

## **Computed Ligand Effects on the Oxidative Addition of Phenyl Halides to Phosphine Supported Palladium(0) Catalysts**

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Supporting Information 2 – xyz coordinates of optimised geometries

PhBr				H	3.79618300	-1.50050300	1.49445100
Br	0.00000000	0.00000000	1.81483700	H	4.47527500	-2.42879700	0.16102800
C	0.00000000	1.21722300	-0.78781500	H	5.09491600	-0.34110400	-1.03023500
C	0.00000000	1.20781700	-2.18469200	H	5.78122400	-0.31595100	0.59253800
C	0.00000000	0.00000000	-2.88494100	C	-1.04747700	3.40516000	1.21828200
C	0.00000000	-1.20781700	-2.18469200	C	-0.51789800	1.97126900	1.02248400
C	0.00000000	-1.21722300	-0.78781500	C	-0.54796400	1.56771300	-0.46785300
C	0.00000000	0.00000000	-0.10758200	C	-1.97536200	1.72653300	-1.03572300
H	0.00000000	2.15274400	-0.23906400	C	-2.50957800	3.15499000	-0.83767300
H	0.00000000	2.15202500	-2.72241700	C	-2.45982400	3.57380700	0.63893700
H	0.00000000	0.00000000	-3.97110800	H	-0.36602300	4.11249600	0.72220500
H	0.00000000	-2.15202500	-2.72241700	H	-1.04034800	3.66288500	2.28564000
H	0.00000000	-2.15274400	-0.23906400	H	-1.13449700	1.28240200	1.61188500
PhCl				H	0.49920400	1.89933800	1.42478600
Cl	0.00000000	0.00000000	2.26485200	H	0.07704700	2.29894700	-1.00577100
C	0.00000000	1.21625600	-0.17816600	H	-1.99155300	1.46207800	-2.10059900
C	0.00000000	1.20765900	-1.57472200	H	-2.65038500	1.02436000	-0.52716100
C	0.00000000	0.00000000	-2.27543900	H	-1.90292500	3.85235400	-1.43418200
C	0.00000000	-1.20765900	-1.57472200	H	-3.53606300	3.22783200	-1.22034000
C	0.00000000	-1.21625600	-0.17816600	H	-3.16192300	2.95158100	1.21408200
C	0.00000000	0.00000000	0.50398300	H	-2.79727100	4.61201000	0.75371500
H	0.00000000	2.15002200	0.37392100	C	-2.59724900	-3.21307100	-0.77508600
H	0.00000000	2.15170400	-2.11264700	C	-1.95250900	-1.88683900	-1.21422200
H	0.00000000	0.00000000	-3.36164000	C	-0.76045000	-1.50826500	-0.30475300
H	0.00000000	-2.15170400	-2.11264700	C	-1.20559500	-1.45945800	1.17021200
H	0.00000000	-2.15002200	0.37392100	C	-1.83890900	-2.79345500	1.60851200
PhI				C	-3.01703300	-3.17969900	0.70205400
I	0.00000000	0.00000000	1.56344400	H	-1.87677300	-4.03066600	-0.92767400
C	0.00000000	1.21648300	-1.25933700	H	-3.46285700	-3.43802900	-1.41194400
C	0.00000000	1.20727300	-2.65682700	H	-2.71194700	-1.09386800	-1.18229500
C	0.00000000	0.00000000	-3.35725400	H	-1.61929600	-1.95550200	-2.25680400
C	0.00000000	-1.20727300	-2.65682700	H	-0.04019400	-2.33609400	-0.39708400
C	0.00000000	-1.21648300	-1.25933700	H	-0.36080900	-1.21285700	1.82547700
C	0.00000000	0.00000000	-0.57627700	H	-1.94888900	-0.66170300	1.30047700
H	0.00000000	2.15618500	-0.71784600	H	-1.07642100	-3.58577900	1.57091900
H	0.00000000	2.15191100	-3.19408900	H	-2.16804800	-2.72676100	2.65397400
H	0.00000000	0.00000000	-4.44350000	H	-3.82602700	-2.44505500	0.83144100
H	0.00000000	-2.15191100	-3.19408900	H	-3.42775500	-4.15181200	1.00409100
H	0.00000000	-2.15618500	-0.71784600	PCy <sub>3</sub> (conformer C)			
PCy <sub>3</sub> (conformer F)				P	0.15725500	-0.37076600	-0.65429000
P	0.22998500	-0.06783000	-1.04415800	C	0.56198000	1.45523200	-0.28657200
C	4.09520900	1.02987900	0.30980400	C	0.88076700	1.86681000	1.16655100
C	2.73482500	1.07525800	-0.40762800	C	1.10393700	3.38562200	1.28858600
C	1.83691900	-0.12808200	-0.03886300	C	2.20712400	3.87383600	0.33898500
C	2.59826700	-1.44567500	-0.30924000	C	1.90997700	3.46467000	-1.11088600
C	3.95938600	-1.49120200	0.40638100	C	1.67681400	1.95006200	-1.23789600
C	4.83477600	-0.28639400	0.03731400	C	-1.69478500	-0.48736900	-0.26725200
H	3.93798600	1.13996900	1.39325000	C	-2.50754400	0.17185100	-1.40492700
H	4.70795700	1.88521100	-0.00394100	C	-4.01832300	-0.06999000	-1.24093200
H	2.23163400	2.02021700	-0.17186900	C	-4.52260800	0.38425000	0.13690400
H	2.90015900	1.07476100	-1.49536900	C	-3.71380900	-0.26753100	1.26793500
H	1.61582100	-0.07677300	1.03790300	C	-2.20566500	-0.00344300	1.10407500
H	2.00125000	-2.30973800	0.00508800	C	0.95141800	-1.31040200	0.79585500
H	2.75437200	-1.55280400	-1.39294200	C	2.49249800	-1.36359100	0.63864200
				C	2.95625400	-2.29325600	-0.49587300
				C	2.38727800	-3.71109200	-0.33342900

C	0.85676500	-3.68598600	-0.20108700
C	0.41462600	-2.75456100	0.93971000
H	-0.35812900	1.98331500	-0.58153300
H	1.79055200	1.35281800	1.50504600
H	0.07909100	1.55619900	1.84524300
H	0.16519800	3.90946700	1.05372800
H	1.35276400	3.64296000	2.32673300
H	3.16848200	3.43733100	0.64874100
H	2.32055800	4.96312500	0.41359300
H	1.01129400	3.99618600	-1.45864400
H	2.73008100	3.77500400	-1.77160300
H	2.61430300	1.42091700	-1.01095200
H	1.42394100	1.69145400	-2.27304000
H	-1.89359400	-1.56828100	-0.33458900
H	-2.16688900	-0.20970200	-2.37527600
H	-2.32141900	1.25623200	-1.41395500
H	-4.56871200	0.44778600	-2.03742000
H	-4.22480200	-1.14329800	-1.36617200
H	-5.58980400	0.15264400	0.24789400
H	-4.43070400	1.47822000	0.21287600
H	-4.05544900	0.10138900	2.24409400
H	-3.89326200	-1.35306500	1.26362500
H	-1.65365100	-0.48613100	1.92015900
H	-2.02810800	1.07693700	1.19882000
H	0.72046700	-0.77476200	1.72459700
H	2.91419800	-1.72851300	1.58821700
H	2.90702800	-0.35918000	0.48975600
H	2.63204100	-1.88174800	-1.46028400
H	4.05342500	-2.32495500	-0.51794800
H	2.81864800	-4.17461100	0.56700500
H	2.68632300	-4.33968800	-1.18209800
H	0.41581900	-3.34898300	-1.14900400
H	0.47418800	-4.69876400	-0.01879500
H	0.80418100	-3.15815800	1.88744300
H	-0.67710400	-2.76132200	1.03775200

#### PH<sub>3</sub>

P	0.00000000	0.00000000	0.12867600
H	0.00000000	1.19674600	-0.64337800
H	1.03641300	-0.59837300	-0.64337800
H	-1.03641300	-0.59837300	-0.64337800

#### PPh<sub>3</sub>

P	-0.00106600	-0.00107600	-1.20502500
C	1.13203300	4.12871200	0.64834400
C	0.14858600	3.36111000	1.27506900
C	-0.20894800	2.11437700	0.75630200
C	0.40966400	1.61795100	-0.40156500
C	1.38873500	2.40702200	-1.02984200
C	1.75420600	3.64708600	-0.50575300
H	1.40754100	5.09917000	1.05284200
H	-0.34277700	3.73192700	2.17112700
H	-0.97502200	1.52654400	1.25289400
H	1.86403300	2.04736800	-1.93971600
H	2.51569100	4.24149900	-1.00403800
C	-4.14408100	-1.08539600	0.64955800
C	-2.98702700	-1.54654000	1.28030500

C	-1.72882300	-1.23301400	0.76096200
C	-1.60877500	-0.45517300	-0.40127500
C	-2.78210000	-0.00828100	-1.03309200
C	-4.03866100	-0.31198300	-0.50870700
H	-5.12210700	-1.33198200	1.05445700
H	-3.06194000	-2.15197000	2.18015000
H	-0.83677400	-1.59777000	1.26122200
H	-2.70902900	0.57875000	-1.94589000
H	-4.93443500	0.04535600	-1.01007400
C	3.01436200	-3.04093300	0.65128900
C	2.83312000	-1.80813000	1.28086100
C	1.93047600	-0.87753100	0.76075600
C	1.19691500	-1.16489700	-0.40086000
C	1.39942500	-2.40434100	-1.03224200
C	2.29244500	-3.33851500	-0.50689900
H	3.71855400	-3.76286400	1.05651300
H	3.39505100	-1.56809500	2.18002900
H	1.79935200	0.07814900	1.25939200
H	0.85563000	-2.63603800	-1.94532800
H	2.43291400	-4.29306000	-1.00747600

#### SPhos (conformer a)

P	0.83048800	0.11026200	-0.49359600
O	-3.45916100	0.63096200	0.39708800
O	-0.55998500	-3.01347000	-0.16419400
C	-1.23004500	-0.74486300	1.27044800
C	0.05124000	-0.15021600	1.18429700
C	0.69901000	0.19960500	2.38305800
H	1.68626200	0.64911500	2.34776800
C	-1.15661600	-0.58914000	3.70384500
H	-1.62834500	-0.76250800	4.66771300
C	-2.01021300	-1.18727600	0.07068200
C	-1.81515200	-0.94657200	2.53067200
H	-2.80109300	-1.40008800	2.58003200
C	-0.75788100	2.35592800	-1.12102400
H	-1.09550600	1.72594000	-1.95335500
H	-1.42129700	2.13353600	-0.27459400
C	-1.66314600	-2.35877600	-0.62958100
C	-3.16168300	-0.48646500	-0.33596700
C	-3.92936200	-0.91992800	-1.42583800
H	-4.80852500	-0.37332900	-1.74450300
C	0.69326000	1.98975300	-0.74253100
H	1.31239600	2.16119700	-1.63759600
C	-4.61337300	1.37803700	0.05377300
H	-4.54428800	1.78801800	-0.96250200
H	-4.65970300	2.19991600	0.77090400
H	-5.52642300	0.77352800	0.13633400
C	2.66954200	-0.11668700	-0.11223400
H	2.98298100	0.54713400	0.70631000
C	0.11213300	-0.01485600	3.62944800
H	0.64353400	0.26719900	4.53506400
C	-3.54673500	-2.07423500	-2.10480100
H	-4.13810900	-2.41519200	-2.95049400
C	1.21027300	2.91436300	0.37509500
H	2.25912700	2.69128500	0.60929800
H	0.63643000	2.72869700	1.29267800
C	-2.42335700	-2.80234700	-1.72008300

H	-2.15137600	-3.70012300	-2.26123900
C	2.94478800	-1.57406200	0.31792400
H	2.36718200	-1.82008500	1.21580100
H	2.59046300	-2.24987800	-0.47439100
C	-0.12261600	-4.17380300	-0.85016400
H	-0.87901100	-4.96967000	-0.82208700
H	0.77265400	-4.51010800	-0.32387300
H	0.13173400	-3.95311800	-1.89487400
C	-0.36818000	4.75864600	-0.38217900
H	-1.00811700	4.64960700	0.50612100
H	-0.43362900	5.81084800	-0.68894000
C	1.07686000	4.40028900	-0.00741700
H	1.42406000	5.03122900	0.82171100
H	1.73650200	4.61646400	-0.86130100
C	3.52173200	0.23584100	-1.35101400
H	3.37525900	1.28476600	-1.63550200
H	3.18260000	-0.36947600	-2.20470800
C	-0.89182500	3.84166900	-1.49687200
H	-0.32427100	4.03532300	-2.41969900
H	-1.94068500	4.07709300	-1.72258000
C	4.44108000	-1.82732600	0.56600000
H	4.77369900	-1.22616800	1.42549100
H	4.60065300	-2.87805000	0.84235600
C	5.28682000	-1.46462300	-0.66281000
H	6.35438000	-1.60682500	-0.44997000
H	5.03776900	-2.14916300	-1.48754500
C	5.01983100	-0.01993400	-1.10860500
H	5.58803400	0.21041300	-2.01950200
H	5.38221600	0.67049000	-0.33228200

SPhos (conformer c)

P	-0.85543000	0.78911500	-1.49062900
O	2.91465300	-1.26329400	-1.13644900
O	-0.35174800	-1.60302500	2.20619900
C	-0.52424900	-1.05298000	-1.34017400
C	0.30652700	-1.83008100	-0.49147100
C	1.26961400	-1.30772900	0.53555000
C	2.61166100	-1.06328000	0.18135600
C	3.55448800	-0.65334900	1.13493700
H	4.58037900	-0.44931300	0.85397000
C	3.15777100	-0.51832900	2.46344500
H	3.88234900	-0.19511300	3.20605300
C	1.85493900	-0.80772400	2.86108300
H	1.57874800	-0.72326700	3.90486700
C	0.92430000	-1.22716300	1.89852000
C	0.30185400	-3.23039000	-0.62413200
H	0.94759000	-3.80759100	0.03242300
C	-0.48987800	-3.88884700	-1.55945700
H	-0.46709100	-4.97338300	-1.62743700
C	-1.28839800	-3.13551200	-2.41694600
H	-1.89868200	-3.61825500	-3.17595500
C	-1.28198400	-1.74748700	-2.30974200
H	-1.87722900	-1.16875000	-3.01125000
C	-0.75721400	-1.58454600	3.56447400
H	-0.13801700	-2.25149500	4.17863700
H	-1.78864500	-1.94149500	3.57125400
H	-0.72338200	-0.57109500	3.98540900

C	4.26243200	-1.11617700	-1.55408800
H	4.61749900	-0.08564900	-1.42418600
H	4.27181100	-1.36826600	-2.61601900
H	4.92810500	-1.79997900	-1.01138500
C	0.45751100	1.75912300	-0.53773700
H	0.74704700	1.23928200	0.38209400
C	-0.05457200	3.16687300	-0.15651300
H	-0.42559900	3.67864900	-1.05787000
H	-0.89965400	3.10039000	0.53715800
C	1.05207700	4.01994000	0.48993200
H	0.65935900	5.01905600	0.72137000
H	1.33700700	3.56618200	1.45071200
C	2.29497200	4.12880300	-0.40365200
H	2.03862300	4.69170300	-1.31354800
H	3.08168700	4.69998100	0.10667800
C	2.80838300	2.73744900	-0.79921800
H	3.18030900	2.21776100	0.09537700
H	3.65968400	2.82948600	-1.48782000
C	1.69802700	1.89746800	-1.45137200
H	2.07878900	0.90886900	-1.72444000
H	1.38656600	2.38038400	-2.38920900
C	-2.43256000	1.03075600	-0.45957000
H	-2.56349200	2.12308900	-0.49844000
C	-3.65939800	0.41922200	-1.16958100
H	-3.69992800	0.75932700	-2.21222200
H	-3.55804800	-0.67421300	-1.19735800
C	-4.96822000	0.78116700	-0.44657100
H	-5.12951600	1.86775900	-0.51151400
H	-5.81869600	0.30894400	-0.95593500
C	-4.93231700	0.36216600	1.03035900
H	-4.88837000	-0.73547400	1.09215400
H	-5.85687100	0.66813000	1.53736600
C	-3.70866700	0.95569800	1.74294200
H	-3.81340100	2.05045200	1.78838200
H	-3.66738600	0.60551500	2.78358100
C	-2.39899900	0.59867500	1.01563700
H	-2.23098300	-0.48289300	1.06643100
H	-1.55097000	1.06262200	1.53402700

1<sub>Cy</sub> [Pd(PCy<sub>3</sub>)] (conformer F)

Pd	-0.61911200	-0.26538000	2.46435900
P	-0.13133100	-0.03837600	0.30135800
C	-3.79581100	1.25025800	-1.40575000
C	-2.55121800	1.20427300	-0.50317300
C	-1.63709800	0.00542900	-0.83995400
C	-2.44670900	-1.30823100	-0.77410300
C	-3.69295500	-1.26022800	-1.67496500
C	-4.59068100	-0.06096100	-1.34283400
H	-3.48546100	1.43688600	-2.44496700
H	-4.43045100	2.09704000	-1.11386400
H	-2.00315100	2.14929800	-0.59393400
H	-2.86003800	1.12313900	0.54872600
H	-1.27250100	0.12890000	-1.87035700
H	-1.82603200	-2.16253400	-1.06847400
H	-2.74869900	-1.48460900	0.26810700
H	-3.37769900	-1.19610600	-2.72731500
H	-4.25419000	-2.19825200	-1.57494000

H	-5.00304700	-0.18619000	-0.33078900
H	-5.44707300	-0.02255300	-2.02830500
C	1.40041500	3.49363900	-1.64119300
C	0.86570400	2.05169600	-1.55169200
C	0.73538200	1.60618600	-0.07901000
C	2.09357000	1.73918500	0.64223100
C	2.63236400	3.17731900	0.55111500
C	2.73903100	3.65126600	-0.90587300
H	0.66114500	4.17904000	-1.20058300
H	1.50633900	3.78463300	-2.69447000
H	1.55212100	1.38497500	-2.08702500
H	-0.09780800	1.99212300	-2.06998800
H	0.05306100	2.31420300	0.41464600
H	1.98962800	1.43483200	1.69080000
H	2.82373100	1.05870100	0.18267000
H	1.95904800	3.84876600	1.10427000
H	3.61059100	3.23978400	1.04511800
H	3.50708700	3.05740300	-1.42390200
H	3.07389800	4.69577500	-0.94464700
C	2.67131300	-3.22213900	0.10345000
C	2.04551700	-1.88850300	0.54660700
C	0.87815500	-1.48679300	-0.38095300
C	1.35636800	-1.41631000	-1.84635300
C	1.97215000	-2.75707800	-2.28937600
C	3.12214300	-3.18111200	-1.36435900
H	1.93178300	-4.02651000	0.23300700
H	3.51897400	-3.47016300	0.75518600
H	2.81828800	-1.10847000	0.53383000
H	1.68470600	-1.95722200	1.57985600
H	0.14413600	-2.30348700	-0.31430800
H	0.53358900	-1.14508900	-2.51906500
H	2.11851600	-0.63266500	-1.94630000
H	1.19235000	-3.53298900	-2.28081100
H	2.32419000	-2.67960800	-3.32637200
H	3.95068700	-2.46452300	-1.46856000
H	3.51556400	-4.15878800	-1.67103200

# **1<sub>Cy</sub> [Pd(PCy<sub>3</sub>)] (conformer C)**

Pd	-1.27736100	-0.54783700	1.88357800
P	-0.08539100	-0.09793800	0.04718200
C	0.72657200	1.62319200	0.02551400
C	1.03571400	2.24409400	-1.35500100
C	1.81532900	3.56445800	-1.20869900
C	1.06373600	4.57229200	-0.32786500
C	0.71789900	3.96299700	1.03841400
C	-0.04896200	2.63739600	0.89581900
C	1.37072200	-1.29269800	-0.15593300
C	2.20814900	-1.37623700	1.13834500
C	3.27093300	-2.48483900	1.04963500
C	4.17504200	-2.31313500	-0.17966800
C	3.34636900	-2.21338800	-1.46824300
C	2.29241200	-1.09382900	-1.37719300
C	-0.97935800	-0.21730100	-1.62148100
C	-2.22590300	0.70267700	-1.69971800
C	-3.46162600	0.14682900	-0.97354900
C	-3.80692900	-1.27298100	-1.44386800
C	-2.59901700	-2.20785400	-1.28765200

C	-1.37227000	-1.65827800	-2.03264700
H	1.68721500	1.43978800	0.53123400
H	0.09621700	2.44947700	-1.88516800
H	1.60404300	1.55152600	-1.98391200
H	2.80001900	3.35546400	-0.76466000
H	2.00609400	3.99200700	-2.20180900
H	0.13491000	4.87181400	-0.83581300
H	1.65909400	5.48563100	-0.20122600
H	1.64684900	3.78228600	1.60001300
H	0.12744200	4.67142200	1.63362200
H	-1.03202700	2.83295400	0.44312900
H	-0.24928000	2.19917200	1.88038400
H	0.86905600	-2.26511400	-0.26588100
H	1.54349000	-1.54837400	1.99335500
H	2.70982500	-0.41380000	1.31920600
H	3.87298000	-2.49636700	1.96734700
H	2.76619000	-3.46086900	0.99487300
H	4.88842400	-3.14436500	-0.24867700
H	4.77282000	-1.39659000	-0.06398100
H	4.00092500	-2.03734700	-2.33180300
H	2.83952500	-3.17258800	-1.65063800
H	1.71227200	-1.05785400	-2.30707500
H	2.81281300	-0.13034500	-1.29083800
H	-0.25523200	0.14561700	-2.36095800
H	-2.47073500	0.82697100	-2.76597700
H	-1.99432500	1.70544700	-1.32246900
H	-3.26457000	0.12803800	0.10820400
H	-4.31128900	0.82315600	-1.13566000
H	-4.11353600	-1.24646300	-2.50116700
H	-4.66404800	-1.66089700	-0.87866500
H	-2.36287200	-2.31523300	-0.21976000
H	-2.83715000	-3.20973800	-1.66842100
H	-1.60436600	-1.63128100	-3.10876400
H	-0.52418800	-2.34432400	-1.92760800

# **1<sub>H</sub> [Pd(PH<sub>3</sub>)]**

Pd	0.00000000	0.00000000	0.65047900
P	0.00000000	0.00000000	-1.54122900
H	0.00000000	1.21878600	-2.26786900
H	1.05549900	-0.60939300	-2.26786900
H	-1.05549900	-0.60939300	-2.26786900

# **1<sub>Ph</sub> [Pd(PPh<sub>3</sub>)]**

Pd	-0.00591600	-0.00640000	2.57430300
P	-0.00109700	-0.00159900	0.35917700
C	3.16354400	-2.85358000	-1.53612700
C	1.92209200	-2.70907100	-2.15717800
C	0.95502700	-1.86203500	-1.60959500
C	1.21840000	-1.15247000	-0.42803000
C	2.46702300	-1.31416100	0.19465800
C	3.43497300	-2.15156400	-0.35891000
H	3.91316900	-3.51500200	-1.96246600
H	1.70158100	-3.25692700	-3.06976200
H	-0.00680600	-1.75914800	-2.10246900
H	2.66797600	-0.78663800	1.12401900
H	4.39629300	-2.26524300	0.13528300
C	-4.05373500	-1.30008100	-1.54803100

C	-3.30350800	-0.29771900	-2.16456500
C	-2.08622200	0.11086400	-1.61335800
C	-1.60714400	-0.47686800	-0.43265000
C	-2.37592900	-1.47678300	0.18546600
C	-3.58531800	-1.89106700	-0.37175100
H	-5.00151100	-1.61445200	-1.97706000
H	-3.66437500	0.17109500	-3.07647500
H	-1.51365300	0.89269700	-2.10281900
H	-2.02292500	-1.91860100	1.11423400
H	-4.16763000	-2.66645900	0.11914300
C	0.90144100	4.16689900	-1.52667500
C	1.40171100	3.01989200	-2.14439100
C	1.14699500	1.75854300	-1.59965000
C	0.39123000	1.63099400	-0.42416600
C	-0.09774800	2.79295900	0.19536500
C	0.14833600	4.05017800	-0.35546500
H	1.10309100	5.14708900	-1.95063000
H	1.99378200	3.10319100	-3.05219200
H	1.54308400	0.87474400	-2.09033700
H	-0.66283000	2.70316700	1.12003600
H	-0.23767300	4.93929500	0.13621300

# **I<sub>SP</sub> [Pd(SPhos)] (conformer a)**

Pd	-0.31526100	-1.22143700	-1.46670500
P	0.89769500	0.26068900	-0.20643500
O	-3.45573800	1.07219300	0.64350900
O	-0.95066000	-2.87215900	0.92048400
C	-1.22403600	-0.21151400	1.70905800
C	0.09488000	0.27813500	1.49309800
C	0.79576100	0.79290800	2.59820200
H	1.80571000	1.16718900	2.46794300
C	-1.06415800	0.38050700	4.07287500
H	-1.51819500	0.41615800	5.05976700
C	-2.05045100	-0.80352300	0.61300400
C	-1.77709400	-0.14054100	2.99597600
H	-2.78665300	-0.51217700	3.14432700
C	-0.58369300	2.49916500	-1.09564000
H	-1.01466800	1.77927200	-1.80246100
H	-1.20800300	2.46089000	-0.19251400
C	-1.67637700	-2.07623500	0.06691000
C	-3.14046600	-0.12754000	0.05869900
C	-3.82060700	-0.63528600	-1.07282200
H	-4.66193300	-0.10397100	-1.49969900
C	0.85781500	2.07638300	-0.74255500
H	1.43207800	2.06199700	-1.68139100
C	-4.54818600	1.81304600	0.12758700
H	-4.38402000	2.10632100	-0.91767100
H	-4.61696200	2.71014200	0.74618800
H	-5.48954800	1.25210800	0.20039500
C	2.71652500	-0.05692500	0.17019900
H	3.06709800	0.66969100	0.91614300
C	0.23386600	0.84581700	3.87366300
H	0.80956400	1.25065800	4.70208300
C	-3.36795800	-1.80126500	-1.66962500
H	-3.87338200	-2.18104100	-2.55377300
C	1.50919000	3.10577800	0.20101200
H	2.55038800	2.83400800	0.41653800

H	0.97600600	3.10736400	1.16052800
C	-2.29035400	-2.54388800	-1.13278600
H	-2.09351800	-3.54288900	-1.50432500
C	2.90953100	-1.47451900	0.74813500
H	2.33065300	-1.58919000	1.67178300
H	2.50278400	-2.20232800	0.03150200
C	-0.45978800	-4.11121300	0.43185900
H	-1.27774400	-4.80296100	0.19016200
H	0.13841400	-4.53477800	1.24065700
H	0.17174200	-3.96241400	-0.45421500
C	0.03284400	4.94383300	-0.75457400
H	-0.55959200	5.02583600	0.16886200
H	0.03185900	5.93930800	-1.21732500
C	1.46574400	4.52397300	-0.39833300
H	1.90936300	5.23792900	0.30808300
H	2.08861600	4.55398100	-1.30489500
C	3.57211100	0.12610600	-1.10230900
H	3.48442000	1.15071000	-1.48375300
H	3.18500400	-0.53640000	-1.88988500
C	-0.62633800	3.91802400	-1.68777200
H	-0.10352100	3.92170100	-2.65614000
H	-1.66620000	4.20371200	-1.89444700
C	4.39229000	-1.78811100	1.00867900
H	4.77242100	-1.12455400	1.79995400
H	4.49255000	-2.81340800	1.38809900
C	5.23893900	-1.60216800	-0.25876700
H	6.29873700	-1.78928500	-0.04265700
H	4.93487200	-2.34745700	-1.00877900
C	5.05465200	-0.19503000	-0.84322200
H	5.62247200	-0.09131400	-1.77694200
H	5.46911700	0.54518600	-0.14246000

# **I<sub>SP</sub> [Pd(SPhos)] (conformer c)**

Pd	-2.53256800	-2.03862100	0.95951900
P	-1.11243400	-0.52184100	0.12987700
O	2.82290100	-1.00112900	1.74166600
O	1.63710700	2.96112900	-0.45486600
C	-0.24578200	0.49518400	1.45674200
C	1.04626000	1.08141700	1.51251400
C	2.16558000	0.89601200	0.52834700
C	3.08010100	-0.16430700	0.69353300
C	4.18138400	-0.31544300	-0.16140300
H	4.86907400	-1.14348500	-0.04283400
C	4.39342000	0.62658500	-1.16551200
H	5.24136400	0.51030100	-1.83505400
C	3.55248500	1.72661500	-1.31284300
H	3.75819100	2.46376500	-2.07918600
C	2.46131000	1.87239200	-0.44349300
C	1.38127200	1.88240300	2.61985300
H	2.37598400	2.31865400	2.64969400
C	0.49631800	2.12018700	3.66582600
H	0.79602500	2.74598000	4.50242200
C	-0.76345400	1.52709400	3.63174900
H	-1.47010600	1.67392000	4.44441700
C	-1.10975400	0.72295900	2.54989900
H	-2.07984900	0.23207600	2.54482200
C	1.90151900	4.00649000	-1.37621000

