

Clusters	Atoms	f^+	DD
ZrO	1(Zr)	0.921	0.035
	2(O)	0.079	-0.035
$(\text{ZrO})_2$	1(Zr)	0.438	-0.065
	2(Zr)	0.511	0.095
	3(O)	0.026	-0.015
	4(O)	0.026	-0.015
$(\text{ZrO})_3$	1(Zr)	0.200	-0.079
	2(Zr)	0.369	0.058
	3(Zr)	0.371	0.060
	4(O)	0.021	-0.011
	5(O)	0.017	-0.017
	6(O)	0.022	-0.011
$(\text{ZrO})_4$	1(Zr)	0.174	-0.001
	2(Zr)	0.235	-0.022
	3(O)	0.015	-0.015
	4(O)	0.015	-0.015
	5(O)	0.017	-0.020
	6(Zr)	0.265	0.049
	7(Zr)	0.265	0.049
	8(O)	0.013	-0.025

Table S3 NPA charges on the $(\text{ZrO})_n$ ($n = 1-4$) subunits of **IS2** and **TS2** during the transmetalation step (in $|e|$).

Clusters	Q_{IS2}	Q_{TS2}	ΔQ
ZrO	0.939	0.997	0.058
$(\text{ZrO})_2$	1.633	1.500	-0.133
$(\text{ZrO})_3$	1.171	1.084	-0.087
$(\text{ZrO})_4$	1.811	1.549	-0.262

Table S4 Fukui function and dual descriptor values of orbital weights for each atom of (ZrO)₁₂ cluster (in |e|).

Cluster	Atoms	f^+	DD
(ZrO) ₁₂	1(Zr)	0.120	0.048
	2(Zr)	0.073	0.001
	3(Zr)	0.053	-0.013
	4(Zr)	0.094	0.019
	5(Zr)	0.053	-0.007
	6(Zr)	0.073	0.001
	7(Zr)	0.148	0.054
	8(Zr)	0.120	0.049
	9(Zr)	0.087	0.012
	10(Zr)	0.054	-0.005
	11(Zr)	0.054	-0.012
	12(Zr)	0.034	-0.059
	13(O)	0.003	-0.009
	14(O)	0.006	-0.003
	15(O)	0.006	-0.003
	16(O)	-0.003	-0.013
	17(O)	-0.003	-0.013
	18(O)	0.003	-0.009
	19(O)	0.003	-0.005
	20(O)	0.005	-0.006
	21(O)	0.004	-0.005
	22(O)	0.005	-0.005
	23(O)	0.004	-0.008
	24(O)	0.004	-0.008

2. Figures

Figure S1 (a) Schematic diagram of possible mechanisms and (b) Gibbs free energy profile of Suzuki-Miyaura reaction catalyzed by $\text{Pd}(\text{PPh}_3)_2$. The spin multiplicities are given as superscript and the related bond lengths are given in Å, while paths **I** and **II** refers to whether the $\text{B}(\text{OH})_3$ is removed or not during the reduction elimination step in b.

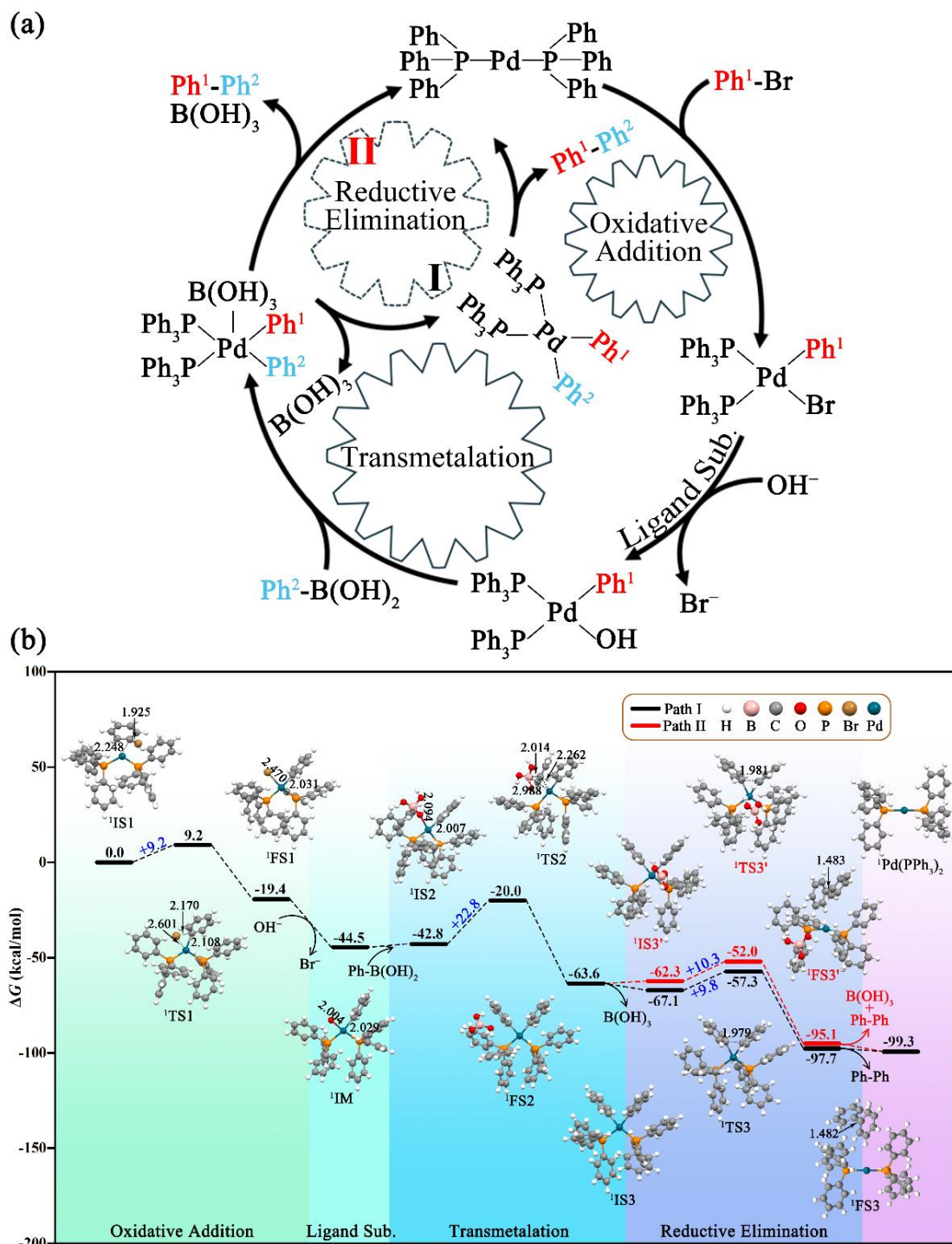


Figure S2 Gibbs free energy profile of Suzuki-Miyaura reaction catalyzed by Pd with corresponding geometric structures, where the spin multiplicities of each structure are indicated by the superscripts and crucial bond lengths are given in Å, while paths **I** and **II** refers to whether the B(OH)₃ is removed or not during the reduction elimination step.

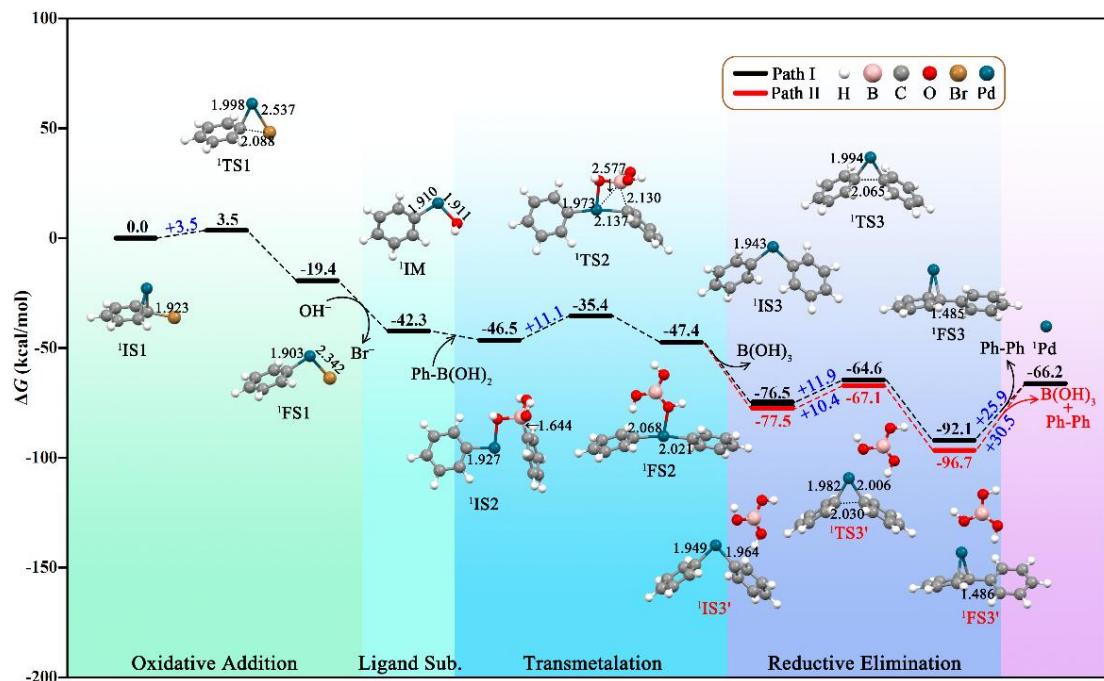


Figure S3 Gibbs free energy profile of Suzuki-Miyaura reaction catalyzed by Pd₂ with corresponding geometric structures, where the spin multiplicities of each structure are indicated by the superscripts and crucial bond lengths are given in Å, while paths **I** and **II** refers to whether the B(OH)₃ is removed or not during the reduction elimination step.

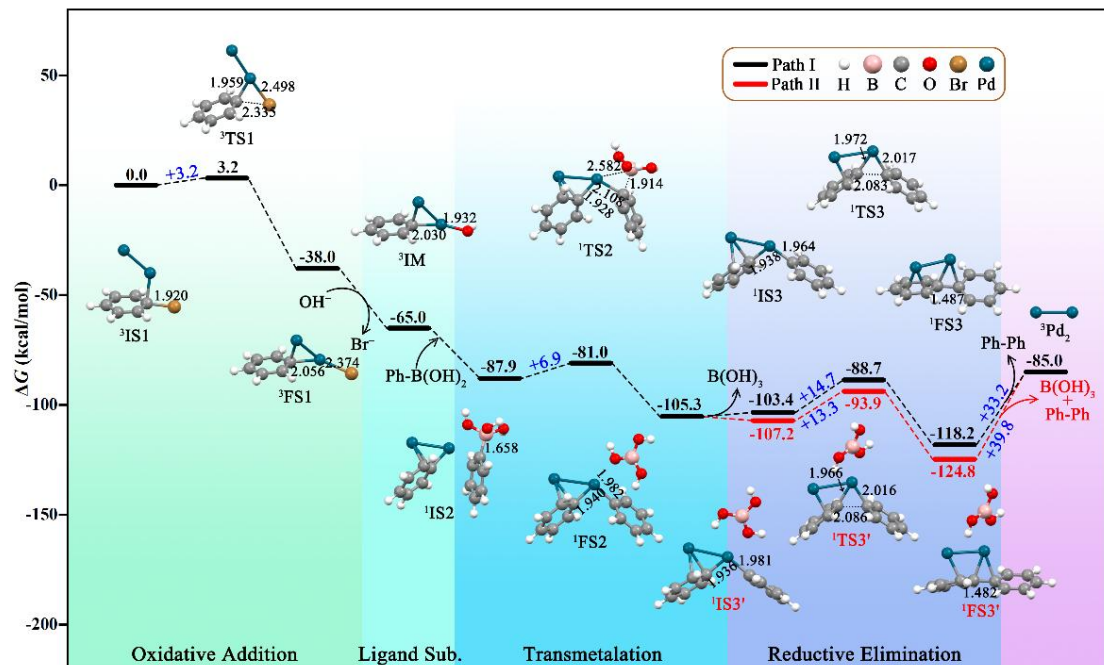


Figure S4 Gibbs free energy profile of Suzuki-Miyaura reaction catalyzed by Pd₃ with corresponding geometric structures, where the spin multiplicities of each structure are indicated by the superscripts and crucial bond lengths are given in Å, while paths **I** and **II** refers to whether the B(OH)₃ is removed or not during the reduction elimination step.

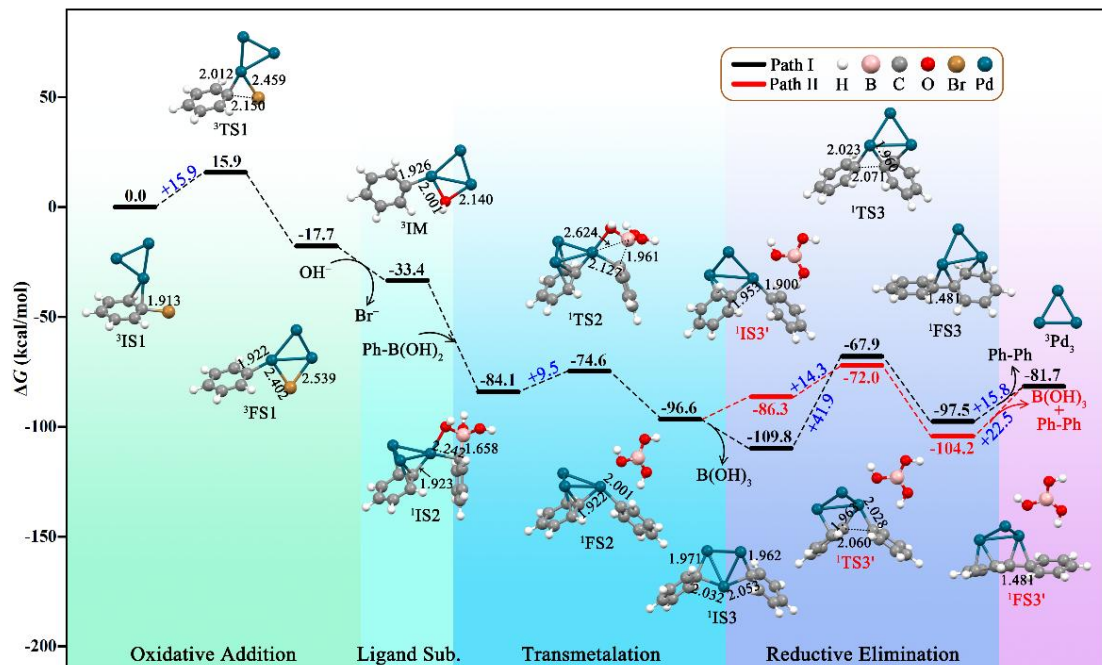


Figure S5 Gibbs free energy profile of Suzuki-Miyaura reaction catalyzed by Pd₄ with corresponding geometric structures, where the spin multiplicities of each structure are indicated by the superscripts and crucial bond lengths are given in Å, while paths **I** and **II** refers to whether the B(OH)₃ is removed or not during the reduction elimination step.

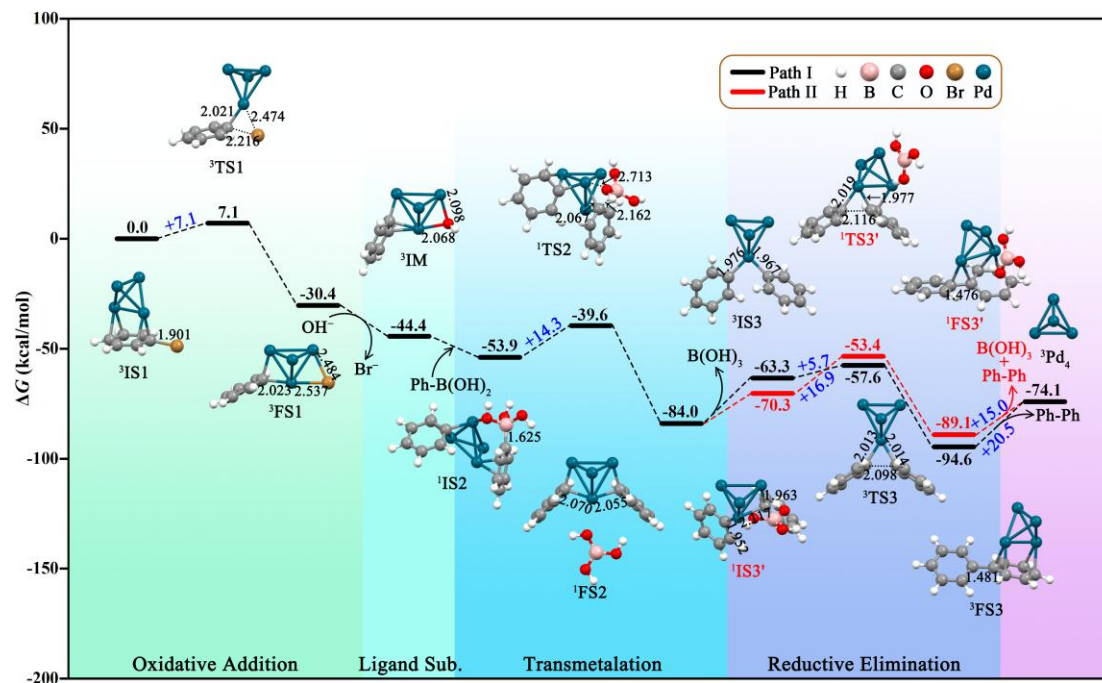


Figure S6 The optimized structures of $(\text{ZrO})_n$ ($n = 1-4$) with different spin multiplicities, symmetric point groups, and relative energies (E_{rel} , in eV).

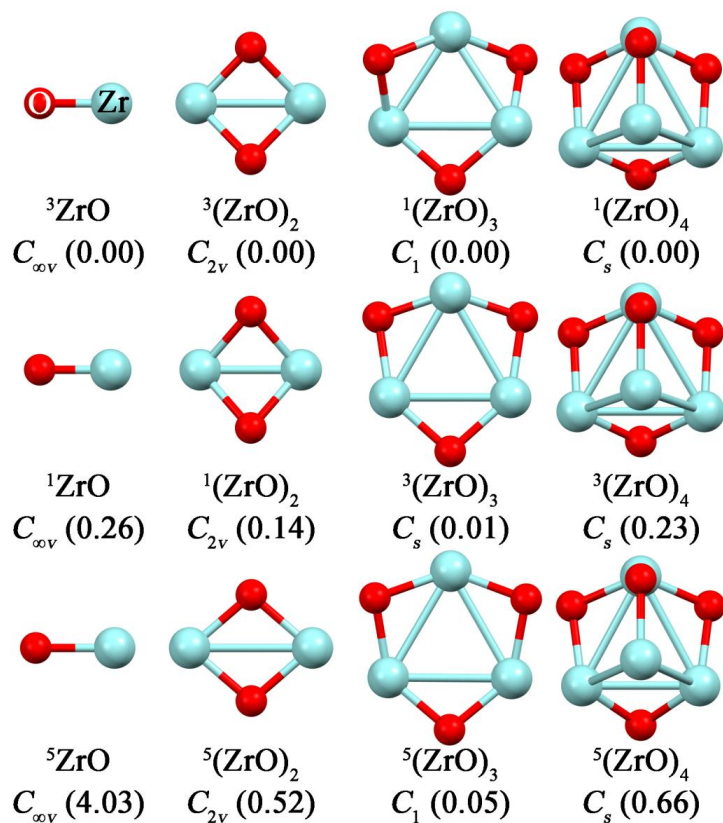


Figure S7 (a) ESP plots as well as (b) Fukui function and dual descriptor values of orbital weights plot of $(\text{ZrO})_n$ ($n = 1-4$) (Isovalue = 0.002 a.u.), where cyan and yellow spheres represent the minima and maxima of the surface electrostatic potential in **a**, and the green and blue regions indicate the positive and negative values in **b**, respectively.

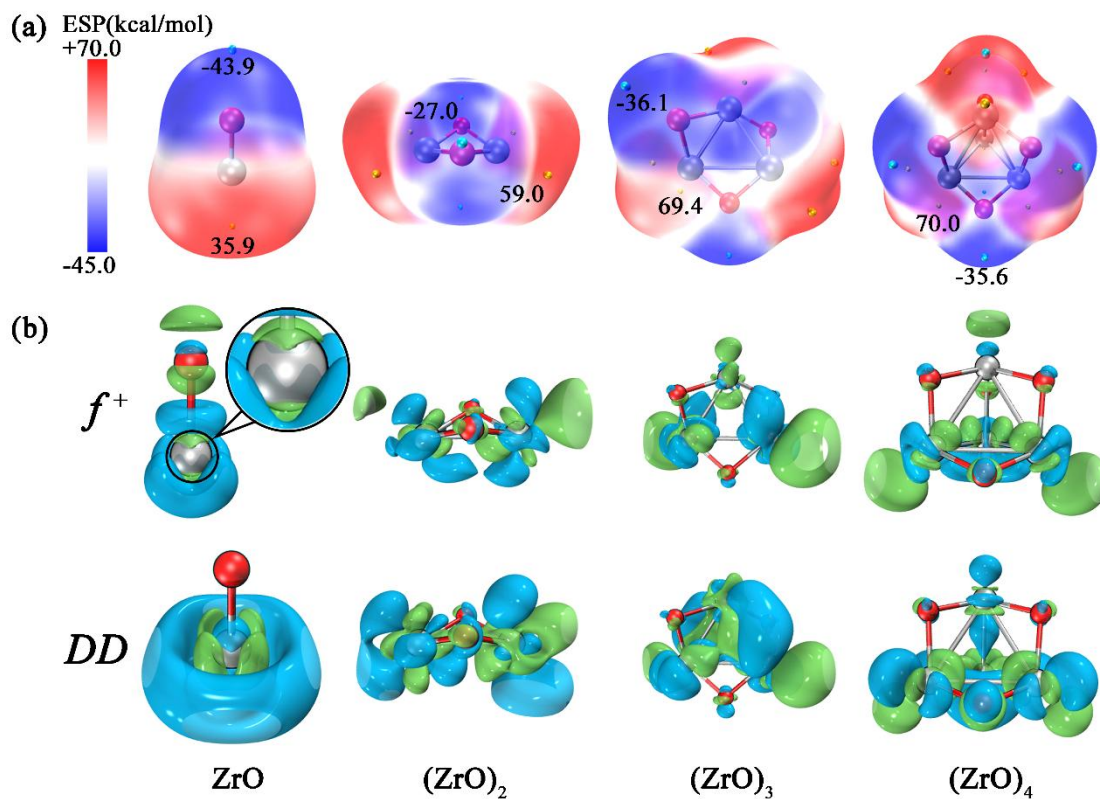


Figure S8 Time evolution of the potential energies and structures of $(\text{ZrO})_{12}$ during the full length of 150 fs ADMP MD simulation.

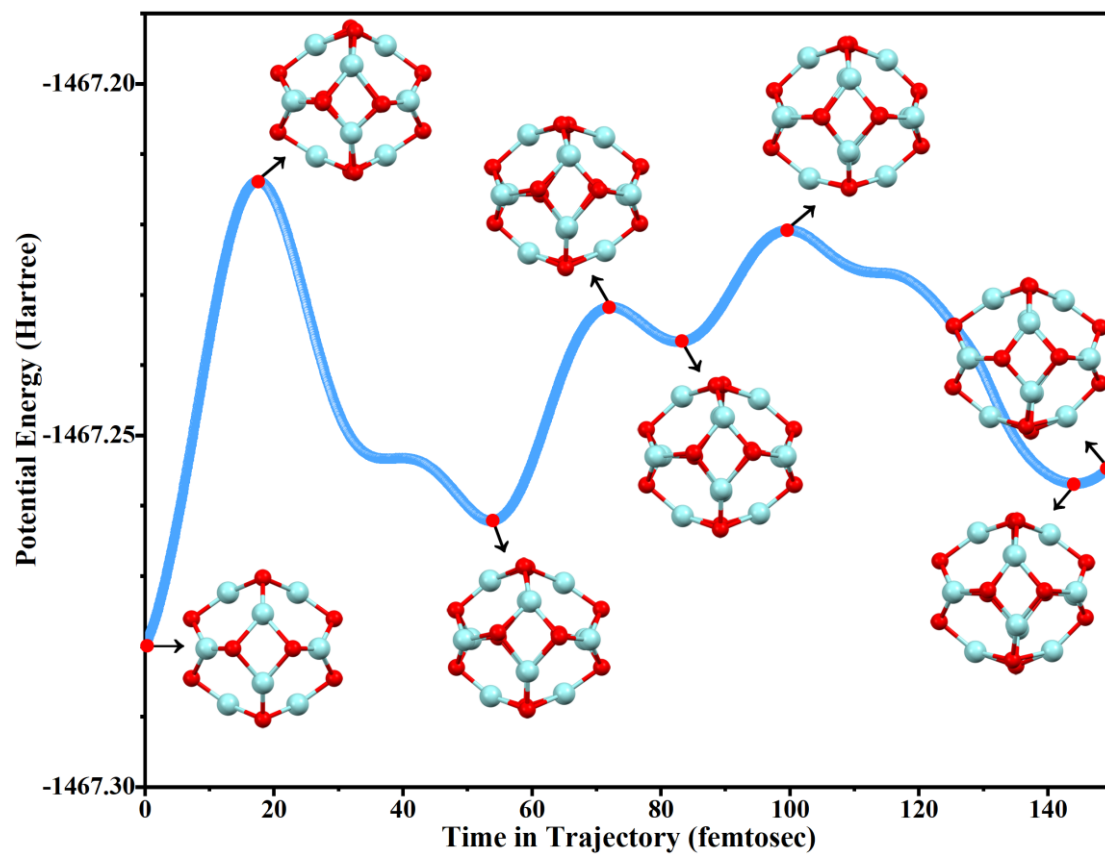
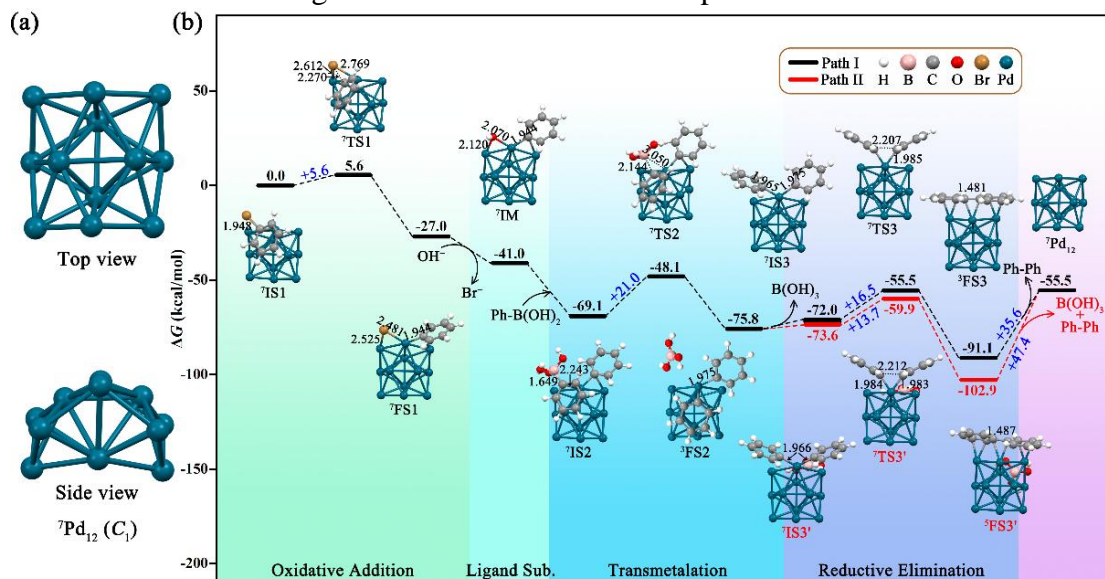


Figure S9 (a) Optimized structure of Pd₁₂ and (b) Gibbs free energy profile of Suzuki-Miyaura reaction catalyzed by Pd₁₂ with corresponding geometric structures, where the spin multiplicities of each structure are indicated by the superscripts and crucial bond lengths are given in Å, while paths **I** and **II** refers to whether the B(OH)₃ is removed or not during the reduction elimination step.



3. Cartesian Coordinates

(1) The optimized structures of $(\text{ZrO})_n$ ($n = 1-4$, and 12) and Pd_n ($n = 1-4$, and 12)

ZrO

Zr	0.00000000	0.00000000	0.28715900
O	0.00000000	0.00000000	-1.43579500

(ZrO)₂

Zr	0.00000000	1.30727200	-0.09000300
Zr	0.00000000	-1.30727200	-0.09000300
O	-1.34091900	0.00000000	0.45001500
O	1.34091900	0.00000000	0.45001500

(ZrO)₃

Zr	0.00194000	1.52604000	0.00018400
Zr	-1.47064300	-0.73217100	-0.19505700
Zr	1.46867500	-0.73536500	0.19469100
O	-1.71732600	0.86461800	0.83329700
O	-0.00208500	-2.01903300	0.00093300
O	1.71954900	0.86189300	-0.83332500

(ZrO)₄

Zr	0.26393600	1.72499700	0.00000000
Zr	1.65799100	-0.79925300	0.00000000
O	-0.80883800	1.23434100	1.56930700
O	-0.80883800	1.23434100	-1.56930700
O	2.12553800	1.09496000	0.00000000
Zr	-0.80883800	-0.71265100	1.47609200
Zr	-0.80883800	-0.71265100	-1.47609200
O	-2.02911400	-1.06585200	0.00000000

(ZrO)₁₂

Zr	0.00000000	-1.54397000	2.49960600
Zr	0.00000000	1.54397000	2.49960600
Zr	2.49960600	0.00000000	1.54397000
Zr	1.54397000	2.49960600	0.00000000
Zr	2.49960600	0.00000000	-1.54397000
Zr	0.00000000	1.54397000	-2.49960600
Zr	1.54397000	-2.49960600	0.00000000
Zr	0.00000000	-1.54397000	-2.49960600
Zr	-1.54397000	-2.49960600	0.00000000
Zr	-2.49960600	0.00000000	-1.54397000
Zr	-2.49960600	0.00000000	1.54397000
Zr	-1.54397000	2.49960600	0.00000000
O	-1.33976400	0.00000000	3.16933100

O	-3.16933100	1.33976400	0.00000000
O	-3.16933100	-1.33976400	0.00000000
O	0.00000000	-3.16933100	1.33976400
O	0.00000000	-3.16933100	-1.33976400
O	-1.33976400	0.00000000	-3.16933100
O	3.16933100	-1.33976400	0.00000000
O	0.00000000	3.16933100	-1.33976400
O	3.16933100	1.33976400	0.00000000
O	0.00000000	3.16933100	1.33976400
O	1.33976400	0.00000000	3.16933100
O	1.33976400	0.00000000	-3.16933100
Pd			
Pd	0.00000000	0.00000000	0.00000000
Pd₂			
Pd	0.00000000	0.00000000	1.24316700
Pd	0.00000000	0.00000000	-1.24316700
Pd₃			
Pd	0.00000000	0.00000000	1.46963500
Pd	0.00000000	-1.25963900	-0.73481800
Pd	0.00000000	1.25963900	-0.73481800
Pd₄			
Pd	0.00000000	-1.26520900	-0.97338500
Pd	1.26520900	0.00000000	0.97338500
Pd	0.00000000	1.26520900	-0.97338500
Pd	-1.26520900	0.00000000	0.97338500
Pd₁₂			
Pd	2.79333500	1.53407200	0.09850700
Pd	0.35502100	2.35881000	1.44679700
Pd	-1.67668600	2.63144200	-0.31704400
Pd	-2.11835600	0.42461900	-1.61122500
Pd	-2.76078800	-1.66021500	-0.09260700
Pd	-0.71917200	-2.11045900	1.52975200
Pd	1.82328000	-2.50160600	0.16012500
Pd	2.49047800	-0.55901800	-1.41416700
Pd	1.10681800	-0.17950200	1.14057900
Pd	-1.54231800	0.39219700	1.09499300
Pd	0.46186100	1.14625800	-0.98796400
Pd	-0.21347300	-1.47659800	-1.04774800

(2) The optimized structures of PhBr@(ZrO)_n (n = 1-4, 12)

Isomer II of PhBr@ZrO

Zr	2.22197500	0.34541900	-0.42652800
O	2.33865500	1.41703100	0.93037100
C	-2.71172300	1.78190800	0.25950300
C	-1.52864600	1.07363600	0.42297200
C	-1.52961500	-0.27023900	0.10493900
C	-2.64654000	-0.93316600	-0.36279100
C	-3.81920700	-0.20604800	-0.52088800
C	-3.85158300	1.14595900	-0.21131100
H	-2.73681300	2.83711900	0.50575900
H	-0.62798300	1.55377300	0.79143400
H	-2.60905500	-1.98905600	-0.60093500
H	-4.70882400	-0.70358600	-0.88964100
H	-4.77035900	1.70658200	-0.33695100
Br	0.12539100	-1.26028900	0.34268400

Isomer II of PhBr@(ZrO)₂

Zr	-1.07214700	2.77834500	0.00000000
Zr	0.83767300	1.22219400	0.00000000
O	0.26411000	2.52437000	1.39668800
O	0.26411000	2.52437000	-1.39668800
C	0.26411000	-4.07172000	0.00000000
C	-0.05339000	-2.72972700	0.00000000
C	-1.34190500	-2.25484100	0.00000000
C	-2.37541400	-3.18230800	0.00000000
C	-2.09736300	-4.54209000	0.00000000
C	-0.78219600	-4.98559500	0.00000000
H	1.29581400	-4.40428700	0.00000000
H	-1.53347200	-1.18036300	0.00000000
H	-3.40269600	-2.83418900	0.00000000
H	-2.90884400	-5.26056100	0.00000000
H	-0.56370600	-6.04759300	0.00000000
Br	1.44523000	-1.43105200	0.00000000

Isomer II of PhBr@(ZrO)₃

Zr	1.67903000	0.81698500	1.37547300
Zr	0.69034000	-1.36906500	0.04620900
Zr	2.41361200	0.64251800	-1.23669200
O	1.44156000	-1.12146300	1.81724600
O	1.56156700	-1.07079100	-1.69332600
O	1.81657500	2.12184700	-0.15490800
C	-4.46020600	-0.01034400	-0.16645100
C	-3.08676300	0.09269600	-0.08878700

C	-2.41388100	1.28838700	-0.06684300
C	-3.16392400	2.45563200	-0.12434300
C	-4.54838500	2.39642500	-0.19781800
C	-5.19402300	1.16784200	-0.21726300
H	-4.95125700	-0.97609200	-0.18611300
H	-1.32372300	1.30024600	0.00225700
H	-2.65565300	3.41366300	-0.11397900
H	-5.12815200	3.31108300	-0.24185500
H	-6.27561900	1.11939100	-0.27286700
Br	-2.06684000	-1.58761100	-0.03343300

Isomer **II** of PhBr@(ZrO)₄

Zr	-1.70676000	-1.71876000	-0.61834200
Zr	0.59861900	0.40874200	-0.88428000
O	-3.18580100	-0.42396800	-1.04712600
O	-1.14552100	-2.05992500	1.25931600
O	-0.18630000	-1.27385600	-1.72081600
Zr	-2.38052100	1.19492000	-0.30743700
Zr	-0.61824000	-0.17651100	1.65218300
O	-2.14637100	1.12910000	1.62602900
C	2.86194500	1.39328200	-1.01574000
C	2.81758000	0.53241800	0.08649500
C	1.83836300	0.61141600	1.12471300
C	0.94939600	1.79132700	1.06386400
C	1.06911700	2.72854300	-0.00388100
C	1.94033800	2.49492800	-1.07865100
H	3.59255000	1.24174400	-1.80151200
H	2.07566900	0.15658700	2.09170500
H	0.43350000	2.11751600	1.97523500
H	0.41590300	3.59527900	-0.01806700
H	1.99356000	3.18708200	-1.91106200
Br	4.00618400	-0.99760500	0.11367800

Isomer **III** of PhBr@(ZrO)₄

Zr	2.52891200	-0.23707700	-1.48469000
Zr	-0.14532400	0.45791900	-0.44801800
O	2.50191800	-2.01071700	-0.61649700
O	3.42283900	1.08999000	-0.33312500
O	0.80741300	0.33220100	-2.17951700
Zr	1.32598400	-1.69875500	0.89866300
Zr	2.17771700	1.21577500	1.15823900
O	2.29064200	-0.49244900	2.07997100
C	-5.44823300	0.65423700	-0.05021400
C	-4.17108100	0.14329200	0.04164500

C	-3.90124100	-1.20438200	0.07722500
C	-4.97004400	-2.08898600	0.01697000
C	-6.26939300	-1.60976800	-0.07741300
C	-6.50785500	-0.24290200	-0.11064800
H	-5.62165900	1.72414300	-0.07616900
H	-2.87283400	-1.55783600	0.14923600
H	-4.78316800	-3.15723100	0.04349000
H	-7.10014000	-2.30419200	-0.12614200
H	-7.52275900	0.13182600	-0.18559100
Br	-2.63332600	1.43964800	0.12101100

Isomer IV of PhBr@(ZrO)₄

Zr	0.44862500	-0.18846900	-0.14697700
Zr	-1.72036000	-0.39339000	1.76080600
O	-0.07406000	1.64525000	-0.64228100
O	-0.48387200	-1.33889700	-1.44383000
O	0.20693300	-0.64067900	1.78186300
Zr	-1.97231800	1.69402700	-0.19338900
Zr	-2.35743900	-1.12840100	-0.94405600
O	-2.76878700	0.64711800	-1.63088100
C	3.68480900	0.76530100	-1.19001500
C	3.27709000	0.08155200	-0.04797200
C	3.00547800	0.74191600	1.14728800
C	3.11340200	2.12866800	1.17288700
C	3.50504300	2.82630500	0.04348200
C	3.79473100	2.14332300	-1.13228800
H	3.90120000	0.22442500	-2.10234900
H	2.69915400	0.18813500	2.02601300
H	2.88445700	2.65551300	2.09139200
H	3.58170900	3.90623700	0.07353800
H	4.09965800	2.68764900	-2.01808100
Br	3.13052800	-1.81821100	-0.10300300

Isomer I of PhBr@(ZrO)₁₂

Zr	1.52365700	-1.58332400	-2.38191800
Zr	1.31804100	-2.88815000	0.37474800
Zr	3.51587500	-0.74031400	-0.14410800
Zr	1.96050600	-0.71720800	2.56337700
Zr	2.64836600	1.95476500	1.08612700
Zr	-0.15442500	1.43018200	2.39275800
Zr	2.31659700	1.44621100	-1.95720500
Zr	0.06117500	2.79216800	-0.41534200
Zr	-0.61773700	0.69954900	-2.56887900
Zr	-2.50508500	0.78603200	0.13126300