H	2.90157400	4.43280800	-1.22425300	H	3.06050900	0.45945700	-2.99418500
H	1.14872100	4.77201000	-1.17986300	H	1.51138800	1.24056500	-2.69905400
H	1.80774400	3.66562700	-2.41555100	H	4.14031000	2.61813200	-3.50145200
C	3.74575500	-2.04198100	2.02534900	H	2.73714100	2.37535600	-4.53779300
H	3.80454600	-2.76676800	1.20334600	H	1.37126700	3.87290600	-3.09855000
H	3.36294600	-2.54018800	2.91755600	H	2.82536200	4.71995500	-3.62349100
H	4.74768600	-1.64328300	2.23073800	C	4.83267200	1.54979600	3.19499700
C	0.13940900	-1.27519700	-1.06126000	C	4.51267800	1.05201300	1.77254700
H	0.92858900	-0.54041200	-1.26024900	C	3.03430200	0.62363400	1.65831600
C	-0.52771700	-1.65495200	-2.40282000	C	2.70261200	-0.45147900	2.71589300
H	-1.37420800	-2.32853800	-2.20276600	C	3.02392100	0.04406400	4.13600000
H	-0.93804900	-0.77144300	-2.90325100	C	4.48653100	0.49665100	4.25750800
C	0.46685200	-2.34709700	-3.35269500	H	4.25865100	2.46727700	3.39368300
H	-0.04773100	-2.62376700	-4.28233300	H	5.89337300	1.82549000	3.26231300
H	1.25425100	-1.63123300	-3.63238100	H	5.16860700	0.20488300	1.53810200
C	1.11275300	-3.58194800	-2.71108500	H	4.75074900	1.84120500	1.04993800
H	0.34126200	-4.34768400	-2.54249100	H	2.42333900	1.50278600	1.91446400
H	1.85028900	-4.02378200	-3.39394000	H	1.64658600	-0.73743700	2.63791600
C	1.76742100	-3.22081200	-1.37086200	H	3.29255400	-1.35712100	2.51853900
H	2.62110700	-2.55128000	-1.55127800	H	2.36073700	0.88648800	4.38281700
H	2.17024200	-4.12306600	-0.89050600	H	2.80843500	-0.74748400	4.86554400
C	0.76718800	-2.53510300	-0.42482800	H	5.14548000	-0.37513200	4.12803300
H	1.24890300	-2.28122500	0.52321900	H	4.68411600	0.89083500	5.26276000
H	-0.04581500	-3.23468500	-0.18213400	C	3.22043800	-3.85654100	-0.94896500
C	-2.02173100	0.77475500	-0.90988500	C	2.70907100	-2.64904100	-0.14445100
H	-2.50479800	0.15267900	-1.67668900	C	3.20729700	-1.32271400	-0.75910900
C	-3.15297300	1.46262200	-0.11875900	C	4.74710400	-1.31726600	-0.83862400
H	-3.79240300	0.70169900	0.34541600	C	5.25982600	-2.52019600	-1.65247200
H	-2.72051400	2.05770900	0.69715500	C	4.75178000	-3.84969600	-1.07461900
C	-3.99000100	2.38248400	-1.02442300	H	2.77406000	-3.83332500	-1.95456100
H	-4.51611100	1.77124500	-1.77302700	H	2.88201600	-4.78917100	-0.47889300
H	-4.76515700	2.88267200	-0.42939400	H	3.06364100	-2.73619300	0.89145200
C	-3.11578800	3.42034200	-1.74307700	H	1.61313900	-2.64685100	-0.10258700
H	-2.68270000	4.10447600	-0.99820500	H	2.82982900	-1.31247800	-1.79320800
H	-3.72609400	4.03553300	-2.41715900	H	5.11839900	-0.38464200	-1.28048800
C	-1.98012900	2.73965300	-2.51983700	H	5.16585200	-1.37650000	0.17401800
H	-2.40849200	2.14359900	-3.33986100	H	4.91947600	-2.42242100	-2.69417900
H	-1.33323200	3.49314400	-2.98951000	H	6.35741400	-2.51142500	-1.68110000
C	-1.14082600	1.82416000	-1.60913500	H	5.19604000	-4.00159100	-0.07928000
H	-0.63144700	2.42861700	-0.85161800	H	5.08842900	-4.68869800	-1.69727600
H	-0.35243000	1.34139400	-2.19979800	C	-3.01867900	-4.00446200	-1.78280500
<b>2<sub>Cy</sub> [Pd(PCy<sub>3</sub>)<sub>2</sub>] (conformer F)</b>				C	-2.51790700	-2.92815200	-0.80375400
Pd	0.00539400	-0.02265700	-0.01152200	C	-3.00334000	-1.51503700	-1.19622100
P	2.31959800	0.18933900	-0.04519500	C	-2.60802200	-1.20763500	-2.65779500
P	-2.31416200	-0.20220600	-0.02389500	C	-3.11125200	-2.28617800	-3.63201300
C	2.83764900	4.12570100	-1.52963600	C	-2.62353600	-3.68404100	-3.23078100
C	2.39579400	2.95152600	-0.64001300	H	-4.11477000	-4.07613500	-1.71505300
C	2.96035500	1.59867200	-1.13062300	H	-2.62391100	-4.98482900	-1.48553400
C	2.59879200	1.37915900	-2.61623200	H	-1.41869600	-2.93018100	-0.78548400
C	3.04132800	2.55891200	-3.49900300	H	-2.84820600	-3.18193700	0.21038100
C	2.46679400	3.89074500	-2.99988800	H	-4.10066000	-1.50008600	-1.12837200
H	3.92725000	4.25691100	-1.44745300	H	-3.00101800	-0.23207200	-2.96778700
H	2.38384300	5.05595200	-1.16353900	H	-1.51252300	-1.13664900	-2.71680000
H	2.70453100	3.14494100	0.39423700	H	-4.21168000	-2.27751200	-3.64791500
H	1.29826500	2.88845000	-0.63071300	H	-2.78310600	-2.04410900	-4.65132800
H	4.05654200	1.63361800	-1.04908100	H	-1.52837500	-3.72676200	-3.32563100
				H	-3.02770800	-4.44188400	-3.91446600

C	-3.18635400	3.91575800	-0.54825200	C	-2.27756100	1.56124300	-2.37607300
C	-2.73730700	2.62667500	0.16171800	C	-3.18194600	0.59609500	-1.57585500
C	-3.16386100	1.37695400	-0.63774100	C	-4.60044900	1.19264800	-1.44297400
C	-4.69118400	1.37667400	-0.85088300	C	-5.20392400	1.51173300	-2.82354400
C	-5.14469900	2.66335800	-1.56656800	C	-4.30110000	2.45191400	-3.63487800
C	-4.70113000	3.92177400	-0.80529600	H	-2.90258200	0.97042900	-4.36199500
H	-2.65473000	4.00220800	-1.50760400	H	-2.22961700	2.59619400	-4.28505900
H	-2.89840200	4.79115500	0.04849700	H	-2.14544500	2.49486200	-1.80978900
H	-3.19038000	2.60004000	1.16184700	H	-1.27653900	1.12706100	-2.48048700
H	-1.64985600	2.62222100	0.30509700	H	-3.26602200	-0.32597000	-2.17193900
H	-2.69675700	1.47949300	-1.62929000	H	-5.26712900	0.51552800	-0.89907700
H	-5.01164200	0.50159600	-1.42850100	H	-4.55447600	2.12115200	-0.85826800
H	-5.19988000	1.31609200	0.11970700	H	-5.34551800	0.57347200	-3.38087200
H	-4.71691100	2.68206600	-2.58009300	H	-6.20150300	1.95332800	-2.69901100
H	-6.23579800	2.65678200	-1.68944500	H	-4.26082700	3.43201400	-3.13615800
H	-5.22976900	3.96340500	0.15885100	H	-4.72946700	2.62590500	-4.63048800
H	-4.99214400	4.82360100	-1.35942800	C	-2.81240200	-4.18617100	-0.42263800
C	-4.87953100	-1.64308700	3.13120900	C	-2.41695100	-2.73551900	-0.74943600
C	-4.54131600	-1.01243400	1.76662700	C	-3.02264600	-1.74377000	0.26759500
C	-3.02983900	-0.72796700	1.65124200	C	-4.55430800	-1.90838400	0.32557500
C	-2.57080300	0.18691300	2.80747200	C	-4.94633300	-3.35807200	0.66718800
C	-2.90095900	-0.44209100	4.17223500	C	-4.33601500	-4.35603300	-0.32778900
C	-4.39728800	-0.76689800	4.29709200	H	-2.35557900	-4.47380900	0.53609900
H	-4.40279500	-2.63233500	3.19933600	H	-2.39997800	-4.86482000	-1.18062100
H	-5.96170400	-1.81372400	3.20521500	H	-2.77003200	-2.49046500	-1.76256400
H	-5.10393400	-0.07541000	1.66453100	H	-1.32567100	-2.62682400	-0.76221600
H	-4.88457600	-1.67360600	0.96234800	H	-2.61746300	-2.02045000	1.25196100
H	-2.50538700	-1.68463000	1.80008600	H	-4.99588300	-1.22282200	1.05932200
H	-1.49505900	0.38241600	2.72367000	H	-4.98821300	-1.64930300	-0.65000000
H	-3.07870900	1.15845300	2.73835800	H	-4.59643200	-3.59638700	1.68262700
H	-2.31573900	-1.36580000	4.29457100	H	-6.03990200	-3.45518800	0.68322000
H	-2.59044900	0.23355700	4.97995300	H	-4.78072200	-4.19165500	-1.32082900
H	-4.96995900	0.17281700	4.30216700	H	-4.58908300	-5.38448400	-0.03933700
H	-4.60337600	-1.26211900	5.25488200	C	3.20712300	-3.29987000	2.51346800
<b>2<sub>Cy</sub> [Pd(PCy<sub>3</sub>)<sub>2</sub>] (conformer C)</b>				C	2.61861600	-2.45920000	1.36794600
Pd	-0.00015800	-0.00064600	-0.01974300	C	3.11534300	-0.99642800	1.40661600
P	-2.32677800	-0.00254700	0.01293900	C	2.80554100	-0.37826500	2.78760200
P	2.32644900	0.00233400	0.01237700	C	3.38456000	-1.21991300	3.93860800
C	-3.20549600	3.30137800	2.51318400	C	2.90290200	-2.67573900	3.88209200
C	-2.61991600	2.46056400	1.36622800	H	4.29713200	-3.38114400	2.38542600
C	-3.11459400	0.99716600	1.40724400	H	2.81046600	-4.32234800	2.46292800
C	-2.80126400	0.38030100	2.78806100	H	1.52171000	-2.45475100	1.43836700
C	-3.37826100	1.22223000	3.93982500	H	2.86265300	-2.92659400	0.40682000
C	-2.89731900	2.67816500	3.88132300	H	4.20571800	-0.99506900	1.26667300
H	-4.29588900	3.38217000	2.38814600	H	3.20414900	0.64075000	2.85426700
H	-2.80941300	4.32399800	2.46098800	H	1.71469500	-0.29808400	2.90112800
H	-2.86861100	2.92699500	0.40585400	H	4.48352700	-1.20079500	3.88369800
H	-1.52275400	2.45772300	1.43254000	H	3.11340600	-0.76437500	4.90000600
H	-4.20522100	0.99420100	1.26926800	H	1.81747600	-2.70543900	4.05878400
H	-3.19887500	-0.63899700	2.85633200	H	3.36804100	-3.26341100	4.68414900
H	-1.71009500	0.30105400	2.89913800	C	2.80857300	4.18615700	-0.42502700
H	-4.47733700	1.20259900	3.88731600	C	2.41391700	2.73510300	-0.75105800
H	-3.10479800	0.76736100	4.90088500	C	3.02140500	1.74409000	0.26562400
H	-1.81143600	2.70835800	4.05512300	C	4.55298500	1.90993400	0.32169700
H	-3.36055200	3.26613300	4.68426400	C	4.94408700	3.35989600	0.66317500
C	-2.87800700	1.88735200	-3.75364500	C	4.33212800	4.35731800	-0.33134600
				H	2.35222000	4.47375600	0.53394600



H	2.39506600	4.86424200	-1.18292500	C	-3.09833800	1.64398300	0.32956300
H	2.76616200	2.48998000	-1.76446900	C	-2.45861200	2.50181000	1.24020900
H	1.32271100	2.62559100	-0.76273000	C	-3.00586200	3.74744900	1.54812300
H	2.61714200	2.02074800	1.25038300	H	-4.61348600	5.13706000	1.16919200
H	4.99620400	1.22445700	1.05453600	H	-5.74812700	3.64292600	-0.46321600
H	4.98570500	1.65171600	-0.65462900	H	-4.79116500	1.42950300	-0.99755400
H	4.59472400	3.59786700	1.67888100	H	-1.52198700	2.18868600	1.69599900
H	6.03758400	3.45795700	0.67839700	H	-2.49920000	4.39888500	2.25556400
H	4.77621500	4.19327900	-1.32471700	C	-4.17958400	-1.27906600	-4.07209900
H	4.58452200	5.38600000	-0.04313000	C	-4.83052300	-1.63111400	-2.88855500
C	2.87753100	-1.89099200	-3.75235100	C	-4.29304000	-1.26073700	-1.65309100
C	2.27795700	-1.56479500	-2.37442400	C	-3.09331300	-0.53656100	-1.58733500
C	3.18153800	-0.59739000	-1.57605900	C	-2.43982900	-0.19834400	-2.78426300
C	4.60054300	-1.19277100	-1.44328400	C	-2.98299400	-0.55983300	-4.01732900
C	5.20369700	-1.51207600	-2.82396000	H	-4.59828900	-1.57006200	-5.03205600
C	4.30147100	-2.45363100	-3.63439600	H	-5.75823000	-2.19668700	-2.92388600
H	2.90032500	-0.97444500	-4.36133100	H	-4.80664200	-1.54294200	-0.73881800
H	2.22962700	-2.60107100	-4.28270500	H	-1.49538300	0.33887800	-2.73927500
H	2.14888300	-2.49820800	-1.80706700	H	-2.46546600	-0.29035200	-4.93440500
H	1.27589200	-1.13283200	-2.47793400	C	4.17969300	1.10604700	4.12268200
H	3.26435900	0.32399100	-2.17338700	C	4.82536500	1.51802100	2.95572900
H	5.26709100	-0.51515800	-0.89986100	C	4.28833600	1.20140400	1.70513400
H	4.55525800	-2.12110500	-0.85820300	C	3.09424300	0.47148900	1.60772900
H	5.34410800	-0.57398800	-3.38187400	C	2.44600400	0.07283400	2.78876700
H	6.20177400	-1.95260400	-2.69963600	C	2.98875500	0.38070600	4.03639700
H	4.26278700	-3.43363300	-3.13537000	H	4.59792400	1.35539100	5.09450600
H	4.72938600	-2.62735800	-4.63024800	H	5.74864800	2.08873700	3.01575300
<b>2<sub>H</sub> [Pd(PH<sub>3</sub>)<sub>2</sub>]</b>				H	4.79800100	1.53026000	0.80438600
Pd	0.00000100	-0.00115000	-0.00048600	H	1.50584600	-0.46922200	2.72051500
P	2.28418200	0.00126000	0.00050200	H	2.47504200	0.06482700	4.94070100
H	3.01282000	-1.18379500	-0.27385400	C	4.16962800	3.03101100	-3.01518600
H	3.00956600	0.83417500	-0.88828300	C	2.97712500	3.31170700	-2.34356000
H	3.00905700	0.35721700	1.16571800	C	2.43813500	2.38053000	-1.45570100
P	-2.28418300	0.00124900	0.00052100	C	3.09202600	1.16105900	-1.21235800
H	-3.00823100	1.20095600	0.21737300	C	4.28686100	0.88710000	-1.89457300
H	-3.01205400	-0.40948400	-1.14453100	C	4.81997100	1.81643100	-2.79182700
H	-3.01117500	-0.78379800	0.93057700	H	4.58497600	3.75174300	-3.71484100
<b>2<sub>Ph</sub> [Pd(PPh<sub>3</sub>)<sub>2</sub>]</b>				H	2.45892200	4.25072600	-2.52026700
Pd	0.00017700	0.00062700	-0.00036800	H	1.49569000	2.58641900	-0.95341800
P	-2.30764800	0.00239400	0.00056200	H	4.80064600	-0.05578000	-1.73274800
P	2.30878000	-0.00091400	-0.00153600	H	5.74408500	1.58793100	-3.31677800
C	-4.16798500	-2.90359100	3.13675700	C	4.18732900	-4.12172200	-1.10706400
C	-4.81798800	-1.69868800	2.86466500	C	4.84352400	-3.30704000	-0.18275500
C	-4.28527900	-0.80673000	1.93006200	C	4.30488400	-2.06674400	0.16923300
C	-3.09067200	-1.10851600	1.25896900	C	3.09820800	-1.62812900	-0.39778000
C	-2.43758300	-2.31791800	1.55082600	C	2.43956000	-2.46216700	-1.31691100
C	-2.97634800	-3.21222500	2.47596600	C	2.98417400	-3.69555000	-1.67489700
H	-4.58326000	-3.59505000	3.86542200	H	4.60701800	-5.08717400	-1.37775300
H	-5.74173700	-1.44884300	3.38045500	H	5.77634700	-3.63573700	0.26835700
H	-4.79925000	0.12869800	1.73000500	H	4.82297200	-1.44413800	0.89279000
H	-1.49606500	-2.54507800	1.05599100	H	1.49009400	-2.14057300	-1.73870900
H	-2.45891500	-4.14396000	2.68979200	H	2.46246000	-4.32888800	-2.38779400
C	-4.19210100	4.16228400	0.93748300	<b>2<sub>SP</sub> [Pd(SPhos)<sub>2</sub>] (conformer ac)</b>			
C	-4.82872400	3.32366000	0.02113400	Pd	-0.72343800	0.30522300	0.06824600
C	-4.28781400	2.07094200	-0.28020400	P	1.59620600	0.54735400	0.21232700
				P	-3.02787600	0.58925800	0.13387000

O	-2.96631900	-3.60125100	1.16049700	C	1.61111200	0.48809500	-2.52045600
O	4.48298200	-2.70179400	-1.16883100	H	0.57080200	0.72238700	-2.30267200
O	5.35933900	1.84830300	-0.42930500	C	-3.60319900	2.11217700	-0.85428900
C	5.22483600	-1.78230300	-0.48233600	H	-4.55290100	2.45871700	-0.41702100
O	-2.42076200	-1.54828800	-3.01799400	C	4.80924500	-4.07585800	-1.03669800
C	-2.64364400	-2.56899000	-0.92067700	H	5.84350900	-4.27591700	-1.34608300
C	-4.01858700	-1.98586900	-0.80261600	H	4.12518700	-4.60708900	-1.70110500
C	-4.31806400	-0.67149100	-0.38488000	H	4.66267300	-4.43031700	-0.00849400
C	3.81653700	-0.09358500	-1.71446600	C	6.70665900	0.22285300	0.78356000
C	-6.70736100	-1.15215400	-0.67803100	H	7.29553800	0.99055700	1.26994300
H	-7.73907700	-0.81307300	-0.62838600	C	-2.54004300	-4.46689900	2.19778800
C	4.88262000	-0.43351700	-0.71318300	H	-2.43752800	-5.50229900	1.84545900
C	-6.40452300	-2.45146600	-1.08493900	H	-3.31864900	-4.42286800	2.96174500
H	-7.19586700	-3.14558600	-1.35613700	H	-1.58676300	-4.13845200	2.63254900
C	-5.07457900	-2.85245500	-1.14191100	C	-5.67294600	-0.28705200	-0.33400900
H	-4.82917900	-3.86296600	-1.45678500	H	-5.93035200	0.72194400	-0.02440100
C	2.29574000	3.23057700	-0.53019800	C	6.22405800	2.88418300	0.01093400
H	3.03215200	2.83155800	-1.23175800	H	6.20599000	2.99364600	1.10323200
H	1.33194300	3.26012000	-1.05938500	H	5.84707100	3.80011800	-0.44618000
C	2.42840500	-0.58709500	1.46913400	H	7.25662900	2.70931200	-0.31761700
H	3.51393800	-0.47476300	1.37733200	C	2.69155300	4.66293400	-0.13032500
C	2.04154200	0.42279400	-3.84394000	H	3.70555800	4.65088400	0.29719000
H	1.34407300	0.62859400	-4.65247200	H	2.73995000	5.29451400	-1.02758600
C	-1.88046300	-2.39160800	-2.08895300	C	-3.68435500	0.89696600	1.89162100
C	5.66900400	0.55893700	-0.09858100	H	-4.77885000	0.96979500	1.81784100
C	4.22866400	-0.17350600	-3.05693400	C	1.72854600	5.26676200	0.89939000
H	5.25998900	-0.44901400	-3.26033900	H	2.06514200	6.26793200	1.19971800
C	2.04044800	-0.24171600	2.92239200	H	0.73727400	5.39271400	0.43903400
H	2.38593700	0.76512500	3.18118700	C	-3.01671600	4.50003500	-1.55646000
H	0.94472100	-0.23903100	3.01638500	H	-3.93178800	4.91558500	-1.10711300
C	-2.16411400	-3.45547000	0.06112100	H	-2.24958000	5.28186400	-1.47741000
C	-0.66725200	-3.07037000	-2.27066400	C	-2.57224500	3.25983200	-0.76225600
H	-0.07274100	-2.92455500	-3.16384300	H	-2.38261300	3.53806900	0.27831400
C	1.18790900	2.92513900	1.71459900	H	-1.61413400	2.88930700	-1.15171700
H	0.18913800	2.94674000	1.25887300	C	-4.28878100	3.00756000	-3.14685400
H	1.09422700	2.29940600	2.60698300	H	-4.43027500	2.72939400	-4.19984400
C	2.47118700	0.25404900	-1.42745500	H	-5.27072000	3.34415100	-2.78063000
C	3.36617400	0.08883300	-4.11674300	C	1.60235000	4.34909800	2.12201200
H	3.72605400	0.02586800	-5.14060000	H	0.87102100	4.75625000	2.83293200
C	-3.16882700	2.19108400	2.54991400	H	2.56663800	4.31579700	2.65236700
H	-3.47623800	3.06696100	1.96792800	C	-3.36364700	1.12385700	4.85812200
H	-2.07003400	2.17998500	2.55484700	H	-2.27280700	1.05327900	4.98385600
C	-0.22249800	-3.93790100	-1.27700100	H	-3.78850400	1.24484800	5.86337700
H	0.71712000	-4.46617400	-1.41527400	C	6.26195400	-2.13085900	0.39409800
C	2.04264800	-2.04662700	1.14706400	H	6.50934300	-3.16844400	0.58143800
H	2.35890900	-2.30530000	0.13179000	C	-3.87940400	-0.16589600	4.20510300
H	0.94764600	-2.13125800	1.16106200	H	-4.97955900	-0.14797000	4.18438100
C	-0.95395800	-4.14096200	-0.10874000	H	-3.59397300	-1.03908500	4.80705500
H	-0.58582700	-4.82284700	0.64799600	C	-3.34309300	-0.32398100	2.77329000
C	2.16841400	2.30058700	0.69537700	H	-2.24954300	-0.43469600	2.80173800
H	3.16259800	2.20551900	1.15570200	H	-3.73565600	-1.24206400	2.32289100
C	-3.84582100	1.77337400	-2.34229700	C	2.64646100	-3.03973400	2.15339500
H	-2.91397100	1.37393000	-2.76710700	H	2.32266300	-4.06020700	1.90559900
H	-4.59413400	0.98233100	-2.44379400	H	3.74346900	-3.02601900	2.06882900
C	-3.69359900	2.34517700	3.98950400	C	-1.73364700	-1.37015200	-4.24515000
H	-3.27733100	3.25747200	4.43712300	H	-0.73582900	-0.94161400	-4.09043600
H	-4.78531300	2.48226400	3.96234000	H	-2.34145300	-0.67562400	-4.82828000

H	-1.63876800	-2.31731400	-4.79354200
C	6.98393800	-1.12007000	1.02449900
H	7.78562100	-1.38455600	1.70874100
C	2.64065900	-1.24362700	3.92534200
H	3.73730600	-1.15471700	3.91073600
H	2.31918000	-0.98271800	4.94245500
C	-3.28497400	4.16198100	-3.02870100
H	-2.33896800	3.86976300	-3.50902700
H	-3.65049000	5.04622500	-3.56729400
C	2.25165100	-2.69042800	3.59458800
H	1.16374100	-2.80890300	3.71144200
H	2.72211800	-3.38415200	4.30409700

**2<sub>SP</sub> [Pd(SPhos)<sub>2</sub>] (conformer ab)**

Pd	-0.00552000	-0.01254200	0.14522400
P	-2.22349100	0.70906600	0.30825200
P	2.21640600	-0.72100300	0.31089900
O	-2.80507700	-1.71242800	-2.98904600
O	-2.61859700	-3.22402500	1.44136700
C	-3.83075000	-1.61414000	-0.41496600
C	-3.79700700	-0.29885800	0.10237500
C	-5.02778900	0.28426600	0.47092600
H	-5.04330900	1.27742800	0.90270300
C	-6.27267400	-1.64998000	-0.23370200
H	-7.21291600	-2.17708300	-0.37377300
C	-2.64614200	-2.45978000	-0.77404200
C	-5.07167900	-2.25691700	-0.58167100
H	-5.07577200	-3.26572200	-0.98525400
C	-2.44793100	1.63386400	-2.35382500
H	-1.55202400	1.01864400	-2.49648800
H	-3.30984400	0.97705400	-2.53034500
C	-2.11442200	-3.34983100	0.17759200
C	-2.20875000	-2.56786500	-2.10567700
C	-1.25177800	-3.52177900	-2.47879000
H	-0.92005600	-3.60888500	-3.50596000
C	-2.48968800	2.15279800	-0.90070700
H	-1.57966400	2.74789500	-0.74071300
C	-2.41704200	-1.76811000	-4.35045900
H	-1.34960500	-1.54433300	-4.47585400
H	-3.00771800	-1.00458600	-4.86014900
H	-2.63453000	-2.74929500	-4.79377700
C	-2.53503700	1.47003600	2.01143800
H	-3.52961900	1.93555400	2.01850600
C	-6.24764800	-0.36769100	0.31045400
H	-7.16847700	0.12662600	0.60974100
C	-0.74116400	-4.38277300	-1.50935300
H	-0.00835400	-5.13232500	-1.79680300
C	-3.70432800	3.08039900	-0.70382700
H	-3.73689400	3.47515600	0.31948700
H	-4.63075700	2.51430400	-0.85921200
C	-1.15767700	-4.30907400	-0.18197000
H	-0.75039900	-4.99394200	0.55149200
C	-2.51788900	0.37262100	3.09676100
H	-3.26673400	-0.39570100	2.87318500
H	-1.53979300	-0.12755100	3.07211600
C	-2.26487800	-4.19424300	2.41243300
H	-2.53145900	-5.20784500	2.08378200

H	-2.83696900	-3.94173700	3.30722600
H	-1.19434600	-4.16088600	2.64904700
C	-3.64700800	3.73804900	-3.15393500
H	-4.58612800	3.20587100	-3.36694100
H	-3.59791700	4.58025600	-3.85691700
C	-3.67964300	4.24896200	-1.70677400
H	-4.55450700	4.89359100	-1.54834600
H	-2.79260500	4.87211500	-1.51867300
C	-2.46276500	2.78580200	-3.37384600
H	-1.52450900	3.35092800	-3.28570300
H	-2.48887000	2.37818100	-4.39393400
C	-2.76198500	0.95748900	4.49760400
H	-3.78107300	1.36987400	4.54894300
H	-2.71212700	0.15814500	5.24888000
C	-1.75189700	2.06472800	4.83057300
H	-1.97161200	2.50226600	5.81335800
H	-0.74537900	1.62567200	4.89947400
C	-1.75216100	3.15441800	3.74879700
H	-0.99198300	3.91459400	3.97580700
H	-2.72160700	3.67547100	3.76098500
C	3.75351400	-4.14963300	-1.83237700
C	3.74219700	-3.02597600	-0.77946400
C	2.51699100	-2.10859400	-0.95551000
C	2.48643300	-1.52947100	-2.38599600
C	2.53682500	-2.63649100	-3.45341300
C	3.73441800	-3.57686800	-3.25635100
H	2.87453400	-4.79522800	-1.68644800
H	4.63680300	-4.78593400	-1.68769800
H	4.66204700	-2.43923300	-0.89233700
H	3.76342400	-3.46547600	0.22579300
H	1.61332500	-2.72196100	-0.83276000
H	1.58129900	-0.92473300	-2.51571400
H	3.33811300	-0.84994000	-2.52147600
H	1.60777900	-3.22169100	-3.40383000
H	2.56994000	-2.18545900	-4.45484800
H	4.66707000	-3.01988200	-3.43093200
H	3.71089400	-4.38821000	-3.99596700
C	6.26852500	1.66642800	-0.06493100
C	6.23450400	0.36947400	0.44267400
C	5.01317000	-0.28937000	0.55691600
C	3.78899000	0.30136600	0.17843200
C	3.83112400	1.63084700	-0.30040500
C	5.07387500	2.28022600	-0.42241900
H	7.21029800	2.19898000	-0.16955200
H	7.14966600	-0.13143900	0.74831800
H	5.02231800	-1.29507100	0.95857900
H	5.08380800	3.29986400	-0.79765300
C	0.76689100	4.43963900	-1.36067300
C	1.30675900	3.62259500	-2.35206300
C	2.25428900	2.65351100	-1.99415300
C	2.65332300	2.48689300	-0.65663000
C	2.09110700	3.33215600	0.31789700
C	1.14388500	4.30637100	-0.02618200
H	0.04217800	5.20145800	-1.63600100
H	1.00562100	3.75581500	-3.38369400
H	0.71447400	4.95761200	0.72511200
O	2.87831200	1.83970600	-2.89753500

O	2.55891000	3.15046200	1.58871600	H	-7.53236800	-2.12248400	-1.46383900
C	2.52325100	1.95070100	-4.26464000	C	-4.69714900	3.89777200	1.92174800
H	3.12729000	1.20907600	-4.79074900	H	-4.52149600	4.42585400	0.97570800
H	1.45945700	1.73167000	-4.42444300	H	-3.89021100	4.13051800	2.61859500
H	2.74963200	2.94928000	-4.66228800	H	-5.65414400	4.22581700	2.34833600
C	-1.50721700	2.56842100	2.34625900	C	-3.14631800	0.76068900	-1.43182000
H	-0.49845100	2.13719500	2.28639400	H	-4.23138400	0.63610500	-1.34329600
H	-1.54414300	3.37134300	1.60002400	C	-2.74257400	0.49665700	-2.90072700
C	2.49774300	-1.55875700	1.98347200	H	-1.64639900	0.53543800	-2.98476600
H	3.49378300	-2.02072500	1.99022300	H	-3.04732500	-0.50625600	-3.21770700
C	2.18828300	4.08530800	2.58778800	C	-3.36745100	1.52872300	-3.85641700
H	2.73655300	3.79393600	3.48567200	H	-3.03902200	1.32259300	-4.88381500
H	2.46990200	5.10853200	2.30469200	H	-4.46140200	1.41026500	-3.84815800
H	1.11224900	4.05127700	2.79716200	C	-3.01476200	2.96816400	-3.46090000
C	1.46866600	-2.67537600	2.24622800	H	-1.93246300	3.12290400	-3.58405900
H	1.52742900	-3.44420600	1.46621500	H	-3.51238800	3.68109300	-4.13161200
H	0.45864200	-2.24732700	2.18188800	C	-3.40118500	3.24122600	-2.00054800
C	1.68632900	-3.32127400	3.62671600	H	-4.49602200	3.20814900	-1.90183400
H	2.65812900	-3.83805600	3.63718000	H	-3.08862500	4.25326500	-1.70823600
H	0.92575000	-4.09447700	3.80307400	C	-2.76963100	2.21011200	-1.05016000
C	1.65705700	-2.28085900	4.75585700	H	-3.05896800	2.41699000	-0.01617700
H	0.64747800	-1.84839600	4.82133900	H	-1.67447500	2.29900100	-1.08720800
H	1.85636000	-2.76133800	5.72282800	C	-2.54725400	-2.13414500	-1.07332500
C	2.66930200	-1.15665500	4.49501000	H	-2.00773300	-2.01845100	-2.02461700
H	3.68904300	-1.56693800	4.55090000	C	-1.83146200	-3.25975200	-0.29876700
H	2.59921900	-0.39151700	5.27959700	H	-0.78802500	-2.97457200	-0.11840400
C	2.45295200	-0.51145700	3.11653300	H	-2.30476400	-3.38652100	0.68471800
H	3.20321200	0.26852800	2.94388500	C	-1.89655500	-4.59330500	-1.06256400
<b>2<sub>SP</sub> [Pd(SPhos)<sub>2</sub>] (conformer cc)</b>				H	-1.32734800	-4.50101300	-1.99996000
Pd	0.00012900	0.00023200	-0.00066800	H	-1.40621400	-5.38161600	-0.47608500
P	-2.27447800	-0.43934100	-0.26670000	C	-3.34341700	-4.99272600	-1.38646900
P	2.27474500	0.43989000	0.26531000	H	-3.87819000	-5.20223700	-0.44786700
O	-4.66157600	2.48976800	1.75010200	H	-3.36307600	-5.92120300	-1.97243500
O	-6.56197000	-1.53677400	0.29158400	C	-4.06955000	-3.86946000	-2.14010600
C	-3.21391100	-0.57711500	1.35809300	H	-3.60972200	-3.74460700	-3.13237100
C	-4.54379200	-0.24782600	1.72860800	H	-5.11814200	-4.14544100	-2.31757100
C	-5.55027500	0.49396500	0.89639600	C	-4.00075100	-2.53385300	-1.37621000
C	-5.60603700	1.90143500	0.95785600	H	-4.55291800	-2.61933800	-0.43411500
C	-6.58174100	2.62337900	0.25580200	H	-4.50768500	-1.75418400	-1.95826600
H	-6.60753800	3.70554200	0.28979600	O	4.65831900	-2.49629400	-1.73693900
C	-7.53540100	1.92842700	-0.48449600	O	6.56608400	1.53415700	-0.29890900
H	-8.29034300	2.48282100	-1.03552100	C	3.21483000	0.57213500	-1.35956500
C	-7.55180000	0.53642900	-0.51545300	C	4.54487600	0.24162200	-1.72838400
H	-8.32283400	0.01893400	-1.07256900	C	5.55075300	-0.49782400	-0.89336700
C	-6.57600000	-0.17417700	0.19953400	C	5.60415900	-1.90567500	-0.94805400
C	-4.98851000	-0.56718400	3.02457600	C	6.57906900	-2.62580500	-0.24303700
H	-6.00810100	-0.30379600	3.29295500	H	6.60310700	-3.70815900	-0.27183000
C	-4.17152600	-1.19036600	3.96194400	C	7.53425500	-1.92884400	0.49339900
H	-4.55547900	-1.42166700	4.95222200	H	8.28857500	-2.48180500	1.04670900
C	-2.85475500	-1.48724900	3.61804400	C	7.55297600	-0.53674500	0.51758700
H	-2.18277800	-1.94942700	4.33673600	H	8.32514600	-0.01782700	1.07180000
C	-2.39415100	-1.16945100	2.34336300	C	6.57795900	0.17199900	-0.20031300
H	-1.35430500	-1.36363900	2.09157000	C	4.99020500	0.55673100	-3.02517700
C	-7.57104200	-2.27468800	-0.37728000	H	6.00990700	0.29242600	-3.29222700
H	-8.57234400	-2.01261200	-0.01107400	C	4.17364700	1.17683400	-3.96496300
H	-7.36870400	-3.32379100	-0.15408500	H	4.55806000	1.40488800	-4.95581600
				C	2.85670700	1.47481000	-3.62266100

H	2.18506600	1.93462600	-4.34318000
C	2.39550100	1.16118300	-2.34715900
H	1.35556400	1.35629400	-2.09642100
C	7.57674200	2.27364500	0.36580700
H	8.57741200	2.00815500	0.00032700
H	7.37599800	3.32198400	0.13763700
H	7.53842700	2.12677400	1.45311300
C	4.69159100	-3.90516200	-1.90184900
H	4.51580700	-4.42841700	-0.95315800
H	3.88379600	-4.14000100	-2.59699800
H	5.64777300	-4.23672700	-2.32754200
C	3.14586000	-0.75666900	1.43459700
H	4.23102900	-0.63467000	1.34383900
C	2.74498500	-0.48541100	2.90296800
H	1.64886400	-0.52151300	2.98892000
H	3.05238700	0.51821600	3.21509600
C	3.36918400	-1.51463100	3.86216800
H	3.04274800	-1.30339000	4.88916200
H	4.46336100	-1.39846300	3.85172200
C	3.01295200	-2.95504300	3.47340500
H	1.93050800	-3.10700300	3.59872500
H	3.51004200	-3.66608500	4.14651200
C	3.39678400	-3.23519300	2.01372200
H	4.49155000	-3.20456400	1.91336800
H	3.08192500	-4.24790400	1.72624800
C	2.76583800	-2.20701200	1.05976200
H	3.05344300	-2.41887800	0.02629200
H	1.67056800	-2.29367100	1.09862500
C	2.54774600	2.13723300	1.06639000
H	2.01046900	2.02397000	2.01923400
C	1.82933600	3.25982100	0.28987200
H	0.78572700	2.97324600	0.11275500
H	2.30033700	3.38375000	-0.69508900
C	1.89514200	4.59588900	1.04920800
H	1.32803500	4.50622200	1.98813100
H	1.40295200	5.38194800	0.46125600
C	3.34240300	4.99743500	1.36870500
H	3.87498800	5.20441400	0.42829900
H	3.36260400	5.92776200	1.95171200
C	4.07103400	3.87710800	2.12429500
H	3.61345400	3.75503400	3.11794500
H	5.11979900	4.15443700	2.29860600
C	4.00158300	2.53906500	1.36474400
H	4.55154200	2.62204400	0.42113900
H	4.51047400	1.76161700	1.94806000

**3<sub>Cy</sub> [Pd(PCy<sub>3</sub>)(PhBr)] (conformer F)**

Pd	0.55591200	-1.02794800	-0.64257400
Br	5.52880600	0.45133100	0.24174700
P	-1.30883500	0.15961800	0.03466700
C	-0.02825400	4.19389000	-0.19710400
C	-0.35814400	2.74762900	-0.60406300
C	-0.96006000	1.93821200	0.56663000
C	-0.01483200	1.99477900	1.78676000
C	0.31795000	3.44199100	2.18974800
C	0.90714700	4.23880900	1.01833900
H	-0.96059100	4.72733800	0.04209100

H	0.42266800	4.72122400	-1.04776500
H	-1.04270700	2.75750500	-1.46036300
H	0.55834500	2.24355100	-0.94200400
H	-1.91569200	2.40147600	0.85155100
H	-0.45908000	1.47915100	2.64596300
H	0.91227100	1.45704500	1.54268900
H	-0.59781500	3.94022200	2.54221600
H	1.01523100	3.43506200	3.03732900
H	1.88160900	3.81025400	0.74203000
H	1.09448100	5.27768700	1.31882300
C	-4.51034000	1.56224000	-2.49611900
C	-3.72124600	1.39017900	-1.18427100
C	-2.56955700	0.37680000	-1.36409100
C	-3.12080200	-0.97552100	-1.86558900
C	-3.91149300	-0.80534200	-3.17404400
C	-5.04338300	0.22123000	-3.02108200
H	-3.85385500	2.01392100	-3.25470800
H	-5.33747200	2.26721200	-2.34080600
H	-4.40727700	1.04550000	-0.40118600
H	-3.34175200	2.36576700	-0.85954400
H	-1.92180400	0.76204000	-2.16643800
H	-2.29616700	-1.68465000	-2.00813200
H	-3.78588400	-1.40738600	-1.10486000
H	-3.22516400	-0.47579300	-3.96829000
H	-4.31620800	-1.77455700	-3.49314500
H	-5.79268300	-0.16997700	-2.31650300
H	-5.56099300	0.36581100	-3.97803800
C	-2.71655000	-2.70802900	2.83127300
C	-2.29467900	-2.11722300	1.47455900
C	-2.14452200	-0.58254300	1.56120400
C	-3.45549100	0.05740400	2.06060200
C	-3.87049700	-0.52797800	3.42327400
C	-4.00279000	-2.05678000	3.36160400
H	-1.90510200	-2.55305600	3.55810500
H	-2.84976200	-3.79375900	2.73943600
H	-3.04915900	-2.37718600	0.72019200
H	-1.34951300	-2.56166900	1.14018200
H	-1.37655100	-0.39891500	2.32775600
H	-3.35803500	1.14694900	2.13772500
H	-4.25769900	-0.13806500	1.33707700
H	-3.11641400	-0.25731000	4.17716400
H	-4.81567000	-0.07565500	3.75070600
H	-4.83999000	-2.31843300	2.69724500
H	-4.25346500	-2.45738600	4.35217700
C	2.14940100	-2.54932300	-1.12326900
C	2.44610700	-1.40900500	-1.90921400
C	2.85458600	-2.75205900	0.08893300
C	3.45021000	-0.50386100	-1.48853200
H	2.03153300	-1.30366700	-2.90805700
C	3.85197700	-1.87175600	0.49089400
H	2.63855700	-3.62902000	0.69280700
C	4.14018800	-0.75743900	-0.31296800
H	3.69182300	0.35961800	-2.09868200
H	4.40320000	-2.04073000	1.40936200
H	1.51961000	-3.34318100	-1.51770000

**3<sub>Cy</sub> [Pd(PCy<sub>3</sub>)(PhBr)] (conformer C)**

Pd	-0.42785400	-1.11584200	-0.48794400	H	2.29151200	-4.21484300	1.31043500
Br	-5.25070400	1.08710100	-0.28803500	H	1.85248200	-3.47524700	3.64171000
P	1.43280200	0.04506800	0.27198600	H	0.33596700	-3.95498100	2.88268200
C	-2.16967000	-2.42035600	-1.00353600	H	-0.23598500	-1.58796600	2.42341500
C	-2.99651700	-2.40012200	0.14915000	H	0.10828700	-1.78189200	4.14438500
C	-3.90294700	-1.36911500	0.36161600	H	2.39957800	-0.92212300	3.84094500
C	-3.98081900	-0.32723900	-0.57707500	H	1.23228500	0.25734400	3.27838100
C	-3.16697000	-0.28953000	-1.69832400	H	-1.62731800	-3.32764500	-1.26157100
C	-2.25022300	-1.34377200	-1.92176900	<b>3<sub>Cy</sub> [Pd(PCy<sub>3</sub>)(PhCl)] (conformer F)</b>			
C	2.74547400	0.40993200	-1.05583100	Pd	0.98466500	-0.97671700	-0.60834700
C	4.20316400	0.61429600	-0.58778300	P	-0.92628300	0.14298100	0.04798000
C	5.11125000	1.03219500	-1.75957200	Cl	5.75661900	0.68148000	0.27729300
C	5.05960000	0.01557000	-2.90855700	C	0.32239200	4.19205800	0.12002200
C	3.61463500	-0.22276100	-3.36968200	C	0.02549200	2.77087000	-0.38862700
C	2.70086600	-0.62752700	-2.20066300	C	-0.62024300	1.88740200	0.70252900
C	0.96592800	1.75623900	0.93384400	C	0.27142400	1.87673900	1.96366500
C	0.13012700	2.54477300	-0.09855100	C	0.57214100	3.29876900	2.46935200
C	-0.41848500	3.85095400	0.50135800	C	1.20308700	4.17088800	1.37616300
C	0.70003900	4.72726800	1.08338000	H	-0.62522700	4.70236400	0.34950300
C	1.54447000	3.94489900	2.09874600	H	0.80433000	4.77401200	-0.67629000
C	2.09836000	2.64264200	1.49099100	H	-0.61874400	2.83034400	-1.27388600
C	2.41491500	-0.71651100	1.70502300	H	0.96094300	2.29400800	-0.71429600
C	2.92374400	-2.14648700	1.38771900	H	-1.59224200	2.32502200	0.97156700
C	1.83903600	-3.23034700	1.48874200	H	-0.20227400	1.30441600	2.76980200
C	1.13454100	-3.20246200	2.85268100	H	1.21330600	1.36260800	1.72565800
C	0.56273900	-1.80762700	3.14524000	H	-0.36270300	3.76738000	2.81225400
C	1.65361400	-0.72906600	3.05424100	H	1.23261800	3.24403500	3.34427800
H	-2.94776500	-3.22373900	0.85610500	H	2.19352400	3.76878400	1.11780900
H	-4.54557800	-1.36734300	1.23525300	H	1.36486300	5.19109800	1.74725400
H	-3.24564500	0.52180000	-2.41382000	C	-4.00612400	1.69315000	-2.54464100
H	-1.73939300	-1.39662500	-2.87905600	C	-3.28135400	1.44432900	-1.20844000
H	2.39786500	1.36444200	-1.47991900	C	-2.12246500	0.44010700	-1.39162400
H	4.58935300	-0.32170200	-0.16266200	C	-2.64798200	-0.88101800	-1.99395100
H	4.26296700	1.36553400	0.20632000	C	-3.37787200	-0.63514900	-3.32574600
H	4.79062100	2.01708100	-2.13067600	C	-4.51495500	0.38509400	-3.16775300
H	6.14233800	1.15399100	-1.40277000	H	-3.31371300	2.18382700	-3.24481900
H	5.49296100	-0.93669400	-2.56777600	H	-4.83902600	2.39138200	-2.38966200
H	5.67843100	0.35745400	-3.74808000	H	-4.00422900	1.05751200	-0.48069200
H	3.22465800	0.69870200	-3.82790200	H	-2.91672000	2.39823200	-0.81026200
H	3.58476700	-0.99494900	-4.14928200	H	-1.43991400	0.87004400	-2.14030300
H	3.01519700	-1.60995600	-1.81894800	H	-1.81665200	-1.58192200	-2.13827400
H	1.66714600	-0.75095400	-2.54399600	H	-3.34701300	-1.35498400	-1.29073800
H	0.28639800	1.51344200	1.76407700	H	-2.65553500	-0.26357400	-4.06773100
H	-0.69156500	1.91776300	-0.46303200	H	-3.76789000	-1.58360300	-3.71731500
H	0.75315600	2.78856600	-0.97239400	H	-5.29586400	-0.04200300	-2.52077800
H	-0.97769900	4.40387000	-0.26430200	H	-4.98821100	0.58418900	-4.13782000
H	-1.13832400	3.60465500	1.29581500	C	-2.43040700	-2.90358900	2.59370900
H	0.27793400	5.62615200	1.55072200	C	-1.94516400	-2.22725200	1.29958400
H	1.34948900	5.07540000	0.26605800	C	-1.83178500	-0.69732400	1.48201300
H	2.37344400	4.56425400	2.46556000	C	-3.18353300	-0.11241100	1.93870700
H	0.92618800	3.69992800	2.97506600	C	-3.66202200	-0.78266000	3.24036600
H	2.68372000	2.10696100	2.24803700	C	-3.75789800	-2.30757100	3.08604300
H	2.79230000	2.90325500	0.68008200	H	-1.66465000	-2.77670400	3.37362500
H	3.29401400	-0.07432600	1.83304200	H	-2.53511500	-3.98433300	2.43245600
H	3.71980500	-2.37630100	2.11295800	H	-2.65127400	-2.45560600	0.48971300
H	3.39462000	-2.18438200	0.39864800	H	-0.97412700	-2.63515500	0.99360300
H	1.09448900	-3.06981200	0.69499400				

H	-1.11565000	-0.54338200	2.30321700
H	-3.11726900	0.97281500	2.08262800
H	-3.93806100	-0.28358100	1.16009700
H	-2.95736000	-0.54199300	4.05015400
H	-4.63356500	-0.36708600	3.53797400
H	-4.55186400	-2.54667000	2.36267600
H	-4.05382000	-2.76847200	4.03715300
C	2.67200600	-2.40309300	-1.05599900
C	2.91947000	-1.25675000	-1.85014800
C	3.36869000	-2.55478400	0.16870200
C	3.86720700	-0.29574600	-1.42573700
H	2.51131000	-1.18370100	-2.85438100
C	4.31053600	-1.61727300	0.57442500
H	3.19003600	-3.43581900	0.77866900
C	4.55259100	-0.49690700	-0.23664800
H	4.07576900	0.57389200	-2.03948200
H	4.85889500	-1.74245700	1.50173800
H	2.09086300	-3.23308400	-1.45059400

### **3<sub>H</sub> [Pd(PH<sub>3</sub>)(PhBr)]**

Pd	1.78098800	0.12559500	0.08019900
Br	-3.37925800	-0.78273700	-0.03879500
P	3.40116600	-1.39249000	-0.28075300
C	0.44644000	1.97109000	0.12083100
C	-0.32224200	1.86889600	-1.06293900
C	-1.45342900	1.06067200	-1.11011100
C	-1.81218900	0.32299200	0.02739200
C	-1.06302000	0.36953300	1.19563000
C	0.07283200	1.20833200	1.25299200
H	1.21660200	2.73409400	0.20005100
H	-0.04527900	2.45633800	-1.93351300
H	-2.05179900	0.99926200	-2.01239600
H	-1.35705600	-0.20647200	2.06599200
H	0.56693700	1.36104100	2.20841800
H	4.65565400	-1.27931500	0.37176500
H	3.20383500	-2.76538800	0.01668100
H	3.93185700	-1.60286600	-1.57980200

### **3<sub>H</sub> [Pd(PH<sub>3</sub>)(PhCl)]**

Pd	1.25512900	0.17560800	0.07956300
Cl	-3.61720800	-1.33123200	-0.08470300
P	3.06442000	-1.10899700	-0.28092600
C	-0.32605200	1.81155800	0.14601500
C	-1.06146300	1.61991900	-1.04797700
C	-2.06850800	0.66368000	-1.11740600
C	-2.33543900	-0.13214900	0.00628400
C	-1.61077500	0.00382900	1.18364500
C	-0.60207300	0.98864400	1.26411400
H	0.33030900	2.67253100	0.24404400
H	-0.85923600	2.25159800	-1.90796100
H	-2.64593800	0.52848100	-2.02550600
H	-1.83557300	-0.62070600	2.04138200
H	-0.14016700	1.19350000	2.22567500
H	4.30407800	-0.80158600	0.33667500
H	3.07017800	-2.48653800	0.05824300
H	3.59252400	-1.28221400	-1.58664100

### **3<sub>Ph</sub> [Pd(PPh<sub>3</sub>)(PhBr)]**

Pd	0.54571600	-1.12730200	0.33134600
Br	5.32944800	1.00439300	-0.04054500
P	-1.42313100	-0.00246800	0.01371400
C	2.28021400	-2.58584400	0.24633000
C	2.95248800	-2.30071000	-0.96693800
C	3.85643200	-1.24807800	-1.05078000
C	4.07736600	-0.44817800	0.08098300
C	3.41393700	-0.67400500	1.27811400
C	2.51170900	-1.76007100	1.37240200
H	1.72269400	-3.51359000	0.34784500
H	2.78583600	-2.93507800	-1.83287100
H	4.38407100	-1.04394500	-1.97589900
H	3.60057600	-0.04760700	2.14337400
H	2.12215200	-2.03519800	2.34874400
C	-2.78226400	-1.00573500	-0.74545700
C	-2.43428500	-1.92938500	-1.74517200
C	-4.13015500	-0.88783100	-0.37467300
C	-3.41149000	-2.70344400	-2.37028600
H	-1.38921500	-2.04312300	-2.02328800
C	-5.10693900	-1.67198700	-0.99417800
H	-4.42006800	-0.18747300	0.40266700
C	-4.75127100	-2.57811300	-1.99419800
H	-3.12550400	-3.41244100	-3.14289800
H	-6.14647700	-1.57311800	-0.69229500
H	-5.51219900	-3.18828000	-2.47363100
C	-2.19731600	0.65701900	1.56115100
C	-2.88698900	1.87700800	1.62277100
C	-2.07983000	-0.11325900	2.73013000
C	-3.45057300	2.31256400	2.82497200
H	-2.98080000	2.49329400	0.73401900
C	-2.65287700	0.31698500	3.92653500
H	-1.52475700	-1.04781000	2.69573600
C	-3.33811700	1.53361500	3.97745600
H	-3.97672400	3.26314500	2.85820900
H	-2.55378300	-0.29157300	4.82165500
H	-3.77544300	1.87520000	4.91191700
C	-1.32988100	1.48132500	-1.08968700
C	-2.37709800	1.88613900	-1.93164100
C	-0.14286500	2.23225800	-1.07591900
C	-2.24156100	3.02103900	-2.73488300
H	-3.29830900	1.31233400	-1.96779000
C	-0.01290400	3.37099800	-1.87121100
H	0.68293000	1.91035200	-0.44613700
C	-1.06194500	3.76694800	-2.70429800
H	-3.05901900	3.31960500	-3.38621400
H	0.91221800	3.94089400	-1.84881400
H	-0.95753900	4.64801300	-3.33204400

### **3<sub>Ph</sub> [Pd(PPh<sub>3</sub>)(PhCl)]**

Pd	1.03696600	-0.94272300	0.40574300
P	-1.01962700	-0.01971900	0.01921600
Cl	5.49897200	1.49457900	-0.17018600
C	2.91184700	-2.21604900	0.40517400
C	3.53897000	-1.95464300	-0.83749200
C	4.33152400	-0.82683200	-1.01135400
C	4.48678100	0.07176300	0.05569400

C	3.86128000	-0.13285100	1.27744200	H	-1.36018700	0.34207700	-2.60663500
C	3.07218900	-1.29108300	1.46469100	H	-2.92596600	0.90367300	-2.03608900
H	2.45228900	-3.18506200	0.58368100	C	-1.46951000	-2.57806000	1.39564000
H	3.42616800	-2.66305400	-1.65310000	C	-2.74969900	-2.40093300	-0.64817500
H	4.82814900	-0.63522500	-1.95644200	C	-2.28162200	-3.65737000	-1.05877500
H	3.99872200	0.57245500	2.08994200	H	-2.59378900	-4.09027800	-2.00132300
H	2.72014200	-1.53121500	2.46417100	C	-1.25738600	2.10850100	-1.34975000
C	-2.34201200	-1.22818200	-0.45091400	H	-0.26768800	2.37998800	-1.74677100
C	-1.99798000	-2.26044600	-1.34047200	C	-4.09708600	-2.16075200	-2.61133200
C	-3.65506200	-1.16832700	0.03798500	H	-3.27515800	-2.30445000	-3.32485900
C	-2.94686400	-3.19935600	-1.74250700	H	-4.78633300	-1.41025500	-3.00252300
H	-0.97641100	-2.32924000	-1.70688300	H	-4.63216200	-3.11061100	-2.48013800
C	-4.60229400	-2.11731700	-0.35691500	C	0.03778200	2.26933300	1.33077300
H	-3.94164900	-0.38281300	0.73039600	H	-0.65503400	3.09548900	1.54328900
C	-4.25252700	-3.13175300	-1.24858400	C	-4.35002200	1.59457000	2.24207600
H	-2.66434100	-3.99082200	-2.43185700	H	-4.86243800	2.44170600	2.69074400
H	-5.61457800	-2.06065900	0.03514400	C	-1.41612900	-4.36263400	-0.22444800
H	-4.99014600	-3.86969100	-1.55284300	H	-1.06393400	-5.34437100	-0.53082800
C	-1.75854100	0.87968800	1.45979600	C	-2.04821300	3.40964100	-1.11410100
C	-2.57310900	2.01450500	1.32828000	H	-1.54296300	4.04796700	-0.37852500
C	-1.48532100	0.38854700	2.74703500	H	-3.03577900	3.16657300	-0.70201300
C	-3.10594500	2.63862800	2.45892900	C	-1.00359500	-3.84087200	1.00002800
H	-2.78758700	2.41821100	0.34349700	H	-0.33937900	-4.41379900	1.63537200
C	-2.02670200	1.00616300	3.87448300	C	0.37208400	1.56956400	2.66530600
H	-0.83589700	-0.47690100	2.85625400	H	-0.54168300	1.17776600	3.12674100
C	-2.83735200	2.13498800	3.73276100	H	1.01270700	0.70152800	2.45356200
H	-3.73069800	3.52042800	2.34189800	C	-0.22374200	-2.64901500	3.43709000
H	-1.80610600	0.61304200	4.86353900	H	-0.59653600	-3.62751000	3.76843900
H	-3.25150400	2.62350300	4.61088100	H	-0.10464700	-1.99774200	4.30453800
C	-1.09128600	1.22678600	-1.34733000	H	0.74719200	-2.77522300	2.94136800
C	-2.20388800	1.38809400	-2.18739400	C	-2.92666300	3.33648100	-3.49837600
C	0.03092300	2.04804200	-1.54336400	H	-3.95152000	3.10554500	-3.17154300
C	-2.19558400	2.35556000	-3.19507300	H	-3.01602400	3.89868700	-4.43699500
H	-3.07672800	0.75429700	-2.06042400	C	-2.23843300	4.19314500	-2.42640200
C	0.03383900	3.02018300	-2.54391400	H	-2.81992300	5.10412400	-2.23290200
H	0.90628000	1.91170200	-0.91283500	H	-1.25665700	4.52202100	-2.79854500
C	-1.07929100	3.17471100	-3.37367400	C	1.31346200	2.87117700	0.70381000
H	-3.06265400	2.46667100	-3.84122000	H	1.07093700	3.41752000	-0.21604600
H	0.91031700	3.64764400	-2.68276800	H	1.98840100	2.05372100	0.41449800
H	-1.07392200	3.92505100	-4.15996900	C	-2.16230900	2.02481200	-3.72924200
<b>3<sub>SP</sub> [Pd(SPhos)(PhBr)] (conformer a)</b>				H	-1.18117700	2.25256300	-4.17280900
Pd	0.54501100	-0.72602100	-0.46296400	H	-2.69428500	1.39737500	-4.45681000
Br	5.82959600	0.14117100	-0.57784400	C	4.19961300	-0.85949700	-0.79426200
P	-0.79369900	1.05259600	0.15405400	C	3.35903400	-0.56602300	-1.85464600
O	-3.63110900	-1.64995700	-1.37367200	C	2.17088500	-1.31709900	-2.02410100
O	-1.15373800	-1.99554900	2.58859600	C	1.85987700	-2.36909000	-1.12197000
C	-2.97822600	-0.57805600	1.08940000	C	2.73237400	-2.60568500	-0.02691200
C	-2.41865900	0.71867900	1.00932700	C	3.89568500	-1.86522600	0.13893900
C	-3.12484700	1.78116300	1.60627200	H	3.61177700	0.21555800	-2.56308600
H	-2.70921800	2.78217300	1.58095600	H	1.60911600	-1.19953200	-2.94630500
C	-4.90677300	0.31794000	2.29636400	H	2.50367800	-3.40776700	0.66974400
H	-5.86288100	0.15123800	2.78562600	H	4.56683300	-2.06328900	0.96763300
C	-2.34080300	-1.83467500	0.57399400	C	1.09396900	2.51516600	3.63956800
C	-4.21941200	-0.74901100	1.72656900	H	0.41216000	3.32795500	3.93275300
H	-4.63923400	-1.74978200	1.77804800	H	1.34583300	1.97423700	4.56133300
C	-1.95531400	1.24430800	-2.42036800	C	2.35888700	3.11582200	3.01032400
				H	3.08787300	2.31282200	2.82676500



H	2.83512500	3.81975800	3.70508200
C	2.03540800	3.81428600	1.68235400
H	2.95409900	4.19390100	1.21691800
H	1.39958100	4.69080900	1.87972100
H	1.08347600	-3.09460000	-1.35756200

**3<sub>SP</sub> [Pd(SPhos)(PhBr)] (conformer c)**

Pd	1.77167200	0.20599900	1.28301500
Br	5.94312800	-0.92839000	-1.72080100
P	-0.39917900	0.52911100	0.52032600
O	-2.00992600	-3.11560800	-1.02266500
O	-4.08880900	0.98029300	-1.94520500
C	-0.64314500	0.00610200	-1.26799900
C	-1.75570400	-0.54722600	-1.95436400
C	-3.03967100	-1.03207000	-1.34423200
C	-3.14815400	-2.36888200	-0.90928800
C	-4.35698600	-2.87754100	-0.41315400
H	-4.42990900	-3.89947800	-0.06216000
C	-5.47862500	-2.05190600	-0.38670000
H	-6.41632600	-2.43881200	0.00303000
C	-5.42643700	-0.74715800	-0.87009100
H	-6.32032500	-0.13574800	-0.86907000
C	-4.21388200	-0.25424500	-1.37517500
C	-1.66666000	-0.74321900	-3.34455200
H	-2.52506200	-1.17217700	-3.85436900
C	-0.52642500	-0.42094700	-4.07294500
H	-0.49996100	-0.58801800	-5.14658000
C	0.58107700	0.09225900	-3.40236000
H	1.49669600	0.32858300	-3.93788100
C	0.51553200	0.28503800	-2.02515500
H	1.39664200	0.64897900	-1.50257600
C	-5.23899600	1.80433400	-2.04376000
H	-6.02666400	1.32568200	-2.63997400
H	-4.90887900	2.71532400	-2.54611700
H	-5.64035900	2.06191500	-1.05492100
C	-2.06681200	-4.49737600	-0.70271500
H	-2.29117800	-4.65859900	0.35958900
H	-1.07421800	-4.89268300	-0.92483900
H	-2.81336600	-5.01979400	-1.31476500
C	-1.69001500	-0.27370000	1.63403000
H	-2.65531400	-0.28779700	1.11534100
C	-1.85358100	0.51410900	2.95401500
H	-0.87127000	0.60635500	3.44107100
H	-2.20835800	1.53215200	2.76193700
C	-2.83795300	-0.18179300	3.91152200
H	-2.90784000	0.39172800	4.84518200
H	-3.84221500	-0.17165200	3.46227900
C	-2.43212800	-1.63237500	4.20341000
H	-1.48419300	-1.63836100	4.76182800
H	-3.17896000	-2.11436500	4.84781900
C	-2.25522400	-2.42141400	2.89916700
H	-3.22935800	-2.52304400	2.39912500
H	-1.90453500	-3.43969500	3.11640500
C	-1.26375600	-1.72438000	1.95254600
H	-1.14911500	-2.29787300	1.02873500
H	-0.27057600	-1.69144700	2.42320900
C	-0.86427300	2.36597900	0.51871200

H	-0.73068900	2.63748900	1.57612200
C	0.14089000	3.21372100	-0.28817700
H	1.16314300	2.98882200	0.03979400
H	0.07999400	2.94124900	-1.35071100
C	-0.14789900	4.71723500	-0.13774000
H	0.02062300	5.01548800	0.90802000
H	0.56233200	5.29335200	-0.74500400
C	-1.59090900	5.06038300	-0.53493200
H	-1.72315500	4.87221800	-1.61084500
H	-1.78802600	6.12866200	-0.37636900
C	-2.59597000	4.20837200	0.25288600
H	-2.54814600	4.48436800	1.31725700
H	-3.62104000	4.42492700	-0.07733200
C	-2.30576500	2.70347900	0.10288700
H	-2.45849500	2.40164000	-0.93847800
H	-3.02710900	2.12935700	0.69714400
C	5.04377700	-0.44288500	-0.09105300
C	5.19051800	0.86558300	0.39714500
C	4.54907800	1.21844300	1.57797600
C	3.77704000	0.27326300	2.29905000
C	3.63321900	-1.03770600	1.77979100
C	4.27139400	-1.38860600	0.56473200
H	5.79663800	1.58574200	-0.14137600
H	4.67088800	2.22252500	1.97483800
H	3.18281300	-1.82403100	2.37914900
H	4.17378100	-2.39483900	0.17230700
H	3.45095300	0.50617500	3.30975300