Zr	-1.17019300	-1.96701900	-1.05593100
Zr	-0.96036400	-1.47772100	2.01621100
O	0.36159400	-3.18883500	-1.53098700
O	-2.33836200	-1.33918700	0.58085800
O	-2.16354900	-0.26704800	-1.76895000
O	1.26144800	0.17075900	-3.34020800
O	0.46032900	2.52324600	-2.36461000
O	-1.37983400	2.34443500	0.97605300
O	3.81441500	1.30448700	-0.63353700
O	0.06019800	-0.25297800	3.46685700
O	3.60761200	0.13715800	1.77014700
O	0.87450000	-2.53216500	2.30379300
O	2.90534000	-2.45472100	-1.00121100
O	1.04310600	3.02515600	1.48743600
C	-5.00039300	0.25785300	-0.01539500
C	-4.67563300	0.87453700	-1.20636600
C	-4.00596100	2.16061000	-1.22544100
C	-4.05638900	2.87722800	0.02145500
C	-4.36914500	2.24311800	1.20574000
C	-4.67895900	0.84064700	1.26577000
H	-4.84618100	0.34310900	-2.14328500
H	-3.91142500	2.69624400	-2.17019200
H	-3.72145600	3.91625500	0.05302300
H	-4.26910500	2.79327100	2.14414000
H	-5.02499800	0.37624300	2.18713300
Br	-5.80053800	-1.45195400	-0.04441400

Isomer II of PhBr@(ZrO)₁₂

Zr	1.32858700	-2.79973700	-0.82859100
Zr	3.09781000	-0.47940400	-1.76008900
Zr	0.26170000	-0.72639300	-2.77116400
Zr	1.35522700	2.10901200	-2.01196000
Zr	-1.62313400	1.28515000	-1.25750300
Zr	0.29842200	2.76862800	0.75597700
Zr	-1.64172000	-1.71626800	-0.45665900
Zr	-1.61520800	0.47572900	1.74645100
Zr	0.27093300	-2.03685000	2.02159000
Zr	1.36587000	0.67916900	2.83134400
Zr	3.10299900	-1.29817400	1.26389100
Zr	3.12075400	1.73073600	0.46417700
O	3.36336200	-2.18530000	-0.52417400
O	3.39226100	0.62216700	2.12266600
O	1.88159800	-1.41140900	3.03332800
O	-0.30805900	-3.18928500	0.25626000

O	-1.75616400	-1.53766500	1.64628800
O	-0.26505200	1.82423900	2.64743400
O	-1.76402500	-0.62365200	-2.15253100
O	1.89896600	3.32740300	-0.30780200
O	-0.29086000	1.38697700	-2.89138400
O	3.38092900	1.51066100	-1.63036100
O	1.85504400	-1.93883600	-2.74164200
O	-1.73631100	2.20554600	0.53800900
C	-8.25494800	-1.22756800	-0.01527200
C	-8.96502500	-0.02571400	-0.01473600
C	-8.28231500	1.19188100	-0.00788800
C	-6.88313000	1.20904800	-0.00130300
C	-6.19648900	0.00555400	-0.00250100
C	-6.85584400	-1.21246300	-0.00902600
H	-8.79339200	-2.18055300	-0.02039200
H	-10.05799100	-0.03804700	-0.01952800
H	-8.84229700	2.13240000	-0.00734500
H	-6.34433500	2.16483400	0.00509000
H	-6.29521900	-2.15607900	-0.00881400
Br	-3.91838000	0.02406800	0.01394400

Isomer **III** of PhBr@(ZrO)₁₂

Zr	-1.76196200	2.23000900	1.73936000
Zr	-1.51710400	2.60862300	-1.27536100
Zr	1.02496100	2.32315200	0.43333600
Zr	0.90361900	0.86403000	-2.33749600
Zr	2.05829800	-0.62834200	0.15935500
Zr	0.22610500	-2.19417700	-1.70959400
Zr	0.47070900	0.21958400	2.70956700
Zr	-0.02458000	-2.54379300	1.27762500
Zr	-2.44774600	-0.80195100	2.29300700
Zr	-2.63942900	-2.21953700	-0.42668800
Zr	-3.66935500	0.62007400	-0.16561900
Zr	-2.04638200	-0.18121000	-2.63436300
O	-3.11966300	2.53650000	0.13231200
O	-3.70034800	-0.86597200	-1.72578800
O	-3.90705600	-1.19052800	0.96470900
O	-1.50087100	0.86810400	3.20910400
O	-0.59503500	-1.61112600	2.97265800
O	-0.98472100	-3.37267500	-0.44536300
O	2.04123100	0.90084400	1.67101700
O	-0.08922200	-0.81791700	-3.16650100
O	2.28808300	1.23623900	-0.92278000
O	-0.98436400	1.64625600	-2.95537900

O	-0.61335400	3.49692200	0.46427100
O	1.61272100	-2.58947200	-0.12607600
C	6.41843600	2.23776900	-0.41425900
C	7.71212000	2.09141000	0.08377000
C	8.15108200	0.84409100	0.52594700
C	7.30271500	-0.26110500	0.47113400
C	6.01747300	-0.08570000	-0.03382300
C	5.55058700	1.14673700	-0.48009700
H	6.06866900	3.21373800	-0.75952200
H	8.38161500	2.95334500	0.12939800
H	9.16302800	0.72318900	0.91964100
H	7.63765700	-1.24096400	0.81620500
H	4.52778700	1.26451100	-0.85422200
Br	4.87549000	-1.61453900	-0.12200500

(3) The optimized structures of the species involved in Suzuki-Miyaura cross-coupling mechanism catalyzed by Pd(PPh₃)₂

Pd(PPh₃)₂

Pd	0.00000600	-0.00051300	0.00045000
P	2.28649700	-0.00012400	0.00014100
P	-2.28649300	-0.00028100	0.00020300
C	3.07722400	-0.08470500	1.66036100
C	2.46342700	-0.89585600	2.62534800
C	4.24256800	0.61315600	1.99941500
C	3.01695000	-1.02378100	3.89689200
H	1.53515800	-1.41697700	2.37067700
C	4.78873700	0.49265800	3.27773900
H	4.72415400	1.26089800	1.26260500
C	4.18089900	-0.32805600	4.22625300
H	2.52968700	-1.66090500	4.63925500
H	5.69579000	1.04661600	3.53293100
H	4.60991600	-0.41969600	5.22731400
C	3.07672700	1.48037600	-0.75645600
C	4.24020200	1.42529500	-1.53315100
C	2.46421900	2.72180000	-0.53361000
C	4.78582000	2.59291800	-2.06788100
H	4.72076300	0.46329000	-1.72806300
C	3.01726400	3.88723000	-1.05843900
H	1.53729300	2.76182500	0.04715700
C	4.17936600	3.82481300	-1.82846100
H	5.69138900	2.53707000	-2.67744200
H	2.53102000	4.84877500	-0.87554500
H	4.60797200	4.73781400	-2.24952900

C	3.07775100	-1.39528000	-0.90328200
C	4.24302700	-2.03771200	-0.46809200
C	2.46445400	-1.82541900	-2.08851400
C	4.78963100	-3.08437600	-1.21149200
H	4.72424800	-1.72351300	0.46146600
C	3.01842400	-2.86248100	-2.83497500
H	1.53620200	-1.34449200	-2.41280000
C	4.18231000	-3.49544000	-2.39677200
H	5.69662000	-3.58225100	-0.85903400
H	2.53154000	-3.18681800	-3.75812300
H	4.61166300	-4.31644900	-2.97657900
C	-3.07753100	1.39186900	0.90844900
C	-2.46435600	1.81762800	2.09532000
C	-4.24255700	2.03615000	0.47532000
C	-3.01820300	2.85217400	2.84535600
H	-1.53627400	1.33533300	2.41805400
C	-4.78904400	3.08029500	1.22233700
H	-4.72366700	1.72539800	-0.45545500
C	-4.18184600	3.48698200	2.40919000
H	-2.53140000	3.17311500	3.76973300
H	-5.69583700	3.57965500	0.87147900
H	-4.61109800	4.30603400	2.99183100
C	-3.07650900	0.09083500	-1.66001700
C	-4.24171600	-0.60565200	-2.00234200
C	-2.46224200	0.90574000	-2.62153900
C	-4.78729800	-0.48012000	-3.28043600
H	-4.72367100	-1.25626200	-1.26830600
C	-3.01518200	1.03867500	-3.89282100
H	-1.53405900	1.42581000	-2.36442400
C	-4.17900700	0.34429200	-4.22544200
H	-5.69425000	-1.03304500	-3.53821000
H	-2.52754600	1.67867800	-4.63245700
H	-4.60756200	0.43987400	-5.22633200
C	-3.07764300	-1.48322300	0.75102500
C	-4.24210500	-1.43062500	1.52642200
C	-2.46490500	-2.72393500	0.52490500
C	-4.78847200	-2.59995800	2.05661700
H	-4.72285800	-0.46923600	1.72388100
C	-3.01867400	-3.89105100	1.04522300
H	-1.53722400	-2.76208500	-0.05478300
C	-4.18176300	-3.83109500	1.81393900
H	-5.69481600	-2.54606200	2.66519900
H	-2.53222300	-4.85201300	0.85983300
H	-4.61094800	-4.74544800	2.23147100

IS1

Pd	-0.01870700	-0.79522900	-0.11617800
P	1.83701400	0.65515500	-0.10723900
P	-2.16199200	0.16129000	0.03064900
C	1.80186300	2.11806300	-1.23136500
C	0.56382100	2.70935100	-1.51165700
C	2.95905400	2.67799700	-1.79246500
C	0.48093100	3.83711100	-2.32659300
H	-0.34321900	2.28141700	-1.08044800
C	2.87454900	3.80123900	-2.61394700
H	3.93469900	2.23008900	-1.58960500
C	1.63614300	4.38408200	-2.88253600
H	-0.49527000	4.28404500	-2.52999500
H	3.78496800	4.22391600	-3.04673400
H	1.57248600	5.26381500	-3.52803200
C	3.44992200	-0.10939800	-0.55467500
C	4.46670900	-0.35333800	0.37549500
C	3.62217300	-0.55249800	-1.87597000
C	5.63216100	-1.01822800	-0.00841400
H	4.35161700	-0.02042600	1.40939100
C	4.79314500	-1.19940500	-2.26058700
H	2.82946400	-0.38740600	-2.61111500
C	5.80198500	-1.43892200	-1.32587000
H	6.41605500	-1.20169700	0.73080900
H	4.91550100	-1.52739600	-3.29612100
H	6.71826200	-1.95371000	-1.62531900
C	2.18922500	1.41716200	1.53535700
C	2.65914500	2.72692900	1.69169800
C	1.94468300	0.64270300	2.67905000
C	2.88553200	3.24845500	2.96541500
H	2.84279300	3.34968800	0.81337300
C	2.18291800	1.16231700	3.95049900
H	1.56060600	-0.37597800	2.56646000
C	2.65125900	2.46814900	4.09704700
H	3.24852300	4.27396000	3.07227100
H	1.99236600	0.54436100	4.83161200
H	2.83031800	2.87896200	5.09397500
C	-3.03825900	0.23113000	-1.58550500
C	-2.25433100	0.25403100	-2.74688800
C	-4.43523500	0.26198500	-1.70821100
C	-2.85274900	0.32912300	-4.00426700
H	-1.16524300	0.19720800	-2.65484800
C	-5.03150800	0.33043400	-2.96598400

H	-5.06157600	0.22236000	-0.81314500
C	-4.24147700	0.36831600	-4.11567000
H	-2.22855400	0.34634600	-4.90104300
H	-6.12117000	0.35259200	-3.04894200
H	-4.71160800	0.42000700	-5.10103400
C	-3.36648700	-0.74090800	1.09646500
C	-3.73738900	-0.28131500	2.36634600
C	-3.85473600	-1.98461300	0.66418100
C	-4.57262900	-1.04556000	3.18157100
H	-3.37650900	0.68576000	2.72355500
C	-4.69488400	-2.74162000	1.47629300
H	-3.58785700	-2.35752800	-0.32802000
C	-5.05426300	-2.27643300	2.74173000
H	-4.85186000	-0.66881800	4.16886700
H	-5.07026500	-3.70352300	1.11792800
H	-5.70991800	-2.87231800	3.38124800
C	-2.30029200	1.88344100	0.67752700
C	-3.21854200	2.82802900	0.20185800
C	-1.41182600	2.25593000	1.69611300
C	-3.24897200	4.11444400	0.73992000
H	-3.90997000	2.56405000	-0.60130200
C	-1.45385300	3.53681400	2.24367200
H	-0.66620500	1.53802600	2.04927300
C	-2.37184200	4.47037700	1.76385600
H	-3.96547300	4.84425800	0.35411900
H	-0.75128100	3.80733300	3.03568400
H	-2.39796500	5.47992300	2.18176100
C	-0.97057500	-3.21961800	-1.69336800
C	-0.57502800	-2.93965300	-0.35375600
C	0.82437500	-2.87879600	-0.08030100
C	1.77249100	-3.16291200	-1.09880600
C	1.34137400	-3.41051400	-2.38438500
C	-0.03884800	-3.43031900	-2.68767600
H	-2.03722300	-3.30013400	-1.91998200
H	-1.28935800	-3.08222300	0.46113700
H	2.83430800	-3.18134000	-0.84860500
H	2.07734200	-3.60617400	-3.16821100
H	-0.36926600	-3.64994000	-3.70570700
Br	1.40220800	-3.12020100	1.73967400

TS1

Pd	0.03248600	-0.86547800	0.07255200
P	1.82792100	0.66692400	0.04638600
P	-2.15659600	0.09577600	-0.17760000

C	1.48809800	2.40529600	-0.46881500
C	0.55266000	3.13257400	0.28426600
C	2.06374900	3.00828700	-1.59375900
C	0.20788200	4.43168900	-0.07622300
H	0.08373500	2.67486000	1.15982300
C	1.70818600	4.30865700	-1.95845400
H	2.79751100	2.46227100	-2.19091500
C	0.78181300	5.02365000	-1.20279000
H	-0.52289300	4.98006500	0.52323900
H	2.16755200	4.76559200	-2.83894700
H	0.50569200	6.04122400	-1.49015800
C	3.21039500	0.18910900	-1.06697200
C	4.56178400	0.22354900	-0.70588100
C	2.86127200	-0.26736100	-2.34636900
C	5.54429400	-0.17558500	-1.61258800
H	4.85328800	0.55681700	0.29247600
C	3.84392700	-0.64927700	-3.25555400
H	1.80483700	-0.34195800	-2.62179200
C	5.18953300	-0.60547000	-2.88989100
H	6.59591400	-0.14904000	-1.31557700
H	3.55523900	-1.00222000	-4.24855400
H	5.96147000	-0.91647700	-3.59837500
C	2.63082400	0.94654100	1.68195200
C	3.45451300	2.05424000	1.93194800
C	2.39552200	0.02873600	2.71290300
C	4.04609900	2.22595800	3.18164000
H	3.62581500	2.79360800	1.14505200
C	2.99142900	0.20103200	3.96262200
H	1.72348700	-0.81736700	2.53796900
C	3.81895300	1.29716700	4.19816500
H	4.68461100	3.09400500	3.36473600
H	2.79780400	-0.52329400	4.75772400
H	4.28141500	1.43509600	5.17886700
C	-2.61865200	0.96141000	-1.73283200
C	-1.61438700	1.65878300	-2.41727500
C	-3.92070600	0.95899900	-2.25201300
C	-1.90894500	2.35399800	-3.58858800
H	-0.59480700	1.65706200	-2.02383700
C	-4.21032900	1.64656400	-3.42991100
H	-4.71246200	0.41147600	-1.73465200
C	-3.20672300	2.34715300	-4.09863000
H	-1.11532200	2.89819300	-4.10632500
H	-5.22844800	1.63404000	-3.82741300
H	-3.43644300	2.88481300	-5.02210400

C	-3.52806500	-1.11723400	0.01560600
C	-4.49719300	-1.03366300	1.02088800
C	-3.56623100	-2.20301800	-0.87223700
C	-5.48485900	-2.01406000	1.13291800
H	-4.48396900	-0.19779800	1.72384600
C	-4.55940200	-3.17153700	-0.76806100
H	-2.80969600	-2.28513800	-1.65846800
C	-5.52128900	-3.08171400	0.23983400
H	-6.23262800	-1.93740500	1.92638000
H	-4.57749800	-4.00799500	-1.47115000
H	-6.29535100	-3.84778700	0.32975600
C	-2.52726300	1.33553700	1.13048600
C	-3.27532600	2.49659300	0.90477500
C	-2.00402200	1.09849800	2.41047400
C	-3.49810800	3.40301900	1.94201600
H	-3.68030000	2.69947800	-0.08945400
C	-2.23772700	1.99970500	3.44706100
H	-1.39788700	0.20391900	2.58576000
C	-2.98298100	3.15637400	3.21390300
H	-4.07991900	4.30882500	1.75263400
H	-1.82509700	1.80241100	4.43954000
H	-3.15825000	3.86845000	4.02429800
C	1.29754300	-3.81764000	-2.15640000
C	0.48617000	-3.23091400	-1.17810600
C	1.07751100	-2.69419200	-0.02054000
C	2.45524900	-2.86767100	0.21002600
C	3.23554200	-3.47334800	-0.76338400
C	2.66743200	-3.94363300	-1.95567300
H	0.83405100	-4.21319300	-3.06439700
H	-0.60023200	-3.22556800	-1.28896700
H	2.90738600	-2.50551300	1.13516800
H	4.31122900	-3.57163200	-0.59530200
H	3.29434700	-4.42543500	-2.70913300
Br	-0.20135500	-2.86039100	1.72531000

FS1

Pd	-0.00001400	-0.12787000	0.00884600
P	2.35776800	-0.09899400	-0.03763000
P	-2.35780600	-0.09905800	-0.03759000
C	3.09261200	-0.21149900	1.64160200
C	2.43150700	-0.98948000	2.60243300
C	4.30071200	0.41390700	1.97896300
C	2.97108300	-1.13312900	3.87898600
H	1.50190400	-1.50036900	2.33288600

C	4.83284500	0.26971500	3.25968800
H	4.82966400	1.02057000	1.24075100
C	4.16881700	-0.50162100	4.21212600
H	2.44834000	-1.74468800	4.61845000
H	5.77390100	0.76470900	3.51223600
H	4.58682400	-0.61157200	5.21601100
C	3.20862800	1.34300900	-0.80011400
C	3.86451900	1.23222300	-2.03267600
C	3.16825600	2.59352600	-0.16508300
C	4.46817800	2.34657000	-2.61580600
H	3.91288200	0.26824700	-2.54285800
C	3.78155900	3.70013100	-0.74488300
H	2.64725600	2.70950800	0.78739800
C	4.43144500	3.58156700	-1.97342500
H	4.97585700	2.24160200	-3.57784500
H	3.73848100	4.66535500	-0.23488200
H	4.90793000	4.45294100	-2.42963500
C	3.08378500	-1.50934900	-0.95784200
C	4.30063200	-2.08720300	-0.58218300
C	2.42333600	-1.97999500	-2.09898300
C	4.85231400	-3.11664700	-1.34372500
H	4.81860700	-1.73914500	0.31445200
C	2.98303700	-2.99915900	-2.86516300
H	1.45562700	-1.55464200	-2.37544500
C	4.19782700	-3.57067400	-2.48740900
H	5.79918700	-3.56801700	-1.03737400
H	2.45810600	-3.36107600	-3.75241400
H	4.63090800	-4.37921900	-3.08163600
C	-3.20830500	1.34329500	-0.79980300
C	-3.16853200	2.59345800	-0.16405400
C	-3.86307000	1.23316100	-2.03301900
C	-3.78132100	3.70037200	-0.74381000
H	-2.64837400	2.70893300	0.78894900
C	-4.46622900	2.34781000	-2.61608500
H	-3.91096100	0.26945100	-2.54375500
C	-4.43009700	3.58246200	-1.97299900
H	-3.73871500	4.66532200	-0.23324800
H	-4.97304600	2.24335800	-3.57863400
H	-4.90618600	4.45407200	-2.42916800
C	-3.08405000	-1.50903600	-0.95819800
C	-4.30132800	-2.08636500	-0.58314300
C	-2.42329800	-1.97988900	-2.09908800
C	-4.85314900	-3.11547600	-1.34503400
H	-4.81953900	-1.73817900	0.31330500

C	-2.98312600	-2.99872200	-2.86561300
H	-1.45524800	-1.55497800	-2.37503300
C	-4.19836100	-3.56969500	-2.48846800
H	-5.80037000	-3.56643100	-1.03914600
H	-2.45796700	-3.36081200	-3.75265900
H	-4.63155400	-4.37797600	-3.08297300
C	-3.09274400	-0.21179300	1.64158100
C	-4.30126800	0.41294300	1.97870400
C	-2.43134800	-0.98930300	2.60258900
C	-4.83352700	0.26855200	3.25935100
H	-4.83044400	1.01925600	1.24036000
C	-2.97103600	-1.13313900	3.87907600
H	-1.50142400	-1.49969800	2.33322700
C	-4.16919300	-0.50230900	4.21196500
H	-5.77491400	0.76301700	3.51170200
H	-2.44805500	-1.74432100	4.61868400
H	-4.58729800	-0.61242400	5.21579100
C	-0.00011500	4.05373700	-1.06309200
C	-0.00009000	4.69431600	0.17596200
C	-0.00005700	3.92701000	1.34126900
C	-0.00004400	2.53091200	1.26445900
C	-0.00006300	1.87580900	0.02237800
C	-0.00009900	2.65984900	-1.13840400
H	-0.00014000	4.64391400	-1.98375900
H	-0.00009600	5.78599300	0.23362500
H	-0.00002800	4.41537100	2.32029000
H	0.00001800	1.94882900	2.19160200
H	-0.00010700	2.18254700	-2.12228000
Br	-0.00010500	-2.64330700	0.33217800

IM

Pd	0.00300800	0.02229200	0.14246200
P	2.32264600	-0.17376000	0.03238900
P	-2.32654300	-0.18290600	0.02919600
C	3.02786500	-0.59886000	1.66943500
C	2.33999700	-1.56257200	2.42415700
C	4.19399100	-0.01498800	2.17672600
C	2.82831800	-1.93442100	3.67428500
H	1.42809700	-2.00466200	1.99606700
C	4.66943500	-0.39036100	3.43381400
H	4.73325700	0.73502800	1.59357900
C	3.98912800	-1.34876700	4.18267600
H	2.29270600	-2.68582800	4.26017300
H	5.57879000	0.07073900	3.82746600

H	4.36423900	-1.63979600	5.16731600
C	3.41040400	1.15302300	-0.61628100
C	4.32960100	0.92186600	-1.64806200
C	3.30994100	2.44162800	-0.07043600
C	5.13560900	1.95746000	-2.12022200
H	4.41983900	-0.07311800	-2.08852400
C	4.12273500	3.47016200	-0.53999400
H	2.58313100	2.64851500	0.71765000
C	5.03608100	3.23214700	-1.56678900
H	5.84695100	1.76215800	-2.92658200
H	4.02837600	4.46834400	-0.10599500
H	5.66765700	4.04281700	-1.93887500
C	2.74352800	-1.61624800	-1.02208500
C	3.77770600	-2.50166000	-0.69857200
C	2.01471100	-1.81719700	-2.20215800
C	4.07807600	-3.56928600	-1.54419300
H	4.34613700	-2.36053600	0.22392000
C	2.31863900	-2.88282300	-3.04651900
H	1.19357300	-1.13862800	-2.44987700
C	3.35126400	-3.76137500	-2.71820400
H	4.88385000	-4.25842000	-1.27943900
H	1.73825200	-3.03306900	-3.96005700
H	3.58522900	-4.60208400	-3.37603600
C	-3.42950800	1.20723100	-0.44150100
C	-3.26302100	2.44939000	0.18705300
C	-4.45136700	1.05598000	-1.38845900
C	-4.10538800	3.51450800	-0.12292900
H	-2.46113100	2.59148800	0.91391500
C	-5.28864000	2.12663500	-1.70004600
H	-4.59702900	0.09540400	-1.88714500
C	-5.11822700	3.35720300	-1.06838300
H	-3.95729200	4.47734400	0.37172800
H	-6.08017300	1.99460200	-2.44200800
H	-5.77350100	4.19621500	-1.31596500
C	-2.68337900	-1.44206000	-1.25592000
C	-3.50366500	-2.55008300	-1.02882100
C	-2.10654600	-1.26500500	-2.52105200
C	-3.74164300	-3.46851100	-2.05237000
H	-3.95384500	-2.70195300	-0.04529700
C	-2.35295500	-2.17709700	-3.54331700
H	-1.45998000	-0.40122100	-2.70284700
C	-3.16972400	-3.28471400	-3.30925700
H	-4.37970900	-4.33512900	-1.86208000
H	-1.90214400	-2.02564200	-4.52746100

H	-3.35829300	-4.00570000	-4.10862400
C	-3.08421300	-0.83754300	1.56613200
C	-4.27950100	-0.32611500	2.08651800
C	-2.42234500	-1.88145900	2.23314900
C	-4.80967100	-0.85201400	3.26472800
H	-4.80001200	0.48630800	1.57482600
C	-2.96594800	-2.40277000	3.40528000
H	-1.48923000	-2.26814100	1.79932800
C	-4.15538800	-1.89013500	3.92507600
H	-5.74139900	-0.44551200	3.66616100
H	-2.45031400	-3.21726500	3.92077000
H	-4.57331000	-2.30039200	4.84815000
C	0.00854500	4.15710500	-1.11825900
C	0.05593300	4.85613000	0.08755600
C	0.08789300	4.14131400	1.28591100
C	0.07155800	2.74387800	1.27181600
C	0.02106500	2.02045300	0.06536200
C	-0.00783900	2.76034400	-1.12630700
H	-0.01621300	4.70412000	-2.06534400
H	0.06812700	5.94924700	0.09403300
H	0.12658700	4.67423900	2.24089700
H	0.10057000	2.20720200	2.22619900
H	-0.04380200	2.24201200	-2.08948700
O	-0.03421700	-2.01986100	0.46361600
H	0.34750800	-2.50761800	-0.27374000

IS2

Pd	-0.10933200	-0.05269900	-0.04538500
P	2.06440000	0.80359300	0.40224000
P	-2.50049700	-0.19066200	0.09252000
C	3.23903700	1.08125200	-0.98232700
C	4.41478400	0.32598800	-1.08637300
C	2.94355600	2.01936100	-1.98503500
C	5.27780300	0.50714400	-2.16602300
H	4.66254500	-0.41273100	-0.32249600
C	3.81504300	2.20112800	-3.05649400
H	2.03282200	2.61847200	-1.93298000
C	4.98265000	1.44517800	-3.15269700
H	6.18856900	-0.09302800	-2.23079600
H	3.56968800	2.93819100	-3.82490300
H	5.66165800	1.58734400	-3.99719400
C	3.07821000	-0.07849400	1.65715600
C	3.77606100	0.61989000	2.65351200
C	3.20009300	-1.47180200	1.58723400

C	4.57987400	-0.06619700	3.56153800
H	3.69595100	1.70629000	2.72452000
C	4.01437700	-2.15120400	2.49198500
H	2.65625900	-2.03127300	0.82681000
C	4.70214500	-1.45306300	3.48249200
H	5.11641900	0.49024700	4.33410200
H	4.10216400	-3.23771500	2.41555000
H	5.33463800	-1.98883100	4.19501300
C	-0.27854400	1.42170100	-1.37746700
C	-0.51707700	2.77813300	-1.13082500
C	-0.08835100	1.02240600	-2.71233000
C	-0.57934000	3.70167500	-2.17877500
H	-0.64506000	3.13867300	-0.10938200
C	-0.15743800	1.94112300	-3.76109100
H	0.13450100	-0.02374400	-2.94549900
C	-0.40453400	3.28851400	-3.49849700
H	-0.76615500	4.75551500	-1.95416800
H	-0.00658800	1.59910200	-4.78881200
H	-0.45773200	4.01125300	-4.31664900
C	-3.48003600	-1.00005000	-1.22717400
C	-3.03492400	-0.93231900	-2.55143400
C	-4.69283900	-1.64004400	-0.94343300
C	-3.79121100	-1.49597700	-3.57687000
H	-2.09248600	-0.43359300	-2.77935300
C	-5.44447600	-2.20710600	-1.97139300
H	-5.05136000	-1.70278800	0.08638300
C	-4.99555300	-2.13710000	-3.28941700
H	-3.43160500	-1.43816200	-4.60710000
H	-6.38673500	-2.70896100	-1.73777900
H	-5.58453400	-2.58520800	-4.09365200
C	-3.05614100	-1.04166400	1.63085100
C	-3.66132800	-0.37154600	2.70328800
C	-2.83247800	-2.42341800	1.72870500
C	-4.01847600	-1.07012400	3.85657600
H	-3.87180100	0.69724900	2.64240900
C	-3.18341100	-3.11194900	2.88765100
H	-2.37190500	-2.95754300	0.89281400
C	-3.77493000	-2.43915800	3.95587600
H	-4.49366300	-0.53501200	4.68273100
H	-2.97485200	-4.18275100	2.94348000
H	-4.04936200	-2.98024300	4.86513500
C	-3.28585400	1.46527300	0.23682400
C	-4.36517200	1.86088800	-0.56015400
C	-2.77307400	2.37107500	1.17643400

C	-4.92293300	3.13131600	-0.41279500
H	-4.77428000	1.17522900	-1.30466700
C	-3.34078900	3.63219100	1.33448600
H	-1.91048300	2.08815800	1.78532800
C	-4.41832300	4.01700900	0.53627200
H	-5.76209800	3.42716300	-1.04717000
H	-2.92872100	4.32319200	2.07423600
H	-4.85989800	5.01000900	0.65106900
C	2.38975400	4.77993300	1.55854100
C	2.59286100	3.58222000	0.87061500
C	1.85125500	2.44475300	1.20222800
C	0.91822900	2.52162800	2.24645600
C	0.72584800	3.71330400	2.93980100
C	1.45747900	4.84989100	2.59099500
H	2.97184100	5.66340200	1.28490000
H	3.33727400	3.53768100	0.07330000
H	0.34627200	1.63007300	2.52186200
H	0.00142100	3.75534400	3.75718300
H	1.30317100	5.78853800	3.12887400
C	2.25013000	-4.62724800	-0.30865600
C	3.44016100	-4.89499200	-0.98896400
C	3.87233200	-4.03817500	-2.00021400
C	3.09740100	-2.92458500	-2.32741200
C	1.91108900	-2.67500000	-1.63712900
C	1.45828900	-3.50518100	-0.59734600
H	1.92335300	-5.33168800	0.46458900
H	4.02890600	-5.78148600	-0.73498800
H	4.80237400	-4.24249300	-2.53779700
H	3.41938400	-2.24809000	-3.12428400
H	1.31044300	-1.80172800	-1.91381100
O	-1.02084200	-2.86274200	-0.73510200
H	-1.17115500	-3.60168800	-1.33138500
B	0.05992900	-3.18080500	0.19105900
O	0.22934900	-1.88001000	1.02110700
H	-0.33349400	-2.00744300	1.79510300
O	-0.35245200	-4.22164300	1.10766400
H	0.39958400	-4.56503100	1.59596000

TS2

Pd	0.00737600	0.26995600	-0.18994600
P	2.36238800	-0.12684500	0.08156000
P	-2.37554900	-0.05748700	0.13847100
C	2.85922600	-0.70635400	1.75946700
C	4.16473400	-1.15854800	2.00632600

C	1.98337800	-0.56366400	2.83649500
C	4.56045100	-1.50229200	3.29564100
H	4.88423900	-1.22666400	1.18681800
C	2.38231500	-0.89521800	4.13169100
H	0.98073300	-0.17883300	2.65062400
C	3.66853100	-1.37524600	4.36203600
H	5.57806500	-1.85964300	3.47166100
H	1.68155000	-0.77740400	4.96192700
H	3.98344200	-1.64015900	5.37444400
C	3.68959800	1.16300600	-0.06768400
C	4.64833900	1.18486400	-1.08541700
C	3.75718400	2.13227500	0.94406000
C	5.65019200	2.15787100	-1.09249500
H	4.63064100	0.43374000	-1.87628100
C	4.76196300	3.09357500	0.94090700
H	3.01522700	2.13588500	1.74651400
C	5.71268100	3.11194500	-0.08076800
H	6.39214700	2.15821900	-1.89497800
H	4.79876600	3.83784900	1.74011100
H	6.50204900	3.86772800	-0.08460500
C	-0.01985300	-1.76564400	0.00928100
C	-0.01043300	-2.44516700	-1.22062300
C	-0.06720300	-2.53846300	1.17461400
C	-0.03786300	-3.83601600	-1.28511300
H	0.01927700	-1.87151000	-2.15108100
C	-0.08894100	-3.93721100	1.11604800
H	-0.09569700	-2.06728500	2.15778300
C	-0.07219600	-4.59170400	-0.11187400
H	-0.03094500	-4.33154100	-2.25951400
H	-0.12161700	-4.51268600	2.04581700
H	-0.09014800	-5.68384100	-0.15731500
C	-2.72181000	-0.43935700	1.90912100
C	-1.78924600	-0.03378000	2.86747400
C	-3.94922600	-0.96155000	2.34362000
C	-2.04979700	-0.18146300	4.23029400
H	-0.86086000	0.43068800	2.52378400
C	-4.20537400	-1.12441100	3.70260700
H	-4.71979300	-1.22663200	1.61608500
C	-3.25412900	-0.74109400	4.64967100
H	-1.31066200	0.14909100	4.96449900
H	-5.16245500	-1.54116500	4.02612500
H	-3.46164900	-0.86427600	5.71555600
C	-3.74666500	1.19012900	-0.06569500
C	-4.59771700	1.22086300	-1.17702100

C	-3.95934100	2.12655000	0.95770800
C	-5.61720000	2.16791100	-1.26871500
H	-4.47839400	0.49374000	-1.97974300
C	-4.97378600	3.07670800	0.86225500
H	-3.33330400	2.11249000	1.85271300
C	-5.80645800	3.10403500	-0.25442800
H	-6.27150100	2.16708300	-2.14416400
H	-5.11514100	3.79595500	1.67275100
H	-6.60465100	3.84642900	-0.33016200
C	-2.98094800	-1.50200000	-0.83130300
C	-3.32060700	-2.72354700	-0.23798800
C	-3.00228200	-1.40098700	-2.23215900
C	-3.71831400	-3.80450000	-1.02330600
H	-3.24605300	-2.85451800	0.84183500
C	-3.41198900	-2.48193200	-3.00978700
H	-2.66734400	-0.47324300	-2.70419100
C	-3.77893700	-3.68516600	-2.40940900
H	-3.97180800	-4.75186800	-0.54127000
H	-3.43047800	-2.38365600	-4.09835800
H	-4.09464200	-4.53369400	-3.02168100
C	3.71572400	-3.64801400	-1.63474100
C	3.34881400	-2.69556300	-0.68507000
C	2.92584900	-1.42459400	-1.08770300
C	2.83942300	-1.13501100	-2.45862200
C	3.21854800	-2.08752600	-3.40199700
C	3.66347800	-3.34463700	-2.99326500
H	4.03566100	-4.63952800	-1.30520200
H	3.36601700	-2.96210800	0.37273600
H	2.43071900	-0.17424900	-2.78478500
H	3.15210600	-1.84860500	-4.46658800
H	3.95465700	-4.09270100	-3.73497000
C	1.34878800	3.10496300	-0.86842000
C	1.65138900	4.38391200	-0.40649500
C	0.71493800	5.08840800	0.35168700
C	-0.52587900	4.50955100	0.61233200
C	-0.81886300	3.24335500	0.10641600
C	0.10043600	2.48045700	-0.64529900
H	2.09502900	2.58807500	-1.47814400
H	2.62419800	4.83042500	-0.63061000
H	0.94743100	6.09006800	0.72456100
H	-1.27728200	5.05666100	1.18934000
H	-1.82497100	2.85456400	0.26153600
O	-1.87143300	1.48581600	-2.42187400
H	-2.46075900	2.23994500	-2.52724600

B	-0.53514500	1.95542600	-2.48720200
O	0.42397200	0.94757300	-2.84969300
H	0.10825100	0.54308900	-3.66630400
O	-0.48624800	3.19547600	-3.15567000
H	0.40794900	3.54473300	-3.17521000

FS2

Pd	-0.03031600	0.00308600	0.20333600
P	-2.37787100	-0.01488800	0.28851500
P	2.31414400	-0.10780000	0.29520700
C	-3.07847100	0.28556200	1.96299100
C	-4.33730900	-0.21204600	2.33062700
C	-2.36032300	1.06230700	2.87954000
C	-4.86032700	0.05907000	3.59338200
H	-4.91179800	-0.81886100	1.62733800
C	-2.88850800	1.33416600	4.14108900
H	-1.39146400	1.47252100	2.59043300
C	-4.13663400	0.83077400	4.50237400
H	-5.84124600	-0.33698900	3.86787700
H	-2.31709200	1.94577200	4.84365600
H	-4.54816300	1.04029300	5.49302000
C	-3.26033600	-1.55421700	-0.21302600
C	-4.07822800	-1.62883000	-1.34528800
C	-3.08785900	-2.70338900	0.57264800
C	-4.69836800	-2.83047300	-1.69252800
H	-4.24568000	-0.74436700	-1.96216300
C	-3.70995600	-3.89806400	0.22711700
H	-2.45443500	-2.66733400	1.46042700
C	-4.51392600	-3.96744200	-0.91135200
H	-5.33414200	-2.87073000	-2.58064000
H	-3.55506600	-4.78399100	0.84722300
H	-4.99735000	-4.90823900	-1.18631800
C	0.02215600	2.08536700	0.42237500
C	-0.29770200	2.94760700	-0.64116000
C	0.46210000	2.71253000	1.60374700
C	-0.20348500	4.33753100	-0.53396400
H	-0.62585600	2.53179400	-1.59749700
C	0.55936500	4.10041200	1.72816800
H	0.76717500	2.10706000	2.46569600
C	0.22234700	4.92488700	0.65617200
H	-0.47070700	4.96732100	-1.38863700
H	0.91033800	4.53868500	2.66739300
H	0.29523700	6.01203400	0.74624800
C	2.82868300	-0.89414400	1.87271900

C	2.00499300	-0.73620500	2.99455500
C	4.03647700	-1.58982600	2.00746500
C	2.38364400	-1.25806600	4.23002300
H	1.05023100	-0.21205800	2.88894500
C	4.41010700	-2.11798400	3.24241600
H	4.68965500	-1.72199800	1.14174400
C	3.58661300	-1.95186200	4.35536400
H	1.72980200	-1.12955100	5.09601500
H	5.35277400	-2.66317500	3.33433200
H	3.88130900	-2.36819800	5.32190100
C	3.20706500	-1.09300100	-0.98773600
C	4.03736700	-0.48508500	-1.94092000
C	3.03888200	-2.48676500	-1.03165500
C	4.66651000	-1.24859700	-2.92562600
H	4.20480500	0.59278700	-1.91672000
C	3.68134000	-3.24445100	-2.00790500
H	2.40498400	-2.98814000	-0.29841200
C	4.49047500	-2.62988700	-2.96272100
H	5.30624000	-0.75398500	-3.66069000
H	3.53448500	-4.32693500	-2.02252000
H	4.98605400	-3.22738400	-3.73197100
C	3.24482900	1.47836000	0.30830700
C	4.16029700	1.80394800	1.31489000
C	3.00186800	2.40244400	-0.71856100
C	4.82480200	3.03039200	1.29306300
H	4.35508900	1.10311900	2.12873800
C	3.67340200	3.62140600	-0.74021100
H	2.27953700	2.16912100	-1.50392700
C	4.58401300	3.94051100	0.26712400
H	5.53324100	3.27378900	2.08888300
H	3.46958300	4.33402200	-1.54278700
H	5.10109500	4.90328700	0.25469000
C	-4.70051800	3.11176600	-1.11358100
C	-4.12985900	2.16084900	-0.26747500
C	-3.18048200	1.26014100	-0.75945300
C	-2.80447600	1.33632700	-2.10740100
C	-3.37958800	2.28162800	-2.95286100
C	-4.33133300	3.17215500	-2.45570900
H	-5.43727300	3.81379400	-0.71534800
H	-4.42330700	2.12706300	0.78364600
H	-2.04113600	0.65807300	-2.49833900
H	-3.05392000	2.33522400	-3.99411200
H	-4.77784100	3.92159700	-3.11407300
C	-0.22277200	-2.60224100	-1.34076600

C	-0.21454100	-3.98048800	-1.56523800
C	-0.00293500	-4.86682700	-0.50839200
C	0.19340400	-4.35485300	0.77394100
C	0.17960300	-2.97261000	0.98877100
C	-0.02426500	-2.05730100	-0.05882300
H	-0.38312600	-1.94325100	-2.20026400
H	-0.37234600	-4.36475200	-2.57751400
H	0.00633000	-5.94639400	-0.68217300
H	0.36212100	-5.03412200	1.61543400
H	0.34456000	-2.60949900	2.00795400
O	1.51147500	0.81213900	-3.51542100
H	1.88121100	-0.03701800	-3.24256200
B	0.28655300	0.70876300	-4.09923900
O	-0.37519200	1.83501900	-4.50362800
H	0.11486600	2.63338000	-4.28160900
O	-0.29812500	-0.51227200	-4.28019600
H	-1.15521700	-0.44120300	-4.71155100

IS3

Pd	0.02104200	-0.92796400	-0.00268600
P	1.94749900	0.52454200	0.07247800
P	-1.90385100	0.57231800	-0.06862500
C	2.26501000	1.82207600	-1.19484300
C	3.54504900	2.35775400	-1.40585500
C	1.20289600	2.28274400	-1.98009200
C	3.74679800	3.34552200	-2.36737100
H	4.39230700	1.98903000	-0.82230000
C	1.40513400	3.27242200	-2.94108800
H	0.20582300	1.86418200	-1.83752700
C	2.67694600	3.80689300	-3.13510100
H	4.74900900	3.75307800	-2.52217800
H	0.56161700	3.62115400	-3.54153400
H	2.83859300	4.57908400	-3.89148900
C	3.57920600	-0.32426300	0.11394400
C	4.38809400	-0.36180300	1.25372500
C	4.00321100	-0.98986400	-1.04487400
C	5.60108300	-1.05236700	1.23455400
H	4.07515000	0.14835800	2.16694000
C	5.21243900	-1.67608900	-1.06114500
H	3.37627100	-0.98244800	-1.93935800
C	6.01504300	-1.71067500	0.08012400
H	6.22322700	-1.07421200	2.13286400
H	5.52364400	-2.19922100	-1.96822600
H	6.96207800	-2.25588500	0.06821800

C	-1.29846900	-2.46346300	0.24501200
C	-1.98882100	-3.08286000	-0.80697300
C	-1.54715800	-2.93390000	1.54414000
C	-2.91352300	-4.10353000	-0.57039600
H	-1.81226200	-2.76969700	-1.83961400
C	-2.46392600	-3.95821000	1.78699700
H	-1.01648300	-2.49626800	2.39545800
C	-3.15970100	-4.54437000	0.72991000
H	-3.44031000	-4.56169200	-1.41275300
H	-2.63515900	-4.29996000	2.81202100
H	-3.87757700	-5.34762200	0.91600800
C	-1.73251400	2.41311600	-0.09418100
C	-0.96257900	3.02488600	0.90519800
C	-2.31867500	3.22014900	-1.07838500
C	-0.79318800	4.40799500	0.92799600
H	-0.48368500	2.41615100	1.67502000
C	-2.13779300	4.60284200	-1.06085300
H	-2.91829100	2.76846500	-1.87100800
C	-1.37737800	5.20138600	-0.05794100
H	-0.18909900	4.86177900	1.71724000
H	-2.59956800	5.21618300	-1.83887000
H	-1.23696200	6.28508000	-0.04697000
C	-2.73234600	0.25049900	-1.67857600
C	-4.10901400	0.41834800	-1.87492200
C	-1.93341900	-0.13261200	-2.76388500
C	-4.67177300	0.20839200	-3.13304900
H	-4.74719800	0.71115300	-1.03782900
C	-2.49580000	-0.33280400	-4.02344900
H	-0.86136900	-0.29272700	-2.60893700
C	-3.86721600	-0.16451000	-4.20943800
H	-5.74817700	0.33660900	-3.27204600
H	-1.86006400	-0.63374200	-4.85970200
H	-4.31164000	-0.33064800	-5.19395500
C	-3.25461100	0.33893900	1.16725800
C	-3.52676700	1.29557500	2.15449900
C	-4.00536900	-0.84715400	1.15268000
C	-4.52122900	1.07194200	3.10593500
H	-2.97074700	2.23409500	2.18096400
C	-5.00418500	-1.06088000	2.10002100
H	-3.81678300	-1.61141600	0.39627200
C	-5.26372600	-0.10651800	3.08209200
H	-4.71901000	1.83234200	3.86564500
H	-5.57545800	-1.99165800	2.06861200
H	-6.04541600	-0.27994700	3.82599700

C	2.46606200	3.31947300	3.10237400
C	2.49585300	2.70521600	1.85028800
C	1.95294600	1.42711500	1.67760600
C	1.37976800	0.77621800	2.78007300
C	1.35731300	1.38851400	4.03204900
C	1.89905000	2.66368300	4.19489600
H	2.88955400	4.31984500	3.22367900
H	2.93343200	3.23257000	0.99979300
H	0.93251000	-0.21392300	2.64507300
H	0.90635300	0.86949400	4.88128600
H	1.87624200	3.14823000	5.17421200
C	1.95291400	-3.12071200	0.82024700
C	2.81980500	-4.19415100	0.60735600
C	2.98704500	-4.72255200	-0.67214000
C	2.27070600	-4.16964500	-1.73257900
C	1.40404000	-3.09656700	-1.51304400
C	1.23733300	-2.54075700	-0.23598100
H	1.84043900	-2.73431300	1.83811600
H	3.36771100	-4.62233400	1.45182900
H	3.66292600	-5.56532400	-0.83925000
H	2.37835300	-4.58191800	-2.74052300
H	0.83998700	-2.69711700	-2.36228100

TS3

Pd	-0.01482100	-0.86123100	-0.01375200
P	-1.95903200	0.54899000	-0.12335700
P	1.92417600	0.60086100	0.10352400
C	-2.37287900	1.78085900	1.18278000
C	-3.68220000	2.23522100	1.40264500
C	-1.34199200	2.27805300	1.98838800
C	-3.94561200	3.17666700	2.39558800
H	-4.50357300	1.84043800	0.79945300
C	-1.60575200	3.22281800	2.97930900
H	-0.32099700	1.92442400	1.83455900
C	-2.90784600	3.67441800	3.18430100
H	-4.97048200	3.52056000	2.55700600
H	-0.78621900	3.60221300	3.59435500
H	-3.11751900	4.41067000	3.96442700
C	-3.54841400	-0.36676700	-0.25347900
C	-4.31181000	-0.41772700	-1.42472300
C	-3.98241500	-1.08039200	0.87268500
C	-5.49319900	-1.15995400	-1.46475300
H	-3.98917700	0.12904800	-2.31347200
C	-5.16501800	-1.81146100	0.83252400

H	-3.38546100	-1.07125900	1.78816100
C	-5.92468700	-1.85410900	-0.33709900
H	-6.08086400	-1.18912800	-2.38593500
H	-5.48699700	-2.36490700	1.71763900
H	-6.85092700	-2.43330500	-0.36959600
C	0.96793200	-2.67016200	-0.29807400
C	1.85422100	-3.22134700	0.64867600
C	1.16487600	-3.03877500	-1.64511300
C	2.88055400	-4.08329600	0.27038300
H	1.73680200	-2.97902200	1.70782500
C	2.18876700	-3.90407900	-2.02514900
H	0.49261000	-2.65233000	-2.41652700
C	3.05620600	-4.43563600	-1.07028100
H	3.55034900	-4.48759400	1.03462000
H	2.30779600	-4.16564700	-3.08043100
H	3.85280900	-5.12367800	-1.36375300
C	1.76173400	2.43018000	0.27651500
C	0.99686900	3.11759700	-0.67751500
C	2.33552800	3.15477300	1.32915100
C	0.81985800	4.49634000	-0.58751900
H	0.52970300	2.56927000	-1.49906500
C	2.14521700	4.53366100	1.42497600
H	2.93430900	2.64013700	2.08366400
C	1.38962000	5.20829000	0.46782400
H	0.22060400	5.01175900	-1.34195000
H	2.59682200	5.08379100	2.25460300
H	1.24180900	6.28829700	0.54556900
C	2.81245700	0.15051900	1.65169000
C	4.20645400	0.18606600	1.77576700
C	2.04151600	-0.22441700	2.76080000
C	4.81485700	-0.14491100	2.98636500
H	4.82176000	0.46939700	0.91846600
C	2.64980200	-0.54384800	3.97318300
H	0.95195400	-0.27594400	2.66215300
C	4.03947700	-0.50734900	4.08704700
H	5.90441700	-0.11919500	3.06857800
H	2.03552900	-0.83331000	4.82946000
H	4.51925000	-0.76759400	5.03390100
C	3.23399100	0.45487800	-1.18345600
C	3.69173500	1.54378300	-1.93697200
C	3.76787300	-0.81751000	-1.43885200
C	4.65854400	1.36326100	-2.92612800
H	3.29932200	2.54504900	-1.74981800
C	4.73914200	-0.99068700	-2.42177400

H	3.43213200	-1.68047600	-0.86087200
C	5.18510800	0.09693800	-3.17216700
H	5.00497000	2.22440100	-3.50333100
H	5.14182300	-1.99045800	-2.60177300
H	5.94385900	-0.04220100	-3.94646600
C	-2.46892500	3.48555700	-3.02091500
C	-2.52623200	2.80240100	-1.80597100
C	-1.95143300	1.53228700	-1.68093700
C	-1.31629100	0.96222100	-2.79414800
C	-1.26832200	1.64146700	-4.01029700
C	-1.84313500	2.90733500	-4.12508700
H	-2.91790600	4.47872900	-3.10410000
H	-3.01244400	3.26857800	-0.94603800
H	-0.84021900	-0.01872800	-2.69302600
H	-0.76917000	1.18396200	-4.86796300
H	-1.79891000	3.44580400	-5.07509500
C	-1.78290100	-3.29355900	-0.67845500
C	-2.75701300	-4.21507600	-0.30626600
C	-2.91786100	-4.57756400	1.03211600
C	-2.09360700	-3.99147500	1.99239400
C	-1.11350200	-3.07379100	1.61741700
C	-0.92691200	-2.70205300	0.27045400
H	-1.67246200	-3.04591600	-1.73753200
H	-3.39917200	-4.65616700	-1.07355500
H	-3.67496800	-5.31034400	1.32177800
H	-2.20312400	-4.26027900	3.04720500
H	-0.45970200	-2.65805000	2.38988200

FS3

Pd	0.88518400	0.86399600	0.01204900
P	2.72747400	-0.48238200	0.22384200
P	-0.96374900	2.18752000	-0.17751500
C	3.82137400	-0.56806100	-1.25435700
C	4.44761600	-1.74333600	-1.68590700
C	4.02300100	0.61634600	-1.97726700
C	5.26931200	-1.73021100	-2.81366300
H	4.28743100	-2.67738600	-1.14162900
C	4.85292200	0.62963500	-3.09554700
H	3.50845700	1.52864400	-1.65939800
C	5.47730100	-0.54509500	-3.51709100
H	5.74885400	-2.65516100	-3.14424500
H	5.00349900	1.56014500	-3.64870700
H	6.12055800	-0.53766100	-4.40070700
C	2.36620700	-2.25064100	0.57786600

C	3.15117400	-3.05035100	1.41757700
C	1.23728400	-2.80947900	-0.03651000
C	2.81557900	-4.38820500	1.62745900
H	4.02544700	-2.62500600	1.91685100
C	0.90889700	-4.14803400	0.16527500
H	0.60278200	-2.18002800	-0.66740100
C	1.69906600	-4.93942100	0.99977700
H	3.43154400	-5.00271400	2.28918400
H	0.02427400	-4.56422800	-0.32374300
H	1.43857000	-5.98751100	1.16850900
C	-3.79746800	-3.10606600	0.50123100
C	-4.51640400	-1.90060700	0.51146000
C	-3.80652700	-3.89181500	1.66429100
C	-5.22338400	-1.49911900	1.64219600
H	-4.53528400	-1.27701400	-0.38561700
C	-4.51387800	-3.49117100	2.79491000
H	-3.22868300	-4.81880200	1.69111600
C	-5.22776100	-2.29330300	2.78849800
H	-5.77826900	-0.55782300	1.62597800
H	-4.49986400	-4.11629700	3.69135800
H	-5.78485300	-1.97895000	3.67462300
C	-0.64986500	3.94507300	-0.62424400
C	0.51055900	4.54311000	-0.11346300
C	-1.50490100	4.70101800	-1.43551900
C	0.79917900	5.87720700	-0.39156400
H	1.19360600	3.94306800	0.49610000
C	-1.20787900	6.03353700	-1.72225700
H	-2.40644800	4.24472400	-1.85209200
C	-0.05922500	6.62480700	-1.19831200
H	1.70616500	6.33222400	0.01433900
H	-1.87952300	6.61248800	-2.36134000
H	0.17208400	7.66856500	-1.42558400
C	-2.18560700	1.65854600	-1.45123000
C	-3.57161300	1.69366500	-1.25623600
C	-1.68234200	1.19102600	-2.67425300
C	-4.43711100	1.27190100	-2.26744100
H	-3.97808900	2.04823600	-0.30569500
C	-2.54802000	0.78343000	-3.68639900
H	-0.59856500	1.13821800	-2.81858300
C	-3.92860000	0.81869400	-3.48346600
H	-5.51737700	1.30020200	-2.10234000
H	-2.14309700	0.42479200	-4.63615400
H	-4.60773000	0.48648800	-4.27249000
C	-1.99577400	2.32030900	1.34059300

C	-2.56546100	3.51817500	1.78831200
C	-2.20619900	1.14689600	2.07921300
C	-3.33725300	3.53906900	2.95072000
H	-2.40129800	4.44299000	1.22993300
C	-2.98957600	1.16741900	3.23049500
H	-1.74250500	0.21262500	1.74769500
C	-3.55422700	2.36546200	3.67063900
H	-3.77103900	4.48157500	3.29468400
H	-3.15248100	0.24210700	3.78833500
H	-4.15885300	2.38507700	4.58101600
C	6.10694800	0.24508200	2.52485900
C	5.28582500	-0.11565700	1.45592800
C	3.89386400	-0.01960300	1.57050200
C	3.33954100	0.45294500	2.76857700
C	4.16068000	0.80147400	3.83805300
C	5.54720600	0.69943600	3.71769900
H	7.19263200	0.17088300	2.42213300
H	5.73311200	-0.46857600	0.52330500
H	2.25284300	0.55708500	2.84830100
H	3.71575300	1.16650600	4.76716100
H	6.19254000	0.98261800	4.55313100
C	-2.97981300	-4.89295900	-1.06133200
C	-2.27717400	-5.30172300	-2.19262400
C	-1.62819800	-4.36206700	-2.99337100
C	-1.69290300	-3.01123100	-2.65304800
C	-2.39563200	-2.60226600	-1.52184200
C	-3.05011600	-3.53695600	-0.70391700
H	-3.50591600	-5.63572100	-0.45662700
H	-2.24449600	-6.36213700	-2.45561700
H	-1.07508900	-4.68143000	-3.87996500
H	-1.18466700	-2.26358400	-3.26698600
H	-2.41411800	-1.54141200	-1.25961700

IS3'

Pd	0.09958900	-0.54086500	-0.79783300
P	2.06035800	0.52178200	0.11518600
P	-1.75097400	0.94057600	-0.22342100
C	2.55632000	2.19814000	-0.46612000
C	3.88508900	2.64674900	-0.42296100
C	1.57075400	3.05841200	-0.96362900
C	4.21147800	3.93078500	-0.85529800
H	4.67271400	1.98263200	-0.05893500
C	1.89709700	4.34411100	-1.39159600
H	0.53513900	2.71914700	-1.01402400

C	3.21847500	4.78319900	-1.33792900
H	5.25121900	4.26553900	-0.81788500
H	1.11157700	5.00124000	-1.77230800
H	3.47737000	5.78888600	-1.67857500
C	3.63419500	-0.41010300	-0.06822100
C	4.27956700	-1.01822600	1.01294800
C	4.17588900	-0.55342500	-1.35365300
C	5.44860800	-1.75406300	0.81260600
H	3.87113300	-0.92187700	2.02104300
C	5.34255500	-1.28438900	-1.54944800
H	3.67392700	-0.09960300	-2.21103500
C	5.98201300	-1.88871900	-0.46609100
H	5.94222500	-2.22498400	1.66648000
H	5.74685400	-1.39478400	-2.55823600
H	6.89480700	-2.46903200	-0.62212400
C	-1.30574600	-1.84904200	-1.50534400
C	-1.88486500	-1.75553700	-2.77926700
C	-1.72206600	-2.91042000	-0.68507900
C	-2.86464200	-2.65655900	-3.20471900
H	-1.57537000	-0.96549100	-3.46824400
C	-2.69277900	-3.82012200	-1.10914800
H	-1.29506300	-3.03443300	0.31357500
C	-3.27747100	-3.69398100	-2.36901700
H	-3.30082000	-2.54943800	-4.20241800
H	-2.99541400	-4.63378600	-0.44311000
H	-4.03753400	-4.40553800	-2.70294200
C	-1.59748200	2.58190200	0.62668900
C	-0.84917200	2.67243000	1.80897700
C	-2.17523300	3.75180100	0.11265400
C	-0.69963500	3.89029300	2.46999600
H	-0.36428800	1.78581600	2.21921800
C	-2.01457100	4.97161500	0.76881100
H	-2.75454700	3.71672400	-0.81142800
C	-1.27988200	5.04555700	1.95050900
H	-0.11224800	3.93097400	3.39028600
H	-2.47195200	5.87145100	0.34955800
H	-1.15525100	6.00296700	2.46245000
C	-2.56481600	1.44018500	-1.79223500
C	-3.93774800	1.69245900	-1.90518500
C	-1.74254800	1.64997800	-2.90686600
C	-4.47537800	2.13811200	-3.11188800
H	-4.59449200	1.54187900	-1.04523400
C	-2.27877700	2.10919800	-4.10837900
H	-0.67233400	1.43251100	-2.83159400

C	-3.64787000	2.34987800	-4.21423300
H	-5.54954300	2.32394600	-3.18915400
H	-1.62434200	2.26706200	-4.96906200
H	-4.07208700	2.69942100	-5.15878900
C	-3.07541900	0.11167400	0.75606700
C	-3.16880000	0.29242400	2.14449300
C	-3.93357300	-0.81054100	0.13881500
C	-4.09429400	-0.43249000	2.89690800
H	-2.52241300	1.00998400	2.65284300
C	-4.86977300	-1.51815400	0.89203200
H	-3.86892700	-0.99229700	-0.93589700
C	-4.95081300	-1.33874300	2.27083400
H	-4.14135800	-0.28465000	3.97843000
H	-5.52515900	-2.23264300	0.38873700
H	-5.67675300	-1.90496100	2.85933300
C	2.46866300	1.79399300	4.04214800
C	2.60724600	1.70201700	2.65774800
C	1.93986900	0.69897100	1.94471500
C	1.13348200	-0.21244000	2.64264900
C	0.99206000	-0.11661000	4.02771400
C	1.65998300	0.88804100	4.72817400
H	2.99193600	2.58418300	4.58676800
H	3.22877400	2.42722400	2.12793600
H	0.58569500	-0.98721400	2.09612400
H	0.33596800	-0.81262500	4.55609600
H	1.54410200	0.96865300	5.81200100
C	1.78931300	-3.04126600	-0.90017800
C	2.61993400	-3.99695200	-1.48803400
C	2.93422200	-3.91927200	-2.84447200
C	2.40175700	-2.87958600	-3.60544500
C	1.56916200	-1.92742400	-3.01254400
C	1.25646700	-1.98138100	-1.64666500
H	1.55697200	-3.13070000	0.16566600
H	3.02429800	-4.81086500	-0.87904600
H	3.58147600	-4.66922100	-3.30676700
H	2.62630300	-2.81246400	-4.67435700
H	1.14654300	-1.13616500	-3.64000700
O	-1.60371300	-2.28023500	5.09950900
H	-1.34306500	-2.66957700	5.94022200
B	-1.23858900	-3.08410700	4.05243600
O	-1.52813000	-2.72665100	2.77280300
H	-2.08997400	-1.94334400	2.69987500
O	-0.56064700	-4.24092100	4.30536800
H	-0.37017900	-4.72200600	3.49368400

TS3'

Pd	0.11156300	-0.50767600	-0.75743500
P	2.08287500	0.47593000	0.19277000
P	-1.74026400	0.99434700	-0.33919200
C	2.73140900	2.06411200	-0.47954500
C	4.08938900	2.41241700	-0.43480500
C	1.82330500	2.96130100	-1.05583600
C	4.52210200	3.63605300	-0.94304800
H	4.81582500	1.71604600	-0.00879700
C	2.25622400	4.18763200	-1.55772000
H	0.76510500	2.69660500	-1.10850600
C	3.60667200	4.52765300	-1.50227200
H	5.58376900	3.89298900	-0.90362400
H	1.53125000	4.87642600	-1.99817300
H	3.94869000	5.48591000	-1.90147800
C	3.57997000	-0.58879900	0.14256300
C	4.13133500	-1.17934600	1.28529200
C	4.15643300	-0.85813300	-1.10683200
C	5.24661200	-2.01170600	1.18118200
H	3.69335500	-0.98595700	2.26702500
C	5.27570100	-1.67844800	-1.20576600
H	3.72170200	-0.42975200	-2.01345700
C	5.82482300	-2.25838700	-0.06186300
H	5.66778200	-2.46439700	2.08255500
H	5.71053900	-1.87910500	-2.18760800
H	6.70062300	-2.90738000	-0.14122100
C	-1.00622900	-2.11809700	-1.45297100
C	-1.76932800	-2.10347200	-2.63697700
C	-1.41305400	-3.01213700	-0.44129900
C	-2.87544600	-2.93391700	-2.80052400
H	-1.48629800	-1.44167200	-3.45894300
C	-2.51556700	-3.84809900	-0.60677000
H	-0.86180800	-3.06069700	0.50103100
C	-3.25588200	-3.81951400	-1.78878600
H	-3.44230600	-2.89387300	-3.73510400
H	-2.79902400	-4.52312800	0.20573500
H	-4.11357300	-4.48290200	-1.92582200
C	-1.59507200	2.72607900	0.29417600
C	-0.79515300	2.96532900	1.42137200
C	-2.21828800	3.81758900	-0.32679200
C	-0.64117900	4.25433800	1.92812100
H	-0.27311800	2.13838700	1.90597300
C	-2.05178300	5.10864400	0.17352500
H	-2.83780100	3.66394700	-1.21218300

C	-1.26733300	5.33162700	1.30377600
H	-0.01379200	4.41274300	2.80852500
H	-2.54393200	5.94672700	-0.32667800
H	-1.13904900	6.34463100	1.69326200
C	-2.60880600	1.26917400	-1.93595400
C	-3.99667300	1.41145400	-2.05605000
C	-1.81339800	1.38680700	-3.08356300
C	-4.57446900	1.65965500	-3.30072600
H	-4.63301200	1.32548600	-1.17209100
C	-2.39015300	1.64908500	-4.32461000
H	-0.72924200	1.25916400	-2.99686700
C	-3.77386800	1.78111800	-4.43597600
H	-5.65963800	1.76099300	-3.38243800
H	-1.75626700	1.73932000	-5.21019900
H	-4.22988900	1.97549500	-5.40997000
C	-3.02482700	0.26566700	0.75944600
C	-3.18469200	0.68080600	2.08971300
C	-3.77217000	-0.83036700	0.30025300
C	-4.06915800	0.01617600	2.93999300
H	-2.61845300	1.53191500	2.47262500
C	-4.66856500	-1.47884600	1.14813900
H	-3.65324300	-1.19047400	-0.72442600
C	-4.81741500	-1.06416700	2.47083300
H	-4.16864000	0.34483800	3.97699900
H	-5.23831400	-2.33019100	0.76840500
H	-5.50941100	-1.58384400	3.13786700
C	2.38706200	2.04745500	4.02416800
C	2.59187100	1.82933400	2.66209000
C	1.90444800	0.80639200	1.99694700
C	1.01045600	0.00521800	2.72297300
C	0.80571500	0.22423200	4.08573700
C	1.49366200	1.24809900	4.73704800
H	2.92681000	2.85241200	4.52982300
H	3.28172900	2.47241300	2.11084400
H	0.44812000	-0.78323900	2.21157400
H	0.08731500	-0.39231100	4.63174300
H	1.32737100	1.42790500	5.80225100
C	1.61930800	-3.16733900	-1.14619900
C	2.58487900	-3.91708900	-1.81131200
C	2.92203600	-3.62928400	-3.13501400
C	2.28214400	-2.56978200	-3.77823900
C	1.30892800	-1.82481700	-3.11392200
C	0.94799100	-2.10456100	-1.78013800
H	1.36520900	-3.42911500	-0.11586400

H	3.08132100	-4.73837300	-1.28701700
H	3.67175100	-4.22675900	-3.65956800
H	2.53177900	-2.32596100	-4.81511400
H	0.80117500	-1.02099100	-3.65537100
O	-1.81158000	-1.88019100	5.21565900
H	-1.58173500	-2.16938900	6.10436600
B	-1.38641800	-2.78426600	4.27972300
O	-1.61544600	-2.57129800	2.95590000
H	-2.16214900	-1.79565400	2.77548300
O	-0.71108100	-3.89793600	4.68821100
H	-0.46849700	-4.45632500	3.94296100
FS3'			
Pd	0.01290200	-0.23982400	-0.49150800
P	-2.18486300	0.32011100	-0.82727300
P	1.91624600	-1.49452700	-0.26995500
C	-2.60383600	1.14921700	-2.41495300
C	-3.70219300	2.00395200	-2.57249000
C	-1.77186800	0.89740300	-3.51475100
C	-3.96609200	2.58951400	-3.81052600
H	-4.35138400	2.21948200	-1.71989800
C	-2.04345200	1.47548700	-4.75326900
H	-0.90008500	0.24817800	-3.38167800
C	-3.14042200	2.32433800	-4.90247000
H	-4.82257200	3.25944200	-3.92131600
H	-1.38897400	1.26957300	-5.60399400
H	-3.34840700	2.78635600	-5.87089600
C	-3.05621800	1.36727900	0.41453600
C	-4.23003200	0.97013800	1.06627600
C	-2.48208700	2.60272000	0.74721200
C	-4.81666000	1.79492900	2.02938200
H	-4.68764900	0.00676400	0.83131100
C	-3.07246900	3.42794900	1.70017400
H	-1.55383900	2.91955400	0.26514400
C	-4.24118200	3.02438000	2.34741500
H	-5.73149200	1.46941600	2.53164200
H	-2.60513900	4.38335400	1.95008600
H	-4.70085700	3.66709900	3.10240900
C	1.60713300	3.59660000	1.46594500
C	1.73365300	4.54482300	2.49421000
C	0.97893700	2.37781100	1.76829500
C	1.25494400	4.28263800	3.77556600
H	2.19127500	5.51398000	2.28094200
C	0.49039700	2.11640700	3.04723800
H	0.86808900	1.60629100	0.99268700

C	0.63079400	3.06773200	4.05761000
H	1.36027400	5.04005600	4.55675500
H	-0.01076100	1.16430700	3.24434100
H	0.24817200	2.86529600	5.06124300
C	2.04918100	-2.83547600	-1.52503300
C	0.85644700	-3.35080200	-2.05204700
C	3.27055400	-3.35892900	-1.96640600
C	0.88477000	-4.38463000	-2.98600100
H	-0.09668000	-2.92009300	-1.72742400
C	3.29652500	-4.38463400	-2.91104200
H	4.20953600	-2.95790200	-1.57754500
C	2.10559100	-4.90213200	-3.41902400
H	-0.05281700	-4.77876800	-3.38595400
H	4.25617000	-4.78021500	-3.25348100
H	2.12925700	-5.70521100	-4.16010100
C	3.57998500	-0.71360700	-0.29285800
C	4.67677500	-1.21763000	0.41967700
C	3.74264700	0.44235200	-1.06629700
C	5.91432600	-0.57988900	0.34796400
H	4.56090300	-2.10872600	1.04223800
C	4.98108800	1.07731600	-1.13916200
H	2.88334200	0.85811900	-1.59966400
C	6.06875000	0.56610800	-0.43240200
H	6.76261600	-0.97849900	0.91035000
H	5.08505300	1.98632500	-1.73640400
H	7.03842600	1.06820200	-0.48017200
C	1.93651200	-2.41740600	1.32566300
C	1.87229100	-3.81225300	1.40945000
C	1.94950500	-1.66615400	2.51296500
C	1.81536600	-4.44405100	2.65377100
H	1.86065100	-4.41251400	0.49675600
C	1.90412100	-2.29979000	3.75269200
H	1.99330700	-0.57385000	2.46476600
C	1.83028800	-3.69345300	3.82630000
H	1.75754800	-5.53432600	2.70244500
H	1.91887500	-1.70058300	4.66663500
H	1.78230700	-4.18995300	4.79833500
C	-5.00216500	-2.61033000	-1.69045900
C	-4.26973400	-1.42326300	-1.74481200
C	-3.21251400	-1.20734300	-0.85398600
C	-2.89949900	-2.20004700	0.08585700
C	-3.64395600	-3.37469600	0.15208800
C	-4.69578600	-3.58420100	-0.74105300
H	-5.82077100	-2.77244900	-2.39641800

H	-4.52108400	-0.66430300	-2.48968500
H	-2.05640600	-2.04099400	0.76445500
H	-3.38955100	-4.12571300	0.90385600
H	-5.27446000	-4.51060500	-0.70076700
C	1.45557900	3.37266300	-1.03424200
C	1.91243600	3.66158700	-2.31807800
C	3.03658900	4.46652400	-2.50125100
C	3.70073100	4.97564500	-1.38530200
C	3.24110200	4.68770800	-0.10249300
C	2.10669200	3.88534800	0.09962500
H	0.57462600	2.73515900	-0.91641600
H	1.37691700	3.25709100	-3.18089900
H	3.39288900	4.69683000	-3.50844100
H	4.58929000	5.59933100	-1.51352700
H	3.78682300	5.07405800	0.76153300
O	-2.46634400	-3.04849800	3.61953600
H	-3.35700000	-3.35128700	3.82209300
B	-2.43680600	-1.68687900	3.49409100
O	-1.26793900	-1.04948600	3.19770600
H	-0.52253900	-1.64719200	3.05918300
O	-3.58475500	-0.97060100	3.66300500
H	-3.46304200	-0.03693100	3.45382700

(4) The optimized structures involved in Suzuki-Miyaura cross-coupling mechanism catalyzed by ZrO superatom

IS1

Zr	1.35509100	0.57317100	-0.00011900
O	2.21661800	2.10290700	0.00005000
C	0.95149400	-1.58583300	-1.21713200
C	-0.24615500	-0.91727900	-1.22398100
C	-0.75683300	-0.28872700	0.00006400
C	-0.24592300	-0.91688800	1.22417900
C	0.95171000	-1.58557400	1.21731300
C	1.74378000	-1.70765800	0.00011400
H	1.33383100	-1.99548900	-2.14494200
H	-0.81204500	-0.81073100	-2.14126400
H	-0.81157400	-0.81029400	2.14160400
H	1.33392500	-1.99494900	2.14530000
H	2.61874000	-2.34190900	-0.00000100
Br	-2.57108300	0.29185800	0.00000900

TS1

Zr	0.12970700	1.49213100	-0.38656700
O	-0.15861600	2.19316800	1.17052300

C	2.13286200	-1.32151700	-1.07113100
C	0.76016400	-1.12375200	-1.11738000
C	0.04689500	-0.81164900	0.07189800
C	0.76143100	-0.72592700	1.29027600
C	2.12988500	-0.91734700	1.29606400
C	2.82875500	-1.23403200	0.12777900
H	2.65748300	-1.55600100	-1.99067300
H	0.22017500	-1.23713000	-2.05094000
H	0.23114500	-0.48679500	2.20263200
H	2.66237100	-0.81879300	2.23513800
H	3.89867500	-1.39349300	0.15515000
Br	-1.87283300	-0.99808600	0.05606200

FS1

Zr	-0.63361700	0.74959300	-0.39391800
O	-0.79677800	2.31144400	0.33176200
C	3.09777200	-1.65877400	-0.33083500
C	1.79069500	-1.19677600	-0.40165800
C	1.44617000	0.10752000	-0.00963400
C	2.47835800	0.92777000	0.47118600
C	3.78608400	0.47364100	0.54543300
C	4.09581200	-0.81953700	0.14283600
H	3.33753600	-2.67134000	-0.63684800
H	1.02475200	-1.88554600	-0.75747600
H	2.25057700	1.93785600	0.79808200
H	4.56791800	1.12431400	0.92227400
H	5.11835900	-1.17574800	0.20412700
Br	-2.42141700	-0.93736700	0.28767100

IM

C	-2.97552900	1.13310200	0.21272600
C	-1.58936400	1.18759900	0.17765300
C	-0.81003700	0.03431600	-0.00063100
C	-1.50012600	-1.18148200	-0.13074400
C	-2.88677700	-1.24747900	-0.09801300
C	-3.62573900	-0.08584900	0.07328500
H	-3.55257800	2.04075400	0.35583700
H	-1.10059600	2.14979500	0.30228100
H	-0.94898100	-2.11410800	-0.24571900
H	-3.39144400	-2.20266200	-0.19903000
H	-4.70903500	-0.13091200	0.10430500
Zr	1.42009500	0.04395800	-0.26481000
O	2.02125300	1.58690600	0.28262300
O	2.26700500	-1.46046500	0.65704900

H	2.91818400	-1.55396700	1.35169900
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IS2

C	-4.44154400	-0.19632200	-0.45509900
C	-3.13896500	-0.60940700	-0.70176400
C	-2.03121800	0.10790200	-0.22481500
C	-2.30738800	1.27268900	0.50708600
C	-3.60519600	1.70163400	0.75285000
C	-4.67655000	0.96102300	0.27402500
H	-5.27680000	-0.77368200	-0.83803000
H	-2.98044200	-1.51001400	-1.28833800
H	-1.49144800	1.88099800	0.89621900
H	-3.78249400	2.61137200	1.31731200
H	-5.69295000	1.28819700	0.46500700
Zr	0.10551800	-0.50652600	-0.64634400
O	0.03464700	-1.73583100	-1.88882000
O	1.39713500	1.09156200	-1.28199300
H	1.81436200	1.09729700	-2.15035200
C	1.57536600	-2.23723100	1.00497600
C	2.37021000	-1.20163200	0.51045300
C	2.12933400	0.13895500	0.85748100
C	1.13836900	0.39051500	1.81814100
C	0.32005000	-0.62873300	2.29488200
C	0.51237300	-1.94170300	1.85588300
H	1.73786800	-3.25540600	0.67260800
H	3.13217300	-1.41364400	-0.23321400
H	0.94869000	1.42076100	2.09963200
H	-0.49966200	-0.40317400	2.96664900
H	-0.15678700	-2.72763200	2.18490400
B	2.57947000	1.32315300	-0.18148100
O	3.74647400	1.07129000	-0.97016000
H	4.51597900	1.49892200	-0.59270500
O	2.44219800	2.58257600	0.44846300
H	2.58077300	3.30835300	-0.16303400

TS2

C	4.45352800	0.89201200	-0.61211000
C	3.19267300	0.50132400	-1.04159000
C	2.20526200	0.05904400	-0.14659300
C	2.56663600	0.02349100	1.21024100
C	3.82683500	0.40561200	1.65309700
C	4.77273900	0.84456400	0.73826600
H	5.19274200	1.23088100	-1.33081700
H	2.97237300	0.53994600	-2.10500100

H	1.85001100	-0.32117500	1.95586800
H	4.07236400	0.36182500	2.70940200
H	5.75824700	1.14664000	1.07630400
Zr	0.13453700	-0.63918900	-0.76548000
O	0.04459300	-0.79939900	-2.50113400
O	-0.90670700	-2.41391500	0.06924000
H	-1.47163600	-2.92323200	-0.52159800
C	-3.60458400	1.89185900	-0.58671300
C	-2.98636200	0.65274100	-0.62324900
C	-1.76945600	0.41598800	0.03059900
C	-1.19803700	1.50377300	0.70940100
C	-1.79895700	2.75918900	0.74006100
C	-3.00961600	2.94850600	0.09533000
H	-4.54722500	2.04504400	-1.10139900
H	-3.46464200	-0.15440000	-1.17021600
H	-0.24793900	1.38646200	1.23632200
H	-1.32655000	3.57929100	1.26981500
H	-3.49066200	3.92009700	0.11659400
B	-1.66705700	-1.67553800	1.04646300
O	-2.99513000	-2.00371000	1.08149100
H	-3.51914100	-1.53254500	1.73006500
O	-0.83368500	-1.29551500	2.08328200
H	-1.20066900	-0.62188400	2.65808900