**3<sub>SP</sub> [Pd(SPhos)(PhCl)] (conformer a)**

Pd	0.87189900	-0.71840600	-0.48931600
P	-0.46628800	1.04705400	0.15651700
Cl	5.96859000	0.23574700	-0.99517000
O	-3.28675100	-1.66151200	-1.34552300
O	-0.79735700	-2.01653000	2.60790600
C	-2.62857200	-0.59739400	1.12003100
C	-2.07779700	0.70273000	1.03342300
C	-2.78233300	1.76050900	1.64061900
H	-2.37249300	2.76377700	1.61145600
C	-4.54710200	0.28667000	2.35170800
H	-5.49611000	0.11414100	2.85265400
C	-1.98997200	-1.85047700	0.59716600
C	-3.86060700	-0.77593100	1.77278300
H	-4.27381300	-1.77920500	1.82911900
C	-1.66623100	1.25222500	-2.40007900
H	-1.07298600	0.35157800	-2.59930300
H	-2.63134600	0.90881600	-2.00450700
C	-1.11534200	-2.59546500	1.41363900
C	-2.40073900	-2.41275500	-0.62603900
C	-1.93065200	-3.66636400	-1.04304500
H	-2.24436300	-4.09622600	-1.98648200
C	-0.95447400	2.11094600	-1.33431700
H	0.02939500	2.38548500	-1.74357500
C	-3.75139500	-2.16629200	-2.58605200
H	-2.92907500	-2.30331400	-3.30044400
H	-4.44286100	-1.41550400	-2.97276100
H	-4.28376800	-3.11845800	-2.46053200
C	0.37618900	2.26146000	1.32814200

H	-0.31636900	3.08480300	1.55212200	C	1.71043900	-0.07451300	1.96519100
C	-3.99831100	1.56648100	2.29166000	C	2.94845800	-0.61782700	1.31149100
H	-4.50978600	2.41031200	2.74759800	C	3.10958100	-2.01095500	1.16778500
C	-1.06056300	-4.37252400	-0.21435700	C	4.29224600	-2.55763000	0.64939200
H	-0.70618100	-5.35181500	-0.52600700	H	4.40444300	-3.62752500	0.52440500
C	-1.74340900	3.40969500	-1.08042600	C	5.33764700	-1.70412800	0.30406100
H	-1.22844700	4.04486100	-0.34881300	H	6.25468300	-2.12190100	-0.10259200
H	-2.72456000	3.16305600	-0.65523600	C	5.23748800	-0.32751600	0.48894500
C	-0.64630500	-3.85486900	1.01138900	H	6.07544900	0.31221200	0.24108700
H	0.02215500	-4.42826800	1.64183900	C	4.05277100	0.20592300	1.01823900
C	0.72811000	1.55713600	2.65578900	C	1.79729400	0.03492200	3.36505100
H	-0.17937800	1.16242000	3.12700400	H	2.73886900	-0.22839400	3.83926600
H	1.36701300	0.69054400	2.43302500	C	0.72697500	0.45193200	4.14920400
C	0.11168600	-2.68639700	3.46575000	H	0.83695900	0.52425100	5.22808200
H	-0.27763100	-3.66277400	3.78410000	C	-0.48682600	0.74792600	3.53349300
H	0.22517300	-2.04244000	4.33942100	H	-1.35050700	1.04900500	4.12041700
H	1.08919300	-2.82188300	2.98543800	C	-0.59545800	0.63546200	2.15022400
C	-2.65475200	3.34891900	-3.45301100	H	-1.55701600	0.82712700	1.68086100
H	-3.67474200	3.11433000	-3.11383900	C	4.97655500	2.41433600	1.06862500
H	-2.75759200	3.91648900	-4.38702400	H	5.86041800	2.13329800	1.65593700
C	-1.95348100	4.20044200	-2.38541800	H	4.63094500	3.39998200	1.38522700
H	-2.53400800	5.10910300	-2.17844800	H	5.24618100	2.45017600	0.00500400
H	-0.97762900	4.53361800	-2.76910900	C	2.17083500	-4.18176100	1.55286600
C	1.64251300	2.86906100	0.68785900	H	2.29503200	-4.55986900	0.52986100
H	1.38703900	3.42012700	-0.22564200	H	1.23738100	-4.56571700	1.96765800
H	2.31445900	2.05426600	0.38447800	H	3.01226700	-4.52221800	2.17017900
C	-1.89160500	2.03989500	-3.70162300	C	1.24047300	-0.57402400	-1.56090800
H	-0.91672100	2.27158300	-4.15679600	H	2.25033300	-0.42056400	-1.16441900
H	-2.43228600	1.41588200	-4.42574700	C	1.20738800	-0.06559900	-3.02065400
C	4.50154300	-0.74036100	-1.05446900	H	0.17807900	-0.13303600	-3.40338500
C	3.58645800	-0.53447000	-2.07437500	H	1.49720300	0.98903000	-3.07507200
C	2.42070500	-1.33284900	-2.13221600	C	2.14556000	-0.88582600	-3.92467000
C	2.20278600	-2.34587500	-1.16117900	H	2.08013200	-0.51251100	-4.95516800
C	3.14654800	-2.49335600	-0.11088600	H	3.18461500	-0.72712000	-3.59964900
C	4.28883300	-1.70535500	-0.05580300	C	1.82838200	-2.38616900	-3.87757600
H	3.77168600	0.21801000	-2.83376400	H	0.83260100	-2.56033900	-4.31173900
H	1.79661600	-1.28000400	-3.01956400	H	2.54258900	-2.94550500	-4.49598200
H	2.99153000	-3.26571700	0.63751200	C	1.84662800	-2.90171900	-2.43209400
H	5.01802500	-1.83383200	0.73712100	H	2.87128500	-2.84599200	-2.03699900
C	1.46091400	2.49975900	3.62467900	H	1.55477200	-3.96047700	-2.40269300
H	0.78213900	3.31093400	3.92913800	C	0.90506100	-2.08248200	-1.53416000
H	1.72461200	1.95574200	4.54131500	H	0.93252200	-2.45863700	-0.50788700
C	2.71735300	3.10401000	2.98210200	H	-0.13076300	-2.20604900	-1.88199700
H	3.44446300	2.30226100	2.78597900	C	0.27472200	2.17808900	-0.92211300
H	3.20200700	3.80523600	3.67380800	H	0.02669100	2.19377900	-1.99344700
C	2.37647400	3.80801000	1.66142500	C	-0.74411500	3.09747400	-0.21755700
H	3.28888700	4.19020700	1.18588700	H	-1.75988900	2.71575900	-0.37742100
H	1.74291700	4.68335400	1.87096300	H	-0.56380200	3.08116400	0.86600500
H	1.43981700	-3.10728800	-1.31197500	C	-0.63269100	4.54587700	-0.72321900
<b>3<sub>SP</sub> [Pd(SPhos)(PhCl)] (conformer c)</b>				H	-0.91889000	4.58130700	-1.78522700
Pd	-2.19856300	-0.27419700	-0.88117700	H	-1.34783400	5.18215200	-0.18569600
P	0.00237100	0.35468300	-0.48503100	C	0.79299900	5.09378000	-0.56425900
Cl	-6.02128300	-0.77477500	2.46703000	H	1.03293400	5.16839200	0.50685700
O	2.04882100	-2.76790800	1.57748200	H	0.86096800	6.11033000	-0.97320700
O	3.89248000	1.53109900	1.30575300	C	1.81543800	4.17362000	-1.24591900
C	0.48749300	0.25735600	1.32690100	H	1.65045700	4.19262700	-2.33391100
				H	2.83504400	4.54734100	-1.08041200

C	1.70174100	2.72342000	-0.73988900
H	1.96954200	2.68163400	0.32159000
H	2.43072200	2.09305600	-1.26326800
C	-5.33561600	-0.65410500	0.84859000
C	-5.57733300	0.50636300	0.09530500
C	-5.04208900	0.60520200	-1.18248100
C	-4.28422100	-0.45523300	-1.73911400
C	-4.04836700	-1.61471900	-0.95995100
C	-4.57490900	-1.70150400	0.35170200
H	-6.17464300	1.30933600	0.51385100
H	-5.23609100	1.49242700	-1.77882700
H	-3.61289100	-2.50329500	-1.40883600
H	-4.40861400	-2.59168400	0.94875600
H	-4.03975000	-0.44089900	-2.79800100

**3<sub>tBu</sub> [Pd(P<sup>t</sup>Bu<sub>3</sub>)(PhMe)] *ipso-ortho***

Pd	-1.03373600	-0.22088100	0.26068300
P	1.25405200	0.02574000	-0.02271800
C	1.67028500	1.82192100	-0.67019800
C	2.19791000	-0.24117600	1.66573900
C	1.96133600	-1.25717500	-1.31300900
C	-3.11838100	-0.16461000	1.17915000
C	-3.43381600	1.21652600	1.16032700
C	-3.88251500	1.82322400	-0.00738300
C	-3.98129500	1.06805200	-1.18774100
C	-3.64709500	-0.28162000	-1.18939900
C	-3.24144500	-0.94498100	-0.00043900
H	-2.94775000	-0.65672300	2.13458100
H	-3.35490800	1.78676300	2.08200200
H	-4.14724100	2.87703000	-0.00957400
C	1.45869400	2.83356500	0.47841100
H	1.48823100	3.84831700	0.05932300
H	0.48312300	2.70051300	0.95742100
H	2.23669800	2.78158300	1.24375800
C	3.08206500	2.03608600	-1.25300200
H	3.87679800	1.80758900	-0.53773000
H	3.19388600	3.09177400	-1.53718500
H	3.25700500	1.44426900	-2.15509800
C	0.62076000	2.19261900	-1.74668800
H	0.76398200	3.24505200	-2.02900400
H	0.70451000	1.59712000	-2.65624000
H	-0.39613100	2.07259300	-1.35896800
C	1.38056800	0.44760800	2.78597300
H	1.83750500	0.20454600	3.75539200
H	1.35594200	1.53404300	2.70036300
H	0.34662400	0.08679000	2.78934300
C	3.65123700	0.27046900	1.72003900
H	3.71445500	1.35598100	1.61072700
H	4.29035100	-0.18464400	0.95934300
H	4.08181600	0.02129200	2.69989100
C	2.19169500	-1.74450200	2.02015800
H	2.54787500	-1.86136300	3.05243200
H	1.18144600	-2.16409000	1.96771100
H	2.85251700	-2.33814800	1.38470400
C	3.49187900	-1.44915200	-1.31561300
H	3.76454800	-2.13980800	-2.12579300
H	4.03479800	-0.51623700	-1.48657200

H	3.85974600	-1.89011900	-0.38562800
C	1.51805200	-0.84772300	-2.73501100
H	1.74451900	-1.67447800	-3.42145600
H	0.44008900	-0.66181100	-2.78323500
H	2.04398500	0.03293300	-3.11048900
C	1.28311600	-2.62278400	-1.04492600
H	1.58533600	-3.32841300	-1.83141400
H	1.56088200	-3.06223900	-0.08670800
H	0.19271500	-2.52545100	-1.06616000
H	-4.31802500	1.53936100	-2.10750000
H	-3.74820000	-0.86384800	-2.10270000
C	-3.22156400	-2.45984700	0.04827400
H	-4.24495100	-2.85439300	0.12038500
H	-2.76966600	-2.88161600	-0.85517900
H	-2.66035400	-2.82874300	0.91063500

**3<sub>tBu</sub> [Pd(P<sup>t</sup>Bu<sub>3</sub>)(PhMe)] *ipso***

Pd	1.01645700	0.18030100	-0.39345800
P	-1.24964200	-0.01931000	0.02538800
C	-2.20147000	1.64967600	-0.31528600
C	-2.03302000	-1.39889000	-1.11634500
C	-1.56922300	-0.52675900	1.88516300
C	-2.27862800	1.88663900	-1.83991000
H	-2.63617100	2.90990100	-2.01707900
H	-1.29361200	1.79266400	-2.30933600
H	-2.97428300	1.21282200	-2.34520400
C	-3.62249500	1.75943200	0.27267400
H	-4.29142700	0.97098600	-0.08108300
H	-4.06149800	2.72028300	-0.02998000
H	-3.62301300	1.73911600	1.36515000
C	-1.33871200	2.81067700	0.23637000
H	-1.80521200	3.76381500	-0.04972400
H	-1.24660100	2.80538600	1.32273800
H	-0.32977200	2.77771500	-0.18758500
C	-1.42280800	-1.24771500	-2.53101900
H	-1.75551800	-2.09207700	-3.15075700
H	-1.72567900	-0.33082800	-3.03758200
H	-0.32864300	-1.26056400	-2.48490800
C	-3.57095000	-1.40068500	-1.23190600
H	-3.95484400	-0.49932300	-1.71644300
H	-4.06977400	-1.50515300	-0.26493800
H	-3.88204300	-2.25322400	-1.85180500
C	-1.58115300	-2.78989100	-0.61806700
H	-1.86211300	-3.53804400	-1.37151600
H	-0.49506000	-2.84006800	-0.48958700
H	-2.05967300	-3.08359800	0.31890100
C	-2.97130000	-1.07748000	2.21607400
H	-3.03216000	-1.27304100	3.29580600
H	-3.77272700	-0.37665900	1.96789000
H	-3.18043800	-2.02355400	1.71022800
C	-1.29737900	0.69045200	2.79707200
H	-1.27414400	0.34613900	3.83973000
H	-0.32752600	1.14888200	2.57758400
H	-2.07228700	1.45791600	2.73231600
C	-0.50702900	-1.58191200	2.27869500
H	-0.59997900	-1.79034200	3.35386400
H	-0.62203900	-2.52926400	1.75165000

H	0.50392200	-1.21000700	2.08278300
C	3.82604800	-1.83444500	0.03491500
C	3.39047300	-1.22299700	-1.13663200
C	3.12627000	0.16960700	-1.16782100
C	3.26552100	0.94831000	0.01122200
C	3.67254800	0.28762000	1.19724900
C	3.96889000	-1.07109800	1.20437100
H	4.05093000	-2.89737900	0.04471500
H	3.29386100	-1.79874500	-2.05310700
H	2.98155100	0.66361100	-2.12722600
H	3.79416200	0.87453300	2.10519100
H	4.30702000	-1.54381900	2.12292300
C	3.24343900	2.46313600	-0.03726900
H	4.26803400	2.86065600	-0.06995900
H	2.71463900	2.83074700	-0.92088500
H	2.75560500	2.88424700	0.84820100

H	2.71355400	-2.81831200	0.17597100
C	3.92830100	-0.56850700	-1.22851000
H	4.45994700	-0.68281500	-2.18350000
H	4.40830300	0.25034100	-0.68648000
H	4.08970600	-1.49006300	-0.66319700
C	2.32617400	0.88779700	-2.48863300
H	2.80127000	0.60692600	-3.43811000
H	1.28159900	1.13807100	-2.70173800
H	2.83630000	1.78415900	-2.12868700
C	1.84980800	-1.51719300	-2.27889500
H	2.40801100	-1.64526300	-3.21685000
H	1.92093300	-2.45379000	-1.72574100
H	0.79535900	-1.35042700	-2.52269900
C	-4.01128800	2.37858800	0.01911700
H	-3.06934400	2.93288100	-0.06738100
H	-4.64121300	2.67888500	-0.82882200
H	-4.51030800	2.70506700	0.93706600

**3<sub>tBu</sub>** [Pd(P<sup>*i*</sup>Bu<sub>3</sub>)(PhMe)] *meta-para*

Pd	-0.94332200	-0.20511400	-0.50256500
P	1.30154900	0.02600700	0.04079500
C	1.68390300	1.82641100	0.69197600
C	1.80702000	-1.24095300	1.43798600
C	2.43563100	-0.30559400	-1.51373900
C	-3.39045900	-1.91864300	-0.02210900
C	-4.03397300	-1.31232600	1.04722600
C	-4.22521300	0.08133100	1.06517300
C	-3.77359400	0.88681900	0.02305700
C	-3.12530200	0.26925200	-1.08243200
C	-2.93902200	-1.13290900	-1.11119700
H	-3.25863000	-2.99685200	-0.04934300
H	-4.39956900	-1.91447500	1.87505200
H	-4.74189900	0.53933600	1.90569300
H	-2.93306500	0.86010000	-1.97601500
H	-2.60912900	-1.62163400	-2.02501100
C	1.09094400	1.99142100	2.10890000
H	1.12269800	3.05556600	2.37833200
H	0.04495800	1.66992200	2.14701900
H	1.65287100	1.45166800	2.87468700
C	3.16958100	2.23809400	0.73363900
H	3.77695900	1.57112400	1.35097100
H	3.24914600	3.24523400	1.16619600
H	3.62014000	2.28390700	-0.26130000
C	0.90958400	2.82843800	-0.19874500
H	1.02762200	3.83729400	0.22077400
H	1.26612300	2.85880500	-1.22853300
H	-0.15777500	2.58438600	-0.22004100
C	0.66791700	-1.27477100	2.48600800
H	0.87314700	-2.08253700	3.20227700
H	0.57726500	-0.34991400	3.05626800
H	-0.29764200	-1.47133200	2.00858400
C	3.14296900	-0.96995800	2.15973000
H	3.12596300	-0.03999300	2.73372000
H	3.99514800	-0.93164700	1.47624400
H	3.33403200	-1.78242300	2.87458600
C	1.85688800	-2.66267900	0.83557500
H	1.94747600	-3.38616900	1.65671800
H	0.94041100	-2.89860800	0.28460000

**3<sub>tBu</sub>** [Pd(P<sup>*i*</sup>Bu<sub>3</sub>)(PhMe)] *ortho-meta*

Pd	-0.93447600	-0.28127000	-0.51731400
P	1.29744800	0.02563100	0.04022200
C	1.61614400	-0.46177100	1.90308700
C	2.45522900	-1.07688600	-1.07983500
C	1.83213700	1.89018800	-0.19365200
C	-2.95365600	-1.14336600	-1.09816000
C	-3.40381300	-1.90648900	0.00809600
C	-4.03144300	-1.27570100	1.07287900
C	-4.20912000	0.11984700	1.06838100
C	-3.75457000	0.90367000	0.01120200
C	-3.12073200	0.26132200	-1.08754500
H	-2.64026200	-1.64984300	-2.00858700
H	-3.28453100	-2.98640300	-0.00281500
H	-4.39662800	-1.86018900	1.91344800
H	-2.92176200	0.83700500	-1.98922900
C	1.55443600	-1.99972500	2.03897200
H	1.53988500	-2.25532300	3.10694400
H	0.64370400	-2.40770000	1.58844900
H	2.41949200	-2.50379700	1.60195000
C	2.93871800	0.02806200	2.52740000
H	3.81978000	-0.31917600	1.98150800
H	3.01611000	-0.36137200	3.55217000
H	2.99023300	1.11751400	2.59792100
C	0.43236400	0.07532200	2.74448300
H	0.52485800	-0.31039100	3.76928500
H	0.40588400	1.16353200	2.80767900
H	-0.52470600	-0.26082500	2.33201100
C	1.78334100	-2.46251400	-1.24167400
H	2.36244000	-3.05250700	-1.96577000
H	1.73947400	-3.03470600	-0.31466400
H	0.76095200	-2.35721800	-1.62018600
C	3.90184500	-1.27587900	-0.58312200
H	3.94951600	-1.83019600	0.35795000
H	4.43725100	-0.33248200	-0.44865200
H	4.45745900	-1.86292400	-1.32765500
C	2.50504700	-0.47560000	-2.50192300
H	2.98399600	-1.20260300	-3.17142400
H	1.50031100	-0.27824000	-2.88995200

H	3.09122300	0.44459700	-2.55792700
C	3.34877100	2.16572900	-0.22195600
H	3.51410800	3.24899400	-0.30502400
H	3.85730700	1.82762600	0.68434700
H	3.84140200	1.70241000	-1.08037500
C	1.20011100	2.74221500	0.92901000
H	1.33536900	3.80336000	0.68021200
H	0.12460800	2.55654000	1.01902200
H	1.66659500	2.58030600	1.90321800
C	1.20278600	2.40805000	-1.51008500
H	1.39021900	3.48803200	-1.58848500
H	1.61741900	1.93926200	-2.40281300
H	0.12044300	2.24166200	-1.51583600
H	-4.71521600	0.59684900	1.90480000
C	-3.96905800	2.39881600	-0.01130200
H	-3.01673100	2.93701900	-0.08695700
H	-4.57979100	2.70131300	-0.87228000
H	-4.47746600	2.74210700	0.89532400

**4<sub>Cy</sub><sup>‡</sup> [Pd(PCy<sub>3</sub>)(Ph··Br)]<sup>‡</sup> (conformer F)**

Pd	-1.27078000	-0.06489300	-0.00536700
Br	-3.23514800	1.71210000	0.11567200
P	1.08769700	0.11283300	-0.04755300
C	-3.25611300	-0.49246400	0.05820000
C	-3.64497100	-1.06669700	-1.16849300
C	-4.24028500	-2.33056600	-1.16118900
C	-4.48480400	-2.99542400	0.04475000
C	-4.12901500	-2.39873300	1.25825800
C	-3.53263900	-1.13524100	1.28150000
H	-3.49380000	-0.52585100	-2.09674200
H	-4.52775000	-2.78862100	-2.10433200
H	-4.96602900	-3.96933700	0.03954500
H	-4.33000800	-2.90934000	2.19682100
H	-3.29757200	-0.64608300	2.22087600
C	1.72026700	4.20182700	0.85512500
C	1.27012200	2.73684000	0.98573600
C	1.71757100	1.88395800	-0.22297100
C	1.21835600	2.52797200	-1.53598700
C	1.66784700	3.99395300	-1.66284600
C	1.22679300	4.83064100	-0.45459600
H	2.81920900	4.24966900	0.88997700
H	1.35549500	4.77556600	1.71667400
H	1.66253900	2.31946300	1.92056600
H	0.17411400	2.69633600	1.05922100
H	2.81720400	1.86481700	-0.24830600
H	1.58022900	1.96649000	-2.40544900
H	0.12053000	2.47722400	-1.56196100
H	2.76418600	4.03170700	-1.75007500
H	1.26653900	4.42057300	-2.59106100
H	0.12895500	4.89036500	-0.43625600
H	1.59658700	5.85978700	-0.54780000
C	3.71186500	-0.54412800	3.30532000
C	3.34060900	-0.16670800	1.85900500
C	1.85512800	-0.47689300	1.57708100
C	1.55652800	-1.96650200	1.85286100
C	1.92935200	-2.34811300	3.29539100
C	3.39633500	-2.01656000	3.60746700

H	3.15023400	0.09762700	4.00029700
H	4.77559400	-0.33781200	3.48083000
H	3.98007800	-0.73076000	1.16975400
H	3.55797800	0.89383200	1.69117400
H	1.26191400	0.09680300	2.30572300
H	0.49693100	-2.17965800	1.66477900
H	2.13526200	-2.59251900	1.15962600
H	1.27633200	-1.80095500	3.99128300
H	1.73643100	-3.41601700	3.45957200
H	4.04918000	-2.65796000	2.99655100
H	3.62506700	-2.24715200	4.65571800
C	1.72326200	-2.74935200	-3.11410400
C	1.25692900	-2.17141700	-1.76650300
C	1.87552600	-0.77827500	-1.51481700
C	3.41435900	-0.85567500	-1.58266900
C	3.87759400	-1.42030600	-2.93819900
C	3.25555800	-2.79683500	-3.21565700
H	1.32433300	-2.12712200	-3.92922200
H	1.30133100	-3.75291000	-3.25371100
H	1.54793700	-2.85980800	-0.96174000
H	0.16232800	-2.10417000	-1.74050000
H	1.54430700	-0.14366600	-2.35086600
H	3.86628300	0.12909000	-1.41320400
H	3.78347500	-1.51426200	-0.78559100
H	3.59019200	-0.72170700	-3.73789800
H	4.97319700	-1.48531000	-2.95951400
H	3.64372000	-3.52113900	-2.48383400
H	3.56102300	-3.15991200	-4.20525100

**4<sub>Cy</sub><sup>‡</sup> [Pd(PCy<sub>3</sub>)(Ph··Br)]<sup>‡</sup> (conformer C)**

Pd	1.10216900	0.16484800	-0.17507800
Br	2.34262700	1.95927500	-1.69487700
P	-1.17161600	-0.27394100	0.34621100
C	3.10281800	0.25192400	-0.53048900
C	3.79994000	0.58399800	0.64899300
C	4.78254000	-0.28894700	1.11974700
C	5.10110100	-1.45286500	0.41096000
C	4.43185400	-1.75243700	-0.77895700
C	3.44493000	-0.89551100	-1.27483400
C	-2.35786200	1.18654300	0.08500100
C	-3.67115200	1.19394800	0.89691600
C	-4.58218400	2.35975100	0.46869700
C	-3.86812100	3.71300300	0.59354300
C	-2.54273700	3.71364500	-0.18142100
C	-1.63478200	2.54433000	0.23563000
C	-1.84368300	-1.62818500	-0.78856300
C	-1.55297800	-1.30237400	-2.27054700
C	-1.91883400	-2.48183600	-3.18788600
C	-3.37869400	-2.91941500	-2.99876000
C	-3.67901700	-3.22871300	-1.52514500
C	-3.31859200	-2.04171800	-0.61267600
C	-1.57252400	-0.91374100	2.08402300
C	-1.09014000	0.05351000	3.19622200
C	0.42415400	-0.00235700	3.45512900
C	0.90029100	-1.43357500	3.74175200
C	0.48624300	-2.38643600	2.61129200
C	-1.03075400	-2.33636700	2.36968800

H	3.57842600	1.50923700	1.17037600	C	1.21835600	2.52797200	-1.53598700
H	5.31182500	-0.04857700	2.03849000	C	1.66784700	3.99395300	-1.66284600
H	5.88108000	-2.11460500	0.77678900	C	1.22679300	4.83064100	-0.45459600
H	4.68885500	-2.64816200	-1.33899400	H	2.81920900	4.24966900	0.88997700
H	2.96129700	-1.09424000	-2.22544700	H	1.35549500	4.77556600	1.71667400
H	-2.62659500	1.08938500	-0.97836700	H	1.66253900	2.31946300	1.92056600
H	-3.44211600	1.30384900	1.96523100	H	0.17411400	2.69633600	1.05922100
H	-4.21148700	0.24754700	0.78859000	H	2.81720400	1.86481700	-0.24830600
H	-4.89585900	2.20821100	-0.57494300	H	1.58022900	1.96649000	-2.40544900
H	-5.49848800	2.35329500	1.07339500	H	0.12053000	2.47722400	-1.56196100
H	-3.66718400	3.91762000	1.65587000	H	2.76418600	4.03170700	-1.75007500
H	-4.52010200	4.52130600	0.23840400	H	1.26653900	4.42057300	-2.59106100
H	-2.75262900	3.63765900	-1.25889800	H	0.12895500	4.89036500	-0.43625600
H	-2.01375900	4.66382300	-0.03422700	H	1.59658700	5.85978700	-0.54780000
H	-1.32694500	2.68346100	1.28253300	C	3.71186500	-0.54412800	3.30532000
H	-0.71458400	2.54606300	-0.35872900	C	3.34060900	-0.16670800	1.85900500
H	-1.21755200	-2.49536000	-0.52993800	C	1.85512800	-0.47689300	1.57708100
H	-0.49588300	-1.03738800	-2.39320800	C	1.55652800	-1.96650200	1.85286100
H	-2.13354300	-0.41964000	-2.57696000	C	1.92935200	-2.34811300	3.29539100
H	-1.73488900	-2.20784700	-4.23453800	C	3.39633500	-2.01656000	3.60746700
H	-1.25391900	-3.32964400	-2.96485300	H	3.15023400	0.09762700	4.00029700
H	-3.59980500	-3.79371400	-3.62410800	H	4.77559400	-0.33781200	3.48083000
H	-4.04483900	-2.11334600	-3.34114700	H	3.98007800	-0.73076000	1.16975400
H	-4.73820100	-3.48675900	-1.39659300	H	3.55797800	0.89383200	1.69117400
H	-3.10223400	-4.11201900	-1.21312700	H	1.26191400	0.09680300	2.30572300
H	-3.53175300	-2.30151100	0.43123500	H	0.49693100	-2.17965800	1.66477900
H	-3.96874400	-1.19389400	-0.86763300	H	2.13526200	-2.59251900	1.15962600
H	-2.66653000	-0.96340200	2.13796600	H	1.27633200	-1.80095500	3.99128300
H	-1.61520600	-0.22793700	4.12198700	H	1.73643100	-3.41601700	3.45957200
H	-1.39290200	1.08402900	2.97721800	H	4.04918000	-2.65796000	2.99655100
H	0.95981600	0.38320000	2.57573500	H	3.62506700	-2.24715200	4.65571800
H	0.67324800	0.66011200	4.29443700	C	1.72326200	-2.74935200	-3.11410400
H	0.46260400	-1.78263200	4.68981700	C	1.25692900	-2.17141700	-1.76650300
H	1.98945100	-1.45086300	3.87254100	C	1.87552600	-0.77827500	-1.51481700
H	1.01899300	-2.10599300	1.69171000	C	3.41435900	-0.85567500	-1.58266900
H	0.78425900	-3.41577000	2.84934700	C	3.87759400	-1.42030600	-2.93819900
H	-1.53893800	-2.69672300	3.27753900	C	3.25555800	-2.79683500	-3.21565700
H	-1.31353200	-3.03436100	1.57374500	H	1.32433300	-2.12712200	-3.92922200
<b>4<sub>Cy</sub><sup>‡</sup> [Pd(PCy<sub>3</sub>)(Ph···Cl)]<sup>‡</sup> (conformer F)</b>				H	1.30133100	-3.75291000	-3.25371100
Pd	-1.27078000	-0.06489300	-0.00536700	H	1.54793700	-2.85980800	-0.96174000
P	1.08769700	0.11283300	-0.04755300	H	0.16232800	-2.10417000	-1.74050000
Cl	-3.23514800	1.71210000	0.11567200	H	1.54430700	-0.14366600	-2.35086600
C	-3.25611300	-0.49246400	0.05820000	H	3.86628300	0.12909000	-1.41320400
C	-3.64497100	-1.06669700	-1.16849300	H	3.78347500	-1.51426200	-0.78559100
C	-4.24028500	-2.33056600	-1.16118900	H	3.59019200	-0.72170700	-3.73789800
C	-4.48480400	-2.99542400	0.04475000	H	4.97319700	-1.48531000	-2.95951400
C	-4.12901500	-2.39873300	1.25825800	H	3.64372000	-3.52113900	-2.48383400
C	-3.53263900	-1.13524100	1.28150000	H	3.56102300	-3.15991200	-4.20525100
H	-3.49380000	-0.52585100	-2.09674200	H	1.47349500	-0.01407900	3.09219100
H	-4.52775000	-2.78862100	-2.10433200	<b>4<sub>H</sub><sup>‡</sup> [Pd(PH<sub>3</sub>)(Ph···Br)]<sup>‡</sup></b>			
H	-4.96602900	-3.96933700	0.03954500	Pd	0.85320600	-0.40434000	-0.00001200
H	-4.33000800	-2.90934000	2.19682100	Br	0.01223600	2.04490300	0.00000500
H	-3.29757200	-0.64608300	2.22087600	P	3.01256900	-1.28437500	0.00001100
C	1.72026700	4.20182700	0.85512500	C	-3.44874400	-1.44799100	0.00000400
C	1.27012200	2.73684000	0.98573600	C	-2.86912700	-1.06033600	1.21178500
C	1.71757100	1.88395800	-0.22297100	C	-1.70936900	-0.28091700	1.22696100