FS2

C	4.04727500	-1.67446300	0.87920000
C	2.88339000	-0.96279000	1.13853700
C	1.91881300	-0.72406200	0.14724200
C	2.20057300	-1.24300500	-1.12612200
C	3.36101000	-1.95558600	-1.40271500
C	4.28858100	-2.17247300	-0.39421500
H	4.76934400	-1.84481500	1.67158000
H	2.71645300	-0.58622200	2.14409100
H	1.49352100	-1.10144700	-1.94508100
H	3.54035900	-2.34628000	-2.39941300
H	5.19595600	-2.73061000	-0.59923900
Zr	-0.00694300	0.44404100	0.46362500
O	-0.01659200	1.01834200	2.11830000
O	0.99448200	2.28763300	-0.78066700
H	1.89220300	2.62540400	-0.81988500
C	-4.07827500	-1.66562600	0.76660300
C	-2.93503100	-0.93146700	1.05379200
C	-1.88722700	-0.79090500	0.13049400
C	-2.06013600	-1.43779900	-1.10299400

C	-3.19723000	-2.17704000	-1.40566000
C	-4.21176200	-2.29001800	-0.46652600
H	-4.86660400	-1.75837800	1.50711800
H	-2.85045200	-0.46225300	2.03059300
H	-1.28079300	-1.38388600	-1.86435400
H	-3.29088500	-2.66887600	-2.36871600
H	-5.10173400	-2.86781700	-0.69233200
B	-0.05957000	3.16846000	-0.70864600
O	0.10331800	4.49515000	-0.83702200
H	-0.67747300	5.04685900	-0.76301000
O	-1.19632000	2.42465400	-0.49928700
H	-2.02329300	2.81954300	-0.21952000

IS3'

C	4.10960600	-1.58206400	0.84465300
C	2.93613100	-0.88626800	1.10381900
C	1.93313500	-0.72811100	0.13465000
C	2.18492400	-1.31379800	-1.11592500
C	3.35395200	-2.01259800	-1.39162200
C	4.32107500	-2.14656300	-0.40617600
H	4.86199000	-1.68901800	1.61974200
H	2.79215800	-0.45861800	2.09243500
H	1.44596100	-1.23944900	-1.91513000
H	3.50964300	-2.45643600	-2.36985600
H	5.23576900	-2.69267800	-0.61107300
Zr	0.00471700	0.43673000	0.44270800
O	-0.00958500	1.02458400	2.09250700
C	-4.01826000	-1.74206200	0.84617800
C	-2.86769100	-1.00905600	1.10641300
C	-1.88183200	-0.79639400	0.13021300
C	-2.12610500	-1.36727800	-1.12845200
C	-3.27226300	-2.10255400	-1.40544700
C	-4.22319900	-2.29008600	-0.41299000
H	-4.75717800	-1.89167300	1.62718900
H	-2.72779400	-0.59625300	2.10199200
H	-1.39922500	-1.25149700	-1.93380000
H	-3.42227200	-2.53362100	-2.39026200
H	-5.11951600	-2.86554300	-0.61876700
O	0.99068100	2.33083700	-0.74146400
H	1.87203600	2.71026100	-0.71127800
B	-0.10220300	3.16502200	-0.69522600
O	0.00971700	4.50079400	-0.77269500
H	-0.79598300	5.01739000	-0.71401700
O	-1.21540200	2.36819400	-0.56796100

H	-2.07338300	2.71854200	-0.32432800
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TS3'

C	1.25229400	3.22087200	0.99818100
C	0.89886200	1.89039400	1.08267200
C	0.88059000	1.06062400	-0.06280600
C	1.32219300	1.63402400	-1.26858600
C	1.69009500	2.96744500	-1.34862900
C	1.64897300	3.77346100	-0.21997900
H	1.22525600	3.83986100	1.88898900
H	0.60017300	1.47402400	2.04022700
H	1.40208400	1.00976100	-2.15465000
H	2.02729600	3.37664100	-2.29554700
H	1.94764000	4.81376000	-0.27749200
Zr	-0.76795200	-0.62246900	0.18804100
O	-1.41880200	-0.53156500	1.82719600
C	3.35047200	-1.82065300	0.87288900
C	2.43093600	-0.82815100	1.07156600
C	1.36434400	-0.60551600	0.15441200
C	1.32687200	-1.47925900	-0.99555400
C	2.31418000	-2.44778200	-1.20022400
C	3.31563600	-2.63676500	-0.27723100
H	4.12206400	-1.98253000	1.61861200
H	2.49948900	-0.19670800	1.95080900
H	0.65666200	-1.27802300	-1.83518900
H	2.28842400	-3.04527100	-2.10635100
H	4.07555200	-3.39206100	-0.43493200
O	-2.46052500	0.76194700	-0.80329800
H	-2.60058200	1.68941400	-0.59361900
B	-3.45298800	-0.11355500	-0.40816200
O	-4.63623100	0.33242800	0.04889300
H	-5.25294100	-0.31849100	0.38739700
O	-3.02027800	-1.41000500	-0.61454100
H	-3.49411300	-2.11846100	-0.17535100

FS3'

C	0.69585600	2.95517700	-1.11086700
C	-0.25123600	1.91618500	-1.12173700
C	-1.01494200	1.59163500	0.06720700
C	-0.49908600	2.17669900	1.27458800
C	0.48425900	3.13260000	1.25949600
C	1.07398500	3.57234600	0.05582700
H	1.14673100	3.25031600	-2.05353800
H	-0.57016300	1.51779600	-2.08038500

H	-0.97277700	1.92435300	2.21693000
H	0.78573400	3.58573000	2.19849500
H	1.82113100	4.35566800	0.06064100
Zr	0.32618500	-0.31661700	-0.09065000
O	0.34108100	-1.38564200	-1.49065200
C	-3.44477900	-1.08349700	-0.96874000
C	-2.68693300	0.04378400	-1.00374500
C	-1.87387200	0.44681900	0.10830000
C	-1.76345800	-0.51517600	1.20442500
C	-2.64687300	-1.63519000	1.22654800
C	-3.44993200	-1.93459200	0.17217100
H	-4.08239800	-1.31895600	-1.81353600
H	-2.73859500	0.69949900	-1.86624600
H	-1.40258400	-0.17513800	2.17216000
H	-2.66983000	-2.25320200	2.11917000
H	-4.10121300	-2.79984700	0.20010400
O	2.74476900	-0.18225300	0.09182400
H	3.34554900	0.21698500	-0.54248700
B	2.81790400	-1.55479000	0.22329900
O	3.80439900	-2.26486400	-0.34874300
H	3.75545300	-3.21975100	-0.27847000
O	1.77552300	-1.97476900	1.02840000
H	1.48195000	-2.88535700	0.94918500

IS3

C	-4.06274700	0.17581900	1.01422000
C	-2.89293800	-0.52587100	0.76256900
C	-1.85912600	0.01985400	-0.01316200
C	-2.06254900	1.31324000	-0.51890400
C	-3.23027700	2.02459000	-0.27527000
C	-4.23270600	1.45232300	0.49384900
H	-4.84452500	-0.26908700	1.62088600
H	-2.77475700	-1.51977300	1.18404100
H	-1.29087400	1.80195700	-1.11449900
H	-3.35686200	3.02412300	-0.67780300
H	-5.14582700	2.00316300	0.69185300
Zr	0.00001000	-1.07971100	-0.59046500
O	0.00011600	-2.55197000	0.33115500
C	4.06286400	0.17570000	1.01388400
C	2.89301600	-0.52592900	0.76223500
C	1.85905700	0.02001300	-0.01315200
C	2.06236600	1.31355600	-0.51853700
C	3.23012700	2.02484600	-0.27489300
C	4.23270900	1.45236200	0.49386600

H	4.84475500	-0.26937700	1.62027900
H	2.77492000	-1.51995200	1.18344300
H	1.29056700	1.80244100	-1.11382700
H	3.35662100	3.02450600	-0.67714100
H	5.14585700	2.00315700	0.69187000

TS3

C	3.15374800	-0.53361600	1.04307200
C	1.86406300	-0.04271900	1.03909700
C	1.02644400	-0.21134300	-0.08415600
C	1.52880200	-0.96084500	-1.16013100
C	2.82206100	-1.45950600	-1.15010300
C	3.64243500	-1.24306300	-0.05281900
H	3.78936900	-0.36644000	1.90593000
H	1.49269800	0.50498500	1.89990600
H	0.88054700	-1.18552000	-2.00358900
H	3.18451000	-2.03724800	-1.99376200
H	4.64959200	-1.64307800	-0.03715400
Zr	-0.42218400	1.60453200	-0.33817800
O	-0.36553800	2.61079800	1.08919700
C	-2.18871800	-1.97379800	1.31816300
C	-1.08570600	-1.16836200	1.33631600
C	-0.71643800	-0.39220000	0.20025500
C	-1.56618100	-0.52640800	-0.97101700
C	-2.65329000	-1.41084100	-0.96908400
C	-2.98442700	-2.11642100	0.16031000
H	-2.46023600	-2.51376100	2.21928200
H	-0.48320900	-1.09372100	2.23453500
H	-1.23794600	-0.16838800	-1.95129300
H	-3.22626400	-1.54233900	-1.88150800
H	-3.83415500	-2.78742200	0.16175500

FS3

C	2.84123500	0.01299000	1.21363000
C	1.43827200	-0.09730600	1.25736500
C	0.73142900	-0.97880700	0.34779200
C	1.52507100	-1.44148700	-0.75851600
C	2.88193700	-1.24276000	-0.81535700
C	3.57434500	-0.54589100	0.19753500
H	3.33724200	0.57952500	1.99516200
H	0.91740900	0.29634600	2.12466100
H	1.05102100	-2.05102400	-1.51968900
H	3.43700300	-1.67057500	-1.64397400
H	4.64986600	-0.43385100	0.15357900

Zr	0.11758500	1.08563300	-0.48800600
O	-0.74859900	2.26748300	0.45214600
C	-2.89170800	-0.70608500	1.31230200
C	-1.54261900	-0.81731600	1.42019100
C	-0.69983900	-0.95213600	0.26574100
C	-1.35173800	-0.80162500	-1.03296400
C	-2.77717500	-0.76143100	-1.08586100
C	-3.53106300	-0.69340000	0.04183300
H	-3.49288300	-0.65433600	2.21287200
H	-1.08153000	-0.86432900	2.40060600
H	-0.85437200	-1.17583400	-1.92396700
H	-3.25572200	-0.79233500	-2.05935700
H	-4.61151800	-0.64723900	-0.01897700

(5) The optimized structures involved in Suzuki-Miyaura cross-coupling mechanism catalyzed by (ZrO)₂ cluster

IS1

C	-0.71872100	2.27011000	-0.64322100
C	0.45751300	1.66600600	-0.95335700
C	1.01742400	0.71803500	-0.00587100
C	0.72168100	0.98511500	1.43522300
C	-0.48821300	1.56942300	1.69334500
C	-1.37148400	2.00172700	0.64983400
H	-1.16332200	2.97893800	-1.33535900
H	0.95114200	1.84645000	-1.90127600
H	1.47285100	0.86607000	2.20809700
H	-0.78576400	1.72924600	2.72600700
H	-2.18802300	2.66020800	0.93862700
Br	2.87257800	0.05782600	-0.26688100
Zr	0.10952500	-1.20668000	0.38050700
Zr	-2.01333000	-0.00845700	-0.46469200
O	-1.83278700	-1.18808800	1.03140500
O	-0.71523200	-1.15714500	-1.40435100

TS1

C	-0.96320900	2.09744900	-0.84304000
C	0.24522900	1.52259200	-1.08170200
C	0.90403300	0.81450700	0.00602700
C	0.64364200	1.37378400	1.35503100
C	-0.57996400	1.90280000	1.56522800
C	-1.56927100	1.98944300	0.49624100
H	-1.46843500	2.63771900	-1.63923900
H	0.69700900	1.54016000	-2.06600200

H	1.40608700	1.34794400	2.12319800
H	-0.84205500	2.27335300	2.55045300
H	-2.41275300	2.65232100	0.68539200
Br	2.77271500	0.23763800	-0.27350000
Zr	0.34651200	-1.33221300	0.35463700
Zr	-2.08847900	-0.13274400	-0.36098500
O	-1.45883200	-1.10500900	1.17212100
O	-0.64479400	-1.19173900	-1.27388200

FS1

C	-2.98347300	0.95226400	-1.20912000
C	-1.65667100	1.32115400	-1.21287500
C	-0.83001300	1.24366200	0.00017900
C	-1.65675200	1.32082500	1.21320500
C	-2.98356000	0.95195400	1.20925900
C	-3.63964200	0.54431200	-0.00000400
H	-3.52706700	0.90305300	-2.14752700
H	-1.19049700	1.55098900	-2.16399800
H	-1.19063200	1.55038200	2.16442100
H	-3.52721900	0.90249900	2.14761500
H	-4.69610900	0.31810700	-0.00007000
Br	3.53378300	0.32937600	0.00001800
Zr	0.96882900	-0.12287600	0.00001800
Zr	-1.60958800	-0.81509100	-0.00009700
O	-0.08876400	-1.07763600	1.31204800
O	-0.08872000	-1.07730100	-1.31227200

IM

C	2.44650400	0.71909000	1.20906100
C	1.18104600	1.25987600	1.21216900
C	0.34505200	1.28510400	0.00112100
C	1.18086000	1.26191800	-1.21010500
C	2.44631300	0.72113900	-1.20812600
C	3.04328700	0.22036200	0.00000000
H	2.98043200	0.60290200	2.14731700
H	0.75171600	1.55065500	2.16426500
H	0.75136800	1.55434400	-2.16162300
H	2.98010400	0.60659300	-2.14666100
H	4.06521800	-0.13006700	-0.00037600
Zr	-1.63921900	0.15117800	0.00025100
Zr	0.85113700	-0.85397600	-0.00070100
O	-0.68305000	-0.93121800	-1.31557600
O	-0.68285200	-0.93356000	1.31414900
O	-3.55727100	0.64439400	0.00016300

H	-4.47856500	0.88561900	0.00049100
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IS2

C	3.29354200	1.19883200	1.37449700
C	1.92236800	1.13099300	1.48032200
C	1.05425600	1.05267000	0.29483100
C	1.71868300	1.64283700	-0.87694600
C	3.09006800	1.71349000	-0.97738200
C	3.93973400	1.28219500	0.09546400
H	3.90360400	1.12467500	2.26979700
H	1.49121100	1.00046900	2.46670100
H	1.12646200	1.91343900	-1.74405200
H	3.54207100	2.03837100	-1.90977400
H	5.01086800	1.40774200	0.03039300
Zr	-0.26574300	-0.77927900	0.01915200
Zr	2.40050700	-0.62011500	-0.18880900
O	0.96713900	-1.05852800	-1.49875700
O	1.16608800	-1.61638700	1.04813600
O	-1.98163200	-1.79792800	-1.03418900
H	-2.34096700	-1.79487300	-1.92213400
C	-2.98277700	2.52338600	1.14966100
C	-2.94411900	1.13723900	1.18165300
C	-2.86943700	0.37579500	0.00773500
C	-2.81271700	1.07893600	-1.20235400
C	-2.84714300	2.46554500	-1.24456300
C	-2.93473100	3.19044000	-0.06541600
H	-3.04088700	3.08600300	2.07493200
H	-2.96731800	0.62451800	2.13791100
H	-2.74598200	0.53371100	-2.14019500
H	-2.80386100	2.98128000	-2.19757300
H	-2.95603100	4.27410800	-0.09336500
B	-2.88973100	-1.25936400	0.05703700
O	-2.01290600	-1.58414500	1.25885500
H	-2.08021500	-2.51528400	1.49121100
O	-4.13845800	-1.91675700	0.02352200
H	-4.84906500	-1.36580000	0.35168800

TS2

C	3.62773000	0.65773900	1.52439900
C	2.26672100	0.72224500	1.72512800
C	1.33851400	1.13753500	0.66320100
C	2.02742200	1.98302000	-0.32431100
C	3.38750000	1.91459300	-0.52456800
C	4.21759300	1.06411300	0.28097500

H	4.26236700	0.22821900	2.29378800
H	1.86968400	0.33008100	2.65491000
H	1.44026200	2.58797800	-1.00639800
H	3.83569100	2.46288800	-1.34776800
H	5.29145000	1.07513200	0.16223100
Zr	-0.23371900	-0.32271500	-0.08742600
Zr	2.41936500	-0.45327000	-0.43101700
O	0.86929000	-0.26762300	-1.70326500
O	1.14827500	-1.64692900	0.53812800
O	-1.72955100	-2.16485300	-0.98153300
H	-2.31097200	-2.17736000	-1.74621700
C	-4.05141900	1.94396200	1.18495700
C	-3.02069800	1.01389300	1.20198400
C	-2.47994100	0.47192500	0.02692700
C	-3.03748400	0.92978100	-1.17574200
C	-4.06533200	1.86352300	-1.21321300
C	-4.57697400	2.37016100	-0.02737700
H	-4.44463400	2.34193500	2.11507100
H	-2.62735500	0.70067300	2.16760700
H	-2.66496800	0.55141400	-2.12851300
H	-4.47034000	2.19435300	-2.16416200
H	-5.38247000	3.09618900	-0.04750300
B	-2.39013700	-1.92172100	0.22463400
O	-1.48319400	-1.82484700	1.30715300
H	-0.74727600	-2.45867300	1.28984800
O	-3.71296500	-2.18943800	0.35196000
H	-4.06326100	-1.97024700	1.21798800

FS2

C	-3.59015700	-0.07642700	1.52728200
C	-2.24037400	-0.00372600	1.79465300
C	-1.26662700	-0.86639700	1.11333500
C	-1.90678100	-2.09763800	0.62468500
C	-3.25409800	-2.15962200	0.35168800
C	-4.11886100	-1.04349200	0.61080700
H	-4.26024800	0.65868500	1.96256300
H	-1.88842700	0.79941400	2.43201500
H	-1.28756600	-2.94505200	0.35237000
H	-3.66309500	-3.04507200	-0.12518400
H	-5.18561200	-1.13125400	0.46329200
Zr	0.36860600	-0.00196700	-0.16635100
Zr	-2.28274700	-0.00837200	-0.65760300
O	-0.66045900	-0.75864300	-1.61851300
O	-1.08239400	1.52093200	-0.33782000

O	1.71214500	1.87207300	-0.00563400
H	2.64775300	1.63536100	0.05134100
C	4.68913500	-1.15499100	1.12614300
C	3.42805900	-0.57782400	1.04078400
C	2.47627200	-0.96611800	0.08254500
C	2.88227800	-1.98852200	-0.79216100
C	4.13956800	-2.57622400	-0.72281800
C	5.04888800	-2.15830400	0.23825600
H	5.38965700	-0.82751400	1.88790600
H	3.18139700	0.19008300	1.77578600
H	2.19797700	-2.34622000	-1.55990000
H	4.41218700	-3.36229200	-1.42000800
H	6.03144400	-2.61385700	0.29687700
B	1.46254400	3.26381600	0.01582800
O	0.21212600	3.71761600	-0.06257600
H	-0.44339400	2.96260800	-0.16249300
O	2.57363600	4.04272200	0.12700500
H	2.35662100	4.97773200	0.13355700

IS3'

C	4.40110000	-1.31630000	0.06430000
C	3.04660000	-1.29500000	0.36260000
C	2.14760000	-0.51000000	-0.36860000
C	2.67380000	0.24930000	-1.42140000
C	4.02910000	0.23770000	-1.73030000
C	4.89350000	-0.54730000	-0.98310000
H	5.07720000	-1.93560000	0.64440000
H	2.68650000	-1.91600000	1.17990000
H	2.02020000	0.87260000	-2.03520000
H	4.40790000	0.83480000	-2.55290000
H	5.95200000	-0.56420000	-1.21800000
Zr	-0.05160000	-0.14890000	-0.19130000
Zr	-2.11970000	-2.08700000	-1.06390000
O	-0.80070000	-0.98530000	-1.83870000
O	-1.52410000	-1.35600000	0.58320000
C	0.06970000	4.36050000	-0.13480000
C	0.39510000	3.01130000	-0.09800000
C	-0.56520000	2.01590000	-0.32720000
C	-1.87320000	2.43960000	-0.59650000
C	-2.20840000	3.78590000	-0.63520000
C	-1.23540000	4.74800000	-0.40360000
H	0.83310000	5.11040000	0.04400000
H	1.42910000	2.74020000	0.10810000
H	-2.65300000	1.70480000	-0.78700000

H	-3.22870000	4.08640000	-0.84840000
H	-1.49380000	5.80090000	-0.43410000
O	-1.37110000	-0.97300000	3.23550000
H	-1.64210000	-1.20570000	2.32160000
B	-0.17460000	-0.37610000	3.26890000
O	0.48180000	-0.03030000	4.40550000
H	-0.00300000	-0.26970000	5.19890000
O	0.50190000	-0.06720000	2.06980000
H	1.39050000	0.27080000	2.23260000

TS3'

C	2.19870000	-1.95280000	2.68230000
C	1.63090000	-0.96420000	1.91090000
C	1.49580000	-1.10900000	0.50910000
C	2.03510000	-2.27270000	-0.06650000
C	2.61710000	-3.26040000	0.71060000
C	2.69620000	-3.11260000	2.08670000
H	2.25820000	-1.82820000	3.75790000
H	1.26180000	-0.06660000	2.40190000
H	2.00500000	-2.39290000	-1.14510000
H	3.02060000	-4.14820000	0.23600000
H	3.15510000	-3.88300000	2.69490000
Zr	-0.33880000	0.08100000	-0.34340000
Zr	-3.01840000	-1.18560000	-0.53070000
O	-1.39200000	-1.25020000	-1.46510000
O	-2.20390000	0.11840000	0.57990000
C	3.55120000	1.95330000	-0.82690000
C	2.81610000	1.18640000	0.03860000
C	1.78860000	0.32260000	-0.43130000
C	1.58040000	0.28720000	-1.86180000
C	2.40710000	1.01780000	-2.72150000
C	3.37180000	1.86090000	-2.22260000
H	4.29760000	2.63170000	-0.42730000
H	3.02400000	1.22320000	1.10350000
H	0.92280000	-0.45540000	-2.32570000
H	2.27730000	0.91130000	-3.79330000
H	3.99710000	2.43860000	-2.89140000
O	-2.29660000	2.56710000	1.64920000
H	-2.46690000	1.65190000	1.32730000
B	-1.05560000	2.98340000	1.37910000
O	-0.55840000	4.19860000	1.72720000
H	-1.20450000	4.73880000	2.18820000
O	-0.15390000	2.13820000	0.69860000
H	0.72290000	2.53040000	0.57690000

FS3'

C	1.89900000	2.05340000	1.96900000
C	0.57260000	1.76470000	1.53820000
C	0.08740000	2.34560000	0.28560000
C	1.09360000	2.90070000	-0.57420000
C	2.37960000	3.06300000	-0.15510000
C	2.79250000	2.66360000	1.14470000
H	2.19320000	1.75730000	2.96990000
H	-0.14930000	1.49820000	2.30900000
H	0.79550000	3.26340000	-1.55170000
H	3.09270000	3.54100000	-0.81710000
H	3.80820000	2.84910000	1.47020000
Zr	0.05610000	0.07540000	-0.10180000
Zr	2.27740000	-1.87200000	-0.51360000
O	1.54290000	-0.32110000	-1.33380000
O	0.91260000	-1.68050000	0.75130000
C	-3.55020000	1.45270000	0.38870000
C	-2.33060000	1.93700000	0.76230000
C	-1.23990000	2.05250000	-0.16200000
C	-1.46970000	1.50010000	-1.48940000
C	-2.75650000	1.05520000	-1.85010000
C	-3.77790000	0.98330000	-0.93360000
H	-4.36240000	1.43990000	1.10670000
H	-2.19050000	2.31730000	1.76830000
H	-0.74750000	1.67940000	-2.28190000
H	-2.92680000	0.73650000	-2.87310000
H	-4.75650000	0.62210000	-1.22380000
O	-1.24780000	-3.11020000	1.35920000
H	-0.34230000	-2.73560000	1.25700000
B	-2.17100000	-2.36890000	0.73930000
O	-3.48820000	-2.69400000	0.66330000
H	-3.67760000	-3.53390000	1.08810000
O	-1.82190000	-1.15160000	0.11410000
H	-2.59880000	-0.70040000	-0.27980000

IS3

C	0.01137300	-4.31061700	-0.42586900
C	-0.35759100	-2.97342000	-0.38097700
C	0.55630200	-1.96778200	-0.03204900
C	1.86403800	-2.37315000	0.27171600
C	2.24092100	-3.70823200	0.23607400
C	1.31295200	-4.67860300	-0.11484000
H	-0.71530300	-5.06730400	-0.70210100

H	-1.38616600	-2.71747000	-0.62711100
H	2.61384200	-1.63157400	0.54077400
H	3.25933600	-3.99310200	0.47787200
H	1.60446800	-5.72275500	-0.14740100
Zr	0.04919900	0.20797900	-0.09658900
Zr	2.14597200	2.22863600	0.09165300
O	0.97379700	1.30552900	1.26669100
O	1.30005900	1.19531500	-1.26180100
C	-4.40273000	1.28135700	-0.64398100
C	-3.05835600	1.36015600	-0.96581400
C	-2.10766800	0.60978900	-0.26729300
C	-2.56621600	-0.20925000	0.76906200
C	-3.91342400	-0.29512200	1.10762400
C	-4.83050100	0.45468400	0.39188200
H	-5.12888900	1.86745900	-1.19714900
H	-2.74617100	2.01709900	-1.77187800
H	-1.86857600	-0.82654500	1.35353500
H	-4.24029000	-0.93701100	1.91808300
H	-5.88455000	0.40096600	0.64048300

TS3

C	1.59162700	3.20696200	-0.98381400
C	1.20759900	1.88840300	-1.06991300
C	1.18953500	1.05042200	0.07090200
C	1.65784600	1.60151200	1.27723600
C	2.06028100	2.92444000	1.35626100
C	2.02296400	3.73676900	0.23346900
H	1.56133400	3.83471800	-1.86755500
H	0.89268000	1.49732800	-2.03611300
H	1.71846100	0.97338800	2.16058000
H	2.41492200	3.32122600	2.30132600
H	2.34288700	4.77011200	0.29416000
Zr	-0.42284900	-0.62513900	-0.14809800
Zr	-3.28083300	-0.04087500	0.04218800
O	-1.84864100	-0.29245200	1.24260200
O	-1.98936200	-0.34432900	-1.32949800
C	3.69813600	-1.77222900	-0.95969400
C	2.81097900	-0.73805500	-1.09668900
C	1.72766600	-0.57440300	-0.19588300
C	1.61287400	-1.55633300	0.85623300
C	2.59020300	-2.54274500	1.03033000
C	3.61475300	-2.66973300	0.12450300
H	4.48820900	-1.89208600	-1.69297200
H	2.93495700	-0.02090900	-1.90129600

H	0.90235900	-1.42743500	1.68316400
H	2.52870400	-3.20570800	1.88669500
H	4.36001900	-3.44587500	0.24594500

FS3

C	1.43260900	2.76633400	-1.27057000
C	1.58860000	1.35697100	-1.23723500
C	2.14491000	0.71192800	-0.05198300
C	2.16215400	1.53849900	1.12363800
C	1.88924500	2.87903400	1.07027700
C	1.56115300	3.52567100	-0.14458300
H	1.17501800	3.23157600	-2.21609200
H	1.63011500	0.84510300	-2.19321100
H	2.48331000	1.10510300	2.06363900
H	1.96462500	3.46306200	1.98103300
H	1.40139600	4.59563100	-0.16954100
Zr	-0.04982300	0.00003900	-0.00001100
Zr	-2.98140800	0.00036100	0.00001300
O	-1.58572300	0.75502100	1.03248400
O	-1.58590700	-0.75459300	-1.03248800
C	1.88820700	-2.87953800	-1.07028200
C	2.16156600	-1.53909100	-1.12365200
C	2.14468100	-0.71252200	0.05197800
C	1.58819200	-1.35738600	1.23724200
C	1.43171600	-2.76669000	1.27058100
C	1.55995800	-3.52607200	0.14458600
H	1.96333200	-3.46358100	-1.98104900
H	2.48282200	-1.10580700	-2.06367000
H	1.62986700	-0.84551500	2.19320900
H	1.17399300	-3.23184600	2.21611000
H	1.39983100	-4.59597600	0.16954500

(6) The optimized structures involved in Suzuki-Miyaura cross-coupling mechanism catalyzed by (ZrO)₃ cluster

IS1

Zr	2.89523800	0.75390200	-0.27504100
Zr	-0.25905700	0.62049600	0.09086800
Zr	1.93841200	-1.65393700	0.43305900
O	1.27722900	1.71801700	-0.61356200
O	0.05474600	-1.35810100	0.31259100
O	3.13864000	-1.05630700	-1.01345000
C	-1.91782300	2.41873600	-0.58075000
C	-1.60682600	2.67110200	0.72099900

C	-1.57766100	1.59496100	1.70727700
C	-2.47268500	0.49594100	1.34514100
C	-2.78358700	0.26261800	0.04024200
C	-2.22119000	1.06254800	-1.04264200
H	-1.81608100	3.20297000	-1.32159300
H	-1.26203900	3.65734600	1.00855000
H	-1.46931900	1.84110300	2.75411800
H	-2.80093600	-0.19775800	2.10879700
H	-2.59917400	0.91925700	-2.04442100
Br	-3.80921400	-1.24873400	-0.43106200

TS1

Zr	1.86163700	1.34535000	-0.79248300
Zr	-0.25578500	0.02943600	0.44524000
Zr	2.60573400	-0.79683800	0.66871700
O	0.23781700	1.90151500	0.21449400
O	0.84404000	-1.34674800	1.33527800
O	3.11680500	-0.21519300	-1.09227600
C	-3.42793300	1.99923400	-0.47574300
C	-3.64037600	2.11312300	0.89759700
C	-3.34712000	1.05099700	1.73825500
C	-2.85110400	-0.14880600	1.22763100
C	-2.67383100	-0.25173300	-0.16495200
C	-2.94429000	0.82338900	-1.02232700
H	-3.63264000	2.83922500	-1.12851500
H	-4.02085700	3.03876600	1.31070000
H	-3.49865600	1.14020500	2.80756900
H	-2.70032100	-1.00731800	1.87149200
H	-2.77573100	0.72505600	-2.08655400
Br	-2.06047500	-1.88821900	-0.92846800

FS1

Zr	2.10139900	-0.73524000	1.33964900
Zr	-0.47048800	0.52104400	-0.00000100
Zr	2.10121200	-0.73574500	-1.33952500
O	0.44018800	0.16177300	1.72303700
O	0.43999500	0.16120100	-1.72302000
O	3.39832600	-0.09899900	-0.00015700
C	-3.99992400	-2.00996500	1.20089900
C	-4.57516700	-2.40168000	0.00023900
C	-4.00028800	-2.00945600	-1.20042800
C	-2.85255400	-1.22896800	-1.19578400
C	-2.24867300	-0.81728200	0.00022800
C	-2.85219600	-1.22946900	1.19624700

H	-4.44719500	-2.31456600	2.14134900
H	-5.47097700	-3.01317000	0.00024400
H	-4.44783800	-2.31365600	-2.14087400
H	-2.42087900	-0.93860400	-2.15071600
H	-2.42023900	-0.93949800	2.15116800
Br	-1.17523000	2.96875000	-0.00038200

IM

Zr	-1.94456300	1.26819100	-0.71542600
Zr	0.54515100	0.11086600	0.97552800
Zr	-1.95858700	-1.38179400	-0.40274400
O	-0.36592100	1.74085100	0.28007100
O	-0.37427900	-1.62755000	0.66778400
O	-3.29847700	0.01463000	-0.01657400
C	4.53737100	1.06534200	-0.93747200
C	5.08067200	-0.16740800	-1.27021700
C	4.36791100	-1.32711500	-1.00177200
C	3.11757800	-1.24887600	-0.40238600
C	2.54142100	-0.02038600	-0.05306500
C	3.28633900	1.13136700	-0.33859300
H	5.09027400	1.97567200	-1.14559100
H	6.05738300	-0.22395600	-1.73862600
H	4.78773800	-2.29372600	-1.26098600
H	2.58172200	-2.17475300	-0.20622000
H	2.88690900	2.11325000	-0.09299500
O	0.85599000	0.33462900	2.86383600
H	0.78967200	0.41498700	3.81021700

IS2

Zr	-0.78453000	-1.46177000	-1.24466600
Zr	0.88594400	0.27656400	0.38164700
Zr	1.42670300	-2.70945600	0.03651600
O	-0.26001400	0.40280800	-1.21838500
O	1.74386200	-1.28422200	1.29407900
O	-0.33346000	-3.27879600	-0.43351700
C	4.69827600	2.69372700	0.62861500
C	4.61766100	3.60551300	-0.41455300
C	3.54055600	3.55672400	-1.28883500
C	2.54973400	2.59972300	-1.11662900
C	2.59934500	1.66218400	-0.07352500
C	3.70237600	1.73955700	0.79094000
H	5.54105300	2.72424300	1.31183000
H	5.39463400	4.35064000	-0.54778800
H	3.47601100	4.26535000	-2.10835500

H	1.72002800	2.57918800	-1.81872600
H	3.80080800	1.02873400	1.60975000
O	-2.69220300	-0.29929500	2.67972700
H	-3.57321000	0.03980500	2.83741300
C	-3.60661400	3.41079000	-0.13053300
C	-2.80148300	2.52405700	0.57000600
C	-3.04939300	1.15105900	0.56389100
C	-4.14955700	0.70283000	-0.17281600
C	-4.96258900	1.58094800	-0.87583500
C	-4.69028900	2.94093500	-0.85797300
H	-3.38464300	4.47240300	-0.11385500
H	-1.95347900	2.90841900	1.12745900
H	-4.37834900	-0.35921700	-0.19521700
H	-5.80901100	1.20412400	-1.44023200
H	-5.31898300	3.63128400	-1.40940000
B	-2.17737500	0.11777800	1.41619400
O	-1.92735300	-1.14806700	0.58109200
O	-0.76393500	0.68134000	1.73614500
H	-0.69597400	0.65886500	2.69685200
H	-1.88001800	-1.90467300	1.17977800

TS2

Zr	-2.36379300	-0.35151400	-1.12915600
Zr	0.35124400	-0.18808300	-0.00382900
Zr	-2.12152600	-1.43644700	1.40039200
O	-0.53871900	-0.27426700	-1.80276000
O	-0.36265300	-0.72287800	1.77556900
O	-3.43847500	-0.30393100	0.62072000
C	3.99723800	-2.76975900	0.62580900
C	4.35575400	-3.21660700	-0.63828700
C	3.57842200	-2.87117900	-1.73505300
C	2.44932000	-2.08121500	-1.56405100
C	2.06009100	-1.61062400	-0.30172600
C	2.86638900	-1.97989100	0.78510500
H	4.59958200	-3.03958400	1.48744000
H	5.23770600	-3.83474400	-0.76798800
H	3.85312700	-3.22116500	-2.72508700
H	1.85247700	-1.83082400	-2.43752300
H	2.60698500	-1.65046800	1.78947800
O	-0.38691400	2.54375600	-2.13136300
H	-0.32061400	1.62283500	-2.42233100
C	2.39637600	2.78864900	2.11698600
C	1.22984800	2.27243300	1.57156500
C	1.10488800	2.00102900	0.19613900

C	2.23460400	2.26293400	-0.59684400
C	3.40682900	2.77908900	-0.06268700
C	3.48706100	3.04393700	1.29702600
H	2.45590600	2.99543200	3.18022300
H	0.38940000	2.08694300	2.23570800
H	2.18529900	2.08448900	-1.66751600
H	4.25755100	2.97709400	-0.70578800
H	4.40087800	3.44780200	1.71895600
B	-0.72762200	2.62515300	-0.79793000
O	-1.74689200	1.67041900	-0.33773600
O	-0.90336200	3.84909200	-0.18493300
H	-2.17778800	1.94817500	0.47940600
H	-0.32419800	4.51968700	-0.55143700

FS2

Zr	1.26559100	-1.60681500	1.22303200
Zr	-0.83097400	0.17259400	-0.11798400
Zr	0.52373100	-2.37824500	-1.30587300
O	-0.00259900	-0.24478800	1.66354400
O	-0.50044200	-0.80917300	-1.81635600
O	2.25191400	-2.44378100	-0.45599000
C	-5.29959500	0.12606300	-0.68543500
C	-5.84610000	-0.01343400	0.58215200
C	-5.00888600	-0.13621300	1.68269600
C	-3.63128100	-0.11867400	1.51142400
C	-3.04596800	0.02116800	0.24533700
C	-3.91992300	0.14100000	-0.84459100
H	-5.94956900	0.22064100	-1.54938000
H	-6.92288600	-0.02787000	0.71244600
H	-5.43294500	-0.24677000	2.67565800
H	-2.99832000	-0.22112800	2.38953000
H	-3.52216000	0.24264100	-1.85307000
O	3.07592900	2.09799300	1.04461000
H	2.11066900	2.11640100	1.01525600
C	0.88875600	4.09042300	-1.76515800
C	0.45105800	2.77857300	-1.64466100
C	-0.07364300	2.28015100	-0.44308000
C	-0.13305100	3.17701500	0.63651400
C	0.30372400	4.49247500	0.52744800
C	0.81631600	4.94979500	-0.67725000
H	1.28906100	4.44646500	-2.70890100
H	0.51811500	2.12810500	-2.51334600
H	-0.53172700	2.84858600	1.59537400
H	0.24518300	5.15914400	1.38150000

H	1.16221900	5.97360300	-0.76771400
B	3.66094700	0.97351300	0.60746800
O	2.91992700	-0.22080300	0.49941400
O	4.98462400	0.99800200	0.30450700
H	5.37802600	0.14595800	0.11267300
H	3.17242100	-0.90432700	-0.16459500

IS3'

Zr	1.83230000	-1.29990000	0.69650000
Zr	-0.85210000	-0.00250000	-0.16990000
Zr	0.89360000	-2.06570000	-1.75660000
O	0.54400000	0.02240000	1.30240000
O	-0.69560000	-0.98470000	-1.89060000
O	2.61360000	-1.36370000	-1.12090000
C	-5.08180000	-1.41010000	0.62080000
C	-5.27340000	-1.20270000	1.97960000
C	-4.23420000	-0.70460000	2.75250000
C	-3.01040000	-0.41640000	2.16320000
C	-2.78340000	-0.61320000	0.79350000
C	-3.85390000	-1.11870000	0.04220000
H	-5.89160000	-1.80000000	0.01260000
H	-6.23100000	-1.42980000	2.43560000
H	-4.37910000	-0.54100000	3.81550000
H	-2.21390000	-0.03110000	2.79660000
H	-3.73260000	-1.29530000	-1.02430000
C	-1.21840000	3.82910000	-2.57390000
C	-1.14140000	2.50030000	-2.17840000
C	-0.89260000	2.13880000	-0.84640000
C	-0.71960000	3.18570000	0.07040000
C	-0.79330000	4.51790000	-0.31430000
C	-1.04440000	4.84100000	-1.64020000
H	-1.41470000	4.07760000	-3.61200000
H	-1.27850000	1.72700000	-2.93040000
H	-0.51700000	2.96830000	1.11720000
H	-0.65380000	5.30490000	0.41970000
H	-1.10330000	5.88020000	-1.94550000
O	2.37120000	1.73380000	2.45930000
H	1.59970000	1.20740000	2.15870000
B	3.51090000	1.46240000	1.81490000
O	3.58390000	0.27710000	1.03540000
O	4.57920000	2.29100000	1.93800000
H	5.40470000	1.97960000	1.56630000
H	4.21650000	0.27350000	0.31030000

TS3'

Zr	2.29000000	-0.46490000	1.05100000
Zr	-0.45210000	-0.15160000	-0.25890000
Zr	1.83460000	-2.00040000	-1.18350000
O	0.58350000	0.39360000	1.44480000
O	0.02370000	-1.45090000	-1.66390000
O	3.45000000	-1.16930000	-0.45450000
C	-4.21540000	-2.40720000	0.62580000
C	-4.65230000	-1.98700000	1.88170000
C	-4.08590000	-0.85390000	2.44830000
C	-3.09550000	-0.15410000	1.78110000
C	-2.61250000	-0.57380000	0.52630000
C	-3.23280000	-1.71180000	-0.04530000
H	-4.64830000	-3.29260000	0.17170000
H	-5.43290000	-2.53050000	2.40080000
H	-4.42470000	-0.50510000	3.41840000
H	-2.68440000	0.74150000	2.23700000
H	-2.90980000	-2.06580000	-1.02060000
C	-3.68320000	2.12550000	-2.16170000
C	-3.33300000	0.90860000	-1.62940000
C	-2.37420000	0.81440000	-0.59580000
C	-1.79070000	2.03550000	-0.14380000
C	-2.19410000	3.26500000	-0.66320000
C	-3.13350000	3.31930000	-1.67070000
H	-4.40320000	2.16110000	-2.97260000
H	-3.80460000	0.00330000	-1.99560000
H	-1.09770000	2.05310000	0.69950000
H	-1.76090000	4.17580000	-0.26330000
H	-3.44730000	4.27260000	-2.07810000
O	1.57710000	2.93920000	1.40630000
H	1.12700000	2.07710000	1.57340000
B	2.63730000	2.83480000	0.59920000
O	3.15750000	1.53570000	0.34910000
O	3.21580000	3.94160000	0.06900000
H	4.02950000	3.80800000	-0.41760000
H	3.73080000	1.40040000	-0.41370000

FS3'

Zr	-1.20260000	-0.08760000	0.63250000
Zr	1.07460000	0.13070000	-1.03940000
Zr	0.04750000	2.78330000	0.20060000
O	-0.71190000	-0.54230000	-1.33110000
O	1.08090000	2.12860000	-1.25890000
O	-1.58330000	1.86710000	0.61220000

C	-0.50820000	-0.61220000	2.97070000
C	-1.54220000	-1.49800000	2.54520000
C	-1.11720000	-2.51300000	1.60610000
C	0.05660000	-2.41400000	0.92330000
C	0.98370000	-1.28190000	1.09420000
C	0.67380000	-0.47410000	2.27820000
H	-0.70030000	0.06720000	3.79470000
H	-2.41710000	-1.65500000	3.15970000
H	-1.77070000	-3.35400000	1.40240000
H	0.30790000	-3.17890000	0.19920000
H	1.38070000	0.27110000	2.61220000
C	4.58100000	-0.44750000	0.29990000
C	3.36570000	-0.46940000	0.92760000
C	2.26910000	-1.25370000	0.44000000
C	2.48850000	-1.86660000	-0.86300000
C	3.79120000	-1.91010000	-1.41790000
C	4.82580000	-1.20850000	-0.87130000
H	5.38260000	0.13830000	0.73550000
H	3.24960000	0.08370000	1.85110000
H	1.75880000	-2.57870000	-1.24280000
H	3.94560000	-2.50190000	-2.31430000
H	5.80940000	-1.22020000	-1.32300000
O	-2.96230000	-1.26080000	-2.41880000
H	-2.03360000	-1.03470000	-2.14300000
B	-3.84630000	-0.99470000	-1.46300000
O	-3.37290000	-0.53690000	-0.20030000
O	-5.18010000	-1.17260000	-1.68190000
H	-5.77340000	-0.98540000	-0.95530000
H	-4.06230000	-0.30260000	0.42450000

IS3

Zr	2.40754500	-0.36900000	1.35382600
Zr	-0.42812300	-0.02192500	-0.00159400
Zr	2.42249200	-0.34045600	-1.33303900
O	0.53688700	-0.10149300	1.73664600
O	0.55544600	-0.05985400	-1.72953200
O	3.40171200	0.69400100	0.02639400
C	-3.51953600	-3.07465000	-1.25302600
C	-4.00967200	-3.59512100	-0.06370300
C	-3.48393600	-3.16232600	1.14551100
C	-2.47168700	-2.21216400	1.15949000
C	-1.95496000	-1.66465900	-0.02328800
C	-2.50744900	-2.12450000	-1.22706800
H	-3.92777800	-3.41032400	-2.20081400

H	-4.80039700	-4.33743500	-0.07913000
H	-3.86451800	-3.56698300	2.07777000
H	-2.07687100	-1.89542600	2.12252500
H	-2.14216100	-1.73713200	-2.17597300
C	-2.28790200	3.94741000	-1.16115400
C	-1.62304500	2.72843900	-1.16875700
C	-1.42481400	1.98773700	0.00514700
C	-1.92715900	2.53785100	1.19292600
C	-2.59438700	3.75525700	1.21200200
C	-2.77572200	4.46215700	0.03163900
H	-2.42634400	4.49825200	-2.08588900
H	-1.24757800	2.35039900	-2.11682700
H	-1.79375600	2.01069700	2.13538500
H	-2.97264300	4.15507600	2.14724200
H	-3.29524100	5.41430300	0.04160900

TS3

Zr	2.60799700	-0.27637100	1.32986700
Zr	-0.14673400	0.04981900	-0.05108800
Zr	2.64255900	-0.17593800	-1.35299600
O	0.72663300	-0.24888400	1.74554300
O	0.74596800	-0.21178800	-1.79774500
O	3.68441100	0.77040600	0.03896600
C	-3.61498100	-2.60389100	-1.05006700
C	-4.24263600	-2.92809000	0.15277000
C	-3.90952500	-2.22059700	1.29899800
C	-2.96057300	-1.21376200	1.25412900
C	-2.28735500	-0.88593500	0.05987400
C	-2.67624700	-1.59699900	-1.10361900
H	-3.86401600	-3.15024200	-1.95391100
H	-4.99000600	-3.71177800	0.18709000
H	-4.40063100	-2.44919700	2.23918800
H	-2.73403700	-0.66044800	2.16055200
H	-2.20490600	-1.36853900	-2.05617900
C	-3.47741200	2.72821100	-1.01029600
C	-3.02734400	1.43523500	-1.11322200
C	-2.15442300	0.88790300	-0.14699000
C	-1.76062200	1.74203100	0.92771600
C	-2.27649100	3.03326700	1.04647500
C	-3.12649000	3.53359900	0.08478700
H	-4.12114200	3.12904500	-1.78606200
H	-3.35210400	0.81386700	-1.94075400
H	-1.13482300	1.37564200	1.74714600
H	-2.00079900	3.63919800	1.90327400

H	-3.52188600	4.53833600	0.17090600
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FS3

Zr	0.44824700	2.74916200	0.33657400
Zr	1.35992200	-0.27800600	-0.51255500
Zr	-1.48980000	0.26777000	-0.41372800
O	1.79210200	1.70255500	-0.47948300
O	-0.19608400	-0.18753300	-1.78859700
O	-1.27176900	2.23330500	-0.29322500
C	2.53618700	-2.49173000	-0.58260800
C	3.31214000	-1.71960300	0.35455200
C	2.69423800	-1.22291700	1.48262000
C	1.28647200	-1.27341600	1.63776800
C	0.49429200	-2.12385500	0.73563100
C	1.19611100	-2.78426800	-0.30569100
H	3.02324800	-2.96205400	-1.42632500
H	4.36868400	-1.56298500	0.18232200
H	3.26962400	-0.64218700	2.19530500
H	0.85344900	-0.88708900	2.54569200
H	0.65221200	-3.38615800	-1.02182800
C	-3.02126400	-1.92309500	-0.57205100
C	-1.76216200	-2.41696400	-0.36265700
C	-0.91422900	-1.91345800	0.69816500
C	-1.59724400	-1.10635100	1.68637700
C	-2.89553200	-0.65899500	1.48188600
C	-3.58448000	-0.92017700	0.27593400
H	-3.58258300	-2.26207900	-1.43556800
H	-1.35760200	-3.11959700	-1.07748900
H	-1.08399100	-0.81467700	2.59030900
H	-3.34281600	-0.00600600	2.22321400
H	-4.59612900	-0.57181300	0.12363000

(7) The optimized structures involved in Suzuki-Miyaura cross-coupling mechanism catalyzed by (ZrO)₄ cluster

IS1

Zr	2.16183900	-0.88896400	-1.19538300
Zr	-0.36246500	-1.23771400	0.35146200
O	3.14363700	-0.62207800	0.50144600
O	1.69168700	0.83632400	-1.90729700
O	0.78305300	-2.23456200	-0.97010800
Zr	1.92736800	0.18736700	1.76121900
Zr	0.29924200	1.40922500	-0.54040200
O	1.50285900	1.88576200	1.06840800
C	-1.72858700	2.21125400	0.58983300

C	-1.64548600	0.80237000	0.97083700
C	-2.23265600	-0.19402100	0.06657600
C	-1.70676700	0.12146400	-1.27500500
C	-1.78883700	1.51394400	-1.71950100
C	-1.91988700	2.52541600	-0.75364800
H	-1.72227900	2.98305800	1.34849800
H	-1.70458300	0.62392100	2.04732100
H	-1.82174000	-0.61671100	-2.06667900
H	-1.85506000	1.74198400	-2.77607400
H	-2.05645400	3.55648500	-1.06212300
Br	-4.07759500	-0.79689700	0.30340200

TS1

Zr	2.01071200	-0.86947100	-1.28662500
Zr	-0.67925600	-1.13002500	0.07764000
O	2.91846500	-1.09880700	0.45966100
O	1.85404500	1.01360200	-1.67989800
O	0.41504200	-1.95304900	-1.40211000
Zr	1.72825400	-0.33461100	1.77173200
Zr	0.48606700	1.55993000	-0.29041000
O	1.65110700	1.51745800	1.40275800
C	-1.43270600	2.50803000	0.97677500
C	-1.63308500	1.06549900	1.06304400
C	-2.11455800	0.36452300	-0.08052000
C	-1.69721000	0.90234600	-1.34172800
C	-1.51096500	2.34393000	-1.45346700
C	-1.48369500	3.11384100	-0.27711400
H	-1.29842000	3.09637200	1.87444400
H	-1.78791500	0.64180000	2.05398500
H	-1.85284900	0.33491300	-2.25328100
H	-1.47494500	2.82008700	-2.42499800
H	-1.38915900	4.19229800	-0.35254100
Br	-3.70010800	-1.07831500	0.18982000

FS1

Zr	0.53778300	-1.89323800	-1.24384200
Zr	-1.29284200	0.50688500	-0.49512700
O	0.03711500	-2.98656700	0.32805400
O	2.22019800	-0.93996000	-1.02378900
O	-0.84828700	-0.70723300	-1.96562100
Zr	-0.23316100	-1.50120300	1.56776100
Zr	1.87048900	0.44364400	0.37088000
O	1.38538000	-0.57333000	2.01056300
C	2.06805900	2.91439500	1.08080300

C	0.74320700	2.67428700	0.79671400
C	0.31249500	2.00892300	-0.42429200
C	1.34466100	2.08120000	-1.46009500
C	2.66838500	2.34852000	-1.18484700
C	3.10905500	2.56236300	0.14958400
H	2.34475900	3.30301900	2.05517600
H	0.00796800	2.87074000	1.57242500
H	1.07837300	1.80437700	-2.47429700
H	3.40234900	2.28011000	-1.98078600
H	4.14018700	2.80686600	0.36121500
Br	-3.71699400	1.10885500	0.11253000

IM

Zr	-1.42258900	-0.90329300	-1.35822700
Zr	-0.51421400	1.86099000	-0.12725500
O	-2.55630200	-1.44656800	0.17601200
O	0.34562500	-1.71840100	-1.37655000
O	-1.30431400	1.01870100	-1.72216000
Zr	-1.45039200	-0.60622200	1.54889700
Zr	1.33225900	-0.92077400	0.16521200
O	0.28787300	-1.39413000	1.79010600
C	3.44038600	0.21629000	1.10658600
C	2.46513100	1.17980000	1.01820000
C	1.64881400	1.36770900	-0.17655300
C	2.31834800	0.80528200	-1.35629500
C	3.31480200	-0.13972200	-1.27457100
C	3.74809600	-0.64555600	-0.01155000
H	3.93424000	0.03983000	2.05640400
H	2.20732700	1.73038200	1.91905700
H	1.94123700	1.06762100	-2.33882000
H	3.69626400	-0.59250100	-2.18384900
H	4.56853200	-1.34613100	0.04977200
O	-1.06600900	3.62957400	0.47390300
H	-1.41858700	4.45651100	0.78691900

IS2

Zr	-0.79374900	-1.80327900	1.56217500
Zr	0.36661600	0.99629000	1.04120200
O	0.51909200	-2.74610900	0.44164600
O	-2.45900000	-1.52355000	0.57377200
O	-0.30086900	-0.17919600	2.52286700
Zr	0.93071700	-1.33655600	-0.88588900
Zr	-2.01929500	-0.23092100	-0.85590300
O	-0.69761200	-1.11018700	-1.98447000

C	-2.73187200	1.97271300	-2.08095100
C	-1.57983600	2.24391600	-1.37561600
C	-1.41072500	1.91032400	0.02178400
C	-2.69561600	1.67395500	0.67289900
C	-3.86569900	1.43629600	-0.02357400
C	-3.86906500	1.38858600	-1.43778400
H	-2.75406700	2.12724500	-3.15479600
H	-0.71553700	2.59923100	-1.93024300
H	-2.71842000	1.57122800	1.75296400
H	-4.76711000	1.17341800	0.51967500
H	-4.77926400	1.20021200	-1.98959700
O	2.30822400	-0.38324200	-2.44838400
H	2.12188600	0.38806600	-2.98455700
C	1.61927800	3.11916700	0.32023300
C	1.99354600	2.15522000	-0.59009400
C	2.47028300	0.83984700	-0.20974600
C	2.83571700	0.78465100	1.20167600
C	2.51585300	1.78321200	2.11389600
C	1.76773800	2.91610600	1.73486000
H	1.16807100	4.03896200	-0.03214400
H	1.81782900	2.35420400	-1.64344100
H	3.32241100	-0.10858700	1.57882500
H	2.75515200	1.63204600	3.16105800
H	1.54395800	3.70611300	2.43628400
B	3.24204300	-0.12475100	-1.29093300
O	4.54047700	0.27960200	-1.66277000
H	4.82526000	1.06498000	-1.19584400
O	3.16152800	-1.55498500	-0.76698900
H	3.72565700	-1.74731600	-0.01779700

TS2

Zr	1.39291200	-1.54822800	-1.58064600
Zr	-0.57623500	0.58888900	-0.81557000
O	0.63811200	-2.81226200	-0.28814200
O	2.96887500	-0.69608300	-0.82941400
O	0.02901100	-0.39294900	-2.42431000
Zr	-0.01584900	-1.62655600	1.14908500
Zr	2.20534800	0.47697100	0.62007300
O	1.53729100	-0.83384700	1.97069900
C	2.27482300	2.81323300	1.69349800
C	1.01644100	2.65119000	1.14732700
C	0.80289000	2.19334300	-0.21158400
C	2.00211600	2.37371300	-1.03067000
C	3.26259600	2.56477900	-0.49466900

C	3.45909700	2.60151500	0.90701700
H	2.37755100	3.03012700	2.75155400
H	0.16096000	2.73832200	1.81329600
H	1.92242600	2.23626800	-2.10415500
H	4.12617600	2.56611300	-1.15116400
H	4.43919700	2.77047500	1.32997900
O	-1.91785000	-0.98866500	2.33258700
H	-2.14424600	-0.26928500	2.92442500
C	-3.98229200	2.67500200	0.14763000
C	-2.96148700	1.77675700	0.43411700
C	-2.82987000	0.53921800	-0.22322400
C	-3.78622400	0.27785200	-1.22658800
C	-4.82254000	1.15576500	-1.51168300
C	-4.92678900	2.35618000	-0.81667800
H	-4.04871100	3.61649500	0.68259800
H	-2.24543600	2.04776600	1.21255300
H	-3.72121700	-0.63979300	-1.81048200
H	-5.54401000	0.91558000	-2.28596700
H	-5.73517000	3.04405800	-1.03693200
B	-2.83680700	-1.19485200	1.26241300
O	-4.16017700	-1.02222500	1.56651900
H	-4.73427600	-0.87189600	0.81328500
O	-2.26311600	-2.28110600	0.55302600
H	-2.62597800	-2.50718400	-0.30343500

FS2

Zr	1.35140100	-2.10516500	-0.86215100
Zr	-0.25981100	0.38907500	-1.35894400
O	0.17580300	-2.70549100	0.60725200
O	2.92437100	-1.20834900	-0.16352300
O	0.45757200	-1.16955500	-2.34348300
Zr	-0.41016100	-1.01678900	1.40485900
Zr	2.21708600	0.50009600	0.62725300
O	1.12420700	-0.13071200	2.16356200
C	2.49179100	3.04765900	0.87191100
C	1.32760100	2.83384100	0.16521800
C	1.25659100	1.94506400	-0.98164900
C	2.58747900	1.70685100	-1.55167000
C	3.75910200	1.94350500	-0.86159100
C	3.73373100	2.43684500	0.46959200
H	2.46340100	3.62025200	1.79313000
H	0.40372000	3.24107600	0.56897600
H	2.65815900	1.22288500	-2.52050900
H	4.70549200	1.63926100	-1.29615600

H	4.64984100	2.65689700	0.99902400
O	-1.88149700	0.08029600	3.06464200
H	-1.74909800	0.85424900	3.61760200
C	-4.58206600	1.98205800	-0.91440600
C	-3.19995600	1.82919500	-0.97300500
C	-2.57877800	0.61066500	-1.30221000
C	-3.46475700	-0.44755500	-1.60151800
C	-4.85027600	-0.31970800	-1.52495200
C	-5.41718000	0.89806400	-1.17069200
H	-5.01238700	2.94850300	-0.66815500
H	-2.58872000	2.69883800	-0.73528700
H	-3.06233300	-1.41268200	-1.90742100
H	-5.48810300	-1.16786000	-1.75349200
H	-6.49442400	1.00852000	-1.11740300
B	-2.91685600	0.13644100	2.14883800
O	-3.82016500	1.12380800	2.14076500
H	-4.34276200	1.20191000	1.32985700
O	-2.81214700	-0.96682800	1.32040000
H	-3.22394700	-0.86697100	0.43783200

IS3'

Zr	-0.97230000	-1.00340000	2.03520000
Zr	1.21850000	0.07710000	-0.00440000
O	-1.60020000	-2.39400000	0.79100000
O	-2.19460000	0.47520000	2.12880000
O	0.92750000	-0.62630000	1.81160000
Zr	-1.58730000	-1.43870000	-0.91670000
Zr	-2.13740000	1.18240000	0.22620000
O	-3.12700000	-0.27070000	-0.77710000
C	-1.67970000	2.21950000	-2.06020000
C	-0.60850000	1.40790000	-1.51800000
C	0.09220000	1.94050000	-0.30400000
C	-0.46310000	3.03570000	0.34880000
C	-1.72100000	3.57180000	-0.00970000
C	-2.25280000	3.21040000	-1.31130000
H	-2.09610000	1.97230000	-3.03040000
H	-0.02180000	0.86600000	-2.25990000
H	0.00180000	3.39430000	1.26330000
H	-2.14320000	4.41030000	0.52750000
H	-3.11930000	3.73800000	-1.69280000
C	5.56370000	1.19010000	-0.84160000
C	4.20110000	0.92920000	-0.92110000
C	3.47740000	0.37670000	0.14730000
C	4.21050000	0.09580000	1.31000000

C	5.57450000	0.34200000	1.40050000
C	6.25540000	0.89210000	0.32320000
H	6.08620000	1.62620000	-1.68740000
H	3.69310000	1.18170000	-1.85160000
H	3.70170000	-0.32940000	2.17150000
H	6.11040000	0.10580000	2.31450000
H	7.32000000	1.08840000	0.39150000
O	1.48350000	-3.05220000	-1.29760000
H	1.19160000	-3.47390000	-0.49010000
B	0.82460000	-1.82520000	-1.58610000
O	1.78580000	-0.79490000	-2.00310000
H	2.69220000	-1.11870000	-2.08460000
O	-0.29220000	-2.02340000	-2.59190000
H	-0.16230000	-2.81050000	-3.13330000

TS3'

Zr	-1.63150000	-0.08850000	2.05120000
Zr	0.65200000	-0.91540000	0.25550000
O	-2.98380000	-0.88620000	0.85700000
O	-1.46320000	1.79010000	1.67550000
O	0.05980000	-1.07020000	2.15330000
Zr	-2.16050000	-0.65280000	-0.91770000
Zr	-0.74820000	1.88660000	-0.23110000
O	-2.31320000	1.25040000	-1.29860000
C	0.73390000	2.25350000	-2.29210000
C	1.06090000	1.05240000	-1.62130000
C	1.47610000	1.08510000	-0.22200000
C	1.64170000	2.35160000	0.37110000
C	1.22800000	3.53130000	-0.27530000
C	0.73150000	3.46600000	-1.60220000
H	0.34230000	2.21460000	-3.30240000
H	1.16890000	0.13360000	-2.19040000
H	1.89110000	2.40130000	1.42750000
H	1.28460000	4.48500000	0.23340000
H	0.38730000	4.36770000	-2.09390000
C	5.17130000	-0.67380000	-0.75700000
C	3.81610000	-0.49170000	-0.98010000
C	2.91150000	-0.39870000	0.08300000
C	3.43310000	-0.45640000	1.38720000
C	4.78820000	-0.65070000	1.61180000
C	5.66430000	-0.75780000	0.54020000
H	5.85110000	-0.75010000	-1.59970000
H	3.45680000	-0.41550000	-2.00300000
H	2.77150000	-0.35520000	2.24620000

H	5.16270000	-0.71080000	2.62850000
H	6.72530000	-0.89660000	0.71360000
O	-0.76260000	-3.87890000	-0.73040000
H	-1.34210000	-3.93860000	0.02800000
B	-0.55090000	-2.54310000	-1.19540000
O	0.86580000	-2.34470000	-1.52830000
H	1.37210000	-3.16420000	-1.56440000
O	-1.50910000	-2.20170000	-2.32540000
H	-1.87400000	-2.98670000	-2.74920000

FS3'

Zr	-1.63800000	-0.20960000	1.99440000
Zr	0.60440000	-0.90790000	0.11820000
O	-3.12280000	-0.77760000	0.80880000
O	-1.19330000	1.65360000	1.77070000
O	0.04960000	-1.21740000	1.99140000
Zr	-2.17380000	-0.49650000	-0.90760000
Zr	-0.43540000	1.87100000	-0.10840000
O	-2.05500000	1.40480000	-1.19460000
C	0.89900000	2.49460000	-2.16850000
C	1.41350000	1.30730000	-1.66670000
C	1.89040000	1.20240000	-0.26420000
C	1.94400000	2.49820000	0.43000000
C	1.37670000	3.63910000	-0.08440000
C	0.70990000	3.63690000	-1.35450000
H	0.48670000	2.49230000	-3.17090000
H	1.52590000	0.45610000	-2.32780000
H	2.39320000	2.52260000	1.41600000
H	1.40160000	4.55010000	0.50170000
H	0.31290000	4.55300000	-1.76590000
C	4.60820000	-1.42890000	-0.59270000
C	3.68430000	-0.45090000	-0.92140000
C	2.91230000	0.18390000	0.06860000
C	3.08450000	-0.25400000	1.39890000
C	4.01660000	-1.22890000	1.71910000
C	4.78670000	-1.82090000	0.72800000
H	5.20190000	-1.88360000	-1.37810000
H	3.57860000	-0.13920000	-1.95370000
H	2.47600000	0.18280000	2.18470000
H	4.12800000	-1.53520000	2.75280000
H	5.50670000	-2.59030000	0.97970000
O	-0.88250000	-3.77000000	-0.93560000
H	-1.38290000	-3.83880000	-0.12370000
B	-0.63920000	-2.42190000	-1.35190000

O	0.79860000	-2.25930000	-1.67740000
H	1.25580000	-3.10730000	-1.72810000
O	-1.58430000	-2.00300000	-2.43670000
H	-2.01400000	-2.75640000	-2.85750000

IS3

Zr	0.00004600	2.23403500	-0.40995700
Zr	0.00000700	0.24705100	1.75741300
O	-1.56774400	1.52134500	-1.33016500
O	1.56780000	1.52126000	-1.33015200
O	0.00004900	2.21657400	1.57490500
Zr	-1.61318800	-0.41251300	-0.86520900
Zr	1.61312100	-0.41260900	-0.86521200
O	-0.00005500	-1.20208200	-1.67838400
C	2.99703700	-2.45533400	-0.07369000
C	2.10462500	-2.15875800	0.93003100
C	1.91436000	-0.81004300	1.44629600
C	3.08223400	0.03028800	1.14286100
C	3.99599500	-0.27493600	0.15999600
C	3.84776800	-1.44350100	-0.64070500
H	3.00586300	-3.45134100	-0.50395000
H	1.42386500	-2.94329200	1.25024200
H	3.18071000	0.98618000	1.64812100
H	4.77698800	0.43769300	-0.08373800
H	4.58667600	-1.70309000	-1.38525000
C	-2.99705200	-2.45531300	-0.07373700
C	-2.10460800	-2.15879100	0.92996800
C	-1.91431700	-0.81010100	1.44628900
C	-3.08220100	0.03025100	1.14293600
C	-3.99600400	-0.27492500	0.16009400
C	-3.84780300	-1.44344700	-0.64067300
H	-3.00589700	-3.45129800	-0.50404700
H	-1.42384400	-2.94334500	1.25012300
H	-3.18066700	0.98611300	1.64825600
H	-4.77701600	0.43771000	-0.08356500
H	-4.58674200	-1.70300300	-1.38519900

TS3

Zr	-1.72810100	-1.49521800	-1.15969900
Zr	0.67051500	-0.96698200	0.55076700
O	-1.69508100	0.23041400	-1.99944300
O	-2.93598400	-1.47749800	0.41585600
O	0.02920500	-2.26313900	-0.81313600
Zr	-0.85743500	1.45532700	-0.59879500

Zr	-2.09130300	-0.25393000	1.64060600
O	-2.31251600	1.45181700	0.81406900
C	5.16529100	-0.07075600	1.02880800
C	3.82450200	0.26254900	1.10815600
C	2.87105800	-0.36986200	0.29828900
C	3.33516700	-1.31677400	-0.63598900
C	4.67757700	-1.65797100	-0.70447600
C	5.59968200	-1.03696700	0.12688700
H	5.88169300	0.42593400	1.67512300
H	3.51219000	1.03437400	1.80671200
H	2.63702400	-1.79440600	-1.32242400
H	5.00660900	-2.40436700	-1.41999900
H	6.65090000	-1.29317800	0.06504800
C	0.57149600	2.92917100	0.88872700
C	0.97132200	1.56206700	0.91024500
C	1.41519900	0.91109000	-0.32574900
C	1.44682800	1.68463400	-1.49505200
C	0.93107400	3.00278200	-1.52743300
C	0.49073700	3.60985300	-0.31993800
H	0.18010900	3.38890900	1.78944000
H	1.23001900	1.10901200	1.87130000
H	1.66231500	1.19114600	-2.43937800
H	0.91806700	3.56718400	-2.45040700
H	0.08940000	4.61585700	-0.34421000

FS3

Zr	1.42576000	-1.44865500	1.34208100
Zr	-0.69814200	-0.85416200	-0.72814500
O	1.22001600	0.33262400	2.04803200
O	2.94939000	-1.64999300	0.08508800
O	-0.32592200	-2.09269900	0.72144500
Zr	0.64683200	1.44508800	0.44913900
Zr	2.27271200	-0.50731000	-1.34277300
O	2.29685800	1.28016700	-0.73100800
C	-4.03107200	-1.42688600	-1.35623500
C	-3.14130400	-0.34203300	-1.29525200
C	-2.80401800	0.26773700	-0.04758200
C	-3.44578600	-0.26798700	1.10299300
C	-4.31280300	-1.32396000	1.01468600
C	-4.60697300	-1.93480800	-0.21777900
H	-4.27369700	-1.84692200	-2.32656100
H	-2.86566400	0.13947300	-2.23171200
H	-3.23665100	0.15656400	2.07653000
H	-4.77810700	-1.69742400	1.92012500

H	-5.28478700	-2.77744300	-0.26620600
C	-0.44213800	3.03724200	-1.18722700
C	-1.14755900	1.82430000	-1.20386000
C	-1.79873100	1.31605100	0.02553500
C	-1.65708900	2.18788600	1.17988800
C	-0.87744800	3.32791900	1.17659100
C	-0.17868700	3.73822300	-0.00307500
H	0.03533400	3.35641800	-2.10631900
H	-1.40803000	1.42082500	-2.17436300
H	-2.13773400	1.89854800	2.10545900
H	-0.79489200	3.91607700	2.08177600
H	0.39665100	4.65250500	-0.01131800

(8) The optimized structures involved in Suzuki-Miyaura cross-coupling mechanism catalyzed by (ZrO)₁₂ cluster

IS1

Zr	0.19561300	-2.80509900	0.30258700
Zr	1.37031100	-0.50705500	2.10063800
Zr	2.22333400	-0.54796400	-0.91599500
Zr	1.50520700	2.13158500	0.42407900
Zr	0.18794100	1.35743000	-2.41575400
Zr	-1.57247500	2.77834700	-0.41262900
Zr	-0.42689000	-1.73647000	-2.44813300
Zr	-2.64972900	0.47743200	-2.09805000
Zr	-2.64895400	-2.15782700	-0.39537600
Zr	-3.38456900	0.62427600	0.93902800
Zr	-1.60586600	-1.37382100	2.45365600
Zr	-0.91057200	1.58571400	2.41295300
O	0.19474200	-2.21091700	2.45231900
O	-2.53439200	0.53630400	2.90562400
O	-3.44155800	-1.44772400	1.32816900
O	-1.05758100	-3.37653400	-1.15278700
O	-2.56594900	-1.51168000	-2.39936300
O	-3.47670200	1.82336600	-0.66955400
O	1.16406200	-0.56115500	-2.76122900
O	-0.22419100	3.14362700	1.03925700
O	2.02018700	1.48779000	-1.41551700
O	1.22566700	1.47696700	2.43817700
O	2.04164100	-1.82123200	0.66680800
O	-1.57558200	2.30537600	-2.52174300
C	3.62887300	0.59740400	0.87123400
C	3.88131600	1.99953900	1.15577700
C	4.36663500	2.85246900	0.18342600
C	4.93551900	2.30925500	-1.01653100

C	5.02930800	0.95592800	-1.18372200
C	4.37112200	-0.00303400	-0.32390700
H	3.70761500	-0.03480400	1.78030900
H	3.71376500	2.37259200	2.17301000
H	4.49965700	3.91422900	0.41101200
H	5.36427700	2.98319100	-1.76092600
H	5.61076200	0.55719700	-2.02095100
Br	5.55230100	-1.53934700	0.11823900

TS1

Zr	0.06339500	-2.53734700	1.28258400
Zr	1.19796400	0.20403100	2.31784500
Zr	2.39856300	-0.94602300	-0.46875200
Zr	1.65412400	2.18224000	-0.07527600
Zr	0.41834500	0.43619700	-2.61367500
Zr	-1.37855200	2.48206900	-1.42905400
Zr	-0.28061600	-2.48413700	-1.70477700
Zr	-2.44346000	-0.22542100	-2.32508200
Zr	-2.70743300	-2.12173100	0.17426600
Zr	-3.39944600	0.96361000	0.43649300
Zr	-1.86021200	-0.42515300	2.64599900
Zr	-1.01113700	2.29825000	1.68665800
O	-0.09261100	-1.23860800	3.07868400
O	-2.72417700	1.55255000	2.40244600
O	-3.60447500	-0.86797600	1.48817500
O	-1.11747800	-3.54120500	0.02127000
O	-2.41084200	-2.19754500	-1.89738100
O	-3.29224300	1.52397500	-1.49087700
O	1.39755900	-1.52100400	-2.22523800
O	-0.13221200	3.26917900	-0.04636600
O	2.12601700	0.84387900	-1.51561900
O	1.10374200	2.20195300	2.01243700
O	1.92774000	-1.50299900	1.44376500
O	-1.25756600	1.32079000	-3.25946600
C	3.79036200	0.89959700	0.99821300
C	3.88653700	2.30833900	1.07061800
C	4.12465500	3.05702600	-0.09585600
C	4.81187700	2.36452400	-1.17299900
C	4.99110900	1.01159300	-1.17084400
C	4.28413400	0.19335100	-0.21981600
H	3.77751700	0.33150100	1.93996500
H	3.66832800	2.81383900	2.01499000
H	4.19437200	4.14635200	-0.03542600
H	5.18095800	2.95168000	-2.01851600

H	5.51989400	0.52401700	-1.99405400
Br	5.16794000	-1.75946300	0.18438400

FS1

Zr	0.17726400	2.28620400	-1.59508200
Zr	1.35790700	-0.56440300	-2.26888700
Zr	2.55465700	0.82671300	0.26820200
Zr	1.80053400	-2.19965900	0.22863100
Zr	0.69571300	-0.31885100	2.64657900
Zr	-1.11980300	-2.48102400	1.71937100
Zr	-0.12933800	2.53503900	1.40792400
Zr	-2.22431000	0.25521100	2.37816200
Zr	-2.64673600	1.83306800	-0.36109100
Zr	-3.24663000	-1.15766900	-0.24572200
Zr	-1.78642300	0.01614000	-2.65189600
Zr	-0.79904000	-2.64114000	-1.44130700
O	-0.04174200	0.81896300	-3.14784800
O	-2.57315800	-1.94133300	-2.09101100
O	-3.58615400	0.50576200	-1.53278200
O	-1.10493300	3.27218100	-0.36354000
O	-2.16159800	2.15163100	1.70822200
O	-3.05308500	-1.59295900	1.71410500
O	1.54084400	1.54805000	1.99278100
O	0.03555300	-3.42416500	0.34877400
O	2.41696500	-0.81917600	1.55497000
O	1.25176900	-2.53563900	-1.84183700
O	1.99974000	1.29251300	-1.63894200
O	-0.97646100	-1.15455800	3.41122100
C	3.69461300	-1.06921200	-1.02491200
C	4.01390200	-2.46150600	-0.66291100
C	5.15105200	-2.73688200	0.14770500
C	5.89697900	-1.73136300	0.71326400
C	5.49637400	-0.37749900	0.50164000
C	4.47599000	-0.00087200	-0.34273500
H	3.57020700	-0.89523200	-2.15028200
H	3.68322400	-3.25421800	-1.34879100
H	5.43166200	-3.78351400	0.30779600
H	6.76071100	-1.96198300	1.34105700
H	6.02187500	0.39984000	1.07199500
Br	1.90929000	3.97725100	0.01364500

IM

Zr	-0.51435200	2.53883500	-1.49468000
Zr	1.47639600	0.11110000	-2.18354500

Zr	2.43225900	1.56945100	0.32992100
Zr	2.43085600	-1.46771100	0.21641100
Zr	0.75465900	0.07377500	2.56975900
Zr	-0.34388400	-2.50985400	1.67721100
Zr	-0.85396800	2.61671400	1.39153000
Zr	-2.18241900	-0.20587500	2.37662000
Zr	-3.08630000	1.21075600	-0.33181700
Zr	-2.74096200	-1.83602200	-0.28614500
Zr	-1.68548400	-0.27598500	-2.62666000
Zr	-0.00893400	-2.53030600	-1.46991900
O	-0.25545400	1.07160100	-3.02482300
O	-1.87789700	-2.38344300	-2.17626700
O	-3.55343000	-0.31394900	-1.56574700
O	-2.14771700	3.04581100	-0.38068000
O	-2.67695300	1.62679700	1.71907900
O	-2.43280400	-2.20360200	1.67798800
O	1.09009600	2.13548500	1.83044300
O	1.05377100	-3.08312000	0.31836800
O	2.66784600	-0.01453200	1.62012800
O	1.94069200	-1.82767900	-1.82943000
O	1.54409300	2.06075600	-1.42457300
O	-0.54898300	-1.21024600	3.38846100
C	3.95347500	0.13323900	-1.05065800
C	4.62235200	-1.14605100	-0.75079900
C	5.81996200	-1.15563600	0.01259200
C	6.32582900	-0.01239500	0.58686600
C	5.60116300	1.20625400	0.43309600
C	4.48340000	1.34429400	-0.36077100
H	3.73288200	0.28758500	-2.16824500
H	4.45981100	-1.98400100	-1.44266000
H	6.34734700	-2.10798500	0.13415800
H	7.23959600	-0.04339100	1.18429900
H	5.94532400	2.07348900	1.01230200
O	0.10856500	4.02795300	0.00119900
H	1.02867400	4.30633300	0.07757800

IS2

Zr	2.44137300	0.61948600	0.32008000
Zr	-0.20152400	1.61079800	1.90105000
Zr	-0.33469800	2.59845400	-0.99264800
Zr	-2.82422700	1.51461100	0.38020400
Zr	-1.79313300	0.15115100	-2.40093400
Zr	-3.13050700	-1.65292300	-0.48935200
Zr	1.45210700	-0.17490400	-2.40481000