C	-1.11540200	0.06437600	0.00000400
C	-1.70937500	-0.28090800	-1.22695300
C	-2.86913200	-1.06032900	-1.21177700
H	-4.36110300	-2.03752700	0.00000400
H	-3.32763600	-1.34988500	2.15380600
H	-1.27892200	0.06174000	2.16186900
H	-1.27893200	0.06175600	-2.16186100
H	-3.32764500	-1.34987100	-2.15379900
H	4.15167400	-0.44227400	0.00020900
H	3.44253500	-2.12695500	1.05532500
H	3.44269000	-2.12667300	-1.05546400

**4<sub>H</sub><sup>‡</sup> [Pd(PH<sub>3</sub>)(Ph···Cl)]<sup>‡</sup>**

Pd	-0.86122700	-0.09081700	0.00001100
P	-3.05151300	-0.93110400	0.00000700
Cl	-0.01615700	2.21774800	-0.00003900
C	3.50663900	-1.07157600	-0.00000200
C	2.90916500	-0.71288200	-1.21213100
C	1.71099800	0.00641500	-1.22741200
C	1.10218700	0.30810500	0.00000300
C	1.71104600	0.00649100	1.22741200
C	2.90921100	-0.71280800	1.21212900
H	4.44781900	-1.61387200	-0.00000300
H	3.38290100	-0.97743300	-2.15395600
H	1.26111500	0.33056100	-2.15984200
H	1.26119400	0.33068800	2.15983900
H	3.38298200	-0.97730300	2.15395200
H	-4.17175500	-0.06456700	-0.00058100
H	-3.49778600	-1.76454400	-1.05546300
H	-3.49813800	-1.76356200	1.05610300

**4<sub>Ph</sub><sup>‡</sup> [Pd(PPh<sub>3</sub>)(Ph···Br)]<sup>‡</sup>**

Pd	-1.19751900	-0.03636800	0.01067500
Br	-2.85076900	-2.08632300	-0.01745200
P	1.14939100	0.10205400	0.00284200
C	-4.84985600	2.36817900	0.01779700
C	-4.44204200	1.80950100	-1.19742900
C	-3.64415800	0.66271000	-1.22034200
C	-3.22250000	0.10684600	0.00315300
C	-3.65876700	0.63648500	1.23311600
C	-4.45624000	1.78359100	1.22555900
H	-5.48639200	3.24842700	0.02355900
H	-4.75864200	2.25605300	-2.13669700
H	-3.36296300	0.19651600	-2.15872000
H	-3.38859300	0.15008800	2.16445500
H	-4.78285900	2.21074000	2.17036300
C	3.13503500	-2.79950200	-3.05053900
C	3.71704600	-1.55022000	-2.82892400
C	3.14329600	-0.65822500	-1.91961300
C	1.97604100	-1.00709000	-1.22344600
C	1.39080500	-2.26173800	-1.46253600
C	1.97108700	-3.15396200	-2.36435100
H	3.58199400	-3.49077200	-3.76011400
H	4.61862800	-1.26549600	-3.36515100
H	3.60316900	0.31239100	-1.75972500
H	0.47213200	-2.53201700	-0.94767200
H	1.50663100	-4.12081500	-2.53871000

C	2.77107800	4.33430900	-1.07596100
C	3.47314000	3.55590100	-0.15422300
C	3.01045700	2.28325000	0.18916400
C	1.83524500	1.77513200	-0.38485200
C	1.13002400	2.57219000	-1.30171800
C	1.59802400	3.83907500	-1.65047400
H	3.13166000	5.32498700	-1.33969800
H	4.38242500	3.93838700	0.30216100
H	3.56291900	1.68979500	0.91137700
H	0.20559000	2.19749400	-1.73548600
H	1.04079600	4.44300300	-2.36166800
C	3.07297300	-0.94940100	4.11127400
C	3.75233600	-1.28582700	2.93912000
C	3.19776600	-0.98341800	1.69325900
C	1.95331200	-0.34109500	1.60665300
C	1.27311500	-0.01749700	2.79185800
C	1.83175700	-0.31317700	4.03541200
H	3.50464100	-1.18907800	5.07937700
H	4.71476100	-1.78812800	2.99172400
H	3.73215300	-1.25618200	0.78815800
H	0.29737200	0.45934000	2.73417200
H	1.29265500	-0.05741600	4.94369700

**4<sub>Ph</sub><sup>‡</sup> [Pd(PPh<sub>3</sub>)(Ph···Cl)]<sup>‡</sup>**

Pd	-1.37173500	0.38760400	0.00171300
P	0.95453600	-0.04231500	0.00399400
Cl	-2.69055600	2.49090300	-0.14731600
C	-5.42489700	-1.43775200	0.11506600
C	-4.92265600	-0.87556300	1.29277800
C	-3.91091600	0.08708600	1.24494500
C	-3.37686100	0.43434800	-0.00692400
C	-3.90436300	-0.07946100	-1.20325000
C	-4.91632000	-1.03975100	-1.12538900
H	-6.22487400	-2.17109700	0.16280700
H	-5.32868000	-1.17357400	2.25616000
H	-3.54489200	0.56378800	2.14823200
H	-3.53315700	0.27024900	-2.16092000
H	-5.31837500	-1.46469200	-2.04171200
C	3.60747500	3.74260800	-0.53616400
C	4.12725000	2.64344000	0.15124700
C	3.35042300	1.49759000	0.33176100
C	2.04263400	1.43951300	-0.17546300
C	1.52381500	2.55453800	-0.85208100
C	2.30493200	3.69635600	-1.03689700
H	4.21248200	4.63513900	-0.67207100
H	5.13704100	2.67813600	0.55186200
H	3.76020500	0.65176400	0.87616600
H	0.50033300	2.53060800	-1.21769500
H	1.88971500	4.55327000	-1.56036800
C	2.47032900	-2.01514300	3.94105600
C	2.99230800	-2.45040600	2.72215200
C	2.55703900	-1.87640300	1.52485200
C	1.58946400	-0.86099100	1.53481200
C	1.06226500	-0.43770800	2.76659900
C	1.50463300	-1.00552500	3.96099200
H	2.80898800	-2.46426200	4.87087800
H	3.73933700	-3.23958600	2.69942700

H	2.96783900	-2.22540000	0.58231100
H	0.29918700	0.33697100	2.78510500
H	1.08833000	-0.66651100	4.90586800
C	2.18503200	-2.96613000	-3.40737800
C	3.05238700	-1.92903000	-3.06071500
C	2.71174200	-1.03718000	-2.04065500
C	1.49450200	-1.17170900	-1.35667400
C	0.62350400	-2.21205200	-1.72191300
C	0.96897800	-3.10700400	-2.73429800
H	2.45131000	-3.65691000	-4.20292400
H	3.99649700	-1.80940000	-3.58573000
H	3.39265600	-0.23143500	-1.78464300
H	-0.33298700	-2.31306700	-1.21363300
H	0.28409700	-3.90641800	-3.00422100

**4<sub>SP</sub><sup>‡</sup> [Pd(SPhos)(Ph··Br)]<sup>‡</sup> (conformer a) *trans* phenyl**

Pd	1.06894100	0.46210800	0.32334600
Br	2.45156400	-0.18778700	2.52642300
P	-1.23863900	0.52801000	-0.22017300
C	-0.24007500	-2.52235500	-0.92979400
C	0.96294200	-2.56786000	-1.66154400
C	2.09826300	-3.20932000	-1.14685000
C	2.02705500	-3.80357500	0.11182800
C	0.85515600	-3.77341200	0.86353100
C	-0.27600600	-3.13736000	0.33491800
C	-1.48412900	-1.99372400	-1.57812100
C	-2.01003400	-0.69315800	-1.39984700
C	-3.17357300	-0.34600700	-2.11269600
C	-3.81380800	-1.23965600	-2.96854400
C	-3.29709100	-2.52341000	-3.13156500
C	-2.14440600	-2.88474700	-2.44122100
H	3.02002300	-3.25312400	-1.71427300
H	0.83082800	-4.23831800	1.84096000
H	-3.59328700	0.64815300	-2.00748800
H	-4.70943500	-0.93099100	-3.50145100
H	-3.78248800	-3.23609100	-3.79310800
H	-1.72890000	-3.88039100	-2.56934500
C	3.03913300	0.81261100	0.66107300
C	3.20506400	2.21047200	0.75505300
C	3.82910700	0.04994200	-0.22349700
C	4.10770600	2.84407700	-0.10359000
H	2.65548000	2.77494500	1.50080100
C	4.72360100	0.70977700	-1.06871800
C	4.86737500	2.10050600	-1.01131100
H	5.32510200	0.12979300	-1.76504200
C	-1.59435500	-3.69887700	2.25380500
H	-0.91570800	-3.24485700	2.98689300
H	-2.62714000	-3.54079500	2.57007500
H	-1.39540200	-4.77677100	2.19334700
C	2.10734400	-1.93281600	-3.66563500
H	2.91088200	-1.39046000	-3.15167300
H	2.45145300	-2.94477000	-3.91836900
H	1.84413600	-1.40312800	-4.58286000
H	2.90441700	-4.30045600	0.51685600
O	-1.48030400	-3.07819100	0.98216500
O	0.92319200	-1.96343800	-2.88527300
C	-1.65431500	2.19370500	-1.00213000

C	-1.22300600	3.36566400	-0.09334600
C	-0.97984300	2.32047500	-2.38638300
H	-2.74195400	2.26473800	-1.13654200
C	-1.51112200	4.72813600	-0.74824600
H	-0.14695000	3.27850700	0.11431300
H	-1.73346100	3.31267800	0.87498100
C	-1.26638100	3.68354000	-3.03861700
H	0.10556300	2.19525300	-2.26246900
H	-1.31161700	1.51324300	-3.04858700
C	-0.85030700	4.84731900	-2.12837800
H	-1.16517900	5.53366100	-0.08751500
H	-2.59878300	4.85769500	-0.85430000
H	-0.74584600	3.74669200	-4.00292900
H	-2.34172700	3.76208700	-3.25910400
H	-1.10734000	5.80795300	-2.59301300
H	0.24301600	4.83848100	-2.00755400
C	-2.39133000	0.32390800	1.27632100
C	-1.75106500	0.81857200	2.59103600
C	-3.81964000	0.88171800	1.12191200
H	-2.46207600	-0.77108700	1.34158000
C	-2.62623700	0.45978300	3.80461200
H	-1.62107500	1.90926600	2.55948200
H	-0.74866600	0.39147000	2.70472700
C	-4.69157600	0.52585900	2.34102000
H	-3.78280400	1.97587400	1.02301700
H	-4.29025000	0.49277600	0.21224100
C	-4.05480500	1.00157500	3.65469200
H	-2.16431200	0.84628800	4.72222600
H	-2.66379700	-0.63499600	3.91102500
H	-5.69252600	0.96076500	2.22052600
H	-4.82734800	-0.56520700	2.37737300
H	-4.67269300	0.69727300	4.50947900
H	-4.02676200	2.10156400	3.66524900
H	3.73676100	-1.03030000	-0.23529100
H	4.23015800	3.92285500	-0.04497500
H	5.58228900	2.59999400	-1.65914400

**4<sub>SP</sub><sup>‡</sup> [Pd(SPhos)(Ph··Br)]<sup>‡</sup> (conformer c) *trans* phenyl**

Pd	1.06885000	0.46229000	0.32319900
Br	2.45162200	-0.18661000	2.52650300
P	-1.23873800	0.52772300	-0.22026800
C	-0.23967500	-2.52260700	-0.92934500
C	0.96323900	-2.56817100	-1.66126200
C	2.09872300	-3.20932700	-1.14654800
C	2.02778800	-3.80320600	0.11232400
C	0.85600200	-3.77296300	0.86420000
C	-0.27532800	-3.13723200	0.33556000
C	-1.48389800	-1.99434800	-1.57765300
C	-2.01000800	-0.69382700	-1.39963800
C	-3.17366800	-0.34704400	-2.11246700
C	-3.81383800	-1.24100800	-2.96803400
C	-3.29693100	-2.52472100	-3.13078000
C	-2.14411800	-2.88569700	-2.44046000
H	3.02039600	-3.25320200	-1.71410900
H	0.83188700	-4.23756700	1.84177800
H	-3.59353800	0.64707200	-2.00746200
H	-4.70956400	-0.93262100	-3.50093400



H	-3.78227600	-3.23764700	-3.79209800
H	-1.72845800	-3.88130100	-2.56838400
C	3.03899500	0.81320100	0.66086600
C	3.20481400	2.21110600	0.75443800
C	3.82897500	0.05035000	-0.22354500
C	4.10736900	2.84453500	-0.10442100
H	2.65520400	2.77574700	1.50004000
C	4.72336300	0.71002000	-1.06901100
C	4.86704300	2.10077300	-1.01198500
H	5.32485900	0.12988900	-1.76521700
C	-1.59331800	-3.69836300	2.25480600
H	-0.91460900	-3.24406800	2.98766600
H	-2.62607100	-3.54030500	2.57119300
H	-1.39425700	-4.77625200	2.19461700
C	2.10734900	-1.93327800	-3.66556200
H	2.91076000	-1.39070800	-3.15163000
H	2.45169800	-2.94516000	-3.91826200
H	1.84400100	-1.40369300	-4.58280700
H	2.90527600	-4.29985200	0.51736600
O	-1.47953100	-3.07801700	0.98297700
O	0.92321600	-1.96415200	-2.88518200
C	-1.65473500	2.19316900	-1.00255700
C	-1.22356900	3.36539600	-0.09405500
C	-0.98038600	2.31978500	-2.38688200
H	-2.74239400	2.26397900	-1.13691000
C	-1.51207300	4.72766800	-0.74919400
H	-0.14746600	3.27851400	0.11347600
H	-1.73388500	3.31248500	0.87435100
C	-1.26729800	3.68264300	-3.03938400
H	0.10505900	2.19484700	-2.26301300
H	-1.31201500	1.51233000	-3.04888600
C	-0.85144200	4.84672500	-2.12942800
H	-1.16623800	5.53340900	-0.08866900
H	-2.59977600	4.85695700	-0.85514800
H	-0.74684400	3.74571800	-4.00374300
H	-2.34267700	3.76088200	-3.25981500
H	-1.10878500	5.80718900	-2.59424000
H	0.24189700	4.83821000	-2.00872200
C	-2.39130900	0.32378400	1.27635500
C	-1.75090200	0.81868500	2.59091100
C	-3.81966200	0.88151300	1.12199100
H	-2.46200800	-0.77120100	1.34179300
C	-2.62593700	0.46011800	3.80464400
H	-1.62090200	1.90937200	2.55914600
H	-0.74848800	0.39160600	2.70456300
C	-4.69145800	0.52598600	2.34129900
H	-3.78289000	1.97564000	1.02275500
H	-4.29037200	0.49227800	0.21249700
C	-4.05449900	1.00193700	3.65479500
H	-2.16389500	0.84675000	4.72214500
H	-2.66352600	-0.63464300	3.91123100
H	-5.69238100	0.96096300	2.22083100
H	-4.82733400	-0.56505900	2.37790400
H	-4.67229500	0.69782900	4.50971900
H	-4.02641200	2.10192700	3.66513000
H	3.73673000	-1.02990500	-0.23502100
H	4.22974300	3.92333800	-0.04611300

H	5.58188500	2.60013800	-1.65999300
<b>4<sub>sp</sub><sup>†</sup> [Pd(SPhos)(Ph···Br)]<sup>†</sup> (conformer c) <i>trans</i> halide</b>			
Pd	2.25810600	-0.17022800	-0.01091800
Br	4.26882600	0.65198100	-1.56547800
P	-0.09632700	0.19132400	-0.09429400
O	-3.48451100	1.90056500	1.42159500
O	-3.58292000	-2.68107100	0.42178300
C	-0.96613500	-0.47694500	1.43125800
C	-2.34350700	-0.62194800	1.74431200
C	-3.50638100	-0.37103000	0.83135300
C	-4.09814700	0.90082800	0.72047800
C	-5.25304500	1.10055600	-0.05021700
H	-5.69310700	2.08491700	-0.15091300
C	-5.84412000	0.00921900	-0.68091800
H	-6.73878600	0.15987500	-1.27891800
C	-5.31776000	-1.27437700	-0.55075200
H	-5.80565300	-2.11024400	-1.03673900
C	-4.15869400	-1.45948700	0.21509700
C	-2.70653500	-1.08473500	3.02111200
H	-3.76457400	-1.19354900	3.24293300
C	-1.76557600	-1.40866900	3.99400500
H	-2.09002300	-1.76100300	4.96972600
C	-0.41302600	-1.28303700	3.69312600
H	0.34795800	-1.53800700	4.42580900
C	-0.03516500	-0.82874800	2.43158600
H	1.02454300	-0.74046400	2.20182100
C	-4.23567000	-3.83634300	-0.08253200
H	-5.25240900	-3.93037100	0.32014100
H	-3.63376200	-4.68397700	0.24936500
H	-4.27971400	-3.83176300	-1.17933600
C	-4.13857800	3.15742000	1.51654600
H	-4.19148200	3.66357200	0.54383600
H	-3.53351800	3.75624600	2.19880000
H	-5.15198300	3.05015800	1.92387400
C	-0.52917100	2.02197900	-0.17105700
H	-1.61253300	2.12163300	-0.30851200
C	0.20144400	2.68381800	-1.36126200
H	1.28021400	2.49965500	-1.26176500
H	-0.10389700	2.22791400	-2.31039400
C	-0.05096400	4.20055300	-1.41640100
H	0.50431900	4.63395200	-2.25811600
H	-1.11729400	4.38777600	-1.61526400
C	0.34760300	4.88527900	-0.10248900
H	1.43459400	4.79292000	0.03787200
H	0.12723400	5.95981400	-0.14795000
C	-0.37457700	4.24064000	1.08816100
H	-1.45304000	4.43896900	1.00159000
H	-0.04748700	4.70053900	2.03000700
C	-0.14036700	2.72127800	1.14907600
H	-0.70626500	2.29150300	1.98201500
H	0.92412700	2.53064500	1.35128600
C	-0.74901100	-0.54757100	-1.70527400
H	0.07087100	-0.26108500	-2.38199100
C	-0.74665400	-2.08955900	-1.63748400
H	0.21347500	-2.44249700	-1.23887100
H	-1.52297700	-2.42510100	-0.93916700

C	-0.99359800	-2.70659000	-3.02505700
H	-0.13909500	-2.47650800	-3.67863800
H	-1.03669400	-3.80074100	-2.94305500
C	-2.27929500	-2.16785800	-3.67033700
H	-3.14890100	-2.50228500	-3.08441400
H	-2.40314900	-2.58434300	-4.67855000
C	-2.27442100	-0.63299300	-3.72419200
H	-1.47640300	-0.29796800	-4.40375400
H	-3.21858900	-0.26338600	-4.14509800
C	-2.05246400	-0.01512800	-2.33106400
H	-2.90599100	-0.25499200	-1.69308300
H	-2.02360800	1.07691500	-2.41908700
C	5.37154800	-2.22300400	2.18975400
C	5.24277100	-0.84521400	2.39356100
C	4.69222800	-0.02786400	1.40353400
C	4.22871400	-0.62083400	0.21072700
C	4.38729500	-2.00327000	-0.01937200
C	4.94131000	-2.79602300	0.98883000
H	5.81992100	-2.84597900	2.95855300
H	5.58695200	-0.39691000	3.32238600
H	4.63290400	1.04717800	1.53666200
H	4.09611400	-2.43439200	-0.97137100
H	5.04999000	-3.86532100	0.82501400

**4<sub>sp</sub><sup>+</sup> [Pd(SPhos)(Ph···Cl)]<sup>+</sup> (conformer c) *trans* phenyl**

Pd	0.95469600	-1.02750100	-0.35122300
P	-1.22270900	-0.21862800	0.21299400
Cl	1.48400200	-3.24080700	-1.48125900
C	0.65447800	2.39188000	0.71719000
C	1.88912200	1.96270300	1.24416500
C	3.08771100	2.19805600	0.55735700
C	3.04848200	2.87502400	-0.65898000
C	1.84822000	3.32967000	-1.20081500
C	0.65650600	3.09086300	-0.50349100
C	-0.59743400	2.25228100	1.52851100
C	-1.49634200	1.16373500	1.43702900
C	-2.63061700	1.17104600	2.26926100
C	-2.88130000	2.20500700	3.16996500
C	-1.99147400	3.27344900	3.25580100
C	-0.86526700	3.28773000	2.43772200
H	4.03340600	1.84292200	0.94623900
H	1.84890600	3.86512600	-2.14223400
H	-3.34071000	0.35309200	2.22297800
H	-3.76824400	2.17142500	3.79737400
H	-2.16999500	4.08834700	3.95238000
H	-0.16419500	4.11561700	2.49760200
C	2.78600300	-1.74938900	-0.82663200
C	3.51777600	-2.08434600	0.33089500
C	3.37348200	-0.99151900	-1.85870900
C	4.80879700	-1.57437400	0.48371000
H	3.08380200	-2.74386000	1.07536900
C	4.66377600	-0.49189600	-1.67824200
C	5.38484700	-0.78078400	-0.51470600
H	5.11400200	0.11288700	-2.46168100
C	-0.63452400	4.30043500	-2.11997500
H	-0.29072700	3.73619500	-2.99700400
H	-1.68710000	4.55979200	-2.24883300

H	-0.04260300	5.22041600	-2.02863300
C	3.02736300	0.92430500	3.07513000
H	3.55123200	0.17339000	2.47238500
H	3.69308800	1.77839400	3.25853900
H	2.73309900	0.48466500	4.02989800
H	3.97581200	3.05416100	-1.19625000
O	-0.57035700	3.52218900	-0.93581400
O	1.81856200	1.33597000	2.45366400
C	-2.22225300	-1.64797200	0.93209100
C	-2.31963800	-2.82448300	-0.06489500
C	-1.58391000	-2.12378900	2.25730800
H	-3.24617000	-1.30870700	1.13880900
C	-3.07325400	-4.02006500	0.54401000
H	-1.30945200	-3.13709800	-0.36013500
H	-2.82938100	-2.50912200	-0.98182200
C	-2.33770900	-3.32110300	2.85999200
H	-0.54172700	-2.41337900	2.05947200
H	-1.54645100	-1.30236100	2.98192600
C	-2.43971300	-4.48333100	1.86267900
H	-3.09471500	-4.84497600	-0.17958200
H	-4.12102100	-3.73595300	0.72565300
H	-1.83436100	-3.64734500	3.77931100
H	-3.34978200	-3.00436700	3.15447700
H	-3.01921300	-5.30917900	2.29513100
H	-1.43263600	-4.87641000	1.66060600
C	-2.20363200	0.45139800	-1.26347300
C	-1.80232700	-0.20918700	-2.59963300
C	-3.73543600	0.47271300	-1.09247100
H	-1.86093200	1.49474100	-1.30131800
C	-2.49227400	0.48256400	-3.78822300
H	-2.07668300	-1.27200000	-2.59611700
H	-0.71256800	-0.17599200	-2.71897100
C	-4.41868400	1.16235200	-2.28773900
H	-4.11794000	-0.55451200	-1.01390400
H	-4.00863600	0.98746400	-0.16388600
C	-4.01877400	0.51295400	-3.62051100
H	-2.22089400	-0.02559000	-4.72260300
H	-2.11794000	1.51419200	-3.87306800
H	-5.50876400	1.13377400	-2.16001800
H	-4.13348900	2.22478600	-2.30060300
H	-4.48500100	1.04604800	-4.45923900
H	-4.40525700	-0.51673900	-3.65115400
H	2.82692800	-0.81213000	-2.77875400
H	5.37566100	-1.81980000	1.37899900
H	6.39957400	-0.41058300	-0.39730600

**4<sub>sp</sub><sup>+</sup> [Pd(SPhos)(Ph···Cl)]<sup>+</sup> (conformer c) *trans* halide**

Pd	-0.56759900	-1.16361100	-0.46409400
P	0.03486100	0.94452600	0.29295200
Cl	-1.20494200	-3.31406200	-1.39035200
C	2.65834700	-1.01355900	0.42282000
C	2.29236800	-2.28791100	0.90095300
C	2.46979400	-3.43329300	0.11352800
C	3.02123600	-3.30133700	-1.15861800
C	3.40634900	-2.05902200	-1.65839500
C	3.22977700	-0.92159700	-0.85963600
C	2.60130100	0.17449600	1.33571700

C	1.52280200	1.08753300	1.41444200	C	-3.17532900	-1.34970500	-2.01853800
C	1.61769200	2.14239600	2.34180800	C	-3.28934600	-2.26438500	0.24453500
C	2.72819700	2.30721500	3.16771200	C	-4.46187700	-0.83662900	-1.86142300
C	3.78839700	1.40782600	3.08121800	H	-2.63555500	-1.22997000	-2.95141600
C	3.71513500	0.35707400	2.17148800	C	-4.57597200	-1.74113100	0.37622600
H	2.17671200	-4.41077200	0.47546100	H	-2.83995000	-2.84739100	1.04080400
H	3.83793400	-1.98650000	-2.64899800	C	-5.16802600	-1.02299600	-0.66763600
H	0.80753800	2.85709900	2.43187500	H	-4.91967600	-0.29672000	-2.68665600
H	2.75991300	3.13495000	3.87157500	H	-5.12373500	-1.91199600	1.29980600
H	4.66317900	1.51948400	3.71643900	H	-6.17626300	-0.63368900	-0.56130000
H	4.53400700	-0.35343900	2.10060900				
C	4.22001800	0.49841200	-2.51440000				
H	3.55375300	0.19918200	-3.33405500	<b>4<sub>sr</sub><sup>*</sup> [Pd(SPhos)(PhCl)]<sup>‡</sup> (conformer c) ???</b>			
H	4.44617600	1.56272200	-2.60326900	Pd	2.49773600	0.04649400	-0.11220000
H	5.15267700	-0.07702200	-2.57908400	P	0.10470200	0.23354500	-0.18053100
C	1.32024000	-3.54680800	2.68724300	Cl	4.33324900	1.44287700	-1.10801900
H	0.51483900	-3.96573400	2.07109700	O	-3.32059600	1.91662100	1.27862000
H	2.13525400	-4.27848600	2.76969500	O	-3.19930900	-2.74030800	0.72703800
H	0.93630700	-3.32325800	3.68418600	C	-0.67953700	-0.31674600	1.43329100
H	3.15720500	-4.18688100	-1.77363600	C	-2.03708900	-0.50253000	1.80492400
O	3.59816700	0.33915000	-1.24949800	C	-3.23590200	-0.40066700	0.91008900
O	1.77949900	-2.31027600	2.16536300	C	-3.89686000	0.82322700	0.69607700
C	-1.32566400	1.79967800	1.27931600	C	-5.08090500	0.88736700	-0.05345300
C	-2.60689900	1.98121300	0.43727800	H	-5.57544700	1.83377700	-0.23424200
C	-1.63677300	0.99995700	2.56328300	C	-5.62974000	-0.28872700	-0.55705300
H	-0.97822600	2.80131900	1.56684100	H	-6.54669200	-0.24233600	-1.13824100
C	-3.73609900	2.62887500	1.25905400	C	-5.03256300	-1.52533300	-0.32072700
H	-2.93795600	1.00446300	0.06438800	H	-5.48737500	-2.42814900	-0.70924800
H	-2.40169200	2.59976300	-0.44375500	C	-3.84539500	-1.57565700	0.42234000
C	-2.76654100	1.64956100	3.38015400	C	-2.33716400	-0.85442300	3.13234900
H	-1.93199600	-0.01862300	2.27664200	H	-3.38066600	-0.99635000	3.39958000
H	-0.73711500	0.90312100	3.18118600	C	-1.35194300	-1.02873100	4.09985600
C	-4.03625200	1.83615000	2.53818600	H	-1.62807000	-1.29876200	5.11582600
H	-4.63861900	2.70957200	0.63950700	C	-0.01761400	-0.86047300	3.74328800
H	-3.44868900	3.65670200	1.52824500	H	0.77658500	-0.99851700	4.47202300
H	-2.98054900	1.03652600	4.26550500	C	0.29795400	-0.51407600	2.43147400
H	-2.43079800	2.62891400	3.75377100	H	1.34381800	-0.38782800	2.15937300
H	-4.81476900	2.34012300	3.12579400	C	-3.80636900	-3.97206800	0.36758300
H	-4.43533500	0.84961000	2.26220400	H	-4.80518800	-4.07153400	0.81160100
C	0.55215500	2.14790300	-1.08079800	H	-3.15288700	-4.75019900	0.76564900
C	-0.22142500	1.92685300	-2.39799400	H	-3.88121600	-4.08611700	-0.72164100
C	0.57334200	3.64084800	-0.69961400	C	-4.04527700	3.13822400	1.28421200
H	1.59043700	1.83407600	-1.25996300	H	-4.15099700	3.55409300	0.27382700
C	0.35849300	2.78743600	-3.53400500	H	-3.46034100	3.82753800	1.89475600
H	-1.28144900	2.18174000	-2.26301100	H	-5.04053600	3.00910000	1.72813100
H	-0.19042500	0.86418100	-2.66607400	C	-0.45558500	2.00853700	-0.46070200
C	1.14809700	4.49910700	-1.84207300	H	-1.54591000	2.02459300	-0.58060800
H	-0.44732700	3.98391400	-0.47863400	C	0.20776000	2.56391100	-1.74185700
H	1.16732600	3.79646900	0.20805300	H	1.29752900	2.45386100	-1.65438800
C	0.39115300	4.27635500	-3.15925500	H	-0.09430600	1.98175000	-2.62081000
H	-0.22580800	2.63692300	-4.45125900	C	-0.13549700	4.04640600	-1.96753500
H	1.38185600	2.44868500	-3.75620500	H	0.37649900	4.40765900	-2.86856000
H	1.12064800	5.55985700	-1.55993100	H	-1.21494100	4.14830000	-2.15786200
H	2.20803200	4.24139100	-1.98453400	C	0.24901400	4.90198900	-0.75328300
H	0.84869700	4.86428500	-3.96557500	H	1.34167400	4.88465800	-0.63114500
H	-0.64026400	4.64438600	-3.05124400	H	-0.03300600	5.95008500	-0.91829900
C	-2.56918300	-2.01596600	-0.93791100	C	-0.41312700	4.36503900	0.52285400