Zr	-0.74997800	-2.59644800	-2.10786900
Zr	1.82125600	-2.35132500	-0.25951400
Zr	-0.82523200	-3.24614300	0.98105300
Zr	0.95946100	-1.30606100	2.48092400
Zr	-2.05482700	-0.80531500	2.35554000
O	1.62454800	0.57003100	2.30807200
O	-0.87705300	-2.32594500	2.92487100
O	1.26655900	-3.18895200	1.49023300
O	3.07571400	-0.89465400	-1.04215900
O	1.22370900	-2.25443400	-2.31213800
O	-2.02286600	-3.45487400	-0.62533000
O	0.07091900	1.32843100	-2.59873200
O	-3.64740900	-0.34717800	0.97910100
O	-2.24751000	2.03097800	-1.49587500
O	-2.13906200	1.29744200	2.39318200
O	1.10866600	2.23992500	0.39645200
O	-2.64214300	-1.66057100	-2.59120100
C	-1.60371300	3.71725400	0.85019700
C	-3.05149600	3.81917800	1.10300400
C	-3.83521100	4.74813600	0.37302700
C	-3.30241700	5.51071000	-0.64288100
C	-1.92952400	5.33455200	-0.97881800
C	-1.06044500	4.51952000	-0.28323900
H	-0.96743000	3.75276600	1.80477000
H	-3.42922700	3.49330400	2.08177200
H	-4.89187600	4.85627800	0.64085900
H	-3.92683900	6.20900100	-1.20438400
H	-1.55720000	5.86177900	-1.86754800
O	2.71472000	1.46563200	-1.74300200
H	2.52572100	2.39597000	-1.91158800
C	5.21364400	0.03379000	1.02125000
C	4.92949900	0.14811100	2.38625100
C	4.58655800	1.39070800	2.92462100
C	4.51042400	2.50753600	2.09175500
C	4.80932700	2.39097100	0.72988300
C	5.18000700	1.15396000	0.16515500
H	5.48996200	-0.93954200	0.60790200
H	4.98479000	-0.73223400	3.03164800
H	4.34618100	1.48097600	3.98572800
H	4.21524700	3.47614800	2.50196400
H	4.77514500	3.27613100	0.08976200
B	5.57133300	1.02054200	-1.37244400
O	5.34294000	-0.10457400	-2.07884600
O	6.21702600	2.08916600	-1.92081200

H	6.38742300	1.93163600	-2.85682100
H	4.55861300	-0.59012600	-1.70257300

TS2

Zr	2.42769500	0.40934200	0.23720400
Zr	-0.01513000	1.61553700	1.92116700
Zr	-0.23777700	2.63440100	-0.96922000
Zr	-2.70664200	1.70161500	0.51092500
Zr	-1.86610700	0.26788100	-2.30050800
Zr	-3.27855200	-1.44433000	-0.35603000
Zr	1.27325100	-0.33952900	-2.49036400
Zr	-1.04370100	-2.55881000	-2.06626800
Zr	1.63546500	-2.54089700	-0.35142500
Zr	-1.03541100	-3.20892400	1.01970100
Zr	0.93347200	-1.41674900	2.43916500
Zr	-2.00602000	-0.68815300	2.42494300
O	1.73680900	0.40805400	2.23612700
O	-0.95968000	-2.30756100	2.96850000
O	1.06442200	-3.30173100	1.42958400
O	2.87844600	-1.10291700	-1.20915100
O	0.93225500	-2.38469300	-2.36877100
O	-2.31832500	-3.31854000	-0.53917300
O	0.09395600	1.33815400	-2.57011100
O	-3.63148300	-0.09337800	1.12520500
O	-2.19289400	2.17919400	-1.40248900
O	-1.94753300	1.42227200	2.47771700
O	1.25738900	2.13296200	0.31873500
O	-2.87415400	-1.45752000	-2.47171000
C	-1.32090300	3.80627200	0.95120400
C	-2.74252900	4.00639300	1.27854700
C	-3.48143000	5.02621100	0.62585700
C	-2.93875300	5.78325400	-0.38851100
C	-1.60825800	5.50184900	-0.81216000
C	-0.77772800	4.59065900	-0.19353800
H	-0.63618900	3.78331600	1.87632200
H	-3.09510000	3.67883500	2.26613700
H	-4.50960500	5.21066500	0.95534200
H	-3.52814000	6.55661500	-0.88569000
H	-1.24154400	6.02588400	-1.70493300
O	2.89166500	1.35935400	-1.95803600
H	2.68777700	2.30151200	-2.05600600
C	5.41481700	-0.29527700	0.63944600
C	6.45740100	-0.30272000	1.56872100
C	6.80292100	0.87453700	2.23071800

C	6.10249200	2.05225300	1.95878100
C	5.06021500	2.04494500	1.03266700
C	4.68315400	0.87340900	0.34042500
H	5.17929000	-1.22694300	0.11061900
H	7.01026600	-1.22550400	1.76682000
H	7.62131300	0.87732900	2.95561200
H	6.37263200	2.97876900	2.47318200
H	4.53028300	2.98428400	0.83597000
B	4.37030900	1.22400400	-1.90322500
O	4.90708600	0.07048600	-2.37881200
O	4.95765300	2.45518200	-2.04593300
H	5.91596100	2.38162700	-2.08907000
H	4.34653500	-0.66695000	-2.04620800

FS2

Zr	-2.41452300	1.29182000	-0.39325100
Zr	0.53977200	2.25791600	-1.11423000
Zr	0.61841600	2.04378500	1.91320700
Zr	3.04254500	1.27103200	0.25620900
Zr	1.74746400	-0.95715200	2.21805200
Zr	2.97832100	-1.98920000	-0.25213900
Zr	-1.38368000	-1.10227600	2.18664900
Zr	0.38593800	-3.18452700	0.83140600
Zr	-1.95285800	-1.80543900	-0.60728500
Zr	0.60139100	-2.52965100	-2.23294400
Zr	-0.89776100	0.06633200	-2.88602100
Zr	2.14771700	0.05572800	-2.50310000
O	-1.34515400	1.86901900	-2.09262300
O	0.83657800	-0.94486900	-3.64860000
O	-1.39541100	-1.98708200	-2.55541300
O	-2.81282100	-0.32832600	0.80584900
O	-1.62213000	-2.95902700	1.18667500
O	1.63403900	-3.55295000	-0.83082000
O	-0.08781500	0.27680000	2.79533600
O	3.70845600	-0.26585100	-1.02365600
O	2.41158600	1.06367400	2.18691800
O	2.46317100	1.96972400	-1.65434100
O	-0.86699000	2.28089900	0.51588600
O	2.38594500	-2.77256900	1.67335300
C	2.06514900	3.62665500	0.68041900
C	3.52830400	3.65165400	0.51006800
C	4.35482300	4.12109000	1.55754000
C	3.84160700	4.49729100	2.78232900
C	2.44168800	4.37658800	2.99862500

C	1.53841400	3.99262300	2.02603500
H	1.50054200	4.10485000	-0.19989200
H	3.93117600	3.68032600	-0.51085700
H	5.43209900	4.19252800	1.37262900
H	4.50002200	4.84511500	3.58107900
H	2.06938600	4.57094400	4.01363400
O	-3.29774800	-1.70293300	3.47701600
H	-3.18424700	-2.14320900	4.32951600
C	-5.61033700	1.78612800	-0.20650400
C	-6.84435500	2.39975200	-0.43200100
C	-6.93791200	3.46691200	-1.32456600
C	-5.79564000	3.91055200	-1.99186900
C	-4.56808800	3.28795600	-1.76113900
C	-4.43314400	2.21042000	-0.85982200
H	-5.58076600	0.94935100	0.50162700
H	-7.73677900	2.04425100	0.09132200
H	-7.90147000	3.95270600	-1.50136700
H	-5.86463500	4.74520300	-2.69559100
H	-3.68926100	3.65431100	-2.30509200
B	-4.63591600	-1.82622600	3.03619500
O	-5.01431500	-1.28103900	1.87718300
O	-5.45566900	-2.51221000	3.87142600
H	-6.35441500	-2.56792300	3.53037600
H	-4.26857900	-0.82392900	1.40138300

IS3'

Zr	-1.19056000	-0.05702700	-2.15830400
Zr	-0.88914700	2.31474700	-0.03771800
Zr	-2.36215300	-0.65090200	0.79992500
Zr	-0.12109700	1.14080900	2.70073200
Zr	0.29030300	-1.94428100	2.23518000
Zr	2.73797100	-0.18486200	2.36351200
Zr	-0.45488000	-2.64049800	-0.85772900
Zr	2.55751900	-2.41327000	0.34599700
Zr	1.65754000	-1.16250000	-2.41668400
Zr	3.65017500	0.39764600	-0.54700800
Zr	1.35533900	1.93634600	-2.08678700
Zr	1.97146400	2.55494000	0.90132100
O	-0.63559200	2.08936800	-2.24475800
O	3.04225200	2.42035800	-0.77081600
O	2.86835900	0.46605900	-2.50038500
O	-0.28214800	-1.75247500	-2.82710800
O	1.61258800	-2.99021600	-1.33592300
O	4.05592400	-0.95676900	0.88091900

O	-1.28684400	-2.45488000	1.00071300
O	1.91981800	1.59786000	2.82058100
O	-1.25356500	-0.51369400	2.68953700
O	-0.03974800	2.98509600	1.66528800
O	-2.24814200	0.86085200	-0.58304200
O	2.27128000	-2.27467000	2.48482900
C	-5.64853600	-0.40998700	0.87913300
C	-6.90866400	-0.24554700	1.45600400
C	-7.03859700	-0.18527800	2.84474100
C	-5.90317600	-0.28981400	3.64634600
C	-4.64624700	-0.44948400	3.05565500
C	-4.47679500	-0.51437800	1.65625000
H	-5.57970700	-0.46779800	-0.21314500
H	-7.79723200	-0.16975700	0.82184900
H	-8.02503600	-0.06038500	3.30039100
H	-5.99742100	-0.24878700	4.73590500
H	-3.77032100	-0.53062800	3.71105600
C	-2.74280700	-3.25724900	-1.32951900
C	-2.85731600	-3.88028300	-2.58334200
C	-3.13621700	-3.15545600	-3.74014600
C	-3.45652200	-1.79706400	-3.60012700
C	-3.36750000	-1.15422500	-2.36220400
C	-2.85518400	-1.80251300	-1.15667600
H	-2.78617300	-3.90213000	-0.43794100
H	-2.77236300	-4.97159900	-2.64172700
H	-3.19745800	-3.64842200	-4.71184000
H	-3.84640900	-1.24345800	-4.46171300
H	-3.84169800	-0.16220500	-2.27886200
O	-2.08532800	4.25278600	-0.37917600
H	-2.36696700	4.82011900	0.35170600
B	-2.58405700	4.70676100	-1.62780700
O	-2.26141500	4.07870700	-2.75725300
O	-3.38061100	5.80176200	-1.55026200
H	-3.70414500	6.07298900	-2.41543100
H	-1.64302200	3.29880600	-2.66041800

TS3'

Zr	1.52170400	0.50724400	1.73360500
Zr	0.43193500	2.47415400	-0.52486700
Zr	2.05077200	-0.27072900	-1.23505000
Zr	-0.56941000	0.83104600	-2.86665800
Zr	-0.33705800	-2.20635100	-2.06585000
Zr	-3.01219100	-0.86885800	-1.82739600
Zr	1.04903400	-2.38705400	0.80845000

Zr	-2.09245900	-2.80648200	0.31805800
Zr	-1.02360700	-1.04803500	2.72373600
Zr	-3.47170900	-0.13081700	1.16816500
Zr	-1.30928700	1.92029400	2.02830600
Zr	-2.52759600	2.08732300	-0.86738100
O	0.61889300	2.45423600	1.74453400
O	-3.20406300	1.96360000	1.02990300
O	-2.43403400	0.34326600	2.98934600
O	1.08543000	-1.28318500	2.57121200
O	-0.71134900	-2.99948200	1.76039100
O	-3.87973900	-1.67544100	-0.05653200
O	1.56419800	-2.32284400	-1.16254500
O	-2.70572400	0.94687000	-2.63484200
O	0.83538800	-0.59723800	-2.96201900
O	-0.87081100	2.79718300	-2.03283200
O	2.16097300	1.39564500	-0.03441200
O	-2.22139400	-2.87498000	-1.83910200
C	5.09381200	0.67124200	-0.97048700
C	6.32520500	0.78979900	-1.60852300
C	6.87891200	-0.30218300	-2.28111300
C	6.18150600	-1.51156300	-2.31141000
C	4.95108300	-1.63014600	-1.66976300
C	4.36535200	-0.53968000	-0.99328100
H	4.67617800	1.53933000	-0.45144100
H	6.86081700	1.74308900	-1.57848600
H	7.85163900	-0.21326800	-2.77092100
H	6.60567700	-2.37391900	-2.83326700
H	4.43274700	-2.59374800	-1.69460100
C	3.56287700	-2.46308400	0.95625500
C	4.11950000	-2.93354900	2.14839300
C	4.53238300	-2.07037600	3.16410800
C	4.44400500	-0.69847400	2.91968100
C	3.89124700	-0.19505900	1.74081000
C	3.37865600	-1.04225900	0.66231500
H	3.41814700	-3.18754100	0.14280000
H	4.23596000	-4.01486800	2.27780700
H	4.94440600	-2.45280600	4.09880900
H	4.82581200	0.01095100	3.66141800
H	4.03315500	0.87628000	1.53584500
O	1.17153500	4.67204800	-0.56120100
H	1.12368000	5.21239400	-1.36113500
B	1.62362900	5.40698500	0.56086600
O	1.66431300	4.84929700	1.77030800
O	1.99428100	6.68541700	0.29005700

H	2.27969600	7.14809300	1.08450700
H	1.29844200	3.91857900	1.83961900

FS3'

Zr	-1.65972800	0.71510800	-1.66984100
Zr	-0.21080600	2.50768500	0.53339200
Zr	-2.05246800	0.03211700	1.40499900
Zr	0.71637100	0.80690300	2.86318800
Zr	0.12337600	-2.20333900	2.07422100
Zr	2.89399600	-1.18330000	1.73206600
Zr	-1.45851400	-2.19778100	-0.73462300
Zr	1.66216600	-3.01145100	-0.36264400
Zr	0.72870700	-1.11737200	-2.73303700
Zr	3.28373700	-0.48247000	-1.30183900
Zr	1.35840700	1.77183600	-2.09467300
Zr	2.69436500	1.81098600	0.77683100
O	-0.48428800	2.53012900	-1.70369700
O	3.26383900	1.63262300	-1.15708900
O	2.26950700	0.10410100	-3.11429600
O	-1.36530200	-1.09788900	-2.49603600
O	0.21410500	-3.01153500	-1.74861800
O	3.56139700	-2.05684100	-0.07205900
O	-1.83179600	-2.03983200	1.24721900
O	2.82964400	0.66249600	2.54690600
O	-0.83435700	-0.46160500	3.02965800
O	1.17500300	2.72132600	1.99487000
O	-2.08489100	1.64428900	0.12664800
O	1.89686000	-3.10218000	1.79814700
C	-4.62223800	0.82910100	1.06797100
C	-5.08860700	1.11223500	2.35935400
C	-5.33150300	0.09823400	3.27914200
C	-5.08131300	-1.22221000	2.87936800
C	-4.61885200	-1.51837700	1.60491400
C	-4.38674900	-0.50860700	0.61852200
H	-4.48386400	1.66467200	0.38463600
H	-5.27113500	2.15569100	2.62992300
H	-5.69548400	0.32237800	4.28328700
H	-5.25057900	-2.04467500	3.57899900
H	-4.43163500	-2.56159200	1.35919100
C	-3.84554000	-2.25339900	-1.17318800
C	-4.04625800	-2.54460600	-2.54234300
C	-4.16427700	-1.57858700	-3.52855400
C	-4.22019600	-0.22778800	-3.12879600
C	-4.07835200	0.16751300	-1.80278000

C	-3.84818800	-0.81709900	-0.71381500
H	-4.20014800	-3.01835600	-0.47348600
H	-4.13477300	-3.60012600	-2.82324300
H	-4.27099500	-1.85406400	-4.57806900
H	-4.45372100	0.54179500	-3.87265700
H	-4.43658700	1.16867100	-1.53723800
O	-0.47892600	4.80598400	0.56542700
H	-0.21579500	5.30909300	1.34761300
B	-0.81465800	5.62761600	-0.53524300
O	-1.05670000	5.08986900	-1.73099200
O	-0.86262000	6.95719900	-0.26290000
H	-1.07458600	7.47364000	-1.04712800
H	-0.89118800	4.10433800	-1.80154900

IS3

Zr	-1.05570600	1.65608300	1.36609800
Zr	-0.27523100	-1.08580300	2.73800400
Zr	-2.73915300	-0.59586300	-0.16892300
Zr	0.19391600	-3.12515100	0.14474100
Zr	-0.30755700	-1.19870600	-2.25869100
Zr	2.48404800	-1.94956300	-1.61548800
Zr	-1.19921500	1.82845600	-1.55027000
Zr	1.76558200	0.83643400	-2.58604100
Zr	1.35397300	2.74583600	-0.12469500
Zr	3.57730700	0.58528900	-0.02397500
Zr	1.95242300	1.12569000	2.46906800
Zr	2.38513900	-1.66192800	1.49479700
O	0.05349400	0.89857500	3.15939800
O	3.64137200	-0.16430500	1.99813800
O	2.96626400	2.31143800	1.04398500
O	-0.66598900	3.15902500	0.04351800
O	0.72014700	2.50993100	-2.15538800
O	3.53353500	-0.15131700	-1.91200200
O	-2.06774800	-0.00218800	-2.01304700
O	2.23784000	-3.22966900	-0.04299300
O	-1.40373200	-2.21365700	-0.63664900
O	0.47885100	-2.85955700	2.17929300
O	-1.81001000	-0.38307200	1.65558600
O	1.39865500	-1.17695000	-3.32251400
C	-6.03613200	-0.68558700	0.22184600
C	-7.28721100	-1.29980900	0.29154300
C	-7.40582400	-2.67338900	0.07275600
C	-6.26882400	-3.42584800	-0.21630500
C	-5.02143500	-2.79893700	-0.28246000

C	-4.86315000	-1.41339900	-0.06494600
H	-5.96842400	0.39409200	0.39237000
H	-8.17796800	-0.70532200	0.51559600
H	-8.38560500	-3.15627100	0.12623300
H	-6.35429800	-4.50243600	-0.39136000
H	-4.14746700	-3.42206100	-0.51630200
C	-3.53503000	2.45076400	-1.14449600
C	-3.64671200	3.84095500	-1.06012300
C	-3.56531800	4.51420300	0.16737000
C	-3.49637300	3.75094400	1.33139500
C	-3.36340900	2.35255400	1.29409000
C	-3.24883500	1.60965500	0.02658800
H	-3.87091200	1.97723000	-2.08010800
H	-3.87527000	4.40983900	-1.96854700
H	-3.64810500	5.60121000	0.21436500
H	-3.59959600	4.24590500	2.30378800
H	-3.62529600	1.80814700	2.21681500

TS3

Zr	1.44070100	1.31351600	-1.58797200
Zr	0.10276700	-1.43406200	-2.42620100
Zr	2.14041300	-1.17804400	0.10586200
Zr	-0.59013500	-3.00932500	0.03702100
Zr	0.07175800	-1.20614300	2.52204800
Zr	-2.77664600	-1.39209600	1.61090200
Zr	1.41553000	1.49917000	1.49991000
Zr	-1.62384400	1.28315900	2.51518800
Zr	-0.89025900	2.87299400	-0.11448200
Zr	-3.39400300	1.18098500	-0.06075400
Zr	-1.59367300	1.21127800	-2.56028300
Zr	-2.75110400	-1.53153300	-1.53431600
O	0.21725700	0.65387600	-3.17051100
O	-3.45944000	0.30363500	-1.97930900
O	-2.50458700	2.71138400	-1.28004000
O	1.23957500	2.73376900	-0.15821400
O	-0.25777800	2.65411800	1.98754000
O	-3.54219900	0.57890800	1.85409700
O	1.95873900	-0.38181900	2.05911000
O	-2.72525400	-2.79063300	0.16306600
O	1.01243100	-2.64257800	1.17950000
O	-1.18144100	-2.92030300	-2.05256500
O	2.00115500	-0.68483500	-1.87131000
O	-1.68927400	-0.71544900	3.34769500
C	5.10937000	-1.37971400	-1.16237900

C	6.29915800	-2.10194200	-1.12418300
C	6.89035800	-2.42160100	0.10047500
C	6.27679200	-2.01175200	1.28567700
C	5.08929700	-1.28445600	1.24589000
C	4.46565400	-0.96446200	0.02177400
H	4.66013000	-1.14317500	-2.13169100
H	6.77158300	-2.41859800	-2.05842500
H	7.82855400	-2.98102000	0.13018700
H	6.73101700	-2.25605300	2.25001300
H	4.62994400	-0.96559500	2.18703100
C	3.91360000	1.59051600	1.15606100
C	4.53085300	2.84167300	1.07873400
C	4.81463100	3.45019400	-0.14406400
C	4.52544900	2.73096300	-1.30579200
C	3.90615200	1.48062500	-1.26267000
C	3.53318500	0.80972100	-0.01795400
H	3.87988300	1.10227200	2.14035800
H	4.80155200	3.34831100	2.01119200
H	5.27926100	4.43592300	-0.19042100
H	4.79728300	3.14574800	-2.28209800
H	3.88015800	0.89703100	-2.19490300

FS3

Zr	1.57750100	1.38042900	-1.52979000
Zr	0.00071600	-1.15451000	-2.59066300
Zr	2.07547300	-1.40608400	-0.16966500
Zr	-0.72796600	-2.98456600	-0.31082900
Zr	0.12957500	-1.52701100	2.35570900
Zr	-2.73714200	-1.43412300	1.54079600
Zr	1.66294800	1.18761800	1.54339000
Zr	-1.37198400	1.04067000	2.70022000
Zr	-0.66113000	2.87018700	0.22498800
Zr	-3.23776900	1.35495700	0.18149000
Zr	-1.54752800	1.57843900	-2.35144500
Zr	-2.82689400	-1.19758300	-1.60459900
O	0.21204400	0.97722600	-3.09140900
O	-3.44100400	0.71220400	-1.82638900
O	-2.31998000	2.98374700	-0.89061000
O	1.42438900	2.61642800	0.05543900
O	0.05442300	2.37126700	2.24175400
O	-3.34564000	0.52964100	2.01901200
O	2.04868300	-0.77910700	1.82797100
O	-2.83215000	-2.65322100	-0.06878400
O	0.93310300	-2.87215800	0.79842300

O	-1.36197200	-2.60010000	-2.34926100
O	1.97301000	-0.59614000	-2.04603300
O	-1.56310600	-1.04377900	3.30859900
C	4.58353200	-1.33734100	-1.19412200
C	5.05199200	-2.65884200	-1.17778400
C	5.39574000	-3.28857600	0.01284600
C	5.24722100	-2.56516400	1.20432000
C	4.78324100	-1.25778800	1.20444000
C	4.44851600	-0.56259800	0.00048800
H	4.36568000	-0.88827800	-2.16136500
H	5.15469900	-3.18710600	-2.12942200
H	5.76084600	-4.31708100	0.02184900
H	5.49838200	-3.03215300	2.16009600
H	4.67355800	-0.75412400	2.16239300
C	4.02342200	1.61603800	1.28115200
C	4.23022100	3.01670000	1.19187800
C	4.24217800	3.72250800	0.00392200
C	4.18851100	2.99090100	-1.20472900
C	4.05052200	1.60987900	-1.23350800
C	3.91366600	0.80860300	0.00744200
H	4.48382900	1.13499200	2.15184800
H	4.40862100	3.55652300	2.12880600
H	4.35404900	4.80703000	-0.00733600
H	4.34513700	3.51346900	-2.15463400
H	4.31624800	1.09582300	-2.16406200

(9) The optimized structures involved in Suzuki-Miyaura cross-coupling mechanism catalyzed by Pd

IS1

Pd	-0.51510300	1.35232700	-0.18128700
C	0.16944000	-0.59094000	0.01748700
C	-0.60508100	-0.33990400	1.18700800
C	-1.92233400	-0.84233200	1.24166600
C	-2.44905700	-1.56721800	0.19424400
C	-1.68923500	-1.78636600	-0.95935700
C	-0.40072600	-1.30489800	-1.06288700
H	-0.12111700	0.00448100	2.09386000
H	-2.50138800	-0.68347700	2.14451500
H	-3.45342700	-1.96745000	0.26348700
H	-2.11041300	-2.34624900	-1.78653300
H	0.20279800	-1.50912700	-1.93824900
Br	2.08743500	-0.48900700	0.11009100

TS1

Pd	0.71411700	-1.20485600	-0.00007200
C	-0.52351500	0.36415200	0.00001800
C	-1.21823200	0.34227600	-1.21911400
C	-2.60141700	0.24355400	-1.20172200
C	-3.29607400	0.19681600	-0.00002900
C	-2.60144900	0.24340400	1.20168800
C	-1.21826500	0.34212300	1.21912900
H	-0.67682100	0.42644300	-2.15256100
H	-3.13974100	0.21285300	-2.14261800
H	-4.37752300	0.13304700	-0.00004800
H	-3.13979800	0.21258700	2.14256600
H	-0.67687900	0.42617100	2.15260200
Br	1.36900200	1.24623800	0.00010100

FS1

Pd	0.65975900	0.95612700	-0.19377000
C	-1.03828400	0.11425000	-0.02394200
C	-1.72925100	0.30373600	1.16395300
C	-3.07843700	-0.02936600	1.20579900
C	-3.69888400	-0.57696600	0.09228700
C	-2.97514100	-0.80284300	-1.07007800
C	-1.62600100	-0.47474600	-1.13310600
H	-1.23396400	0.69857400	2.04357500
H	-3.63727300	0.12670600	2.12185800
H	-4.74751500	-0.84731000	0.13686900
H	-3.45471400	-1.25017800	-1.93365700
H	-1.05023400	-0.67652100	-2.02815700
Br	1.96145100	-0.94964300	0.20467000

IM

Pd	1.35034200	-0.32183100	0.13805900
C	-0.52610600	-0.00670600	-0.02959800
C	-1.26964500	-1.15881500	-0.25365000
C	-2.65853900	-1.08677800	-0.22769700
C	-3.28574700	0.12988600	-0.00703500
C	-2.52870000	1.27693000	0.19100400
C	-1.14066900	1.21866400	0.17877100
H	-0.78738800	-2.11231900	-0.45602700
H	-3.24460800	-1.98334900	-0.39600200
H	-4.36784600	0.18597100	0.00374800
H	-3.02075800	2.22831500	0.36188700
H	-0.54206400	2.10799200	0.33265600
O	2.05916200	1.33945500	-0.48624000
H	1.83007300	1.42290300	-1.41780600

IS2

Pd	0.17311100	-0.19906300	-0.15935600
C	2.08295400	0.00838500	-0.00938500
C	2.78449300	1.06350800	0.54665500
C	4.16420300	0.95252900	0.67818700
C	4.82335100	-0.19289300	0.25312900
C	4.10913100	-1.24006400	-0.31027200
C	2.72911900	-1.13568900	-0.45172100
H	2.26492400	1.95143900	0.88799200
H	4.72562000	1.76732900	1.12241600
H	5.89945600	-0.26888300	0.35796600
H	4.62046800	-2.13309200	-0.65190900
H	2.17518800	-1.95387500	-0.91394800
C	-2.55549600	-0.44789300	1.28744700
C	-2.76719200	-1.80566400	1.43945800
C	-2.59520800	-2.66792100	0.35754300
C	-2.23509800	-2.15567400	-0.87532600
C	-2.03195300	-0.77794500	-1.02760200
C	-2.17522800	0.11286000	0.05501900
H	-2.71081000	0.21107000	2.13601700
H	-3.07012900	-2.20346600	2.40196100
H	-2.75951500	-3.73273100	0.47894500
H	-2.13596200	-2.81426600	-1.73170600
H	-1.85017100	-0.36737600	-2.01714600
O	-2.17349500	2.13801000	-1.48081400
H	-2.56660200	3.01274500	-1.45866000
B	-1.89444900	1.71962200	-0.14801600
O	-0.26917300	1.76625800	0.01840600
H	0.05072500	2.23489000	-0.76170500
O	-2.44537600	2.60205700	0.82255200
H	-2.02814900	2.52319700	1.68026700

TS2

Pd	-0.27202500	-0.01596200	-0.02542600
C	-2.23890000	-0.17227500	0.00258600
C	-3.15081600	0.81254900	-0.35282200
C	-4.51049800	0.52314100	-0.37488300
C	-4.96171300	-0.74488600	-0.03574800
C	-4.05376200	-1.72870900	0.32792100
C	-2.69381100	-1.43815700	0.35303600
H	-2.80787100	1.80597700	-0.62655400
H	-5.22013000	1.29224500	-0.66144600
H	-6.02288100	-0.96617900	-0.05175000

H	-4.40060800	-2.71984200	0.59993700
H	-1.99384900	-2.21878400	0.65328300
C	2.38807200	-0.61003600	-1.26604600
C	3.36858700	-1.59036000	-1.32566900
C	3.85680900	-2.15151500	-0.15349000
C	3.36176400	-1.72841400	1.07201100
C	2.37850200	-0.74881100	1.12018200
C	1.85909500	-0.17398100	-0.04579700
H	2.03886300	-0.16662900	-2.19493500
H	3.75971100	-1.91095500	-2.28547100
H	4.62878600	-2.91206500	-0.19531300
H	3.74762200	-2.15710000	1.99104200
H	2.02070100	-0.40471500	2.08661300
O	1.93442400	2.19659900	1.40965300
H	2.87878900	2.36148200	1.38887300
B	1.43731700	1.90455900	0.14663700
O	-0.03620000	2.00960700	0.12862200
H	-0.34805000	2.30432600	0.99223300
O	2.08548800	2.42060200	-0.96623500
H	1.55581200	2.39797200	-1.76412100

FS2

Pd	0.13963900	-0.37583300	0.02386000
C	2.15782200	-0.48468000	0.02562400
C	2.95581500	0.19425200	0.94534700
C	4.33466400	0.00786000	0.97338600
C	4.93593500	-0.85671100	0.07137400
C	4.15677400	-1.53244200	-0.85786000
C	2.78069800	-1.33850100	-0.88381400
H	2.50561700	0.86402700	1.67626900
H	4.93772300	0.53581500	1.70499600
H	6.01014400	-1.00264300	0.08967100
H	4.62192400	-2.20697000	-1.56933100
H	2.19243200	-1.87023600	-1.63012300
C	-2.60518400	-0.71735600	1.26855600
C	-3.91734300	-1.17249600	1.31820100
C	-4.59141100	-1.47159500	0.14280100
C	-3.94953500	-1.30849400	-1.07642200
C	-2.63702900	-0.85274600	-1.11436800
C	-1.91910200	-0.56834200	0.05542900
H	-2.10538700	-0.47839000	2.20519600
H	-4.41671600	-1.28726200	2.27487000
H	-5.61807700	-1.81930900	0.17620100
H	-4.47449200	-1.53027800	-2.00003200

H	-2.16404600	-0.72098800	-2.08553200
O	-0.10747000	4.00212300	-0.35777600
H	-0.79873700	4.66547200	-0.41809700
B	-0.60608800	2.74507500	-0.22431700
O	0.34200500	1.72305700	-0.13234500
H	1.26258300	1.99992500	-0.19492600
O	-1.91669100	2.46383300	-0.17551200
H	-2.10127500	1.50917400	-0.08959900

IS3

Pd	0.00005800	-1.33749100	0.00000400
C	-1.45594400	-0.05289500	0.06231600
C	-2.55237800	-0.36963200	-0.73847200
C	-3.71350700	0.39229200	-0.66633900
C	-3.78068500	1.47936700	0.19102000
C	-2.68398000	1.80297500	0.97776200
C	-1.52171800	1.04526600	0.91520600
H	-2.51338700	-1.20494400	-1.43129300
H	-4.56153500	0.13689500	-1.29272400
H	-4.68375900	2.07692400	0.24262100
H	-2.73049500	2.65347100	1.64969700
H	-0.67205500	1.31126600	1.53101200
C	3.71377600	0.39201400	0.66567500
C	3.78058400	1.47963700	-0.19101800
C	2.68355100	1.80373000	-0.97710000
C	1.52132000	1.04596900	-0.91455200
C	1.45591000	-0.05272400	-0.06232900
C	2.55268200	-0.36996200	0.73780100
H	4.56206500	0.13622400	1.29154600
H	4.68362800	2.07723800	-0.24261200
H	2.72978100	2.65464800	-1.64851900
H	0.67140900	1.31234100	-1.52985500
H	2.51399300	-1.20571800	1.43011100

TS3

Pd	-0.00016500	1.60850700	0.00004300
C	1.03250500	-0.09703600	0.00003700
C	1.62402800	-0.49622800	-1.20082700
C	2.79129600	-1.24569700	-1.19846700
C	3.37991100	-1.62326800	0.00016300
C	2.79063400	-1.24649000	1.19873500
C	1.62336300	-0.49706400	1.20096900
H	1.16862800	-0.22815700	-2.14750200
H	3.23983900	-1.54067600	-2.14110600

H	4.28715700	-2.21638400	0.00017800
H	3.23865500	-1.54210500	2.14140300
H	1.16736200	-0.22978100	2.14753500
C	-2.79103900	-1.24598000	1.19843800
C	-3.37968100	-1.62352300	-0.00018600
C	-2.79050100	-1.24662700	-1.19877300
C	-1.62330800	-0.49706500	-1.20103200
C	-1.03234000	-0.09716500	-0.00011400
C	-1.62379000	-0.49647200	1.20077500
H	-3.23950900	-1.54109000	2.14108100
H	-4.28676600	-2.21693700	-0.00021900
H	-3.23853700	-1.54227900	-2.14144000
H	-1.16741100	-0.22964100	-2.14760800
H	-1.16828000	-0.22857000	2.14740200

FS3

Pd	1.00872500	1.31734300	-0.03256200
C	0.19435500	-0.67606700	-0.03877900
C	0.79739400	-1.31425000	-1.15516300
C	2.08981000	-1.79035400	-1.10144200
C	2.86456300	-1.62279600	0.04994100
C	2.33553000	-0.96549900	1.14047200
C	1.00787900	-0.48805300	1.12398400
H	0.19533100	-1.49468600	-2.03839600
H	2.50227200	-2.30792300	-1.96007400
H	3.87804300	-2.00496200	0.08420700
H	2.92508800	-0.83843700	2.04158600
H	0.55096400	-0.17907800	2.05923000
C	-3.38118300	-0.55536000	1.19455100
C	-4.06231200	-0.14700400	0.05822000
C	-3.35177700	0.08953100	-1.11086800
C	-1.97784400	-0.07521900	-1.13949600
C	-1.27681000	-0.47850000	0.00063000
C	-2.00533200	-0.72265800	1.16524600
H	-3.92492100	-0.75561400	2.11114400
H	-5.13808500	-0.01711200	0.08110600
H	-3.87150300	0.41122900	-2.00656700
H	-1.43259200	0.13449200	-2.05308000
H	-1.49157000	-1.06833800	2.05490400

IS3'

Pd	-0.01972300	-0.92698200	-0.25289500
C	-1.90046000	-0.46689800	-0.03078200
C	-2.68475800	-0.00455200	-1.08868600

C	-4.06184300	0.11435500	-0.95236700
C	-4.67771500	-0.20716100	0.24871500
C	-3.90729800	-0.64496000	1.31562000
C	-2.52941300	-0.76465300	1.18043400
H	-2.22056700	0.26914000	-2.02967000
H	-4.65555800	0.46881300	-1.78860200
H	-5.75214800	-0.10759400	0.35565500
H	-4.37794000	-0.88962500	2.26226400
H	-1.94504400	-1.09729500	2.03283500
C	0.77731700	2.98492900	1.20243700
C	1.29160400	3.63302400	0.09055600
C	1.35366500	2.96170400	-1.12218800
C	0.91233000	1.64820900	-1.22252400
C	0.40124600	0.98519400	-0.10551100
C	0.32379600	1.67271500	1.10589100
H	0.71471100	3.50245500	2.15382800
H	1.63782600	4.65744700	0.16626400
H	1.74871000	3.46118100	-2.00060200
H	0.97031600	1.14290200	-2.18023400
H	-0.10076600	1.19171100	1.97924700
O	4.33317600	-2.06293900	0.14149200
H	5.08053500	-1.70781900	0.62811500
B	3.22816500	-1.27314100	0.23854700
O	2.10325400	-1.69769300	-0.46337100
H	2.28353200	-2.48607300	-0.98272500
O	3.21323500	-0.14435700	0.97277900
H	2.39468900	0.37010200	0.90726800

TS3'

Pd	0.24111800	-0.96113500	-0.11601300
C	-1.65109500	-0.38833000	0.02029000
C	-2.43770200	-0.48764000	-1.13231400
C	-3.79989800	-0.73375100	-1.04546900
C	-4.41074000	-0.86383000	0.19378300
C	-3.64670200	-0.74665900	1.34676100
C	-2.28449400	-0.50243500	1.26220800
H	-1.98390700	-0.36949900	-2.11010300
H	-4.38838600	-0.81797100	-1.95294200
H	-5.47737400	-1.04528000	0.26100300
H	-4.11521300	-0.84114500	2.32066800
H	-1.70959800	-0.39558000	2.17537100
C	0.39507900	3.03068000	1.14678000
C	0.46094800	3.74023800	-0.04292400
C	0.20403100	3.08290800	-1.23847300

C	-0.11239700	1.73303600	-1.24665600
C	-0.17278600	1.00053800	-0.05610300
C	0.07379300	1.67948200	1.14328800
H	0.58957200	3.53003100	2.09001400
H	0.70476600	4.79620000	-0.03888200
H	0.24932000	3.62551200	-2.17681800
H	-0.31936700	1.24578600	-2.19242400
H	0.00795600	1.15116700	2.08780000
O	4.66554200	-1.48244200	0.02282000
H	5.37055200	-0.86170000	0.22013800
B	3.43302400	-0.90898300	0.09511200
O	2.34596700	-1.72852000	-0.18462700
H	2.60600600	-2.62012700	-0.42972600
O	3.25906400	0.38729800	0.42199200
H	2.33631800	0.68361400	0.41842100

FS3'

Pd	0.57026500	-0.92215000	-0.15972000
C	-1.47815200	-0.37072900	0.11514800
C	-1.33159100	-1.15253200	-1.07140700
C	-1.63389100	-2.53447000	-1.04580000
C	-2.07624300	-3.13944400	0.10749000
C	-2.20847300	-2.38661700	1.28209700
C	-1.90352100	-1.04608000	1.29354900
H	-1.21372800	-0.66500800	-2.03412300
H	-1.54301800	-3.10529400	-1.96321300
H	-2.32298800	-4.19480300	0.10864400
H	-2.56179800	-2.86115400	2.19057200
H	-2.05342900	-0.46786600	2.19821400
C	-1.05147500	3.25029200	1.13107200
C	-1.51727800	3.92058900	0.00763700
C	-1.97239500	3.18826600	-1.07782000
C	-1.95834100	1.80212600	-1.04441500
C	-1.48098100	1.11466800	0.07213100
C	-1.03527900	1.86664200	1.16373500
H	-0.69091300	3.81035600	1.98675100
H	-1.52754400	5.00402600	-0.01868900
H	-2.35099000	3.69817400	-1.95679100
H	-2.34094900	1.24448900	-1.89150900
H	-0.64614000	1.35589200	2.03743800
O	4.75040900	0.40430500	0.24466200
H	5.13121900	1.27563800	0.11460700
B	3.40793700	0.38615100	0.02715900
O	2.74583300	-0.82096800	0.18975200

H	3.30588500	-1.54902500	0.46787700
O	2.71175900	1.48715900	-0.33334500
H	1.76423000	1.30246600	-0.43750900

(10) The optimized structures involved in Suzuki-Miyaura cross-coupling mechanism catalyzed by Pd₂ cluster

IS1

Pd	-0.11384700	-0.79106300	0.07966100
Pd	-2.57341200	-0.32109800	-0.11177300
C	1.44578900	0.65749600	-0.01305600
C	1.22882800	1.44784100	-1.15476300
C	0.43610200	2.57172000	-1.04649700
C	-0.13681100	2.92978700	0.17592100
C	0.07353400	2.15331700	1.29600500
C	0.86878000	1.00084800	1.22756900
H	1.69276400	1.17463100	-2.09346900
H	0.26142500	3.18082900	-1.92570000
H	-0.74614800	3.82297600	0.24355300
H	-0.36069000	2.43287100	2.24869000
H	1.16265100	0.48153900	2.13100600
Br	2.80304500	-0.69998400	-0.05822800

TS1

Pd	-0.28047400	-0.68206100	-0.00094200
Pd	-2.64036200	0.20051900	0.00027600
C	1.24180300	0.55147100	0.00011800
C	1.42335100	1.20342200	-1.22015500
C	1.66857200	2.56750200	-1.20459000
C	1.78802900	3.24979900	0.00000300
C	1.66685400	2.56794700	1.20466400
C	1.42157300	1.20388000	1.22039000
H	1.36723000	0.65405200	-2.15086100
H	1.78207500	3.09621300	-2.14425900
H	1.99865700	4.31266300	-0.00003900
H	1.77905700	3.09700300	2.14429600
H	1.36407500	0.65489200	2.15121500
Br	2.02303700	-1.64937200	0.00079100

FS1

Pd	0.91257000	-0.14546800	-0.28533600
Pd	-1.16124900	1.42393000	-0.07873800
C	-1.06521300	-0.66593600	-0.06966300
C	-1.68583200	-0.46648600	1.19571400
C	-3.01640000	-0.86482100	1.40336800

C	-3.71934300	-1.48536800	0.39404100
C	-3.11465100	-1.71065300	-0.84635200
C	-1.81725300	-1.30455800	-1.08133700
H	-1.09873400	-0.15065600	2.05227700
H	-3.46963800	-0.71799900	2.37763700
H	-4.73791400	-1.81487000	0.56465000
H	-3.67303600	-2.20383400	-1.63471200
H	-1.36909200	-1.47933800	-2.05281200
Br	3.20856500	-0.38444700	0.27045000

IM

Pd	1.49357400	-0.44522400	0.05983800
Pd	-0.38921200	1.41424900	-0.20077300
C	-0.52638400	-0.64286600	0.05621500
C	-1.30417100	-0.26559500	1.18790400
C	-2.68627700	-0.50584900	1.22310000
C	-3.30633000	-1.14058400	0.16823500
C	-2.56237700	-1.52789000	-0.94987700
C	-1.20788100	-1.27262200	-1.01449700
H	-0.81554000	0.08501900	2.09181700
H	-3.25582000	-0.21907800	2.10059400
H	-4.37003700	-1.34659700	0.20657900
H	-3.05623900	-2.02345800	-1.77890200
H	-0.65305000	-1.56981200	-1.89860400
O	3.38282200	-0.78588300	0.28026500
H	3.84799700	-1.08176000	-0.50709900

IS2

Pd	-0.41890700	-0.47231700	-0.30541000
Pd	2.06385900	-1.38228900	-0.17040900
C	1.16505400	0.57740400	0.01652000
C	1.86171800	0.22916800	1.21986800
C	3.14701100	0.77731700	1.46332900
C	3.69791800	1.67068000	0.57677200
C	2.99521800	2.04890000	-0.57874100
C	1.75185300	1.52747000	-0.85262000
H	1.32940700	-0.23835400	2.04475100
H	3.65933200	0.53293300	2.38741400
H	4.66775300	2.10907900	0.78248400
H	3.43965800	2.76273200	-1.26389000
H	1.20907600	1.84615700	-1.73427600
C	-2.00708300	1.09539000	-1.12892500
C	-1.62601900	2.43789100	-1.28108100
C	-1.52436400	3.24859900	-0.17351700

C	-1.77513900	2.72952300	1.10266000
C	-2.14544600	1.41304300	1.25832300
C	-2.32319300	0.55392700	0.14572700
H	-2.20998400	0.50717000	-2.02028300
H	-1.43368800	2.83631700	-2.27163100
H	-1.24599100	4.29072800	-0.28630800
H	-1.68015200	3.37432300	1.96985500
H	-2.35444900	1.00592600	2.24188400
O	-2.89609700	-1.43391700	1.64903100
H	-3.75763500	-1.73622900	1.94220400
B	-3.02150600	-0.94185500	0.30434700
O	-2.08441900	-1.76056900	-0.62500700
H	-2.01592000	-2.64349000	-0.25137600
O	-4.39035200	-1.02016400	-0.11799300
H	-4.50590700	-0.76484700	-1.03307100

TS2

Pd	-0.25682300	-0.73278200	-0.13885700
Pd	2.38413700	-1.01920600	-0.38199900
C	1.08167900	0.62059500	0.16660900
C	2.00285300	0.33969200	1.22978100
C	3.13774400	1.16952500	1.41244600
C	3.33015800	2.26651400	0.60811200
C	2.40488000	2.57522500	-0.40200400
C	1.30462500	1.77888600	-0.61930000
H	1.72382200	-0.34150700	2.02995500
H	3.81844800	0.96265200	2.23120700
H	4.18458100	2.91388100	0.77012700
H	2.56028900	3.45510500	-1.01710300
H	0.58415400	2.04108300	-1.38558000
C	-2.32945700	0.92086500	-1.25416400
C	-2.73019200	2.23630800	-1.41038200
C	-2.83303800	3.06083700	-0.29527300
C	-2.53247100	2.56726700	0.96729200
C	-2.12966500	1.24998200	1.11539700
C	-2.03828400	0.38301800	0.01470900
H	-2.26107300	0.28264300	-2.13081000
H	-2.96453100	2.62419100	-2.39602700
H	-3.14962400	4.09170400	-0.41243800
H	-2.61012100	3.21458600	1.83418000
H	-1.91186100	0.85660900	2.10210700
O	-2.54559600	-1.65504200	1.75063400
H	-3.40256800	-1.63822600	2.18172300
B	-2.70446800	-1.37441400	0.37588700

O	-1.79088700	-2.19316500	-0.46301700
H	-1.63697300	-3.02567300	-0.00557400
O	-4.05466600	-1.36027500	-0.03007000
H	-4.15243200	-1.31794600	-0.98157200

FS2

Pd	-0.28376600	-0.45977100	-0.15162700
Pd	2.37581100	-1.19606700	-0.31510800
C	1.30878000	0.61782800	0.10286400
C	2.12032800	0.29780000	1.23969200
C	3.33213500	0.99112500	1.46553800
C	3.72603100	1.99679300	0.61415100
C	2.93447000	2.33024900	-0.49383200
C	1.76144900	1.65588000	-0.75196300
H	1.71697300	-0.30972100	2.04517400
H	3.92286500	0.75243900	2.34360100
H	4.64294700	2.54289700	0.80580200
H	3.25010600	3.12901900	-1.15655900
H	1.15453900	1.93651400	-1.60452800
C	-2.31912400	1.31230700	-1.26714000
C	-3.26490400	2.32959000	-1.28319100
C	-3.44957700	3.13304300	-0.16676800
C	-2.67707900	2.91434600	0.96302800
C	-1.72201000	1.90200500	0.97850700
C	-1.53534300	1.07689000	-0.13347500
H	-2.19843100	0.69244500	-2.14957200
H	-3.86277800	2.49150400	-2.17426900
H	-4.18963700	3.92518600	-0.17930000
H	-2.80845200	3.53861500	1.84078300
H	-1.11735600	1.76052800	1.86699700
O	-3.69023500	-3.31437800	0.42222900
H	-4.47722400	-3.31559300	0.97181400
B	-3.07841800	-2.09667900	0.40134600
O	-1.93954900	-1.98763600	-0.38946000
H	-1.73202000	-2.81095700	-0.83904600
O	-3.54381300	-1.04798400	1.10734300
H	-3.04564400	-0.22806200	0.96678800

IS3

Pd	-0.46452000	-1.00409700	0.04045900
C	0.68279700	0.55762300	0.06027600
C	1.56729500	0.70894600	1.17387200
C	2.44427000	1.81710400	1.22050600
C	2.42624700	2.76183600	0.22154100

C	1.54697100	2.62814300	-0.86194500
C	0.69790900	1.54787300	-0.95224900
H	1.42332800	0.12198700	2.07549800
H	3.09657200	1.93771100	2.07869000
H	3.08289900	3.62263500	0.27835100
H	1.53541200	3.38391800	-1.63978200
H	0.01384300	1.46306100	-1.78763400
C	-2.86672600	0.16052800	-1.15845800
C	-4.17997700	0.61434700	-1.16933900
C	-4.87523500	0.77069700	0.02096500
C	-4.25061800	0.47309800	1.22325400
C	-2.93710000	0.01942000	1.23810600
C	-2.23693800	-0.15806000	0.04456000
H	-2.33715000	0.05334300	-2.09963800
H	-4.65881000	0.85085600	-2.11394800
H	-5.89815800	1.13018500	0.01196800
H	-4.78442400	0.60062600	2.15933100
H	-2.46167400	-0.19447100	2.18894300
Pd	2.26614600	-0.83023300	-0.20390000

TS3

Pd	-0.33445600	-1.36234100	-0.35496600
C	0.18679900	0.53282900	-0.19889700
C	0.88335400	0.87339100	1.00033200
C	1.71371800	2.02372200	1.02068300
C	1.82207800	2.83075200	-0.09216000
C	1.12350800	2.50882500	-1.26083800
C	0.34408800	1.37343700	-1.32257200
H	0.59224200	0.42342000	1.94608200
H	2.21841800	2.28984200	1.94277200
H	2.43842000	3.72178900	-0.05679000
H	1.19958500	3.15338100	-2.12948000
H	-0.18816200	1.14119000	-2.23734600
C	-2.66687900	0.27727400	-1.03565300
C	-3.98276900	0.64381900	-0.78950900
C	-4.45350100	0.72792900	0.51283400
C	-3.59990400	0.44002800	1.56865100
C	-2.28581600	0.06810600	1.32451900
C	-1.80577000	-0.03442800	0.01817200
H	-2.31246200	0.23712100	-2.05981400
H	-4.64090200	0.87122100	-1.62142000
H	-5.47822300	1.02497600	0.70490100
H	-3.95698500	0.50887300	2.59073200
H	-1.63024500	-0.14188300	2.16257800

Pd	2.24934500	-0.52513700	0.23071400
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FS3

Pd	-0.51573900	-0.95640800	-0.66117800
C	-0.11384200	1.08117500	0.07879600
C	0.86984300	0.73204900	1.07661900
C	2.19862700	1.24723800	0.97881700
C	2.55935200	2.06187000	-0.09553800
C	1.60737600	2.39390500	-1.05398000
C	0.30920600	1.92497400	-0.97235100
H	0.52682500	0.34291500	2.02959400
H	2.86916800	1.14895300	1.82735600
H	3.56509700	2.45988300	-0.15785400
H	1.87834800	3.05379300	-1.87065000
H	-0.41943200	2.26339600	-1.69887700
C	-2.40220600	0.62446700	-0.85940100
C	-3.74708400	0.29143400	-0.70006200
C	-4.27991100	0.09093100	0.55888100
C	-3.45753600	0.22285800	1.67633800
C	-2.12074900	0.53338600	1.53822500
C	-1.54972600	0.74448900	0.26688100
H	-2.03781100	0.87778000	-1.84858500
H	-4.37635900	0.20392700	-1.57888400
H	-5.32781200	-0.15775400	0.67778800
H	-3.87033700	0.08318900	2.66937400
H	-1.50640700	0.64331800	2.42365300
Pd	2.02570900	-0.83950700	0.28221600

IS3'

Pd	0.44473000	0.24929300	-0.05778600
C	-1.01329500	-1.01578200	0.09208300
C	-1.90022000	-0.82991300	1.20317200
C	-3.07931600	-1.60644300	1.31082700
C	-3.36735200	-2.56394900	0.36789200
C	-2.49668000	-2.77200500	-0.71250400
C	-1.35687300	-2.01422300	-0.85459000
H	-1.57385300	-0.26769300	2.07328000
H	-3.72671300	-1.46944900	2.17036400
H	-4.25862100	-3.17335800	0.46701500
H	-2.72681000	-3.53930900	-1.44404500
H	-0.69062300	-2.19982800	-1.68927100
C	2.32534300	-1.79623000	-1.05696700
C	3.46298400	-2.59432400	-1.01729300
C	4.24820500	-2.63811300	0.12524600

C	3.88890800	-1.87728500	1.22785100
C	2.75288100	-1.07597800	1.18903300
C	1.96172100	-1.02112700	0.04204400
H	1.72387800	-1.78172600	-1.96005600
H	3.73207400	-3.18802000	-1.88505200
H	5.13208500	-3.26527100	0.15792700
H	4.49146400	-1.90913700	2.12999100
H	2.48568500	-0.49680200	2.06664000
Pd	-2.23197000	0.76396800	-0.22712900
O	1.80627400	2.00988100	-0.20558500
H	2.74190700	1.87976800	-0.38299400
B	1.39788200	3.31545500	-0.01349900
O	0.10280400	3.57324300	0.30047300
H	-0.43470800	2.77130800	0.39682700
O	2.31835700	4.30528200	-0.14965600
H	1.95052500	5.17723300	0.01036800

TS3'

Pd	0.20670500	-0.77384500	-0.48163600
C	-0.83509600	0.87018500	-0.20688800
C	-0.56074600	1.57669200	1.00391900
C	-0.85891100	2.95995100	1.09256400
C	-1.44504900	3.61933800	0.03190600
C	-1.74014200	2.92372600	-1.14451500
C	-1.42799400	1.58569200	-1.26829000
H	-0.36412400	1.02884700	1.92141600
H	-0.67093400	3.47938900	2.02562700
H	-1.69085100	4.67169500	0.11646000
H	-2.21430200	3.44093600	-1.97144600
H	-1.66574100	1.06745300	-2.18989100
C	-2.61993900	-1.38412300	-0.95077600
C	-3.77319000	-2.08978200	-0.63506200
C	-4.06615200	-2.39843700	0.68500900
C	-3.19483000	-1.99779700	1.68813700
C	-2.03878300	-1.29786100	1.37405800
C	-1.72569900	-0.99851200	0.04851500
H	-2.42002500	-1.13657100	-1.98724700
H	-4.44955400	-2.39248700	-1.42750600
H	-4.97233500	-2.93971700	0.93198900
H	-3.41620400	-2.22833400	2.72488500
H	-1.37518000	-0.98778200	2.17352100
Pd	1.36594300	1.69777500	0.15037600
O	1.92121900	-2.18869300	-0.72222600
H	1.90919400	-2.99127100	-1.24919000

B	3.03323500	-2.07260500	0.10133000
O	3.17448000	-1.00054400	0.91138500
H	2.43201900	-0.36291100	0.85538700
O	3.95621000	-3.07052800	0.04294700
H	4.69397500	-2.92332100	0.63900100

FS3'

Pd	0.45858500	0.45650200	-0.50425500
C	0.34447500	-1.63840000	-0.00621000
C	-0.66772600	-1.51808800	1.02266100
C	-1.89956700	-2.23730600	0.91151000
C	-2.17110300	-2.97823600	-0.23425800
C	-1.21523500	-3.05392000	-1.25176000
C	0.00245400	-2.41789400	-1.14337400
H	-0.36982400	-1.15483900	1.99982000
H	-2.55144900	-2.31534100	1.77553200
H	-3.10301700	-3.52473100	-0.31730600
H	-1.42069700	-3.65286200	-2.13193400
H	0.74663300	-2.57560600	-1.91448600
C	2.58001900	-0.89939300	-0.87589100
C	3.88702400	-0.45959500	-0.67812800
C	4.39329000	-0.30440600	0.59806800
C	3.57875500	-0.58989800	1.69229200
C	2.27878600	-1.01459500	1.51504900
C	1.73736900	-1.18897600	0.22445900
H	2.23699300	-1.08857700	-1.88611400
H	4.50959400	-0.24941100	-1.54091000
H	5.41373100	0.02792300	0.74780300
H	3.96986300	-0.48381000	2.69821700
H	1.67445200	-1.24834000	2.38298600
Pd	-2.05076700	-0.12307100	0.25700600
O	0.24523700	2.63754300	-0.85435300
H	0.81466900	3.11360100	-1.46296400
B	-0.48566800	3.46321500	-0.01402600
O	-1.28014100	2.93528200	0.94192800
H	-1.25091100	1.95294200	0.96145600
O	-0.36496200	4.80694900	-0.20421700
H	-0.89363200	5.31117100	0.41811400

(11) The optimized structures involved in Suzuki-Miyaura cross-coupling mechanism catalyzed by Pd₃ cluster

IS1

Pd	-0.18855800	-0.34948500	-0.19376900
Pd	2.27000600	-1.24097600	0.08853600

Pd	1.86160400	1.16669500	0.05964600
C	-2.20999600	0.30276100	0.05704900
C	-2.27665900	1.08235900	1.22707600
C	-1.97250900	2.42374900	1.15591600
C	-1.60674200	3.01337600	-0.05986100
C	-1.53033600	2.25239400	-1.20477900
C	-1.82924700	0.87748200	-1.17499100
H	-2.57777300	0.62311500	2.15963900
H	-2.02081100	3.02492700	2.05634400
H	-1.38841200	4.07396500	-0.09924500
H	-1.26374800	2.70694200	-2.15182500
H	-1.95040700	0.32616900	-2.09928000
Br	-2.96075200	-1.45641700	0.06368300

TS1

Pd	-0.23386500	-0.16523100	-0.00026400
Pd	2.11360600	0.99176000	0.00090500
Pd	2.09404900	-1.54671500	-0.00042600
C	-2.23423300	0.05428000	0.00007500
C	-2.75099900	-0.39426600	-1.21786900
C	-3.75506900	-1.35142200	-1.20167800
C	-4.25974500	-1.82762000	0.00111100
C	-3.75517400	-1.34995700	1.20338300
C	-2.75109200	-0.39282300	1.21851300
H	-2.37520500	0.00667700	-2.15028200
H	-4.14956100	-1.71985500	-2.14211200
H	-5.05262600	-2.56607500	0.00152600
H	-4.14975500	-1.71725600	2.14422400
H	-2.37530700	0.00917900	2.15047100
Br	-1.36154400	2.01962100	-0.00099900

FS1

Pd	-0.48541500	-0.33603800	0.03822200
Pd	2.06755700	0.83952800	0.18535600
Pd	1.93772700	-1.67888900	-0.14476200
C	-2.40409400	-0.21889600	0.03354800
C	-3.09937900	-0.13451100	-1.16332100
C	-4.47013400	-0.36584000	-1.15679100
C	-5.12944600	-0.63763200	0.03380000
C	-4.42459300	-0.67342100	1.22847200
C	-3.05346500	-0.44248200	1.23903500
H	-2.58664800	0.09947300	-2.08936300
H	-5.02340200	-0.32089200	-2.08848200
H	-6.20026400	-0.80553900	0.03285900

H	-4.94115000	-0.86650000	2.16226800
H	-2.50689900	-0.44301500	2.17654400
Br	-0.14768400	2.03547300	-0.14593600

IM

Pd	0.49581100	-0.12675100	-0.06228100
Pd	-1.93298600	1.21484000	0.03591500
Pd	-2.01806600	-1.35116300	-0.05153100
C	2.41565300	0.00779300	0.01714200
C	3.00759000	-1.21470300	0.29683000
C	4.39377700	-1.32540800	0.27031600
C	5.16933000	-0.21129500	-0.01585800
C	4.56336500	1.00980600	-0.27864700
C	3.17844400	1.13029000	-0.26054000
H	2.40287100	-2.08846200	0.53870200
H	4.86225900	-2.27981800	0.48422600
H	6.24997700	-0.29460100	-0.03052600
H	5.17195300	1.87891700	-0.50476900
H	2.69972700	2.07961500	-0.46987300
O	0.10969100	1.80741600	0.27340300
H	0.30779700	1.96753600	1.20285200

IS2

Pd	0.67693500	-0.27086400	-0.27601800
Pd	-1.40173100	-1.57441200	0.91024200
Pd	-1.85535400	-0.13479900	-1.34824100
C	-0.81557900	0.83932800	0.21055800
C	-1.45532900	1.84985500	-0.58089000
C	-2.75303700	2.24350200	-0.23352400
C	-3.37302400	1.75790800	0.92819100
C	-2.71885900	0.89728900	1.78165200
C	-1.41730000	0.42354000	1.46030900
H	-0.91394800	2.37111100	-1.36262100
H	-3.26287500	2.98056900	-0.84384600
H	-4.36386800	2.11674700	1.18299800
H	-3.15891900	0.63966000	2.73841000
H	-0.73863400	0.18707400	2.28983600
C	2.67886900	1.07589500	1.47803100
C	2.36902400	2.40559300	1.67783400
C	2.06142100	3.23111200	0.59233800
C	2.04353100	2.71214500	-0.68459900
C	2.36160900	1.36261700	-0.89249700
C	2.72733900	0.51369500	0.18089500
H	2.94834100	0.43840800	2.31316400

H	2.37546500	2.81996800	2.68059100
H	1.83673500	4.27932700	0.75713800
H	1.81348200	3.35049600	-1.53130100
H	2.48864600	0.99861000	-1.90842100
O	4.26632900	-1.02289900	-1.24202000
H	5.13991600	-0.76959900	-0.94200300
B	3.32515500	-0.99940100	-0.13806900
O	2.11451300	-1.76767900	-0.69455500
H	2.29366500	-1.95510200	-1.62039800
O	3.77993500	-1.55793000	1.10008200
H	4.06490000	-2.46363700	0.96374700

TS2

Pd	0.57054400	-0.57677600	-0.20693500
Pd	-1.90110900	-1.41510700	0.74051000
Pd	-1.80012800	0.26698400	-1.38140800
C	-0.64573400	0.80419400	0.33262300
C	-0.96727200	1.99874300	-0.39318500
C	-2.13709000	2.69337100	-0.06315000
C	-2.93148200	2.29723200	1.02289200
C	-2.57500300	1.22841200	1.81657500
C	-1.42296100	0.45817200	1.50417100
H	-0.25872800	2.42332700	-1.09699600
H	-2.39822800	3.58624900	-0.62022100
H	-3.81217100	2.87937600	1.27036800
H	-3.13033000	1.01391900	2.72279500
H	-0.90063100	-0.04013100	2.33052000
C	2.62225500	0.87028500	1.42339100
C	3.06755000	2.16642500	1.63584200
C	3.34056400	2.98951400	0.55223100
C	3.17585400	2.51037600	-0.74261600
C	2.73586300	1.21332400	-0.94460800
C	2.45480200	0.34955400	0.13062600
H	2.44027000	0.22223000	2.27335300
H	3.20346900	2.53671300	2.64642600
H	3.69041400	4.00340500	0.71506800
H	3.40131500	3.14876600	-1.59048700
H	2.64844600	0.84033900	-1.96000800
O	4.08112100	-1.43483200	-1.01590400
H	4.92078100	-1.37919200	-0.55685400
B	3.01800100	-1.51535800	-0.09614600
O	1.86440800	-2.19650300	-0.70731300
H	2.04149400	-2.33601100	-1.64198100
O	3.31517200	-1.97088100	1.20498800

H	2.68612400	-2.63671600	1.48612900
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FS2

Pd	0.60401000	-0.25616500	-0.22751000
Pd	-1.80518200	-1.32005100	1.04546800
Pd	-1.97108500	-0.11159900	-1.35621700
C	-0.84992900	0.94271100	0.14907400
C	-1.40870300	1.90243400	-0.75761400
C	-2.63741700	2.50093300	-0.45675800
C	-3.29800200	2.22177500	0.74472700
C	-2.74376300	1.37178200	1.67942000
C	-1.51533700	0.71415300	1.41368900
H	-0.82193700	2.26917400	-1.59378500
H	-3.05593300	3.22739000	-1.14459300
H	-4.23767900	2.71818200	0.96037100
H	-3.21270900	1.24904000	2.64948600
H	-0.89911500	0.41357100	2.27070500
C	2.39520600	1.59502200	1.30512200
C	3.46238900	2.47401200	1.46595500
C	4.20385300	2.88244700	0.36847300
C	3.87331700	2.40297400	-0.89124100
C	2.81285100	1.51964300	-1.05041700
C	2.05555600	1.09303600	0.04561100
H	1.82378500	1.30024900	2.17914100
H	3.70768000	2.84383200	2.45624200
H	5.03288600	3.57003300	0.49242600
H	4.44555600	2.71614100	-1.75863400
H	2.57867700	1.15628100	-2.04581400
O	3.67210100	-3.55275400	-0.32001900
H	4.51327200	-3.71743300	0.11200700
B	3.22071600	-2.28517800	-0.09985400
O	2.01852400	-1.94223300	-0.70726400
H	1.65376400	-2.66457400	-1.22484100
O	3.89680500	-1.40699200	0.66533000
H	3.49243800	-0.52620100	0.70589700

IS3

Pd	-0.01077300	0.94673700	0.17008100
Pd	-1.15872200	-1.49196200	0.66587600
Pd	1.09354200	-1.43140800	-0.72043100
C	1.88434600	0.25137300	-0.06619800
C	2.37101000	1.10372400	-1.08629900
C	3.51313400	1.86944400	-0.87545000
C	4.18746700	1.80624000	0.33402100

C	3.71612200	0.98099800	1.34952100
C	2.57685700	0.21386300	1.16536100
H	1.86661400	1.14095700	-2.04594600
H	3.87612500	2.51499200	-1.66814500
H	5.07766300	2.40458900	0.49090900
H	4.23903500	0.93900100	2.29914400
H	2.21362500	-0.42196800	1.96295800
C	-2.37846400	1.10465100	1.00790300
C	-3.40799700	1.99960200	0.70923400
C	-3.99435000	2.00102400	-0.54278300
C	-3.54794100	1.11211500	-1.51925100
C	-2.51609100	0.22997200	-1.25594500
C	-1.91637900	0.19868400	0.02168200
H	-1.99204000	1.05625500	2.02111600
H	-3.75961500	2.68007200	1.47750700
H	-4.79712500	2.69402400	-0.76676600
H	-4.00046100	1.12252100	-2.50524000
H	-2.15628700	-0.43547900	-2.03054200

TS3

Pd	-0.35977700	-0.98376400	-0.57090400
Pd	1.75517000	0.97826300	-0.01912500
Pd	2.08942500	-1.61955700	0.21505200
C	-2.19446800	-0.35762500	0.00640500
C	-3.16571600	-0.28042800	-0.99311500
C	-4.50616600	-0.48134300	-0.69195700
C	-4.89961600	-0.72627600	0.61531700
C	-3.94341600	-0.77540200	1.62065200
C	-2.60248500	-0.58706400	1.32046200
H	-2.88114500	-0.06909000	-2.01806200
H	-5.24622400	-0.43734300	-1.48391800
H	-5.94775400	-0.86966600	0.85191900
H	-4.24257500	-0.96093000	2.64673400
H	-1.86904500	-0.62727000	2.11810400
C	-0.85906800	1.91096100	-1.13681700
C	-0.62418600	3.24191200	-0.89405600
C	-0.04338100	3.65922400	0.31680500
C	0.26797400	2.73595300	1.28826500
C	0.01142300	1.35394400	1.07507000
C	-0.57313200	0.92019400	-0.15948300
H	-1.30340200	1.60886500	-2.07725800
H	-0.88193600	3.97833500	-1.64694000
H	0.14496000	4.71258700	0.48979300
H	0.68196900	3.05344000	2.23843100

H	0.03691900	0.67945300	1.92483600
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FS3

Pd	-0.61775700	-0.63188400	-0.61155300
Pd	1.84408600	0.57568300	0.08063400
Pd	1.52808900	-1.99083900	0.12132200
C	-2.14748300	0.70293500	0.24809700
C	-2.87406000	0.32837300	-0.90728700
C	-4.07411000	-0.37428200	-0.78899700
C	-4.58136800	-0.69230400	0.45466800
C	-3.88676400	-0.30449000	1.60087000
C	-2.69002200	0.37105100	1.50515900
H	-2.55040800	0.65724800	-1.88820100
H	-4.61217300	-0.65699800	-1.68670400
H	-5.51856900	-1.22905600	0.54237100
H	-4.29123100	-0.53520200	2.58004900
H	-2.16964600	0.66992200	2.40694300
C	-0.63013800	2.33221200	-0.95465300
C	0.46442800	3.15565800	-0.95662300
C	1.40994400	3.13916200	0.09243100
C	1.21616900	2.30006100	1.18597200
C	0.16826800	1.32895700	1.13265300
C	-0.83638100	1.37089200	0.08482400
H	-1.38248300	2.44344700	-1.72522200
H	0.59340700	3.86435600	-1.76701200
H	2.22671700	3.85053200	0.09363000
H	1.81397600	2.40592800	2.08400900
H	-0.04374100	0.74432300	2.01891400

IS3'

Pd	-0.51628500	-0.22234700	-0.04254200
Pd	2.39248000	0.09194600	-0.78998700
Pd	1.38798800	-2.07211900	0.29264500
C	-1.97662700	1.12970900	-0.07860500
C	-2.66273800	1.35389500	-1.27575100
C	-3.73936400	2.23083300	-1.33053700
C	-4.15745100	2.89960400	-0.18844400
C	-3.48783600	2.68756200	1.00666300
C	-2.40275800	1.81701800	1.06078600
H	-2.35827700	0.83776100	-2.18069300
H	-4.25604500	2.38811300	-2.27187800
H	-4.99936100	3.58136100	-0.23077400
H	-3.80299000	3.20645600	1.90613100
H	-1.88271000	1.67957500	2.00236000

C	0.87798700	2.43888400	-0.33365500
C	1.83048100	3.36685800	0.01686000
C	2.84010200	3.05739500	0.94658100
C	2.89156100	1.80709200	1.50793300
C	1.90816600	0.83781100	1.18057100
C	0.85246800	1.13968300	0.25298500
H	0.10615200	2.70574400	-1.04492300
H	1.80266900	4.35529400	-0.42960500
H	3.57287200	3.80889200	1.21805600
H	3.65633200	1.55766500	2.23535700
H	1.82858600	-0.04442400	1.81481800
O	-3.88825600	-1.26118900	0.78889700
H	-3.49776700	-0.37559100	0.73726100
B	-3.15914700	-2.21650100	0.17898400
O	-3.57888300	-3.51119100	0.10548900
H	-4.43804100	-3.63668200	0.51472900
O	-1.93491400	-1.92398700	-0.40912500
H	-1.51559900	-2.69285100	-0.80550400

TS3'

Pd	-0.52700100	-0.18439300	-0.56548600
Pd	2.33367500	-0.57118700	-0.36447200
Pd	0.61512600	-2.11530000	0.97450800
C	-1.14496000	1.56555200	0.25278500
C	-1.89287900	2.41338300	-0.57033800
C	-2.84992600	3.26681400	-0.03156100
C	-3.05360100	3.31232300	1.33872200
C	-2.29745800	2.49292000	2.16705900
C	-1.35336200	1.62977200	1.63242000
H	-1.72969000	2.41695400	-1.64253600
H	-3.42979900	3.90391800	-0.69081300
H	-3.79173800	3.98471400	1.76018700
H	-2.44662600	2.52211900	3.24118200
H	-0.77948900	0.99194000	2.29505800
C	1.18244900	2.11513500	-1.33567000
C	2.36809200	2.80846700	-1.30033100
C	3.27686600	2.62098800	-0.24544700
C	2.97329000	1.75403800	0.77840600
C	1.73696100	1.04843300	0.78613400
C	0.81181000	1.22505300	-0.29429900
H	0.50009800	2.27357900	-2.16281200
H	2.60812700	3.50236700	-2.09834100
H	4.21127800	3.17036300	-0.23256300
H	3.65129000	1.63179200	1.61549900

H	1.39721000	0.59875600	1.71660800
O	-3.99710000	-0.33484000	-0.59194100
H	-3.34946100	0.37938400	-0.51004800
B	-3.46009100	-1.56006400	-0.77789800
O	-4.22508200	-2.68541900	-0.81275000
H	-5.15543600	-2.49822500	-0.66897100
O	-2.09402500	-1.71728700	-0.95655400
H	-1.80215900	-2.63375500	-0.95956700

FS3'

Pd	-0.47769600	0.12940900	-0.61962500
Pd	2.13497400	-0.76717100	-0.24363100
Pd	0.18651200	-1.85233700	1.15659500
C	-0.55693800	2.08782800	0.45523200
C	-1.53407200	2.48962300	-0.48840300
C	-2.83302500	2.79917100	-0.08640000
C	-3.19505700	2.72361100	1.24586500
C	-2.24025600	2.34507100	2.18792800
C	-0.95276300	2.03128300	1.80665700
H	-1.26342200	2.63048200	-1.52761100
H	-3.55584500	3.11547700	-0.83103100
H	-4.20326000	2.97064500	1.55593000
H	-2.50800200	2.29867300	3.23761300
H	-0.23160100	1.74963700	2.56336900
C	1.35215200	2.30274100	-1.18578600
C	2.68034500	2.16450500	-1.51018100
C	3.57994100	1.49382600	-0.66550600
C	3.12925600	0.96291400	0.54099700
C	1.72770000	0.98686000	0.84003800
C	0.80249400	1.72037700	-0.00416400
H	0.72269000	2.91646300	-1.81706900
H	3.05055200	2.61620100	-2.42372600
H	4.63395800	1.45614900	-0.91309100
H	3.83500500	0.63039600	1.29455700
H	1.41101100	0.72247300	1.84186100
O	-3.82775400	-0.46482800	-0.92783400
H	-3.29201700	0.33237400	-0.82066300
B	-3.09773400	-1.59135400	-1.10466400
O	-3.66843700	-2.82531400	-1.10258400
H	-4.61060000	-2.79157100	-0.92256800
O	-1.73068900	-1.51578300	-1.32442900
H	-1.25780200	-2.34552800	-1.18674100

(12) The optimized structures involved in Suzuki-Miyaura cross-coupling mechanism

catalyzed by Pd₄ cluster

IS1

Pd	2.19346500	-0.24102100	1.12675900
Pd	-0.42232800	-0.56198200	0.54359100
Pd	0.80964000	1.33400600	-0.56663200
Pd	1.60563200	-1.16784100	-1.11269400
C	-2.34236800	0.34601100	0.00042300
C	-1.96072100	0.92824400	1.24540300
C	-1.23441000	2.12669400	1.23427200
C	-0.84699100	2.73078200	0.03279400
C	-1.21308400	2.12446700	-1.20253900
C	-1.98193400	0.95324600	-1.20959900
H	-2.38367100	0.55567400	2.16985500
H	-0.98935400	2.60014700	2.17731900
H	-0.42109900	3.72726000	0.04660700
H	-1.05445700	2.65027300	-2.13710600
H	-2.31673500	0.52453600	-2.14498400
Br	-3.65521300	-1.02914300	-0.00866700

TS1

Pd	-2.24788700	-0.66514000	-0.85853800
Pd	0.44294500	-0.28156200	-0.36535800
Pd	-1.32180100	1.64835700	-0.30408800
Pd	-1.35788500	-0.12753000	1.51941700
C	2.40888500	0.04770000	-0.02957700
C	2.97113500	0.49198100	-1.22659200
C	3.78957300	1.61464300	-1.20162500
C	4.08587700	2.24442200	-0.00276000
C	3.55658600	1.75414400	1.18678600
C	2.72914500	0.64417000	1.18958700
H	2.78103200	-0.03568600	-2.15304600
H	4.21342200	1.98026800	-2.13034000
H	4.74110900	3.10718500	0.01023800
H	3.79316100	2.23937500	2.12734900
H	2.32617600	0.24889300	2.11286200
Br	2.03402200	-2.13520400	0.02663200

FS1

Pd	-0.66149300	-1.35349500	1.19129600
Pd	0.13145500	1.01347000	0.30020600
Pd	0.99505300	-1.27973100	-0.74000500
Pd	-1.79753700	-0.35352000	-1.00839500
C	2.03838200	0.40770800	0.00076900
C	2.83547700	0.11081900	1.12298200

C	4.17632300	0.46481200	1.15123500
C	4.75939300	1.10253500	0.06397700
C	3.99637200	1.38863100	-1.05919900
C	2.65248700	1.04202800	-1.09919900
H	2.39307600	-0.38567400	1.97848700
H	4.77120500	0.23826400	2.02965200
H	5.80867800	1.37354600	0.09153400
H	4.44696600	1.88720900	-1.91069000
H	2.06459200	1.28080000	-1.97970200
Br	-2.31254600	1.69363700	0.30070400

IM

Pd	-0.73649400	-0.91225300	1.30334600
Pd	0.42587200	1.25679500	0.11079700
Pd	0.10626300	-1.29915600	-1.14117800
Pd	-2.19758000	0.44506500	-0.39005700
C	1.65987500	-0.40881600	-0.36547200
C	2.37537700	-0.98860500	0.71190800
C	3.62460100	-0.52408000	1.05994300
C	4.20735800	0.54558200	0.37055900
C	3.54039800	1.12916400	-0.68104900
C	2.26943600	0.66151700	-1.06885300
H	1.93804400	-1.81826000	1.25690500
H	4.15583800	-0.98660400	1.88475000
H	5.18742000	0.90652500	0.66087100
H	3.99918100	1.93565400	-1.24287300
H	1.84828700	1.01658200	-2.00535000
O	-1.38621600	2.20476700	0.41516500
H	-1.61212300	2.25861700	1.34833300