H	-1.50297600	4.48932000	0.43901900	C	-2.15804600	-0.93555500	-0.81394200
H	-0.09787300	4.95301700	1.39485100	C	-2.03450300	-2.34670400	-0.19136200
C	-0.08686800	2.88017300	0.75849800	C	-2.99097200	-3.33903700	-0.87515800
H	-0.61431500	2.51832700	1.64722400	C	-4.44385500	-2.84232600	-0.84686700
H	0.99008500	2.77719900	0.95650300	H	-4.32257600	-1.47306900	-2.52123700
C	-0.51672000	-0.73478400	-1.67726500	H	-5.59796900	-1.07350800	-1.37453500
H	0.26381500	-0.46532000	-2.40605400	H	-3.92504900	-0.34168200	0.29825100
C	-0.39185400	-2.25399000	-1.43628400	H	-3.71658600	0.55155300	-1.20664800
H	0.60047200	-2.48692200	-1.02883800	H	-1.89475800	-1.04309300	-1.87644100
H	-1.12607200	-2.56563400	-0.68326800	H	-1.00400300	-2.72221500	-0.27676100
C	-0.61797100	-3.04325000	-2.73751600	H	-2.25778000	-2.30430800	0.88220800
H	0.20166300	-2.82583800	-3.43847800	H	-2.67432400	-3.47995100	-1.91893200
H	-0.57333700	-4.12074500	-2.53126700	H	-2.91077800	-4.31916400	-0.38984800
C	-1.95542900	-2.68027700	-3.40014000	H	-4.80064700	-2.82143200	0.19358400
H	-2.78229200	-3.00826800	-2.75222800	H	-5.09423100	-3.54262000	-1.38538000
H	-2.06916400	-3.21930900	-4.34969400	C	-1.67593100	0.74335100	3.90828000
C	-2.07142100	-1.16610900	-3.62842000	C	-1.52597400	0.03856800	2.54868900
H	-1.31629800	-0.85260000	-4.36486700	C	-1.30816400	1.06436800	1.41391900
H	-3.05004700	-0.91962800	-4.06039400	C	-2.47260500	2.08018500	1.38034100
C	-1.86972100	-0.37706100	-2.32096000	C	-2.60628800	2.79229400	2.73904200
H	-2.68927300	-0.60635600	-1.63609500	C	-2.79964900	1.79057800	3.88625600
H	-1.92634900	0.69699800	-2.53039800	H	-0.72573300	1.23427700	4.16459800
C	5.94067100	-2.39622700	1.21839500	H	-1.86307300	-0.00226400	4.69102400
C	5.65527000	-1.22915700	1.93480200	H	-2.43521800	-0.54410500	2.34689200
C	4.93420700	-0.18982700	1.34277600	H	-0.69467300	-0.67602800	2.58243300
C	4.45744100	-0.36285100	0.03077500	H	-0.39107100	1.62016200	1.66044600
C	4.78075800	-1.50712000	-0.72056200	H	-2.32861100	2.82408300	0.58968300
C	5.50325000	-2.53111000	-0.10284400	H	-3.41334700	1.56374100	1.15745800
H	6.51812200	-3.19056900	1.68282200	H	-1.70194400	3.39031600	2.92413000
H	6.00779900	-1.11741500	2.95729000	H	-3.44557400	3.49838900	2.70309000
H	4.74603500	0.73769600	1.87366300	H	-3.76685100	1.28126300	3.76140200
H	4.47716000	-1.58137700	-1.75969100	H	-2.84679600	2.31753700	4.84732800
H	5.73732300	-3.43156100	-0.66548100	C	2.29482100	0.32517800	0.47539000
<b>5<sub>Cy</sub> [Pd(PCy<sub>3</sub>)(Ph)(Br)] (conformer F)</b>				C	3.18698100	0.83115100	-0.47647700
Pd	1.05565200	-1.12646000	-0.03724000	C	2.34774200	0.77606700	1.79779900
Br	2.64316100	-2.98465300	0.01639700	C	4.11545400	1.80948100	-0.10227000
P	-0.81318900	0.24234200	-0.20221300	H	3.17708800	0.45840700	-1.49593100
C	-0.40988400	2.23907400	-3.91986000	C	3.28339100	1.75303000	2.16077500
C	-0.36839900	1.11577400	-2.86869600	H	1.68672700	0.36066900	2.55247900
C	-0.81663600	1.62374700	-1.47864600	C	4.16335600	2.27677200	1.21289800
C	0.05353700	2.82955400	-1.05469900	H	4.80987500	2.19509000	-0.84501100
C	0.00120500	3.95215000	-2.10610800	H	3.32451400	2.09351900	3.19286300
C	0.42882100	3.45061600	-3.49173400	H	4.88943100	3.03290600	1.49885700
H	-1.45316800	2.55378100	-4.07186700	<b>5<sub>Cy</sub> [Pd(PCy<sub>3</sub>)(Ph)(Br)] (conformer C)</b>			
H	-0.05803200	1.84936100	-4.88323400	Pd	1.42098000	-0.12029900	0.04336100
H	-0.99861300	0.28505600	-3.20672900	Br	3.85887400	-0.15892800	0.32834600
H	0.65396700	0.72109900	-2.79329100	P	-0.85125900	-0.48782300	-0.31402900
H	-1.85994800	1.96517300	-1.56069000	C	1.21776300	1.77964100	0.56935700
H	-0.26838800	3.22542300	-0.08543700	C	1.28656700	2.77134100	-0.41507700
H	1.09088800	2.49881600	-0.92809300	C	1.18258700	4.11919700	-0.05129600
H	-1.02243300	4.35230700	-2.16289600	C	1.01681000	4.48049400	1.28715900
H	0.64313700	4.78164300	-1.78429900	C	0.96740000	3.48670000	2.26656600
H	1.49012700	3.16444800	-3.46088300	C	1.06987400	2.13536100	1.91386400
H	0.34183800	4.25466200	-4.23317500	C	-1.75520700	-0.99115000	1.26332900
C	-4.56445800	-1.43475500	-1.44895400	C	-3.06308100	-1.79134500	1.07498600
C	-3.61797400	-0.44112400	-0.75079100	C	-3.77719000	-2.01075500	2.42165400

C	-2.85961200	-2.68763200	3.44968300	Cl	1.53316800	3.79692100	-0.44188200
C	-1.55152900	-1.90294000	3.62750000	C	0.69494700	-1.63084900	4.01366100
C	-0.82953900	-1.69011300	2.28636800	C	0.29092100	-0.66260800	2.88782000
C	-1.87310700	0.90856000	-1.08150300	C	-0.05898700	-1.41750500	1.58440600
C	-2.24892900	1.99969000	-0.05122000	C	1.12443400	-2.32093200	1.16553300
C	-2.83528800	3.23614100	-0.75319500	C	1.51460800	-3.29124500	2.29408300
C	-4.05539300	2.87474600	-1.61098700	C	1.85299900	-2.54399900	3.59055000
C	-3.72676600	1.74690300	-2.59941200	H	-0.17327600	-2.24809000	4.28900100
C	-3.13036400	0.51522200	-1.89158700	H	0.96528100	-1.05606100	4.90828500
C	-1.01222100	-1.92151500	-1.53792300	H	-0.55341700	-0.05091900	3.22664800
C	-0.35978700	-3.23226900	-1.03793900	H	1.11666100	0.03218000	2.68434900
C	1.17372000	-3.21964000	-1.10516100	H	-0.93075500	-2.06008500	1.78233600
C	1.67341100	-2.91429500	-2.52287200	H	0.88134300	-2.89349500	0.26401700
C	1.07533700	-1.60228700	-3.04701900	H	1.98601600	-1.69160400	0.91448100
C	-0.45914700	-1.57919300	-2.94759300	H	0.68374900	-3.98830200	2.48141800
H	1.43663700	2.50666400	-1.45772800	H	2.36698200	-3.90137100	1.97013000
H	1.24261400	4.88515200	-0.82107400	H	2.75559800	-1.93630100	3.43245000
H	0.93912400	5.52793300	1.56577100	H	2.08906100	-3.25545400	4.39179200
H	0.85791500	3.75664000	3.31435800	C	-4.63069700	0.24956900	1.56642700
H	1.04935600	1.37515700	2.68901200	C	-3.44721500	-0.42509900	0.84920200
H	-2.01888700	-0.01816500	1.70161000	C	-2.20514200	0.48930200	0.85812400
H	-2.83661200	-2.76911100	0.62852800	C	-2.53614400	1.85453100	0.20928500
H	-3.73847100	-1.27950700	0.38095900	C	-3.72908600	2.52695100	0.91103200
H	-4.10882600	-1.03845100	2.81488100	C	-4.96285400	1.61312500	0.94261000
H	-4.68356300	-2.60893300	2.26364500	H	-4.38089800	0.38368500	2.62919600
H	-2.62727800	-3.70841700	3.11152300	H	-5.50645600	-0.41090700	1.53261600
H	-3.37793300	-2.78816900	4.41138600	H	-3.73909300	-0.63457400	-0.18805200
H	-1.77350700	-0.92369100	4.07707600	H	-3.22792100	-1.39130300	1.31942900
H	-0.88450000	-2.42333700	4.32578600	H	-1.96029700	0.69778900	1.90982300
H	-0.50482200	-2.66457400	1.89858600	H	-1.66818400	2.53007500	0.25531000
H	0.08115300	-1.09853100	2.43154600	H	-2.76601500	1.71823000	-0.85554600
H	-1.15607800	1.36237300	-1.78125000	H	-3.43939000	2.78366500	1.94043300
H	-1.38204800	2.28945900	0.54733500	H	-3.96461500	3.47266900	0.40828900
H	-3.00359500	1.59993100	0.64103000	H	-5.32928300	1.46116300	-0.08355300
H	-3.10553500	3.98854300	-0.00198400	H	-5.77768500	2.09587800	1.49618000
H	-2.05767100	3.69081600	-1.38315600	C	-1.38387200	-1.30956000	-3.78127500
H	-4.41953200	3.75745400	-2.15148800	C	-1.41268800	-0.48470000	-2.48275500
H	-4.87599100	2.55054700	-0.95360900	C	-0.85112000	-1.30133200	-1.29715900
H	-4.62531800	1.45044500	-3.15543300	C	-1.64069900	-2.61871400	-1.12758900
H	-3.00552400	2.11382300	-3.34453900	C	-1.59754600	-3.44360900	-2.42742500
H	-2.90591400	-0.25318100	-2.63757800	C	-2.13044000	-2.64259700	-3.62432900
H	-3.88745900	0.09037300	-1.21917300	H	-0.33777600	-1.50862200	-4.05644000
H	-2.09148100	-2.09670900	-1.62820900	H	-1.81616600	-0.72272400	-4.60118800
H	-0.72540100	-4.04091400	-1.68861800	H	-2.45026600	-0.19122600	-2.26949000
H	-0.69844800	-3.48301400	-0.02817700	H	-0.84182200	0.44333400	-2.60972000
H	1.58572300	-2.46935900	-0.40126900	H	0.18233400	-1.57254700	-1.56073400
H	1.56847200	-4.18096100	-0.75373300	H	-1.24105500	-3.21586000	-0.30087800
H	1.38690600	-3.74292000	-3.18781300	H	-2.68567200	-2.40048400	-0.88158700
H	2.76770300	-2.85908000	-2.53325900	H	-0.56021600	-3.75082000	-2.62598300
H	1.49811900	-0.76608700	-2.46967600	H	-2.17685900	-4.36637700	-2.29678100
H	1.37095700	-1.43774600	-4.09077100	H	-3.20199500	-2.44198800	-3.47592400
H	-0.86766000	-2.33321300	-3.63712100	H	-2.04864400	-3.23432400	-4.54451900
H	-0.83724100	-0.61282700	-3.29975700	C	2.35937000	0.65821800	-0.57127800
5 <sub>Cy</sub> [Pd(PCy <sub>3</sub> )(Ph)(Cl)] (conformer F)				C	3.38633000	0.65483800	0.37941200
Pd	0.69942300	1.65339100	-0.17912800	C	2.55300600	0.05136400	-1.81583200
P	-0.57797600	-0.22987100	0.22236000	C	4.59732600	0.01696400	0.08713500
				H	3.25780600	1.15831400	1.33235600

C	3.77104800	-0.57925400	-2.09896400
H	1.77643200	0.08041900	-2.57438300
C	4.79185000	-0.60520200	-1.14799700
H	5.39297200	0.02115100	0.82845500
H	3.91757200	-1.04270200	-3.07190000
H	5.73618200	-1.09396600	-1.37187800

# 5<sub>H</sub> [Pd(PH<sub>3</sub>)(Ph)(Br)]

Pd	0.73386600	0.64395100	-0.00014200
Br	2.00691800	-1.40615200	-0.00008100
P	-0.26058900	2.70815900	0.00041500
C	-3.61475700	-1.31444100	0.00005700
C	-2.97877800	-1.02212500	-1.20757600
C	-1.70811000	-0.43384400	-1.21713200
C	-1.08814100	-0.14530700	-0.00006700
C	-1.70745300	-0.43497800	1.21705300
C	-2.97814600	-1.02321800	1.20761900
H	-4.59950000	-1.77330800	0.00010300
H	-3.46246200	-1.25600700	-2.15261500
H	-1.21118700	-0.22762700	-2.16004900
H	-1.21001100	-0.22969200	2.15990000
H	-3.46131100	-1.25798600	2.15270200
H	0.54429900	3.87202300	0.00130500
H	-1.11900600	3.04251000	1.07055600
H	-1.11964300	3.04476400	-1.06848100

# 5<sub>H</sub> [Pd(PH<sub>3</sub>)(Ph)(Cl)]

Pd	-1.12235700	0.01166600	-0.00483200
P	-0.96181700	2.28446600	0.01714300
Cl	-1.51310900	-2.24127400	-0.00610800
C	3.63949700	-0.21740900	0.00117200
C	2.93815800	-0.19856100	1.20781600
C	1.54076300	-0.11057300	1.21595600
C	0.86135600	-0.04197500	-0.00144900
C	1.54602700	-0.06471500	-1.21770100
C	2.94338200	-0.15340900	-1.20695100
H	4.72361500	-0.28814500	0.00219900
H	3.47173300	-0.25954300	2.15297700
H	1.00040200	-0.11711400	2.15748500
H	1.00994500	-0.03459700	-2.16127400
H	3.48104400	-0.17868200	-2.15142600
H	-2.14254200	3.06413100	0.00838900
H	-0.27452600	2.92731200	-1.03550500
H	-0.30625300	2.90452600	1.10308200

# 5<sub>Ph</sub> [Pd(PPh<sub>3</sub>)(Ph)(Br)]

Pd	-1.19138200	-0.91525200	0.01693300
Br	-3.14192400	-2.37381300	0.07512500
P	0.92192900	0.00999400	-0.01892000
C	-3.44167600	3.29132000	-0.08642100
C	-3.34746900	2.50298500	-1.23535000
C	-2.67201000	1.27784200	-1.20351200
C	-2.08744100	0.84868500	-0.00834400
C	-2.18260700	1.62368700	1.15002600
C	-2.86253300	2.84794200	1.10365500
H	-3.97002300	4.24044700	-0.11634200

H	-3.80677700	2.83220500	-2.16428800
H	-2.61722600	0.66625200	-2.09823200
H	-1.73617200	1.29150400	2.08199800
H	-2.93739300	3.44907500	2.00676800
C	3.64359600	-3.64538900	-0.93088800
C	4.07195800	-2.69213300	-0.00419600
C	3.27665100	-1.58158000	0.28217200
C	2.04055200	-1.41316300	-0.36096300
C	1.61463900	-2.38025700	-1.28934500
C	2.41452200	-3.48764800	-1.57427000
H	4.26349300	-4.51125600	-1.14645400
H	5.02656200	-2.81326500	0.50051400
H	3.61674100	-0.84993200	1.00826500
H	0.65478300	-2.26816800	-1.78916800
H	2.07120200	-4.22885700	-2.29026300
C	1.93385100	3.26604200	-3.17526100
C	0.99623100	3.51461700	-2.16964700
C	0.70305900	2.53371900	-1.22328500
C	1.35657200	1.28912100	-1.26799800
C	2.29896600	1.04746800	-2.27880900
C	2.58260600	2.03208100	-3.22793100
H	2.15571100	4.03068000	-3.91473000
H	0.48399800	4.47160100	-2.12397300
H	-0.03411100	2.73662800	-0.45325000
H	2.81435800	0.09398100	-2.32743500
H	3.31396900	1.83152500	-4.00613100
C	2.35183000	1.63610200	4.08869200
C	2.89972100	2.16442300	2.91813500
C	2.47561000	1.69963200	1.67158300
C	1.49532200	0.69886300	1.58674200
C	0.94473000	0.17718400	2.76915500
C	1.37454000	0.64095100	4.01266700
H	2.68139100	2.00237900	5.05712200
H	3.65715700	2.94162700	2.97263000
H	2.90361100	2.12075000	0.76707700
H	0.17371700	-0.58772700	2.71192000
H	0.93965700	0.23074500	4.91982100

# 5<sub>Ph</sub> [Pd(PPh<sub>3</sub>)(Ph)(Br)]

Pd	-1.19138200	-0.91525200	0.01693300
Br	-3.14192400	-2.37381300	0.07512500
P	0.92192900	0.00999400	-0.01892000
C	-3.44167600	3.29132000	-0.08642100
C	-3.34746900	2.50298500	-1.23535000
C	-2.67201000	1.27784200	-1.20351200
C	-2.08744100	0.84868500	-0.00834400
C	-2.18260700	1.62368700	1.15002600
C	-2.86253300	2.84794200	1.10365500
H	-3.97002300	4.24044700	-0.11634200
H	-3.80677700	2.83220500	-2.16428800
H	-2.61722600	0.66625200	-2.09823200
H	-1.73617200	1.29150400	2.08199800
H	-2.93739300	3.44907500	2.00676800
C	3.64359600	-3.64538900	-0.93088800
C	4.07195800	-2.69213300	-0.00419600
C	3.27665100	-1.58158000	0.28217200
C	2.04055200	-1.41316300	-0.36096300

C	1.61463900	-2.38025700	-1.28934500
C	2.41452200	-3.48764800	-1.57427000
H	4.26349300	-4.51125600	-1.14645400
H	5.02656200	-2.81326500	0.50051400
H	3.61674100	-0.84993200	1.00826500
H	0.65478300	-2.26816800	-1.78916800
H	2.07120200	-4.22885700	-2.29026300
C	1.93385100	3.26604200	-3.17526100
C	0.99623100	3.51461700	-2.16964700
C	0.70305900	2.53371900	-1.22328500
C	1.35657200	1.28912100	-1.26799800
C	2.29896600	1.04746800	-2.27880900
C	2.58260600	2.03208100	-3.22793100
H	2.15571100	4.03068000	-3.91473000
H	0.48399800	4.47160100	-2.12397300
H	-0.03411100	2.73662800	-0.45325000
H	2.81435800	0.09398100	-2.32743500
H	3.31396900	1.83152500	-4.00613100
C	2.35183000	1.63610200	4.08869200
C	2.89972100	2.16442300	2.91813500
C	2.47561000	1.69963200	1.67158300
C	1.49532200	0.69886300	1.58674200
C	0.94473000	0.17718400	2.76915500
C	1.37454000	0.64095100	4.01266700
H	2.68139100	2.00237900	5.05712200
H	3.65715700	2.94162700	2.97263000
H	2.90361100	2.12075000	0.76707700
H	0.17371700	-0.58772700	2.71192000
H	0.93965700	0.23074500	4.91982100

# 5<sub>Ph</sub> [Pd(PPh<sub>3</sub>)(Ph)(Cl)]

Pd	-0.82045500	-1.59893700	0.05206800
P	0.68520900	0.13241200	-0.02476100
Cl	-1.92298700	-3.62162700	0.18123500
C	-4.66378100	1.22453600	-0.06669400
C	-4.26413500	0.50944800	-1.19780700
C	-3.12454500	-0.30150700	-1.16030700
C	-2.38286000	-0.38705200	0.02161600
C	-2.77857300	0.31447000	1.16299200
C	-3.92265700	1.12177400	1.11161600
H	-5.55121000	1.85082500	-0.10112100
H	-4.84226100	0.57133800	-2.11665500
H	-2.83161600	-0.86560500	-2.03988900
H	-2.21119700	0.24421300	2.08568800
H	-4.22979700	1.66619300	2.00147900
C	4.71170200	-2.03337000	-0.86668400
C	4.68051800	-0.99137100	0.06268200
C	3.48658600	-0.31789400	0.32581100
C	2.30758400	-0.68248000	-0.34215700
C	2.34688000	-1.73617300	-1.27356600
C	3.54370800	-2.40371600	-1.53626200
H	5.64208500	-2.55847600	-1.06444000
H	5.58696700	-0.70172500	0.58720600
H	3.47371100	0.48795500	1.05269300
H	1.43964400	-2.03586900	-1.79387900
H	3.55848400	-3.21789800	-2.25517800
C	0.21549300	3.42571300	-3.26966800

C	-0.74564700	3.26981000	-2.26765600
C	-0.59424700	2.28240900	-1.29498100
C	0.53371700	1.44221600	-1.30873600
C	1.49612100	1.60671000	-2.31590100
C	1.33432400	2.59274800	-3.29175600
H	0.09096900	4.19189600	-4.03005300
H	-1.62174600	3.91188900	-2.24562800
H	-1.35411400	2.16543100	-0.52897700
H	2.37339000	0.96887600	-2.34084000
H	2.08699700	2.70826500	-4.06693200
C	1.29282000	2.31902000	4.02633300
C	1.53670400	3.00802000	2.83672600
C	1.34775500	2.37488000	1.60649500
C	0.91020400	1.04258700	1.55723700
C	0.66266700	0.35795600	2.75871300
C	0.85708900	0.99244300	3.98571200
H	1.43734800	2.81536100	4.98204800
H	1.87290100	4.04097200	2.86329800
H	1.53656100	2.91999800	0.68690900
H	0.31161300	-0.67095400	2.72912300
H	0.66031500	0.45282600	4.90790000

# 5<sub>SP</sub> [Pd(SPhos)(Ph)(Br)] (conformer a)

Pd	-0.50524600	-0.99216700	-0.20217300
Br	-1.97444800	-2.92263300	-0.75338900
P	0.92614000	0.79154800	0.18197300
O	-2.54777600	1.68267500	-1.77997600
O	-2.08334300	0.36278900	2.70089900
C	-1.46746800	2.18139700	0.72522400
C	-0.06333500	2.26193800	0.69807500
C	0.55894800	3.46746000	1.07429000
H	1.64092200	3.53726700	1.08824900
C	-1.57808400	4.51268700	1.44367200
H	-2.17412800	5.37622700	1.72649600
C	-2.27967300	0.94687900	0.43330100
C	-2.20437700	3.32075600	1.09403300
H	-3.28877700	3.25575000	1.11337900
C	0.87155600	1.51255300	-2.54935600
H	0.20008800	0.65123000	-2.64114700
H	0.23329700	2.37964000	-2.33291700
C	-2.74878300	0.16814500	1.52908700
C	-2.99269200	0.85567900	-0.79448600
C	-4.09143500	0.00491600	-0.93051500
H	-4.61164200	-0.09234300	-1.87444100
C	1.85255200	1.29661600	-1.37640700
H	2.44212400	0.39585900	-1.59868300
C	-3.15778400	1.59477900	-3.06228500
H	-3.05719400	0.58669200	-3.48145200
H	-2.62477900	2.30858600	-3.69225800
H	-4.21914000	1.87035700	-3.01979100
C	2.22953700	0.68004000	1.53386100
H	2.59680300	1.70608000	1.68139400
C	-0.18465600	4.58532100	1.44195000
H	0.32112000	5.50408900	1.72621100
C	-4.50037400	-0.75229100	0.16492700
H	-5.34382200	-1.42681600	0.05358900
C	2.82286600	2.49062700	-1.26780600

H	3.53714300	2.34740300	-0.44836600	H	-5.83398600	-2.35108800	1.41244800
H	2.25582400	3.40317800	-1.04526700	C	-5.11929400	-0.50438500	0.58694300
C	-3.84922400	-0.68181900	1.39339200	H	-5.91664800	0.08132500	1.02749600
H	-4.18484500	-1.29919200	2.21635400	C	-4.13886100	0.09671400	-0.21575600
C	1.58927400	0.21556200	2.86019300	C	-2.55318400	0.00693800	-3.05771800
H	0.74217300	0.85960800	3.12246000	H	-3.56217700	-0.33553300	-3.26884400
H	1.18265800	-0.79548300	2.72231100	C	-1.75351200	0.47034500	-4.09709100
C	-2.43406500	-0.44341700	3.81959400	H	-2.14159900	0.49914100	-5.11160500
H	-3.46771000	-0.25817400	4.13773500	C	-0.44832800	0.87128100	-3.82198900
H	-1.75250500	-0.15039100	4.61959700	H	0.21036400	1.21207400	-4.61587400
H	-2.30393100	-1.50882100	3.59611800	C	0.01799800	0.81753700	-2.51159700
C	2.62391800	2.90166500	-3.76747000	H	1.04801400	1.10182700	-2.31191700
H	2.07267700	3.84290300	-3.62402200	C	-5.19958700	2.23854800	-0.05945800
H	3.18579200	3.00727800	-4.70412700	H	-6.16985100	1.88195900	-0.42798300
C	3.58641800	2.69803200	-2.58896600	H	-5.00701000	3.23735400	-0.45478100
H	4.26073200	3.55875100	-2.49295700	H	-5.22312200	2.28178400	1.03715100
H	4.22190400	1.82155700	-2.78274300	C	-2.05319300	-4.15428900	-1.08500500
C	3.44219300	-0.20235000	1.17274500	H	-1.93375200	-4.46661400	-0.04011900
H	3.92155700	0.15346400	0.25353100	H	-1.17560100	-4.46570600	-1.65285200
H	3.10695800	-1.22589600	0.97645000	H	-2.95364100	-4.62026700	-1.50523100
C	1.62439600	1.74077600	-3.87144500	C	-0.76952400	-0.28958600	1.60575700
H	2.16450000	0.82133100	-4.14167300	H	-1.84765400	-0.16864800	1.45115300
H	0.90477300	1.92736400	-4.67898100	C	-0.40027400	0.32533100	2.97686100
C	2.62314700	0.20168000	3.99901700	H	0.68894900	0.27376500	3.11956500
H	2.95113500	1.23183700	4.20416000	H	-0.67828900	1.38290400	3.02476100
H	2.15229400	-0.16390900	4.92072300	C	-1.10251600	-0.42022900	4.12711200
C	3.84364700	-0.65932500	3.64472300	H	-0.79886000	0.02333400	5.08388700
H	4.58693300	-0.61674000	4.45110200	H	-2.18840400	-0.26654900	4.04088500
H	3.53237100	-1.71065100	3.55964100	C	-0.80280400	-1.92450600	4.11278400
C	4.47230500	-0.21135700	2.31706800	H	0.26505400	-2.08392800	4.32206000
H	5.30883100	-0.86908400	2.04951000	H	-1.35845000	-2.42899100	4.91357500
H	4.89413600	0.79818500	2.43795800	C	-1.14826600	-2.53506600	2.74824100
C	3.11825800	-4.01307200	-1.17958100	H	-2.23502600	-2.48963500	2.58956500
C	2.68005800	-3.11136200	-2.14979000	H	-0.86970500	-3.59685300	2.72583000
C	1.63683200	-2.21986500	-1.87015000	C	-0.42867800	-1.79575900	1.60811900
C	1.02372400	-2.21893700	-0.61178600	H	-0.67174600	-2.24621200	0.64298700
C	1.45298200	-3.13908900	0.35457800	H	0.65331400	-1.90945200	1.73565200
C	2.49628700	-4.02679200	0.07121300	C	-0.07498100	2.43616200	0.59246000
H	3.92493900	-4.70750800	-1.39941700	H	0.40817500	2.51249200	1.57704300
H	3.13956200	-3.10346900	-3.13591400	C	0.73076800	3.33710300	-0.36992600
H	1.29286500	-1.54656100	-2.65022400	H	1.77692300	3.00607100	-0.43126600
H	0.96385400	-3.18298100	1.32315400	H	0.31524000	3.25724500	-1.38264300
H	2.81271600	-4.73872200	0.83046600	C	0.68506200	4.80791400	0.07909400
<b>5<sub>SP</sub> [Pd(SPhos)(Ph)(Br)] (conformer c)</b>				H	1.19928600	4.90754600	1.04613300
Pd	2.41420900	0.36640600	0.04456200	H	1.24294300	5.42517700	-0.63572100
Br	4.82144600	0.81723100	0.04770100	C	-0.75848700	5.31209800	0.21240700
P	0.10081400	0.59312500	0.19111800	H	-1.23177100	5.31878800	-0.78055600
O	-2.10066100	-2.73865200	-1.20406300	H	-0.76886000	6.34854500	0.57246000
O	-4.13529400	1.42548100	-0.52994500	C	-1.57150300	4.41265300	1.15386200
C	-0.78843000	0.38723300	-1.43517800	H	-1.17154800	4.50130400	2.17504300
C	-2.10386600	-0.05317200	-1.72601900	H	-2.61526100	4.75051000	1.19940100
C	-3.08708900	-0.65954600	-0.76787900	C	-1.52569500	2.93719000	0.71529300
C	-3.09608700	-2.05539900	-0.56987900	H	-2.02811700	2.82163700	-0.25182900
C	-4.07820700	-2.66893000	0.22056900	H	-2.08975300	2.32406200	1.42788100
H	-4.07717800	-3.74038000	0.37809200	C	2.67235100	-4.30998600	-0.90026100
C	-5.07244200	-1.88087600	0.79632600	C	3.19506000	-3.78127300	0.28215000
				C	3.08703600	-2.41417200	0.55872700



C	2.43726100	-1.57378100	-0.35417300
C	1.91673500	-2.09225200	-1.54145800
C	2.04075300	-3.46214600	-1.81056200
H	2.76862600	-5.37114700	-1.11486500
H	3.70730000	-4.42718100	0.99139300
H	3.52540600	-2.01065100	1.46533400
H	1.41720900	-1.45284300	-2.26105200
H	1.64310900	-3.85658300	-2.74329000

**5<sub>SP</sub> [Pd(SPhos)(Ph)(Cl)] (conformer a)**

Pd	-0.30421700	-1.16673200	-0.54381500
P	0.62938600	0.73755000	0.36266400
Cl	-1.21966000	-3.08954900	-1.53798800
O	-2.89743400	1.29472500	-1.64010300
O	-2.25432200	-0.99545900	2.40537700
C	-2.04778200	1.36508700	0.99468000
C	-0.70443300	1.76502900	1.12027500
C	-0.40625500	2.94385300	1.82912500
H	0.62569800	3.25126100	1.95757400
C	-2.74456000	3.35106100	2.23248900
H	-3.54145800	3.95730300	2.65485700
C	-2.52102400	0.09372300	0.34099800
C	-3.05115500	2.17714400	1.55154200
H	-4.08736900	1.86632900	1.45140600
C	0.49579100	2.08125600	-2.11768200
H	0.06552100	1.13663300	-2.46923700
H	-0.34725600	2.69359900	-1.77075600
C	-2.80748000	-1.03284100	1.16155400
C	-3.14232100	0.15476100	-0.93728200
C	-3.96969800	-0.87497800	-1.38836700
H	-4.41166600	-0.84680400	-2.37585200
C	1.45524100	1.81969300	-0.93621000
H	2.26313100	1.17041300	-1.30272600
C	-3.42754900	1.40566000	-2.95507300
H	-3.05100900	0.60634000	-3.60449500
H	-3.08772500	2.37241500	-3.32997000
H	-4.52475500	1.38484800	-2.94745700
C	1.87474400	0.58848900	1.76388800
H	1.96167700	1.59583900	2.19588800
C	-1.41102200	3.73413400	2.38032100
H	-1.15327800	4.64035800	2.92172100
C	-4.20241800	-1.96847000	-0.55711600
H	-4.83017900	-2.77853400	-0.91574000
C	2.08331000	3.14613500	-0.46117900
H	2.77650700	2.98200800	0.37258300
H	1.29257700	3.81309300	-0.09518700
C	-3.64075600	-2.06077800	0.71252300
H	-3.82791300	-2.93515200	1.32193800
C	1.33277400	-0.34801800	2.86599200
H	0.34205000	-0.01595900	3.19664900
H	1.20140900	-1.35321300	2.44342300
C	-2.41316000	-2.12942400	3.24965200
H	-3.46830500	-2.29690900	3.50012600
H	-1.85859200	-1.89905200	4.16060800
H	-1.99842000	-3.03107200	2.78377100
C	1.88767800	4.09922800	-2.80872100
H	1.11176100	4.82066200	-2.51242400