IS2

Pd	0.14481900	2.45073400	-0.59962200
Pd	0.12180200	-0.95031000	-1.15711800
Pd	1.91346100	0.65837700	-0.21609500
Pd	-0.51776100	0.61758000	1.09917600
C	1.59497800	-1.46549600	-0.02025600
C	2.94055200	-1.27396000	-0.46029800
C	4.00959700	-1.52804000	0.42530700
C	3.76916200	-1.98584300	1.69977700
C	2.45432500	-2.22603200	2.12064600
C	1.38935500	-1.98190600	1.28247500
H	3.16056100	-1.13294600	-1.51564200
H	5.02760400	-1.40100900	0.07291300
H	4.59619600	-2.18738000	2.37071500

H	2.27251700	-2.60941700	3.11895700
H	0.37742800	-2.20703500	1.60315800
C	-2.54369800	0.66680000	0.32723300
C	-2.58249500	1.22765800	1.62897900
C	-2.84785400	0.38655800	2.72993700
C	-3.06711400	-0.95847800	2.51986000
C	-2.99950300	-1.50693000	1.22668500
C	-2.72656700	-0.73119600	0.11399400
H	-2.50443400	1.31522800	-0.54173700
H	-2.57302700	2.30419800	1.75971300
H	-2.89560300	0.80501900	3.72851700
H	-3.28232800	-1.60440100	3.36450900
H	-3.12472100	-2.57834400	1.10449200
O	-1.42014900	-2.47383500	-1.13325200
H	-1.45125900	-3.09751800	-1.86557900
B	-2.46704500	-1.37953200	-1.35331200
O	-1.73799900	-0.33968400	-2.16480500
H	-1.85490700	-0.52042100	-3.10116900
O	-3.56983600	-1.91254000	-2.08803500
H	-4.40006200	-1.83216300	-1.62126100

TS2

Pd	-0.00637500	-2.31434600	0.39067900
Pd	0.32489400	0.00679900	-1.21918400
Pd	-2.07761300	-0.75789100	-0.17451000
Pd	-0.02170500	-0.01315500	1.75338200
C	-1.24911700	1.06870500	-0.68157000
C	-2.33734200	0.94980200	-1.60640000
C	-3.47219200	1.76756800	-1.48337800
C	-3.54155500	2.71670700	-0.48469000
C	-2.47933000	2.86607100	0.40923100
C	-1.35724100	2.06424500	0.32279500
H	-2.22720700	0.35806200	-2.51310600
H	-4.27651100	1.66918000	-2.20436000
H	-4.41342500	3.35544200	-0.40123700
H	-2.53102200	3.62269800	1.18472000
H	-0.52657500	2.23966600	1.00019100
C	1.96802300	0.05400700	1.05966000
C	2.13472500	0.61620700	2.34886700
C	2.18710600	2.00873000	2.47774500
C	2.12216500	2.82425000	1.35245000
C	1.88135600	2.27921700	0.09535900
C	1.81079900	0.89706000	-0.09080100
H	2.17360300	-1.00798300	0.91281000

H	2.35285700	-0.02158800	3.19863800
H	2.32111700	2.44980000	3.45930000
H	2.23632600	3.89743200	1.46320700
H	1.76278200	2.93570800	-0.76000300
O	2.89034100	1.11084900	-2.77353900
H	3.66965300	1.67051400	-2.78819000
B	2.97830500	0.16835600	-1.75870900
O	2.16143700	-1.01619400	-1.95953100
H	2.06382400	-1.17436200	-2.90437800
O	4.21706200	0.01421800	-1.15263800
H	4.26471600	-0.76751900	-0.60089100

FS2

Pd	-1.94622200	-0.20854100	-1.58338700
Pd	0.44185300	0.08261600	-0.28512400
Pd	-1.93625900	1.21343900	0.65173800
Pd	-1.61104300	-1.52776000	0.69505700
C	-0.13336000	1.93435600	0.43947600
C	0.17609300	2.69896200	-0.70746400
C	1.11849300	3.72010000	-0.62854600
C	1.74147400	4.01626500	0.57675000
C	1.42282700	3.28523000	1.71796800
C	0.50723800	2.24669700	1.65703400
H	-0.34061400	2.50557200	-1.64093800
H	1.35234300	4.29792400	-1.51650500
H	2.46865300	4.81824800	0.63048500
H	1.90884500	3.51428700	2.66035100
H	0.29785900	1.65428900	2.54083500
C	0.74580800	-2.56851800	-0.65781200
C	1.85281600	-3.40493500	-0.55233400
C	2.52714400	-3.53722200	0.65536300
C	2.09725800	-2.82107200	1.76947100
C	1.01098300	-1.96553100	1.68139300
C	0.31030100	-1.82663900	0.46324800
H	0.19704500	-2.50668600	-1.59096200
H	2.17837700	-3.96930100	-1.41986400
H	3.38235700	-4.19887900	0.73121900
H	2.62529600	-2.91943300	2.71189800
H	0.70526100	-1.38495100	2.54473700
O	5.29795300	1.09699700	-0.97489500
H	6.09522000	0.62729600	-1.22897300
B	4.29106800	0.23775600	-0.63093200
O	3.08349700	0.74539000	-0.23190900
H	3.05276500	1.70733800	-0.20842800

O	4.49359100	-1.10723600	-0.68648300
H	3.73532400	-1.63049600	-0.40126200

IS3

Pd	-1.13858500	-0.00814600	1.54760500
Pd	0.41011400	-0.02354700	-0.50641200
Pd	-2.01714600	-1.30896200	-0.49209100
Pd	-2.02039100	1.22805300	-0.52644900
C	1.85967700	-1.34380900	-0.26466300
C	1.58776800	-2.43203100	0.55971000
C	2.49022100	-3.48516300	0.65271100
C	3.67031800	-3.45807900	-0.07555400
C	3.94702400	-2.37123000	-0.89172000
C	3.05469200	-1.30907300	-0.97803400
H	0.66054300	-2.47075600	1.12486300
H	2.26552000	-4.32896700	1.29668400
H	4.37419400	-4.27961000	-0.00394500
H	4.86996000	-2.34011400	-1.46128300
H	3.29913700	-0.45750400	-1.60173700
C	1.71471300	2.45605500	-1.01185800
C	2.51450600	3.57038900	-0.78414800
C	3.30093300	3.64326300	0.35583100
C	3.28966800	2.59432100	1.26396500
C	2.50208200	1.47275900	1.03638900
C	1.70272300	1.40297300	-0.10004400
H	1.09659600	2.42207400	-1.90462500
H	2.51680300	4.38360400	-1.50230200
H	3.92199900	4.51364400	0.53466200
H	3.90509800	2.64225700	2.15624300
H	2.52055400	0.65278300	1.74389700

TS3

Pd	-1.25671900	-0.00005100	1.53465900
Pd	0.33152100	0.00000700	-0.49627400
Pd	-2.07805900	-1.27306600	-0.54251800
Pd	-2.07804800	1.27311400	-0.54243000
C	2.00924300	-1.04908200	-0.12391300
C	2.20578000	-1.62330100	1.13001100
C	2.99375700	-2.75600500	1.26917300
C	3.60693300	-3.32462700	0.16149900
C	3.42796500	-2.74879400	-1.08794100
C	2.64483600	-1.61223400	-1.22990800
H	1.74096300	-1.18698900	2.00733400
H	3.13026100	-3.19530200	2.25156100

H	4.22697300	-4.20663100	0.27271500
H	3.90612700	-3.18087800	-1.96045300
H	2.53427400	-1.16799600	-2.21361500
C	2.64485900	1.61221800	-1.22991000
C	3.42799300	2.74877400	-1.08794800
C	3.60695400	3.32461900	0.16148800
C	2.99376600	2.75601200	1.26916200
C	2.20578300	1.62331100	1.13000600
C	2.00925300	1.04908200	-0.12391400
H	2.53430400	1.16796900	-2.21361300
H	3.90616600	3.18084600	-1.96046000
H	4.22699700	4.20662100	0.27270000
H	3.13026200	3.19531900	2.25154700
H	1.74095400	1.18701200	2.00732900

FS3

Pd	1.48340200	-1.53999000	0.92104600
Pd	-0.30284900	-0.26058100	-0.63166700
Pd	1.30396800	1.13314200	0.71242500
Pd	2.31481500	-0.49419900	-1.18450000
C	-2.02721200	0.98409900	0.12161400
C	-1.48465300	1.35595400	1.36607700
C	-0.46153600	2.30621500	1.47232500
C	0.04028000	2.94130300	0.30164900
C	-0.48836300	2.58041800	-0.94362500
C	-1.48730300	1.60586800	-1.05123900
H	-1.90735500	0.93438600	2.27006800
H	-0.18703100	2.67674300	2.45349500
H	0.69710400	3.79995000	0.38051000
H	-0.12818600	3.07010800	-1.84035600
H	-1.95894300	1.43859300	-2.01280900
C	-4.24665200	0.39457700	-0.87338900
C	-5.38158400	-0.39903600	-0.93007800
C	-5.52809700	-1.47306900	-0.06554500
C	-4.52814100	-1.74766800	0.85726700
C	-3.39340600	-0.95700100	0.91375500
C	-3.23374200	0.12868800	0.04869200
H	-4.15785100	1.24687800	-1.53738100
H	-6.15953300	-0.17056800	-1.64983000
H	-6.41524400	-2.09400200	-0.11091200
H	-4.62755500	-2.59099700	1.53124900
H	-2.60242000	-1.19825200	1.61503700

IS3'

Pd	-0.75964800	0.45373600	-1.56728700
Pd	0.62931200	-0.09059400	0.75436800
Pd	-1.82016100	-1.11612800	0.34868200
Pd	0.28702400	-1.97454100	-0.91404400
C	0.52128700	1.55758600	-0.57026300
C	1.65551200	1.84229500	-1.36386700
C	2.20068900	3.11328100	-1.37070100
C	1.66695000	4.11616600	-0.56647900
C	0.56718600	3.84997900	0.23449600
C	-0.01546800	2.58843600	0.23364800
H	2.11099600	1.05099200	-1.94519500
H	3.06603800	3.31942500	-1.99119000
H	2.11236600	5.10447800	-0.56572300
H	0.14400100	4.63154400	0.85622400
H	-0.90075600	2.40565700	0.83162000
C	3.22882300	0.60071200	1.73152000
C	4.58298500	0.42409100	1.99039500
C	5.28184500	-0.61033300	1.38431500
C	4.62560300	-1.46944300	0.51462700
C	3.27074700	-1.29895300	0.25514400
C	2.56847900	-0.27717800	0.87873500
H	2.69830600	1.42873700	2.19292900
H	5.09320600	1.10644400	2.66195500
H	6.33957600	-0.74126800	1.58274900
H	5.16799400	-2.27518500	0.03136500
H	2.76450200	-1.97293100	-0.43739100
O	-5.23212900	1.19323700	1.98215200
H	-5.54354400	2.06721300	1.73661300
B	-4.16069100	0.79816800	1.23990300
O	-3.62378100	-0.45194100	1.49897100
H	-4.05411000	-0.92714100	2.21329500
O	-3.61333700	1.57386600	0.27815500
H	-2.84925000	1.13627000	-0.14950000

TS3'

Pd	0.70183600	0.07395400	1.59989600
Pd	-0.56970400	-0.03471600	-0.90499000
Pd	2.02193900	-0.81752800	-0.61079600
Pd	0.24604700	-2.25251400	0.43947700
C	-1.30009600	0.97435700	0.63029100
C	-1.41343000	0.30602700	1.88587900
C	-1.37592300	1.05202900	3.08626600
C	-1.26258500	2.42768500	3.05474600
C	-1.20356900	3.08807700	1.82278800

C	-1.20062300	2.38122300	0.63777900
H	-1.73867400	-0.72901900	1.92027500
H	-1.47313400	0.52848600	4.03075700
H	-1.23777800	2.99405400	3.97811100
H	-1.14658300	4.17082000	1.79588000
H	-1.12785100	2.91935200	-0.30002200
C	-3.08087300	1.22229000	-1.75358700
C	-4.37308700	1.11768000	-2.25093300
C	-5.18237800	0.05551400	-1.87549400
C	-4.69051700	-0.90551800	-1.00260000
C	-3.39659700	-0.80786600	-0.51257300
C	-2.56945300	0.24610800	-0.89847800
H	-2.47313200	2.07478200	-2.03807400
H	-4.75084700	1.87744100	-2.92689300
H	-6.19563300	-0.01845300	-2.25362300
H	-5.31836300	-1.73679800	-0.69983800
H	-3.02622700	-1.56619200	0.16966000
O	4.18493800	2.73340400	-2.00153900
H	4.00762200	3.67168700	-1.90557000
B	3.24616900	1.96257200	-1.38762200
O	3.41593600	0.58595100	-1.46600100
H	4.18919100	0.30976800	-1.96374200
O	2.19057900	2.47800300	-0.72615000
H	1.61827400	1.78369200	-0.34882200

FS3'

Pd	0.66557900	-0.74218100	1.34478600
Pd	-0.77778900	0.36395600	-0.71450800
Pd	1.84897700	-0.47397800	-1.00682600
Pd	0.09779300	-2.22574400	-0.69482300
C	-1.70862300	0.71642200	1.34119800
C	-1.41167600	-0.57286100	1.92639300
C	-0.60640700	-0.69029100	3.08952500
C	0.06257100	0.44606200	3.56407200
C	-0.22545300	1.69691900	3.00090100
C	-1.12024700	1.84165700	1.95855100
H	-1.97699400	-1.43312800	1.59222000
H	-0.55944600	-1.63090200	3.62565200
H	0.72067200	0.37137000	4.42053700
H	0.24497200	2.58090700	3.41675400
H	-1.36730900	2.83435600	1.60493300
C	-2.55785700	1.94639700	-0.66311700
C	-3.45202200	2.07825400	-1.73110500
C	-4.47527700	1.17167500	-1.91041100

C	-4.61786100	0.10903000	-1.01461400
C	-3.73946700	-0.05471400	0.03217600
C	-2.68428600	0.85970400	0.24340800
H	-1.85142800	2.74594000	-0.46998900
H	-3.33862300	2.91549500	-2.41063000
H	-5.17034900	1.28676400	-2.73358700
H	-5.43110100	-0.59679100	-1.14196400
H	-3.87744800	-0.87869400	0.72195400
O	4.02822400	3.31770900	-0.63149700
H	3.78055600	4.15825200	-0.24035200
B	3.02508300	2.39884600	-0.56011400
O	3.28557000	1.14487200	-1.09774600
H	4.17461700	1.04106300	-1.44519300
O	1.82674300	2.66476900	-0.00375600
H	1.23202800	1.88837500	-0.01454400

(13) The optimized structures involved in Suzuki-Miyaura cross-coupling mechanism catalyzed by Pd₁₂ cluster

IS1

Pd	-0.13629700	-3.10898500	-0.65802700
Pd	-2.30070500	-1.85578500	-1.20747100
Pd	-3.37393100	-0.47117300	0.95856400
Pd	-1.70752000	1.24000000	1.95501500
Pd	-0.92551300	3.13187400	0.16357700
Pd	0.17470800	2.00515500	-1.96285800
Pd	2.42860600	0.85310200	-1.34086700
Pd	1.81805200	-1.47002000	0.39861200
Pd	0.18216600	-0.69643600	-1.65494500
Pd	-1.85809600	0.82561600	-0.75585800
Pd	-0.82398600	-1.15534300	0.97473700
Pd	0.77592900	1.07353600	0.67178100
C	3.25591000	-1.58201900	2.10896800
C	2.54358100	-1.67718400	3.32099700
C	1.86204500	-0.57989900	3.84958300
C	1.88781400	0.65488000	3.19694100
C	2.53933300	0.81822700	1.95174400
C	3.21418100	-0.34157200	1.39854800
H	3.95231700	-2.37173100	1.81577100
H	2.55800700	-2.62550100	3.86347200
H	1.33276000	-0.67859600	4.79939900
H	1.44792400	1.53463800	3.67279400
H	2.86578500	1.81845200	1.63868400
Br	4.58197100	0.04220700	0.06586300

TS1

Pd	0.00790100	-3.13565400	-0.51761600
Pd	-2.24043800	-2.00662700	-1.00504600
Pd	-3.28708200	-0.62177000	1.12791200
Pd	-1.68608100	1.24096600	1.95080700
Pd	-1.10591500	3.10173000	0.02694100
Pd	-0.03426400	1.93112100	-2.09000600
Pd	2.31036300	0.86167500	-1.50265400
Pd	1.96340500	-1.29822300	0.34644500
Pd	0.12529500	-0.76010900	-1.67186000
Pd	-1.93267800	0.70074200	-0.72097800
Pd	-0.67196800	-1.16815000	1.06460400
Pd	0.68800500	1.13010100	0.51289400
C	3.46332800	-1.13133400	2.57662300
C	3.18992200	-0.83212800	3.90683800
C	2.57425100	0.37671600	4.26677100
C	2.24940300	1.30994400	3.29213600
C	2.48215000	1.04262900	1.92701200
C	3.03530600	-0.22608500	1.57957100
H	3.97986500	-2.05404500	2.30271700
H	3.46829800	-1.55208700	4.68089300
H	2.38886300	0.59860400	5.31972700
H	1.84135600	2.28450900	3.57174600
H	2.52620200	1.88802100	1.21187800
Br	4.38709400	-0.09401000	-0.23905600

FS1

Pd	2.26928600	-1.56768400	-0.77527800
Pd	-0.10918900	-2.28249100	-1.66234100
Pd	-1.75702200	-2.96642300	0.35694900
Pd	-2.20374100	-0.88381300	1.91518200
Pd	-3.35120000	1.14448800	0.61815000
Pd	-1.76657500	2.01482200	-1.37152700
Pd	0.58552000	2.87696900	-0.45071600
Pd	2.23422600	0.83672900	0.41260200
Pd	0.36738000	0.37439600	-1.47456800
Pd	-2.03381400	-0.60828400	-0.83639400
Pd	0.24977700	-1.24222400	0.89025800
Pd	-0.69570700	1.25519400	1.05295900
C	4.42364900	-0.88251400	-0.43078800
C	5.36018300	-1.93208000	-0.28261100
C	5.50012900	-2.58057100	0.93412300
C	4.72338400	-2.18416700	2.03633800
C	3.79117300	-1.16306000	1.91952900

C	3.60349300	-0.51799000	0.67419700
H	4.46026300	-0.25598500	-1.32829600
H	6.00140100	-2.19718400	-1.12727600
H	6.23263000	-3.38326700	1.04579800
H	4.85139300	-2.68698200	2.99856600
H	3.19806300	-0.85779300	2.78526400
Br	2.75865500	3.23331900	0.78453000

IM

Pd	-2.64580100	-1.10265600	0.30125100
Pd	-0.53294000	-2.01335200	1.64861700
Pd	1.23086900	-3.08842600	-0.07211200
Pd	2.22164600	-1.23512100	-1.67513700
Pd	3.51791900	0.69169800	-0.33412000
Pd	1.86507600	1.98857500	1.30042200
Pd	-0.26613500	3.04839800	0.07109300
Pd	-2.15557300	1.25579400	-0.76892100
Pd	-0.51900500	0.65400300	1.26871600
Pd	1.73815100	-0.70971400	1.00324200
Pd	-0.37229800	-1.10318100	-0.97748900
Pd	0.97983500	1.17568300	-1.14725400
C	-4.90227000	0.98646800	0.20274900
C	-6.10775600	0.32596500	0.38819400
C	-6.37726900	-0.88233900	-0.27904000
C	-5.44097800	-1.41746700	-1.14829500
C	-4.20349200	-0.76501100	-1.35979700
C	-3.91627800	0.43971000	-0.65515500
H	-4.70257300	1.92887000	0.71826100
H	-6.85627400	0.75170300	1.06178600
H	-7.33455100	-1.38630300	-0.12673100
H	-5.66317100	-2.33044400	-1.70686000
H	-3.56060500	-1.10182900	-2.17851600
O	-2.12620300	3.32038100	-0.90963900
H	-2.02514600	3.61285700	-1.82495100

IS2

Pd	-1.38049100	2.52310000	-0.30903200
Pd	1.07805800	2.58007700	-1.22104800
Pd	2.96800200	2.11067800	0.75321500
Pd	2.58363400	-0.24782600	1.79555000
Pd	2.76736900	-2.26150600	0.01120100
Pd	1.10530700	-1.92399500	-1.97514200
Pd	-1.42481200	-2.15635500	-1.32071900
Pd	-2.00601000	0.04856200	0.57772600

Pd	-0.34020500	0.31926200	-1.56234300
Pd	2.25461700	0.16531100	-0.88222000
Pd	0.49153500	1.21264600	1.08550200
Pd	0.20224000	-1.53626000	0.71742900
C	-4.18656400	1.35704800	-0.86948300
C	-5.00930900	2.41648800	-1.22081900
C	-4.96741700	3.62942000	-0.51034500
C	-4.11479600	3.77118900	0.57218400
C	-3.26753500	2.70565600	0.95973600
C	-3.27647800	1.50005300	0.20377300
H	-4.24249200	0.40520600	-1.40152400
H	-5.70243900	2.30278700	-2.05847800
H	-5.62736700	4.45119500	-0.79804000
H	-4.11495000	4.69245200	1.16051800
H	-2.74276500	2.76367900	1.91822800
C	-3.05632600	-0.71959300	2.33929700
C	-2.10857500	-0.30874700	3.33806300
C	-0.91230400	-0.97077500	3.49203700
C	-0.60823300	-2.10710000	2.67180800
C	-1.54539200	-2.52997600	1.69098600
C	-2.80338700	-1.83610700	1.49555600
H	-4.06320000	-0.29406100	2.33743300
H	-2.35641800	0.53031700	3.99359100
H	-0.20557600	-0.66537000	4.26731400
H	0.18370600	-2.78832900	3.00000400
H	-1.46885600	-3.54011600	1.27394300
O	-4.27906400	-3.87056200	0.96482500
H	-4.88914100	-3.85538700	1.70658700
B	-3.97502400	-2.51258100	0.55195500
O	-3.40658800	-2.73132000	-0.86030400
H	-3.59252800	-3.65901400	-1.05615400
O	-5.08372300	-1.60203400	0.53689100
H	-5.77524400	-1.94429100	-0.03669400

TS2

Pd	-1.68427400	2.42003500	-0.09018300
Pd	0.80739200	2.82920500	-0.87030000
Pd	2.67642300	2.23538400	1.11905700
Pd	2.50729700	-0.25565700	1.82180800
Pd	3.01557100	-1.96221400	-0.25400900
Pd	1.33992200	-1.55759500	-2.24210700
Pd	-1.13578400	-2.00776100	-1.62904500
Pd	-1.96274900	-0.20332300	0.44279800
Pd	-0.33872100	0.55526500	-1.64561400

Pd	2.19305500	0.47321100	-0.79591700
Pd	0.29172500	1.13084600	1.18801300
Pd	0.39377400	-1.54796100	0.45795400
C	-4.20043100	1.06382100	-1.04926100
C	-5.20166600	2.00493900	-1.25338000
C	-5.43873100	3.01882500	-0.31107100
C	-4.67748200	3.07950100	0.84637700
C	-3.66510200	2.12494600	1.08980000
C	-3.40597800	1.10755500	0.12744100
H	-4.01236100	0.29240700	-1.80068600
H	-5.80169000	1.96020500	-2.16611800
H	-6.22982600	3.75148900	-0.48633700
H	-4.87884400	3.84586600	1.59953000
H	-3.19831500	2.08575200	2.07856600
C	-2.58461600	-1.43578600	2.89274500
C	-1.83710900	-1.83830200	4.00210400
C	-0.74717200	-2.69968800	3.85188600
C	-0.43313700	-3.19940500	2.58931600
C	-1.17437700	-2.79227500	1.45833400
C	-2.27488900	-1.87785600	1.58802800
H	-3.44300800	-0.77333200	3.03977500
H	-2.10131700	-1.46869600	4.99710200
H	-0.16350200	-3.00527300	4.72360800
H	0.35044800	-3.95333100	2.47527600
H	-1.09042400	-3.40367600	0.54537300
O	-3.94708600	-3.88904000	0.83400200
H	-4.59886200	-3.90465100	1.54158300
B	-3.83784600	-2.60569200	0.31299100
O	-3.18981200	-2.64228400	-0.99815200
H	-3.37195900	-3.52509300	-1.34684100
O	-4.91235000	-1.76246900	0.53795200
H	-4.80006300	-0.89450700	0.13696600

FS2

Pd	2.00157400	-2.04099500	-0.69976800
Pd	-0.27298800	-1.95838400	-2.11772800
Pd	-2.30474800	-2.66045300	-0.44950200
Pd	-2.47234200	-0.67486100	1.49413100
Pd	-3.29117600	1.69347100	0.16420800
Pd	-1.27873400	2.38744300	-1.39538500
Pd	1.20104400	2.65518500	-0.05597400
Pd	2.20759000	0.24465400	1.00699000
Pd	0.61956400	0.40276000	-1.29972900
Pd	-2.05864600	-0.14625200	-1.21432500

Pd	-0.16068000	-1.48389600	0.60548300
Pd	-0.73577000	1.31600800	1.02644900
C	4.69910300	-0.94889300	0.45294600
C	5.65670100	-1.91685700	0.17683000
C	5.37323000	-3.27601900	0.38001800
C	4.13574700	-3.65634100	0.87650600
C	3.15198800	-2.68594200	1.17697900
C	3.42128900	-1.31179900	0.95300200
H	4.94284200	0.10696400	0.29357900
H	6.63740500	-1.61352600	-0.19879600
H	6.13107100	-4.03141600	0.15926500
H	3.91577400	-4.71053700	1.06353600
H	2.25851200	-3.00391600	1.72072900
C	0.22103100	-1.26751100	2.70195600
C	-1.13325600	-1.20874800	3.21147800
C	-1.77879400	0.05141900	3.38967900
C	-1.00786700	1.26697900	3.20968300
C	0.37196900	1.20032700	2.86754200
C	0.95172400	-0.05192500	2.47377800
H	0.77079800	-2.20771200	2.82787000
H	-1.55853400	-2.11075800	3.65961200
H	-2.69159400	0.11410800	3.99146400
H	-1.42103300	2.20484700	3.58957900
H	1.00099100	2.08733600	2.97576700
O	5.30271500	3.88501500	-1.23966300
H	6.16840500	3.68281300	-0.87081100
B	4.29237800	3.37541600	-0.49371700
O	2.99516900	3.60425600	-0.92610600
H	2.93961500	4.04738000	-1.77991500
O	4.51002200	2.66808800	0.63923300
H	3.68778200	2.33502200	1.04347300

IS3

Pd	1.61032200	-2.40255500	-0.31052300
Pd	-0.83072800	-2.39434600	-1.43376700
Pd	-2.73884100	-2.29422400	0.47240200
Pd	-2.54994500	-0.02759200	1.84639800
Pd	-2.91303000	2.10551600	0.31449900
Pd	-1.03729700	2.23272300	-1.58694400
Pd	1.41852800	2.41198600	-0.63351300
Pd	2.24166300	0.06724500	0.57704800
Pd	0.45808100	-0.03167000	-1.42535800
Pd	-2.15107800	-0.11667200	-0.90239500
Pd	-0.29933200	-1.31811100	1.04902300

Pd	-0.38201600	1.35573100	0.94070000
C	4.57427100	-1.51742700	-0.39955100
C	5.32208700	-2.67681000	-0.54582500
C	5.03111800	-3.82063000	0.21770900
C	3.99846700	-3.78755900	1.14038500
C	3.23238900	-2.61071300	1.31424400
C	3.50513700	-1.45056300	0.53130500
H	4.81530100	-0.64050700	-1.00500700
H	6.14435400	-2.70123800	-1.26614900
H	5.62701100	-4.72774000	0.09163900
H	3.78474100	-4.66004000	1.76344000
H	2.54225700	-2.55752000	2.16203600
C	3.68412900	2.43185200	-0.38662100
C	3.21648400	1.76120500	0.78019400
C	3.27303300	2.45677000	2.01461800
C	3.74842900	3.75949300	2.07522400
C	4.17359200	4.42429300	0.91324800
C	4.14841200	3.76603700	-0.30664600
H	3.84290700	1.87466300	-1.31755300
H	2.94406000	1.95896500	2.92988900
H	3.78704300	4.27539300	3.03850900
H	4.53942700	5.45200400	0.97481700
H	4.51648400	4.26080300	-1.20950100

TS3

Pd	-1.52076200	2.30494400	-0.60133400
Pd	1.00416900	2.34243100	-1.45795100
Pd	2.89623000	2.20311700	0.42661200
Pd	2.56320500	-0.00016700	1.86527900
Pd	2.89620300	-2.20320200	0.42586300
Pd	1.00425700	-2.34173000	-1.45891300
Pd	-1.52027300	-2.30451900	-0.60173300
Pd	-2.06339600	0.00016800	0.87635900
Pd	-0.40131600	0.00040900	-1.34854100
Pd	2.21854100	0.00021300	-0.87781700
Pd	0.37592500	1.35887600	1.00400300
Pd	0.37566800	-1.35915200	1.00320600
C	-4.33254800	-1.72173100	1.67823900
C	-4.96994800	-2.94956200	1.52016000
C	-4.98927900	-3.59182000	0.27604300
C	-4.40098600	-2.97956900	-0.82509400
C	-3.75453200	-1.73213300	-0.68327300
C	-3.68840100	-1.10388400	0.59150200
H	-4.32248600	-1.24384300	2.66129300

H	-5.45332700	-3.42015200	2.38061000
H	-5.48713100	-4.55792200	0.16560900
H	-4.46299300	-3.44306100	-1.81346800
H	-3.47629700	-1.17146400	-1.58527900
C	-4.33493100	1.72015800	1.67723400
C	-3.68904200	1.10312000	0.59115200
C	-3.75441600	1.73144800	-0.68357200
C	-4.40205500	2.97817500	-0.82596600
C	-4.99235600	3.58954600	0.27451800
C	-4.97364900	2.94718500	1.51854700
H	-4.32537100	1.24220500	2.66020900
H	-3.47485300	1.17107100	-1.58525000
H	-4.46344000	3.44172300	-1.81429900
H	-5.49135500	4.55497500	0.16360300
H	-5.45865200	3.41703300	2.37843700

FS3

Pd	-1.69615300	2.22307700	-0.74465400
Pd	0.90578500	2.25980300	-1.51350600
Pd	2.83428800	2.22774400	0.32590900
Pd	2.54564300	0.11812900	1.80990800
Pd	2.79521000	-2.27739100	0.34398200
Pd	0.89420900	-2.39676000	-1.41608000
Pd	-1.69204400	-2.23589000	-0.59993000
Pd	-1.92488200	0.03277200	1.01247000
Pd	-0.44149200	-0.02282900	-1.30321700
Pd	2.15135800	-0.06825000	-0.85726800
Pd	0.29591000	1.47640200	1.02886600
Pd	0.34248100	-1.36497700	1.07651200
C	-4.17104500	-1.47044300	1.66892200
C	-4.17828700	-2.86196100	1.66572300
C	-3.97814700	-3.58830600	0.48618000
C	-3.79666600	-2.91053300	-0.73193000
C	-3.69562800	-1.48994100	-0.73895400
C	-3.90462400	-0.72572400	0.48278400
H	-4.40635000	-0.94975300	2.59723900
H	-4.35647300	-3.39353200	2.60303500
H	-4.01642900	-4.67961100	0.49923400
H	-3.85414400	-3.45556900	-1.67808200
H	-3.75494600	-0.96922600	-1.69701600
C	-4.03513000	1.50852900	1.67963300
C	-3.88138300	0.75502400	0.47657000
C	-3.72289800	1.51302800	-0.75694500
C	-3.78878700	2.93550200	-0.74608000

C	-3.86781000	3.61960600	0.48047300
C	-4.00120300	2.90186400	1.67323500
H	-4.22747200	0.99777100	2.62326800
H	-3.86326600	0.99460800	-1.70789400
H	-3.89816500	3.48122800	-1.68731400
H	-3.87600500	4.71158000	0.49209000
H	-4.09147900	3.43841100	2.62012700

IS3'

Pd	-1.78475500	-2.16709200	-0.04249100
Pd	0.63007400	-2.53109700	1.08741500
Pd	2.58184600	-2.41803900	-0.71647000
Pd	2.70691700	-0.01889000	-1.91743500
Pd	3.12738800	1.93153400	-0.15501800
Pd	1.19469200	2.05377100	1.67343900
Pd	-1.21075500	2.53416200	0.61074000
Pd	-2.17545300	0.40874000	-0.77447900
Pd	-0.42258300	-0.05169400	1.22752800
Pd	2.19592900	-0.32349400	0.81331000
Pd	0.28594500	-1.10796000	-1.28410700
Pd	0.58894000	1.43528600	-0.97239300
C	-2.80044700	3.01633700	-2.10856300
C	-3.12631400	4.36455300	-2.08392300
C	-3.58356100	4.97251600	-0.90189500
C	-3.74270300	4.21470100	0.24779200
C	-3.43171800	2.83386000	0.24044000
C	-2.93135900	2.21546800	-0.94447800
H	-2.44215500	2.56276300	-3.03565800
H	-3.01989200	4.96283400	-2.99299900
H	-3.83110200	6.03677600	-0.89631800
H	-4.14117900	4.67003700	1.15856000
H	-3.73792300	2.22071300	1.09545600
C	-3.37824500	-1.53209000	-2.70867900
C	-3.34829300	-1.05030000	-1.37503200
C	-4.00532700	-1.82232500	-0.37001900
C	-4.62264900	-3.05101500	-0.70339400
C	-4.61719200	-3.50224700	-2.01482100
C	-4.00782700	-2.73007800	-3.01789500
H	-2.90220300	-0.95065700	-3.50171500
H	-4.18155400	-1.39881700	0.62483500
H	-5.13111300	-3.62393900	0.07677900
H	-5.10058300	-4.44786200	-2.27179300
H	-4.02122000	-3.08127000	-4.05336000
O	-1.90037400	-1.33602900	5.37885100

H	-2.20969300	-2.18435600	5.71226000
B	-1.72444000	-1.35762900	4.03135100
O	-1.27400700	-0.20405000	3.41597600
H	-1.08858800	0.51681600	4.02725100
O	-1.98130200	-2.46288700	3.29254800
H	-1.78785400	-2.32794700	2.34191200

TS3'

Pd	-1.58191900	-2.22196900	-0.09493500
Pd	0.89737700	-2.51702000	0.91050500
Pd	2.90173700	-2.14020900	-0.79874400
Pd	2.76602200	0.28349500	-1.88016800
Pd	3.04839100	2.19113300	-0.06929800
Pd	1.03401800	2.13643700	1.67521600
Pd	-1.43031300	2.32542300	0.67231600
Pd	-1.95390900	0.33349800	-1.23630000
Pd	-0.43509600	-0.10078200	1.08596900
Pd	2.22086900	-0.15548200	0.80535000
Pd	0.46578900	-1.06634200	-1.37760500
Pd	0.54169000	1.54996200	-0.95576400
C	-4.15252800	2.23348900	-1.78592400
C	-4.77643900	3.42618100	-1.42984000
C	-4.83737500	3.83172900	-0.09072100
C	-4.30596900	3.01492400	0.90095100
C	-3.67170300	1.80090400	0.55719100
C	-3.55996600	1.41450000	-0.80773600
H	-4.10992900	1.94160500	-2.83837900
H	-5.21684200	4.05651400	-2.20716500
H	-5.32469300	4.77248500	0.17556700
H	-4.40384200	3.29081500	1.95448600
H	-3.44104700	1.07895700	1.35137000
C	-4.19349800	-1.21739900	-2.36990100
C	-3.60437500	-0.76588200	-1.17563900
C	-3.75406900	-1.55981700	-0.00294600
C	-4.40822100	-2.81024400	-0.07245900
C	-4.93216000	-3.25889900	-1.28120700
C	-4.84425900	-2.44851600	-2.41911800
H	-4.12418300	-0.60896800	-3.27534900
H	-3.54161600	-1.12495900	0.98163900
H	-4.53268500	-3.40297300	0.83787900
H	-5.43500800	-4.22719400	-1.33489500
H	-5.28020800	-2.78962600	-3.36201800
O	-1.10307200	-1.72375400	5.28480300
H	-1.12695800	-2.62489000	5.62238200

B	-1.19460600	-1.68901300	3.92945200
O	-1.15968300	-0.45283700	3.30844900
H	-0.99558500	0.27516400	3.91786000
O	-1.33124700	-2.81754100	3.19241300
H	-1.33321400	-2.63928400	2.22729700

FS3'

Pd	-1.57500400	-2.35198500	0.23548900
Pd	1.02234300	-2.30970300	1.10737400
Pd	2.88520100	-1.98448600	-0.75204500
Pd	2.66101300	0.28636900	-1.95967700
Pd	2.69046900	2.52585700	-0.26209900
Pd	0.78056600	2.35808400	1.46413000
Pd	-1.79274600	2.18853400	0.59011200
Pd	-1.89641200	0.08082600	-1.27829600
Pd	-0.52295600	-0.03996500	1.13298700
Pd	2.11283300	0.13370800	0.69627200
Pd	0.40752500	-1.19531700	-1.33254800
Pd	0.31987600	1.51904300	-1.11694000
C	-4.67504900	1.56009500	-1.36568000
C	-4.85204000	2.90983100	-1.04765300
C	-4.46892200	3.41271900	0.19177600
C	-3.92659600	2.54208200	1.16004400
C	-3.71827800	1.17367200	0.84017100
C	-4.08078600	0.66298400	-0.45966300
H	-5.02069600	1.19644900	-2.33473100
H	-5.30950100	3.57435100	-1.78438100
H	-4.62661200	4.46546100	0.43585400
H	-3.82330100	2.87771300	2.19604400
H	-3.49168900	0.46576800	1.64173400
C	-3.76662400	-1.17577500	-2.17383100
C	-3.81602500	-0.75700500	-0.81213500
C	-3.66743600	-1.78542000	0.20453900
C	-3.57710400	-3.15545200	-0.16717900
C	-3.53185800	-3.51572000	-1.53731400
C	-3.62015200	-2.53593400	-2.51323900
H	-3.97167400	-0.46189600	-2.97413900
H	-3.94051200	-1.53470900	1.23290200
H	-3.72533200	-3.93159200	0.58960700
H	-3.45512100	-4.56894200	-1.81541700
H	-3.59154400	-2.81385400	-3.56925000
O	1.19801900	-1.28797200	4.40412500
H	1.90150300	-1.92120700	4.22785900
B	0.04243600	-1.57930100	3.75604800

O	-1.03397200	-0.74279300	3.83953600
H	-0.81942100	0.07258100	4.30587100
O	-0.09408300	-2.77203400	3.05751000
H	-0.95736100	-2.82200500	2.60046700