H	2.44270200	4.55845400	-3.63655100
C	2.82159900	3.84772400	-1.61630800
H	3.24914400	4.79353900	-1.25931200
H	3.66762200	3.22315900	-1.93858500
C	3.28484300	0.14707800	1.31758500
H	3.68954700	0.83535200	0.56666900
H	3.23074700	-0.83857800	0.84280300
C	1.21780000	2.79738800	-3.27178900
H	1.98233100	2.12580800	-3.68945600
H	0.50676700	3.00196900	-4.08256500
C	2.29808900	-0.41683100	4.06145100
H	2.34529000	0.56938200	4.54735900
H	1.90574200	-1.11472000	4.81248600
C	3.70881300	-0.83768000	3.62609100
H	4.39023900	-0.83611500	4.48646400
H	3.67818500	-1.87102800	3.25090200
C	4.24409300	0.08312800	2.52028200
H	5.23036100	-0.25903500	2.18231800
H	4.38684400	1.09532700	2.92870200
C	3.93644800	-2.92384300	-1.99490200
C	3.30643500	-1.92167700	-2.73303300
C	2.08213700	-1.39135100	-2.30723800
C	1.47868600	-1.85661100	-1.13349200
C	2.10193600	-2.87973300	-0.40645200
C	3.32612800	-3.40468200	-0.83402000
H	4.88534600	-3.33669400	-2.32745000
H	3.75887700	-1.55249400	-3.65101800
H	1.59481700	-0.63033400	-2.90976500
H	1.62741800	-3.28446100	0.48261500
H	3.79548600	-4.20125100	-0.26067900

**5<sub>SP</sub> [Pd(SPhos)(Ph)(Cl)] (conformer c)**

Pd	2.57912500	0.85857800	0.04273400
P	0.27264200	0.67782900	0.18910300
Cl	4.75943000	1.64618700	0.05333300
O	-1.41169500	-2.94501300	-1.21559600
O	-4.05764000	0.85929500	-0.52711900
C	-0.57912800	0.33904500	-1.43675300
C	-1.81733400	-0.28927800	-1.72455000
C	-2.69489700	-1.03755800	-0.76377700
C	-2.49058200	-2.41891200	-0.56762000
C	-3.35875700	-3.17367600	0.23357400
H	-3.19236300	-4.23194100	0.39224300
C	-4.45633400	-2.54622200	0.81873100
H	-5.13019800	-3.12603500	1.44351200
C	-4.71703800	-1.19451200	0.60623700
H	-5.59142600	-0.73756900	1.05247100
C	-3.84838100	-0.45177000	-0.20665400
C	-2.27741600	-0.29075300	-3.05370800
H	-3.22655100	-0.77624000	-3.26205400
C	-1.55924000	0.28832500	-4.09466600
H	-1.95207300	0.26305200	-5.10746000
C	-0.32607800	0.87610100	-3.82319200
H	0.27122100	1.31369500	-4.61815900
C	0.14884000	0.88840600	-2.51475100
H	1.12454300	1.32534400	-2.31803300
C	-5.23086700	1.49820500	-0.04658300

H	-6.13748500	0.99115900	-0.40051700	Cl	-0.27063800	4.76110100	1.18108900
H	-5.20290200	2.51190900	-0.44987100	C	-0.58602300	4.00165800	-0.37832500
H	-5.24700300	1.54513000	1.04996900	C	0.29927600	3.00240400	-0.83574600
C	-1.14580500	-4.33576200	-1.09155500	C	0.06012200	2.42353100	-2.10417200
H	-0.95945300	-4.61814700	-0.04787800	C	-1.04588800	2.85141700	-2.87515300
H	-0.24245100	-4.51382700	-1.67628600	C	-1.88496800	3.85182400	-2.39987200
H	-1.97208900	-4.93741000	-1.49125300	C	-1.65869400	4.43790500	-1.14274900
C	-0.41557100	-0.35370200	1.60187500	H	1.21887200	2.80660400	-0.29705200
H	-1.50525800	-0.38751800	1.48473900	H	0.81433600	1.78107800	-2.55144500
C	-0.08743100	0.28808300	2.97148100	H	-1.21371100	2.41374500	-3.85517400
H	1.00277500	0.39279700	3.07064100	H	-2.72371400	4.19302200	-3.00057100
H	-0.51206400	1.29399000	3.05035100	H	-2.30654500	5.22517700	-0.77179400
C	-0.62965900	-0.56605900	4.13256800	C	6.62903700	1.38699800	1.11432300
H	-0.35440600	-0.09666500	5.08560700	C	5.51544600	0.35669500	0.85107700
H	-1.72904300	-0.56817400	4.09037000	C	4.18828200	1.04690000	0.47784200
C	-0.11956500	-2.01147700	4.07814800	C	3.77350400	2.03692600	1.59177900
H	0.96721600	-2.01948400	4.24635500	C	4.88319900	3.06862400	1.86120600
H	-0.56733900	-2.60203100	4.88763700	C	6.21925800	2.39161900	2.20172400
C	-0.42488200	-2.64517100	2.71450000	H	6.84770300	1.92887000	0.18205400
H	-1.51207000	-2.75459800	2.59454200	H	7.55573000	0.87184500	1.40007500
H	0.00183800	-3.65550100	2.66206900	H	5.37226100	-0.24281000	1.75973800
C	0.13943300	-1.79439000	1.56440300	H	5.83030000	-0.33752600	0.06277000
H	-0.07151600	-2.26216000	0.60037700	H	4.38881800	1.66872100	-0.40890600
H	1.23055800	-1.75378600	1.65361500	H	2.84395200	2.55115400	1.31970800
C	-0.21926400	2.45715700	0.61015500	H	3.56305700	1.49065700	2.52061400
H	0.28254700	2.62272200	1.57440700	H	5.01287900	3.69818400	0.96820600
C	0.36565300	3.48783600	-0.38095400	H	4.57847300	3.74043000	2.67395600
H	1.45016900	3.35029300	-0.49228800	H	6.12118700	1.86243000	3.16157400
H	-0.07465700	3.33155700	-1.37421500	H	7.00480400	3.14562300	2.34057100
C	0.07446700	4.92635700	0.08018800	C	1.76033700	-2.26067900	3.31670500
H	0.60476300	5.11799200	1.02445900	C	2.18895900	-1.06491700	2.44902900
H	0.47851800	5.63426700	-0.65392300	C	2.53406400	-1.50289300	1.00935700
C	-1.42898700	5.16158900	0.28212600	C	3.62274500	-2.59784100	1.03107200
H	-1.94128000	5.08429800	-0.68834900	C	3.18937000	-3.79635100	1.89679100
H	-1.60914500	6.17886200	0.65197500	C	2.82729400	-3.36503000	3.32506500
C	-2.02267100	4.12952400	1.25101900	H	0.81740600	-2.67042400	2.92456100
H	-1.59946200	4.28872400	2.25411900	H	1.55212300	-1.92355600	4.34079200
H	-3.10720100	4.27284500	1.34576000	H	3.06831800	-0.59493300	2.91005200
C	-1.72997700	2.68725100	0.79836600	H	1.39611100	-0.30696200	2.43270600
H	-2.24426700	2.48297600	-0.14707500	H	1.62069500	-1.96377800	0.60364400
H	-2.14158200	1.98153700	1.52964700	H	3.84590800	-2.94767000	0.01679000
C	3.64247700	-3.69736900	-0.92108500	H	4.55852500	-2.19058600	1.43238700
C	4.09037000	-3.07836900	0.24808300	H	2.31696400	-4.28050500	1.43259800
C	3.74664300	-1.75119200	0.52651400	H	3.98856100	-4.54902300	1.91661100
C	2.93313300	-1.04568100	-0.36919100	H	3.73076300	-2.98952800	3.82871500
C	2.48697700	-1.65386600	-1.54398400	H	2.48063800	-4.22783600	3.90843300
C	2.84834200	-2.98017100	-1.81626500	C	4.37005400	-0.36717000	-4.05260500
H	3.92142900	-4.72536800	-1.13750500	C	3.85923300	0.26919000	-2.74807100
H	4.72594700	-3.61960100	0.94506400	C	3.45373600	-0.79365200	-1.70279600
H	4.12775400	-1.27011800	1.42112100	C	2.42893400	-1.77116400	-2.32224200
H	1.86343300	-1.11685200	-2.25003300	C	2.93975800	-2.40608000	-3.62677200
H	2.50671500	-3.44348900	-2.73946600	C	3.34641300	-1.33969400	-4.65247100
				H	5.30544600	-0.90854300	-3.84660100
				H	4.61916900	0.42079500	-4.77525300
				H	2.99129400	0.90684200	-2.97424500
				H	4.63471700	0.93176000	-2.34767200
				H	4.35723800	-1.36415800	-1.44178600
<b>6<sub>Cy</sub><sup>‡</sup> [Pd(PCy<sub>3</sub>)<sub>2</sub>(PhCl)]<sup>‡</sup> (conformer F)</b>							
Pd	-0.64090700	0.85645400	-0.56379700				
P	2.72568800	-0.00096000	-0.13849700				
P	-2.35204600	-0.56532700	0.05642700				

H	2.17446200	-2.56402300	-1.60896800
H	1.49428500	-1.22734200	-2.52291100
H	3.80762100	-3.04500600	-3.40460300
H	2.16730300	-3.06506200	-4.04510200
H	2.45307100	-0.77882500	-4.96624900
H	3.75235700	-1.81176800	-5.55642400
C	-3.33410900	-2.17990300	3.93171400
C	-3.57749900	-1.78194800	2.46402000
C	-2.39752000	-0.95791400	1.90958200
C	-2.16005800	0.29180100	2.78629800
C	-1.92200100	-0.09783200	4.25545200
C	-3.07235700	-0.94969200	4.81309300
H	-2.46791000	-2.85645800	3.98354500
H	-4.19467900	-2.74590700	4.31202200
H	-4.49769600	-1.18592800	2.41146800
H	-3.75000100	-2.68119900	1.86023100
H	-1.49172700	-1.57466800	2.01397600
H	-1.30787200	0.86172700	2.39699700
H	-3.03110700	0.95827900	2.73177500
H	-0.98253700	-0.66575100	4.33035000
H	-1.78918300	0.80659600	4.86321000
H	-3.98607500	-0.33809700	4.85694400
H	-2.85481100	-1.25910200	5.84358900
C	-5.45989500	2.26348500	-0.53912200
C	-4.27560000	1.55633300	0.14098900
C	-4.01843000	0.16982400	-0.48677500
C	-5.29434100	-0.69610300	-0.40664200
C	-6.48091900	0.01000800	-1.09059500
C	-6.73214400	1.40445600	-0.49839100
H	-5.19641000	2.47634900	-1.58589700
H	-5.64079300	3.23386800	-0.05846000
H	-4.50201100	1.44114500	1.21014000
H	-3.37140300	2.17133800	0.06793900
H	-3.81800800	0.35139700	-1.55366500
H	-5.13814800	-1.67531000	-0.87353700
H	-5.55420700	-0.88749800	0.64144000
H	-6.27107200	0.10577500	-2.16652900
H	-7.38266200	-0.61034400	-1.00316700
H	-7.06216200	1.29837000	0.54607800
H	-7.55006600	1.90360400	-1.03417400
C	-1.23023700	-4.53762800	-0.99061500
C	-1.20885800	-3.15568800	-0.31452400
C	-2.41616000	-2.28833400	-0.72764300
C	-2.48515300	-2.18329400	-2.26752700
C	-2.50733900	-3.56532300	-2.94257200
C	-1.30693700	-4.42184500	-2.51879300
H	-2.09922000	-5.10606900	-0.62673400
H	-0.33985500	-5.10778000	-0.69398000
H	-0.28538500	-2.62749000	-0.59000000
H	-1.18154100	-3.29026100	0.77317900
H	-3.32919800	-2.79137400	-0.37755300
H	-3.36927600	-1.61384900	-2.57674700
H	-1.61177700	-1.61523300	-2.61891600
H	-3.43762400	-4.08769700	-2.67300900
H	-2.52425900	-3.44328600	-4.03352400
H	-0.38167900	-3.95903400	-2.89370100
H	-1.36648500	-5.41819100	-2.97559100

**6<sub>H</sub><sup>†</sup> [Pd(PH<sub>3</sub>)<sub>2</sub>(PhBr)]<sup>‡</sup> Fixed Pd—P = 3.3**

Pd	1.08413200	0.29863800	0.05538400
Br	-3.47402700	0.57083600	-0.42658200
P	1.86453800	2.30339800	0.69982700
P	4.05123900	-0.95617300	-0.75359600
C	-2.01000500	-0.59405900	0.00042000
C	-0.94843700	-0.71024200	-0.91383400
C	0.11020000	-1.60544300	-0.61779400
C	0.10888100	-2.30167500	0.61457400
C	-0.95732000	-2.15647500	1.49964200
C	-2.03632900	-1.31554200	1.18805800
H	-1.00844300	-0.22707200	-1.88240500
H	0.83427100	-1.86105400	-1.38761100
H	0.92299400	-2.98298600	0.84162600
H	-0.96659300	-2.70782300	2.43563700
H	-2.87443900	-1.21888100	1.86963200
H	3.21371800	2.69545500	0.48555500
H	1.29343700	3.49385300	0.18044600
H	1.82099800	2.70717000	2.06001500
H	5.32220200	-1.51856000	-1.09444300
H	4.31124900	0.25921200	-1.44294600
H	4.51286700	-0.46365400	0.49735400

**6<sub>H</sub><sup>†</sup> [Pd(PH<sub>3</sub>)<sub>2</sub>(PhCl)]<sup>‡</sup>**

Pd	0.67195700	0.27920800	0.06661600
P	1.63858900	2.22507900	0.63185800
Cl	-3.62832300	0.97191900	-0.85482100
C	-2.49375100	-0.21286900	-0.22264200
C	-1.37838600	-0.56792400	-1.00230500
C	-0.48984900	-1.55645300	-0.51229600
C	-0.70498300	-2.11033200	0.77263700
C	-1.81799300	-1.73172500	1.52035700
C	-2.73161100	-0.79419400	1.01754200
H	-1.28469300	-0.18750700	-2.01332900
H	0.25953700	-1.98582500	-1.17219600
H	-0.02151800	-2.86541300	1.14866200
H	-1.99258600	-2.17339600	2.49734700
H	-3.60927300	-0.51228300	1.58938300
P	3.47771800	-1.26201800	-0.67380900
H	2.98451000	2.52797400	0.28982100
H	1.10097200	3.45248300	0.16541900
H	1.75119500	2.62788300	1.98869900
H	4.68129000	-1.97084300	-0.98714200
H	3.86713400	-0.10978300	-1.40883600
H	3.98972100	-0.77442800	0.55927500

**6<sub>Ph</sub><sup>†</sup> [Pd(PH<sub>3</sub>)<sub>2</sub>(PhBr)]<sup>‡</sup>**

Pd	0.54913800	-0.53292000	-0.85134400
Br	2.32155300	-4.16964500	1.02010800
P	1.97635700	1.11434600	-0.14120600
P	-2.79802300	-0.03359400	-0.15032200
C	1.60766300	-3.49190800	-0.63209100
C	0.33915200	-2.87717700	-0.61562300
C	-0.21049700	-2.42592900	-1.84411600
C	0.55569900	-2.54074400	-3.02986800
C	1.80553700	-3.15023000	-3.00405600

C	2.33560200	-3.65012100	-1.80233700
H	-0.26641700	-2.91533300	0.28394300
H	-1.26169800	-2.16013200	-1.90323400
H	0.13557800	-2.19320000	-3.96936100
H	2.37782500	-3.25943800	-3.92137300
H	3.30271600	-4.14053100	-1.78671300
C	-2.87524700	-0.22385800	1.68737100
C	-1.67758200	-0.05519300	2.40115600
C	-4.04719500	-0.53907200	2.39583700
C	-1.65386100	-0.17926900	3.79219000
H	-0.75819100	0.16027000	1.86177300
C	-4.02075300	-0.67018100	3.78510100
H	-4.97967800	-0.68966800	1.85934200
C	-2.82529900	-0.48741500	4.48576200
H	-0.71682700	-0.04189000	4.32466800
H	-4.93412100	-0.91674600	4.32071700
H	-2.80773400	-0.59193900	5.56760400
C	-3.47015000	1.66664000	-0.44649400
C	-3.32435100	2.19649300	-1.74148200
C	-4.07433900	2.46329700	0.53836100
C	-3.79565200	3.47351700	-2.05035900
H	-2.83664200	1.60457900	-2.51298300
C	-4.52967600	3.74821000	0.23358400
H	-4.18920300	2.08079100	1.54757000
C	-4.39819800	4.25481500	-1.06061700
H	-3.68386100	3.86020400	-3.06008100
H	-4.99220700	4.35218100	1.01008200
H	-4.75823800	5.25287500	-1.29612400
C	-4.19143900	-1.12396400	-0.70968700
C	-4.00295000	-2.51466500	-0.60088600
C	-5.37814200	-0.65709800	-1.29458600
C	-4.97451800	-3.40807100	-1.04976000
H	-3.09226500	-2.90301400	-0.14973300
C	-6.34760600	-1.55342800	-1.75306600
H	-5.55071300	0.40996600	-1.39193200
C	-6.15130000	-2.92931000	-1.63174000
H	-4.81003500	-4.47782400	-0.94980900
H	-7.26110800	-1.17101100	-2.20164700
H	-6.90689300	-3.62405800	-1.98857300
C	1.65398800	2.84200300	-0.73275400
C	0.31710500	3.22442900	-0.92858100
C	2.66751400	3.77802700	-0.99325800
C	-0.00169300	4.51455800	-1.35478700
H	-0.47587000	2.50217200	-0.75445400
C	2.34865300	5.06545200	-1.43067200
H	3.70919100	3.50228800	-0.86115800
C	1.01465300	5.43788400	-1.60866100
H	-1.04353900	4.78856900	-1.49613700
H	3.14534300	5.77689900	-1.63316400
H	0.76958800	6.44052600	-1.94971100
C	2.12277500	1.31732100	1.69714800
C	2.08987000	2.55794600	2.34994000
C	2.25795600	0.15026900	2.47034100
C	2.19278500	2.63080500	3.74246900
H	1.98442900	3.47129200	1.77314500
C	2.37546100	0.22577400	3.85803200
H	2.26964500	-0.82007900	1.97963500

C	2.33953500	1.46814600	4.49946800
H	2.16124600	3.60050200	4.23280800
H	2.48954300	-0.68629900	4.43842600
H	2.42393400	1.52737500	5.58150000
C	3.74140100	0.83421200	-0.63817900
C	3.98867200	0.18691700	-1.85930900
C	4.83452900	1.24022700	0.14343400
C	5.29540600	-0.03217000	-2.29705600
H	3.14727300	-0.15911900	-2.45462900
C	6.14228800	1.01130200	-0.29095200
H	4.66705400	1.73005100	1.09818400
C	6.37600700	0.37822200	-1.51299600
H	5.46929500	-0.53496800	-3.24502600
H	6.97797500	1.32700300	0.32849700
H	7.39411000	0.19834100	-1.84840700

	<b>6Ph<sup>†</sup> [Pd(PPh<sub>3</sub>)<sub>2</sub>(PhCl)]<sup>†</sup></b>		
Pd	-0.64020600	0.94610000	-0.58089500
P	-2.15279900	-0.70760200	-0.11538000
Cl	-2.36076300	4.34280200	1.50545500
C	-1.58879300	3.90223900	-0.01581500
C	-0.35822400	3.21428900	0.02618200
C	0.29436400	2.91201900	-1.19716700
C	-0.34189900	3.23967300	-2.42032700
C	-1.56016700	3.91048200	-2.42187500
C	-2.18482100	4.26625300	-1.21445100
H	0.15215400	3.09444500	0.97640100
H	1.33504800	2.60225900	-1.19497900
H	0.15525200	3.00647200	-3.35755600
H	-2.03106600	4.18152300	-3.36295200
H	-3.12439300	4.80828900	-1.21252700
P	2.69230300	0.01341300	-0.08720200
C	2.90043400	-0.29578000	1.72409900
C	1.74246900	-0.57958900	2.46601800
C	4.13678100	-0.24832800	2.39073200
C	1.81928300	-0.83075000	3.83795200
H	0.77538500	-0.58998100	1.96979100
C	4.21170900	-0.49343700	3.76253500
H	5.04042300	-0.01155000	1.83630800
C	3.05382900	-0.78861000	4.48763700
H	0.91097000	-1.04908200	4.39267000
H	5.17436000	-0.45210400	4.26603600
H	3.11499500	-0.97701800	5.55645900
C	3.24710000	-1.57041100	-0.87305100
C	2.94006600	-1.74857000	-2.23403700
C	3.91461100	-2.60341300	-0.19681800
C	3.31364600	-2.91355200	-2.90647700
H	2.40154600	-0.96974600	-2.76939900
C	4.27387900	-3.77582400	-0.86548300
H	4.15312100	-2.49482300	0.85647700
C	3.98026900	-3.93274900	-2.22147700
H	3.07577700	-3.02769900	-3.96093900
H	4.78748500	-4.56670400	-0.32473900
H	4.26467600	-4.84445500	-2.74027200
C	4.10628500	1.16090000	-0.44366400
C	4.02822700	2.46334300	0.08494000
C	5.19644800	0.84079800	-1.26673700

C	5.01520700	3.40918500	-0.18874000	C	-7.137773	-1.507313	-0.710589
H	3.19371600	2.73591100	0.72763500	C	-6.258815	-0.655272	-1.369204
C	6.18062300	1.79244300	-1.54807300	C	3.224773	2.897631	-0.390871
H	5.28275300	-0.15539700	-1.68870200	C	3.184722	-0.951179	1.469083
C	6.09553000	3.07699700	-1.01056200	C	1.131917	0.370728	-3.367438
H	4.93789700	4.40684200	0.23566900	C	-4.323667	1.815142	-1.602929
H	7.01868600	1.52352000	-2.18626700	C	5.826740	-0.343467	-1.235567
H	6.86236600	3.81483100	-1.23073500	C	3.292773	-0.674568	-3.413380
C	-1.98211000	-2.30181800	-1.04709000	C	3.408467	-0.611993	2.958676
C	-0.68574800	-2.72353800	-1.38385900	C	-3.423642	0.066866	-2.999006
C	-3.07110700	-3.09915900	-1.43364700	C	-3.789767	2.787066	-2.460699
C	-0.47942400	-3.91989400	-2.07214400	C	2.847100	2.676022	2.087795
H	0.16438500	-2.10329500	-1.11312400	C	2.366304	0.009920	-1.267138
C	-2.86515400	-4.29132000	-2.13140000	C	2.174530	-0.199519	-4.093418
H	-4.08374200	-2.78751800	-1.19707400	C	-2.564844	-4.270630	-0.189709
C	-1.57019400	-4.70624500	-2.44890000	C	-3.059255	2.379453	-3.574660
H	0.53295900	-4.22641300	-2.32062400	C	2.467581	-2.309513	1.337918
H	-3.71943000	-4.89467900	-2.42815900	C	-2.869110	1.029168	-3.856196
H	-1.41317000	-5.63402400	-2.99315800	C	3.279115	1.926901	0.805969
C	-2.23506300	-1.25978500	1.65429200	C	-3.392143	-1.225187	3.250887
C	-2.28021700	-2.60438200	2.05042000	C	-2.215558	-5.321764	-1.260959
C	-2.22815000	-0.26310000	2.64662900	C	1.233400	0.454738	-1.979844
C	-2.31974500	-2.94461100	3.40596400	C	-2.666959	-2.168342	2.266914
H	-2.28331800	-3.39049400	1.30194100	C	3.881970	-4.715685	-1.632268
C	-2.28244900	-0.60365500	3.99800500	C	7.040237	-0.892233	-0.795095
H	-2.17625200	0.78308000	2.35418000	C	-2.706806	-1.717106	-4.427740
C	-2.32482000	-1.94777000	4.38222600	C	-5.307233	-2.222519	0.677198
H	-2.34945300	-3.99192500	3.69580700	C	6.812133	1.822717	-1.478637
H	-2.28464100	0.18039900	4.75090000	C	4.079541	4.154206	-0.141370
H	-2.36030300	-2.21429500	5.43541900	C	-2.055346	-2.873378	-0.596048
C	-3.91037600	-0.22317400	-0.45551300	C	3.696724	4.878072	1.156601
C	-4.15164300	0.66480700	-1.51581600	C	-1.323348	-3.094356	4.225593
C	-5.00176600	-0.70266800	0.28541100	C	-1.260022	-2.492270	2.810874
C	-5.45335100	1.04806800	-1.84074200	C	-3.466067	-1.822869	4.666239
H	-3.30722000	1.06466300	-2.07197100	C	3.722504	3.913644	2.349526
C	-6.30367900	-0.30906200	-0.03329000	C	-0.710140	-5.348285	-1.565090
H	-4.83720700	-1.38041000	1.11791600	C	6.060621	-3.108123	-0.893403
C	-6.53289500	0.56343000	-1.09879200	C	-0.199129	-3.951822	-1.949208
H	-5.62317200	1.73574900	-2.66529900	C	-0.542222	-2.908958	-0.872412
H	-7.13820600	-0.68462000	0.55348200	C	3.206662	-3.435681	2.079879
H	-7.54631000	0.87045300	-1.34400200	C	-5.442493	3.473893	-0.280752
<b>6<sub>SP</sub><sup>+</sup> [Pd(SPhos)<sub>2</sub>(PhBr)]<sup>+</sup> (conformer ac)</b>				C	7.138607	-2.269570	-0.621378
Pd	-1.233952	0.481671	0.642833	C	4.139731	-1.745294	3.701743
P	2.184288	0.382964	0.564559	C	-2.071882	-2.176871	5.202383
P	-2.569392	-1.416404	0.526710	C	3.417633	-3.090879	3.559765
O	-3.357300	-1.275955	-3.246022	C	-2.377045	2.355946	1.586009
O	3.757403	-3.301835	-1.653727	C	-1.790450	3.120051	0.549456
O	5.663548	0.989003	-1.486901	C	-1.969863	2.587505	2.919847
C	4.851352	-2.547610	-1.329619	C	-0.864623	4.114250	0.881768
O	-5.064550	2.121040	-0.495064	C	-1.023758	3.563474	3.211341
C	-4.132340	0.439014	-1.841216	C	-0.474360	4.359268	2.193402
C	-4.897725	-0.562551	-1.024425	H	-7.313625	-2.973407	0.866435
C	-4.392190	-1.369081	0.026373	H	-8.183274	-1.549586	-1.004515
C	3.419991	-0.579782	-2.016302	H	-6.624991	-0.028599	-2.177765
C	-6.653954	-2.297117	0.328496	H	3.569084	2.397452	-1.298885
C	4.696586	-1.152053	-1.466631	H	2.184031	3.201764	-0.566758
				H	4.170977	-1.027019	0.997716

H	0.239778	0.744108	-3.862991
H	4.105002	-1.132278	-3.971893
H	3.998878	0.304471	3.056839
H	2.440650	-0.421151	3.446400
H	-3.936815	3.842922	-2.269130
H	1.802572	2.989550	1.972481
H	2.869418	2.019758	2.962952
H	2.121445	-0.281458	-5.176302
H	-3.649607	-4.257599	-0.033408
H	-2.106563	-4.575293	0.762057
H	-2.640189	3.128846	-4.240532
H	2.355443	-2.574731	0.282933
H	1.455004	-2.211416	1.750434
H	-2.322720	0.735829	-4.743892
H	4.318921	1.585987	0.921179
H	-2.839141	-0.277149	3.285287
H	-4.400420	-0.988041	2.893911
H	-2.557644	-6.313457	-0.935652
H	-2.767434	-5.089074	-2.183831
H	0.396002	0.868921	-1.418223
H	-3.217769	-3.116410	2.218638
H	4.676655	-5.058438	-2.307569
H	2.922003	-5.103749	-1.976190
H	4.079714	-5.089929	-0.619820
H	7.898386	-0.261101	-0.599993
H	-3.188403	-1.308824	-5.325802
H	-2.802262	-2.804413	-4.430554
H	-1.643121	-1.447284	-4.428599
H	-4.967793	-2.857488	1.485728
H	7.239292	1.918679	-0.471773
H	6.470759	2.802202	-1.815863
H	7.583012	1.446897	-2.163703
H	5.138957	3.862248	-0.084765
H	3.988982	4.836732	-0.997250
H	-2.548333	-2.603835	-1.537904
H	4.370418	5.727344	1.333291
H	2.685477	5.294401	1.050270
H	-1.831378	-4.069891	4.183789
H	-0.305662	-3.289406	4.589621
H	-0.739710	-3.186808	2.142323
H	-0.665615	-1.568490	2.825631
H	-3.967221	-1.117038	5.341883
H	-4.088973	-2.730105	4.647143
H	3.382323	4.423333	3.261215
H	4.758743	3.594639	2.540622
H	-0.168878	-5.697660	-0.672503
H	-0.496780	-6.072045	-2.363353
H	6.167199	-4.178773	-0.771739
H	-0.656100	-3.651177	-2.904026
H	0.885204	-3.963142	-2.116530
H	0.002572	-3.158548	0.046560
H	-0.191738	-1.917271	-1.175896
H	2.645041	-4.375014	1.982745
H	4.185565	-3.601453	1.606259
H	-4.572469	4.109809	-0.077215
H	-6.091478	3.463350	0.596726
H	-5.996072	3.874749	-1.139742

H	8.076002	-2.699293	-0.278633
H	5.157559	-1.839762	3.294888
H	4.250451	-1.478398	4.761179
H	-1.493481	-1.251245	5.342142
H	-2.148955	-2.650468	6.189841
H	2.440183	-3.034671	4.062464
H	3.984677	-3.883966	4.064933
H	-3.277415	1.787705	1.380455
H	-2.133631	3.013835	-0.472236
H	-2.430292	2.022030	3.724687
H	-0.724457	3.741707	4.241052
H	0.230576	5.149909	2.425103
Br	-0.184175	5.241911	-0.526034

**6<sub>SP</sub><sup>+</sup> [Pd(SPhos)<sub>2</sub>(PhCl)]<sup>+</sup> (conformer ac)**

Pd	-1.24086300	0.70259400	0.56276900
P	2.17030400	0.58473400	0.50061900
P	-2.58369000	-1.19073300	0.56105600
Cl	-0.13162400	5.23723200	-0.66763300
O	-3.32506900	-1.28217700	-3.21494800
O	3.75158600	-3.24748200	-1.47406900
O	5.66631000	1.04160600	-1.53493500
C	4.84265100	-2.47778200	-1.17822000
O	-5.00565300	2.31175400	-0.70805900
C	-4.08813100	0.53177900	-1.93251900
C	-4.88198100	-0.40016900	-1.06227800
C	-4.40166500	-1.14263400	0.04623700
C	3.42504400	-0.55284900	-1.99902100
C	-6.68361000	-2.00372300	0.38865600
C	4.69344100	-1.09244500	-1.39982200
C	-7.14239000	-1.27899200	-0.70765300
C	-6.24109000	-0.49092000	-1.41437200
C	3.21698400	3.02938600	-0.60678000
C	3.14709300	-0.70025000	1.49680700
C	1.15261700	0.31194700	-3.43141400
C	-4.25393500	1.92374000	-1.78236000
C	5.82229200	-0.27365800	-1.20149200
C	3.31025600	-0.73994500	-3.38784100
C	3.34206900	-0.28447300	2.97104200
C	-3.36892900	0.07437000	-3.05255700
C	-3.68448900	2.83026000	-2.68747400
C	2.84605800	2.95914700	1.88378300
C	2.36634700	0.08830800	-1.30053000
C	2.19983200	-0.30797700	-4.10821200
C	-2.62892600	-4.08436600	0.04102700
C	-2.94583800	2.33976000	-3.76187400
C	2.42437700	-2.05991500	1.42076400
C	-2.78160800	0.97114500	-3.95768000
C	3.27410000	2.13449600	0.64802600
C	-3.40644700	-0.79984800	3.26276600
C	-2.29019500	-5.21907600	-0.94439800
C	1.24151600	0.48783700	-2.05155700
C	-2.70199100	-1.82402900	2.34741400
C	3.87086400	-4.65795000	-1.36928400
C	7.02755500	-0.79743000	-0.71077300
C	-2.65001200	-1.80874800	-4.34686200
C	-5.33875500	-1.93106300	0.74531500

C	6.81712400	1.87178000	-1.56268700	H	-1.58169700	-1.55846200	-4.33210500
C	4.06407800	4.30469800	-0.43621000	H	-5.01890800	-2.51454300	1.59939500
C	-2.09454700	-2.72859400	-0.46170800	H	7.23253200	2.02741600	-0.55835000
C	3.67222000	5.10630400	0.81193400	H	6.48254600	2.82992700	-1.96233800
C	-1.38166400	-2.64595600	4.36822800	H	7.59516400	1.45381900	-2.21442600
C	-1.30318700	-2.14522700	2.91512400	H	5.12504800	4.02358700	-0.35776400
C	-3.49480800	-1.29780500	4.71533200	H	3.97179500	4.92988800	-1.33446400
C	3.71072600	4.21944900	2.06282300	H	-2.58291600	-2.51506700	-1.42006400
C	-0.78317100	-5.29333600	-1.22996200	H	4.33660000	5.97238000	0.93398500
C	6.04386000	-3.01372000	-0.69194100	H	2.65646600	5.50357700	0.67961300
C	-0.24735200	-3.93870900	-1.71647900	H	-1.91248900	-3.60988200	4.39214900
C	-0.58144700	-2.80761500	-0.72956900	H	-0.36920400	-2.83928900	4.74740700
C	3.14021300	-3.14954400	2.23589700	H	-0.80207500	-2.89939800	2.29836200
C	-5.36571400	3.68078600	-0.58672000	H	-0.68302300	-1.23989200	2.86487700
C	7.11971100	-2.16216300	-0.45385700	H	-3.97964000	-0.53603800	5.34029400
C	4.04919900	-1.38150500	3.78831800	H	-4.13876200	-2.18944500	4.75729600
C	-2.10945600	-1.64639900	5.27756600	H	3.36869700	4.78188400	2.94231200
C	3.32157900	-2.72870300	3.69998400	H	4.75081900	3.92321100	2.26923000
C	-2.39109100	2.62335600	1.43213100	H	-0.25556400	-5.58125100	-0.30782200
C	-1.75898800	3.30865100	0.36891100	H	-0.57421800	-6.07957100	-1.96802300
C	-2.01883900	2.93060400	2.76099900	H	6.14556900	-4.07550600	-0.50549000
C	-0.82241700	4.30612900	0.66539200	H	-0.69241100	-3.70783400	-2.69599700
C	-1.06419000	3.90692500	3.01991000	H	0.83802900	-3.97947600	-1.87312900
C	-0.46858800	4.62492700	1.97127600	H	-0.04381600	-2.98539100	0.20978700
H	-7.36143400	-2.62820100	0.96530200	H	-0.21632200	-1.84947800	-1.11313500
H	-8.18579100	-1.32193700	-1.00884400	H	2.57429800	-4.08948700	2.17637100
H	-6.58762800	0.08564900	-2.26767900	H	4.12748100	-3.34571900	1.79215500
H	3.56495900	2.47393100	-1.48082400	H	-4.49003500	4.31576100	-0.40606800
H	2.17511100	3.31710100	-0.80216400	H	-6.03100600	3.73526100	0.27683800
H	4.14230500	-0.80534400	1.05045600	H	-5.89706000	4.03480300	-1.47970200
H	0.26641200	0.65398200	-3.95897100	H	8.05080800	-2.57226100	-0.07208400
H	4.12586800	-1.23613500	-3.90718900	H	5.07545900	-1.50251900	3.41059400
H	3.93673400	0.63241800	3.03329400	H	4.13758200	-1.06042000	4.83474300
H	2.36574400	-0.06222300	3.42736300	H	-1.50965100	-0.72714800	5.35499000
H	-3.81029600	3.89868400	-2.56194100	H	-2.19841500	-2.04924100	6.29500100
H	1.79774200	3.25533800	1.75894400	H	2.33363600	-2.64091400	4.17702400
H	2.88259300	2.35927600	2.79801100	H	3.87200200	-3.49744700	4.25839600
H	2.15626000	-0.46151400	-5.18372600	H	-3.29222800	2.05274600	1.23731100
H	-3.71422400	-4.04184000	0.18702500	H	-2.07453600	3.15462100	-0.65614000
H	-2.18225100	-4.32507400	1.01603000	H	-2.51347700	2.42478500	3.58487800
H	-2.49923000	3.03760100	-4.46487700	H	-0.79372000	4.14572200	4.04528300
H	2.33262200	-2.37887500	0.37879600	H	0.24431900	5.41757200	2.17045600
H	1.40377200	-1.93558400	1.80545600	$^{tol}6_{tBu}^{\ddagger} [Pd(P^tBu_3)_2(PhMe)]^{\ddagger}$			
H	-2.22935500	0.61304400	-4.81769300	Pd	0.47492300	0.24225100	-0.08667600
H	4.31330800	1.79879600	0.78020800	P	-2.92931200	-0.37825700	-0.01133500
H	-2.83335700	0.13576900	3.23296300	P	2.54338600	-0.72791100	-0.01434100
H	-4.40915900	-0.56609400	2.88796300	C	-3.04907700	-1.88164800	-1.24754300
H	-2.65220300	-6.17707800	-0.54754500	C	-2.17998900	-3.04257700	-0.71732200
H	-2.83028500	-5.04871400	-1.88759500	H	-1.18061700	-2.69993800	-0.43334900
H	0.40142500	0.94158900	-1.52587300	H	-2.63161800	-3.55914700	0.13315200
H	-3.27547600	-2.75968900	2.36411100	H	-2.06116800	-3.78603600	-1.51737000
H	4.67404500	-5.04130600	-2.01194700	C	-2.37769600	-1.42763800	-2.56744500
H	2.91448200	-5.06234000	-1.70443800	H	-1.36137700	-1.06151400	-2.38449500
H	4.05205100	-4.97431300	-0.33424500	H	-2.31092200	-2.28698900	-3.24903000
H	7.88451700	-0.15751000	-0.54067300	H	-2.93077100	-0.64447300	-3.08787600
H	-3.09746500	-1.45001300	-5.28295500	C	-4.45431700	-2.43632900	-1.55644500
H	-2.76692000	-2.89216000	-4.28440100				

H	-4.35879300	-3.30690700	-2.22088700	H	0.95727600	-2.89300900	1.22549000
H	-4.97896100	-2.76811800	-0.65659700	H	2.42063500	-3.81060000	0.80505100
H	-5.09164400	-1.71236200	-2.07055200	H	1.98268000	-3.57940100	2.49513200
C	-4.41305300	0.82805200	-0.43421500	C	2.19935400	-0.99968100	2.79577800
C	-5.82418300	0.37774500	-0.00511100	H	1.16747200	-0.70945600	2.57653200
H	-6.10607200	-0.58907600	-0.42907900	H	2.19983900	-1.64038100	3.68885600
H	-5.92753200	0.31524100	1.08119900	H	2.75431700	-0.09436000	3.04360300
H	-6.56011000	1.11669600	-0.35364100	C	4.26671000	-2.15716300	1.97533500
C	-4.43731000	1.10620000	-1.95431300	H	4.26031200	-2.78546800	2.87738700
H	-4.78697500	0.25541000	-2.54277600	H	4.76943200	-2.72543900	1.18912300
H	-5.13004500	1.93644000	-2.14697600	H	4.87787000	-1.28071800	2.20515900
H	-3.45554600	1.40955000	-2.33310800	C	0.20088700	3.67269700	-1.92732000
C	-4.11132600	2.19866800	0.22204000	C	-0.50850100	2.76592000	-1.12991300
H	-4.90231900	2.90733400	-0.06045400	C	-0.38565900	2.81053100	0.26399700
H	-4.08411300	2.16558100	1.31146600	C	0.43821600	3.76905400	0.88538400
H	-3.16098000	2.61158900	-0.12643100	C	1.13168200	4.67069900	0.07338500
C	-3.23900900	-1.06433200	1.79026500	C	1.01721400	4.62550800	-1.32162100
C	-4.37291200	-2.09256300	1.97664500	H	0.10691500	3.63673900	-3.00937800
H	-5.35223000	-1.70216100	1.68886200	H	-1.17762600	2.04231300	-1.58676600
H	-4.19637800	-3.01131200	1.41204000	H	-0.98620100	2.14124900	0.87823300
H	-4.43211100	-2.37508600	3.03754000	H	1.76581000	5.42441400	0.53530800
C	-1.90959800	-1.69714700	2.26778200	H	1.56362600	5.34208400	-1.92964800
H	-1.69542400	-2.65391200	1.78986000	C	0.55214100	3.81976700	2.39138200
H	-1.06039700	-1.03286600	2.07285500	H	1.18296700	4.65326900	2.71687100
H	-1.96618400	-1.87946500	3.34999700	H	-0.43106900	3.94009500	2.86396300
C	-3.49909500	0.12398000	2.74275400	H	0.98750100	2.89374500	2.78760200
H	-3.47697800	-0.24304800	3.77759000	<b>7<sub>H</sub> [Pd(PH<sub>3</sub>)<sub>2</sub>(PhBr)]</b>			
H	-2.72594900	0.89546500	2.65486300	Pd	-1.68341600	0.11846700	0.11279500
H	-4.47490200	0.59049800	2.59000800	P	-1.91937100	2.41681800	-0.13461000
C	2.87377800	-1.91338800	-1.54049000	P	-3.12314100	-1.35156700	-0.96627300
C	4.06664300	-2.88466600	-1.42296600	Br	3.77186400	0.31044100	-0.50668000
H	5.01635800	-2.37514900	-1.24470500	C	1.39559000	0.44866900	1.09084000
H	3.92530100	-3.62534700	-0.63190600	C	0.18923700	-0.04727100	1.64696100
H	4.16739500	-3.44102700	-2.36562100	C	-0.23146600	-1.36570800	1.34935700
C	1.58943000	-2.73730100	-1.78451400	C	0.56508700	-2.16617600	0.49335200
H	1.35281200	-3.42325200	-0.97063200	C	1.73108700	-1.67156300	-0.06570300
H	0.73046300	-2.07579900	-1.92668000	C	2.13225600	-0.35755500	0.24523700
H	1.71976100	-3.33883900	-2.69537300	H	-0.28629500	0.51240700	2.44711300
C	3.06235600	-1.06403100	-2.81721900	H	-1.03017600	-1.82633800	1.92291400
H	3.02671600	-1.73100500	-3.68941500	H	0.26346700	-3.18949900	0.28542200
H	2.26160400	-0.32560200	-2.93039200	H	2.34001800	-2.28734200	-0.71842900
H	4.02356100	-0.54613900	-2.85047200	H	-3.12871600	3.00016400	-0.59911600
C	3.95596800	0.63350200	-0.04471500	H	-1.73249000	3.36035000	0.91520100
C	3.55543800	1.71105200	-1.07870100	H	-1.08443500	3.09636700	-1.06198000
H	2.56264500	2.11390200	-0.86476500	H	-2.70600600	-1.95552100	-2.18344000
H	4.28089800	2.53529800	-1.02639800	H	-3.61614400	-2.55853800	-0.39334900
H	3.55386100	1.34342000	-2.10489700	H	-4.38879500	-0.93463200	-1.45931800
C	3.99212700	1.36060900	1.31763700	H	1.73839300	1.44651600	1.34316900
H	2.99456300	1.69433200	1.62034000	<b>7<sub>H</sub> [Pd(PH<sub>3</sub>)<sub>2</sub>(PhCl)]</b>			
H	4.41931800	0.75250200	2.11862700	Pd	-1.18513200	0.08750000	0.12821500
H	4.62502300	2.25315800	1.21983400	P	-1.61683700	2.34780200	-0.18895900
C	5.38355500	0.14693500	-0.37092500	P	-2.58117200	-1.53101800	-0.78452800
H	6.07513400	0.99742700	-0.28868400	Cl	4.05295700	0.54976300	-0.86473900
H	5.74090400	-0.62710800	0.31239600	C	1.93064800	0.67449000	0.83734300
H	5.47247700	-0.23388100	-1.39176000	C	0.81044100	0.12973900	1.51282000
C	2.81343100	-1.78709700	1.61360400				
C	1.99479400	-3.09275900	1.51035700				



C	0.46218600	-1.22770700	1.31285900
C	1.24667500	-2.01817400	0.43664000
C	2.32810800	-1.47677800	-0.23613800
C	2.65734800	-0.12315600	-0.02582100
H	0.35894400	0.69770300	2.32080300
H	-0.25773300	-1.70899300	1.96797500
H	1.00372600	-3.06922900	0.30429200
H	2.93236100	-2.08148100	-0.90392300
H	-2.89810700	2.81647400	-0.58582600
H	-1.43294100	3.34848900	0.80729800
H	-0.90587500	3.04852800	-1.20034700
H	-2.20743200	-2.14820700	-2.00918700
H	-2.93500900	-2.74950900	-0.13746400
H	-3.90842700	-1.23192800	-1.19427900
H	2.22401700	1.70494300	1.00938600

**7<sub>tBu</sub>\* [Pd(PtBu<sub>3</sub>)(Ph)(Br)]\***

Pd	-0.82575300	-0.33063000	0.00229500
Br	-2.07205700	-2.41707100	0.02041700
P	1.66305200	0.22028100	0.00236700
C	2.29274300	0.51088600	1.81716800
C	2.66442700	-1.24222900	-0.80149300
C	1.93761200	1.83669100	-1.03973500
C	-4.74599300	2.26484700	-0.00187300
C	-4.23497800	1.78021700	-1.20815000
C	-3.16762100	0.87446200	-1.21301600
C	-2.59259300	0.50069500	0.00508100
C	-3.12905100	0.93141400	1.22196900
C	-4.19711300	1.83616900	1.20899600
H	-5.58316000	2.95756200	-0.00474800
H	-4.67575100	2.08973300	-2.15273200
H	-2.79352700	0.47259800	-2.14998100
H	-2.72509000	0.57388200	2.16464200
H	-4.60832800	2.18926200	2.15161200
C	1.65603900	-0.57530000	2.71910900
H	1.92426800	-0.36377600	3.76290800
H	0.56370000	-0.56736200	2.64177300
H	1.99813100	-1.58480100	2.49294700
C	1.74781400	1.85797800	2.34171700
H	1.95800300	1.91935000	3.41718300
H	2.21898300	2.72496300	1.87331600
H	0.66242800	1.93608700	2.21679700
C	0.80283800	2.83004700	-0.68739500
H	0.89883100	3.71427800	-1.33161100
H	-0.18517000	2.39283700	-0.87198600
H	0.82981600	3.17676700	0.34536000
C	1.76103800	1.52045400	-2.54157100
H	1.74572200	2.46951600	-3.09292900
H	2.57759300	0.92369800	-2.95285600
H	0.81469300	1.00818200	-2.74347300
C	3.30051300	2.53184300	-0.84383200
H	4.14336700	1.87941600	-1.08668300
H	3.43981100	2.90305800	0.17459200
H	3.35607700	3.40149900	-1.51254500
C	3.82363500	0.49500300	2.00265300
H	4.26273300	-0.47904600	1.77257000
H	4.05739500	0.71166200	3.05380100

H	4.33005000	1.24918900	1.39418900
C	1.86367400	-1.76100500	-2.02087000
H	2.38182600	-2.64050500	-2.42575700
H	0.85330700	-2.07075000	-1.73551800
H	1.78023700	-1.03436400	-2.82898400
C	2.72807400	-2.42654400	0.18851800
H	3.14399500	-3.29257300	-0.34212800
H	3.37702900	-2.23437000	1.04573300
H	1.73538300	-2.71275600	0.55065100
C	4.09898300	-0.89008200	-1.24403500
H	4.71482000	-0.51255400	-0.42372700
H	4.58437500	-1.79815100	-1.62623100
H	4.11907300	-0.15355500	-2.05129200

**7<sub>tBu</sub>\* [Pd(PtBu<sub>3</sub>)(Ph)(Cl)]\***

Pd	0.93716400	-0.61241700	0.04683000
P	-1.48711600	0.16950600	-0.00902100
Cl	1.84799900	-2.73081800	0.15893800
C	-2.44246800	-0.72209800	-1.44888000
C	-2.38021300	-0.18198500	1.67973900
C	-1.47132300	2.08433700	-0.33540200
C	5.18076900	1.41155100	-0.06723800
C	4.52388600	1.22707600	1.15161400
C	3.33201700	0.49468500	1.20921200
C	2.78986700	-0.00838100	0.02353300
C	3.46312700	0.11851500	-1.19398100
C	4.65311600	0.85434200	-1.23454500
H	6.11158100	1.97102800	-0.10418500
H	4.94348200	1.63692000	2.06717700
H	2.83892600	0.32486500	2.16241200
H	3.07152300	-0.34428900	-2.09475400
H	5.17387700	0.97439000	-2.18151200
C	-2.04403700	-2.21823700	-1.41962100
H	-2.50756700	-2.71863700	-2.28021400
H	-0.95947300	-2.34684900	-1.49577700
H	-2.37747500	-2.74035800	-0.52354200
C	-1.94548700	-0.18634100	-2.80984500
H	-2.36361300	-0.82242300	-3.60066800
H	-2.27007500	0.83561300	-3.01732300
H	-0.85493800	-0.23755600	-2.89466900
C	-0.37538000	2.38115900	-1.38886500
H	-0.34160800	3.46475300	-1.56415500
H	0.61464400	2.07277000	-1.03268100
H	-0.54973100	1.89973600	-2.35064500
C	-1.02532600	2.82989100	0.94282800
H	-0.84345600	3.88062400	0.68184200
H	-1.78094600	2.82293600	1.73164000
H	-0.08958700	2.42892300	1.34609800
C	-2.80930800	2.68861700	-0.80885400
H	-3.62710800	2.50501300	-0.10692100
H	-3.11416500	2.31538100	-1.78965100
H	-2.69499000	3.77710500	-0.90128900
C	-3.97897600	-0.59577100	-1.40412600
H	-4.41146700	-1.05635400	-0.51267100
H	-4.40396500	-1.11823600	-2.27179500
H	-4.31744100	0.44302100	-1.45032300
C	-1.37653700	0.11559200	2.82094900

H	-1.83669300	-0.17685200	3.77405000
H	-0.45647700	-0.46634500	2.70090500
H	-1.10553300	1.16874200	2.90214700
C	-2.69775400	-1.69010700	1.79060200
H	-3.05088900	-1.89325600	2.80988200
H	-3.48692300	-2.01255800	1.10844500
H	-1.81078700	-2.30972300	1.62156200
C	-3.67636200	0.61812000	1.91787100
H	-4.43639800	0.42365300	1.15657800
H	-4.10154600	0.32953000	2.88843700
H	-3.49764200	1.69515400	1.95087100

**7<sub>tBu</sub>\* [Pd(PtBu3)(Ph)(I)]\***

Pd	-0.66692200	-0.08675000	-0.03876700
I	-2.36678000	-2.06336400	0.00717400
P	1.86869800	0.15553300	-0.00389300
C	2.38943900	1.03962700	1.64737100
C	2.73675800	-1.58389600	-0.09790300
C	2.43610300	1.23827900	-1.51500100
C	-4.07809500	3.15234200	0.01280700
C	-3.67510900	2.59014700	-1.20070700
C	-2.79306500	1.50358800	-1.22102700
C	-2.28319600	1.01968900	-0.01131100
C	-2.72217100	1.53628000	1.21263600
C	-3.60534800	2.62210100	1.21542200
H	-4.77483900	3.98608100	0.02194200
H	-4.06036500	2.98112200	-2.13933900
H	-2.51034900	1.04654700	-2.16449300
H	-2.38518600	1.10381500	2.14992700
H	-3.93628300	3.03738400	2.16429000
C	1.55698500	0.42766300	2.80104300
H	1.76048300	0.99609300	3.71838600
H	0.48310400	0.49087100	2.59518200
H	1.79621700	-0.61582500	3.00464400
C	1.97935300	2.52760300	1.58001500
H	2.10162200	2.96612300	2.57879900
H	2.59857100	3.11271800	0.89648600
H	0.92881300	2.65086700	1.29629700
C	1.42220800	2.39773200	-1.67834800
H	1.66041500	2.94464100	-2.60042900
H	0.39627700	2.02391200	-1.76925600
H	1.44598700	3.11777900	-0.86052800
C	2.32671500	0.40489000	-2.81117200
H	2.47934700	1.07592100	-3.66634900
H	3.08261000	-0.37990900	-2.88111300
H	1.33678300	-0.04930000	-2.92326900
C	3.86046700	1.82177300	-1.42501500
H	4.62568600	1.04909300	-1.31678000
H	3.97235500	2.52946500	-0.59982600
H	4.07862200	2.37172500	-2.35048200
C	3.88717200	0.95930400	2.00537800
H	4.21590500	-0.06409000	2.20305000
H	4.06575100	1.53675200	2.92252100
H	4.52921200	1.37765000	1.22600300
C	1.97887100	-2.44587600	-1.13712300
H	2.40905700	-3.45622300	-1.12803300
H	0.91619500	-2.53396100	-0.88954500

H	2.05861900	-2.06939500	-2.15694500
C	2.57006000	-2.31580100	1.25226800
H	2.90849000	-3.35187200	1.12336700
H	3.17116300	-1.88026800	2.05350200
H	1.52387900	-2.35321600	1.57227100
C	4.23567900	-1.55036700	-0.45753600
H	4.82327600	-0.94486900	0.23715200
H	4.63191500	-2.57395000	-0.41685400
H	4.41698300	-1.18032400	-1.46991000

**8<sub>Cy</sub>\* [Pd(PCy3)<sub>2</sub>(Ph...Br)]\* (conformer F)**

Pd	-0.01676300	-0.78100300	-0.05063600
Br	0.37990500	-3.00277400	1.52266500
P	2.23504400	0.35463600	0.02428100
P	-2.14935900	0.37226900	0.06578000
C	2.76939800	0.78056500	4.20900500
C	2.45952400	0.15167200	2.83986300
C	2.60028900	1.17628800	1.69182900
C	1.69878200	2.39653000	1.97110700
C	2.00565600	3.02926600	3.34054300
C	1.88916400	2.00810000	4.48012200
C	6.04329000	-1.65998300	0.42615500
C	5.06081000	-0.47398800	0.48346000
C	3.70047100	-0.85502700	-0.14523200
C	3.93113800	-1.31671300	-1.60153200
C	4.89424300	-2.51449900	-1.66290000
C	6.24019700	-2.17931100	-1.00491500
C	2.04927600	2.66016700	-3.54512900
C	2.05281200	1.41970300	-2.63514600
C	2.49936600	1.77751000	-1.19916000
C	3.88021000	2.46568600	-1.21890800
C	3.87226500	3.70736300	-2.12969200
C	3.41590400	3.36154300	-3.55470900
C	-2.82185300	0.54263700	4.24963800
C	-2.12614600	0.64872800	2.88166000
C	-3.04287600	0.18544500	1.72744300
C	-3.53379000	-1.25097700	2.00576600
C	-4.24415100	-1.35205100	3.36753100
C	-3.33939700	-0.87780100	4.51282600
C	-3.91805900	-0.99823700	-3.54957300
C	-2.89864900	-0.32340100	-2.61503700
C	-3.46183900	-0.18105500	-1.18212800
C	-4.80701000	0.57312700	-1.20021700
C	-5.82189600	-0.11649100	-2.13049900
C	-5.26723500	-0.26525100	-3.55439800
C	-1.98542700	2.27115000	-0.04774800
C	-3.12818100	3.15948400	0.49619600
C	-0.48944400	-2.79833700	-0.51232100
C	0.45041000	-3.05109200	-1.52999400
C	-1.79390000	-3.32174400	-0.62602800
C	0.03302300	-3.65693400	-2.72377000
C	-1.27826800	-4.10255600	-2.87089900
C	-2.29690400	5.11631200	-0.90921600
C	-1.18134300	4.22461800	-1.47225300
C	-1.58494000	2.73999500	-1.46166000
C	-2.18031600	-3.94714700	-1.80678100
C	-2.72479200	4.64650600	0.48755900

H	3.82816700	1.07950300	4.24279100	H	-3.40022000	2.87290600	1.51714700
H	2.63240400	0.03025900	4.99827500	H	1.49513800	-2.81434200	-1.37578700
H	3.11446200	-0.71192400	2.67732800	H	-2.49004400	-3.22689200	0.19814400
H	1.43570500	-0.24414300	2.83735700	H	0.75971600	-3.82006500	-3.51635500
H	3.63972000	1.53282400	1.67109200	H	-1.59003000	-4.60329100	-3.78301200
H	1.81781700	3.15819300	1.19138000	H	-3.16406000	5.08008500	-1.58551000
H	0.64840100	2.07682000	1.94587000	H	-1.97047600	6.16376300	-0.87660900
H	1.32997500	3.87701700	3.51462900	H	-0.92516800	4.53378100	-2.49414900
H	3.02567500	3.44151700	3.32615600	H	-0.27174300	4.35707700	-0.86720100
H	0.84088700	1.68767300	4.57352500	H	-0.76580200	2.12098800	-1.84497400
H	2.16151600	2.47201800	5.43686500	H	-2.43202100	2.60421500	-2.14664500
H	5.65633200	-2.47380600	1.05681600	H	-3.19627300	-4.32503100	-1.89684800
H	7.00706600	-1.36179600	0.85929400	H	-1.89207200	4.79716000	1.19095800
H	4.94279800	-0.16377800	1.52606900	H	-3.55851700	5.25758700	0.85735700
H	5.49546300	0.38092400	-0.05076700	<b>8<sub>Cy</sub><sup>‡</sup> [Pd(PCy<sub>3</sub>)<sub>2</sub>(Ph···Cl)]<sup>‡</sup> (conformer F)</b>			
H	3.32161400	-1.72702100	0.40928100	Pd	-0.03572800	0.78554500	-0.40373200
H	2.98292600	-1.56866100	-2.08837400	P	2.26513000	-0.20942100	0.02346800
H	4.36681100	-0.49141300	-2.17986600	P	-2.12697800	-0.32533500	0.01199400
H	5.04559200	-2.81695000	-2.70738300	Cl	0.51495700	2.15088000	-2.55886600
H	4.43827700	-3.37377800	-1.14965700	C	2.69271000	-2.55047000	-3.48290100
H	6.75038200	-1.40875200	-1.60239100	C	2.37750000	-1.36358200	-2.55682200
H	6.89635900	-3.05902700	-1.00399500	C	2.63293400	-1.70931400	-1.07222000
H	1.28363500	3.36702200	-3.19341700	C	1.82224500	-2.96230200	-0.68068000
H	1.76235800	2.37128100	-4.56468700	C	2.13324700	-4.15204200	-1.60686300
H	1.05743500	0.96013000	-2.61111900	C	1.90200600	-3.80375600	-3.08355100
H	2.72993100	0.67166900	-3.06436900	C	5.92537300	1.53625300	-1.49000600
H	1.77280600	2.51845100	-0.83236000	C	5.01599500	0.42272000	-0.93485500
H	4.18709200	2.75234900	-0.20581200	C	3.65136300	0.99598000	-0.48755400
H	4.63755300	1.76163300	-1.58826500	C	3.88851200	2.10283000	0.56348400
H	4.87133300	4.16218200	-2.14786700	C	4.78042500	3.22534800	0.00728500
H	3.19348800	4.46167000	-1.70452100	C	6.12775200	2.67423600	-0.48022400
H	4.15979800	2.69817200	-4.02096200	C	2.29532200	-0.55268700	4.25940000
H	3.37609600	4.26817400	-4.17208800	C	2.19779100	0.10727500	2.87320100
H	-3.66513100	1.24904100	4.28456600	C	2.64637500	-0.86520400	1.75881000
H	-2.12631800	0.84894900	5.04215700	C	4.07267800	-1.38466900	2.03466900
H	-1.79282500	1.68164000	2.72353300	C	4.17210600	-2.03874800	3.42520600
H	-1.22175800	0.02446400	2.87757700	C	3.71008800	-1.08373200	4.53537300
H	-3.92666700	0.83827300	1.70440300	C	-2.69780400	-2.58169900	-3.54294700
H	-4.21803900	-1.58733100	1.21757100	C	-2.03043000	-1.99535100	-2.28673500
H	-2.67377800	-1.93279500	2.00183000	C	-2.95731400	-1.00119900	-1.55338000
H	-4.56475200	-2.38773200	3.53889600	C	-3.38370000	0.11020500	-2.53480400
H	-5.15868400	-0.74014600	3.34830700	C	-4.06113900	-0.46711400	-3.79062700
H	-2.48457300	-1.56351400	4.60424900	C	-3.15663000	-1.47939200	-4.50660000
H	-3.87881400	-0.91725000	5.46795800	C	-4.04346800	2.57022600	2.46445500
H	-4.06916200	-2.03668100	-3.22234800	C	-2.97960500	1.56658700	1.98588400
H	-3.50850700	-1.05009900	-4.56677800	C	-3.49303800	0.72833300	0.79210100
H	-1.97020500	-0.90372200	-2.59244500	C	-4.82223900	0.03309800	1.15179700
H	-2.64643900	0.66451000	-3.02080900	C	-5.88059000	1.05094800	1.61453800
H	-3.66589300	-1.20642700	-0.84136500	C	-5.37461400	1.88364000	2.80073500
H	-5.22637400	0.65205800	-0.18989100	C	-1.93023500	-1.91901000	1.04058800
H	-4.64844500	1.59919400	-1.55729200	C	-3.04833200	-2.98648600	0.99727200
H	-6.76135400	0.45182100	-2.14223200	C	-0.57993600	2.78011100	-0.87765300
H	-6.06391100	-1.11138300	-1.72766400	C	0.20697600	3.52723400	0.01812000
H	-5.13687700	0.73449400	-3.99576100	C	-1.87547200	3.22839900	-1.20387200
H	-5.98824300	-0.79485400	-4.19054400	C	-0.36302800	4.60332300	0.71022000
H	-1.11162500	2.44952300	0.59554800	C	-1.67154400	5.00380000	0.44675400
H	-4.02969200	3.03247900	-0.11490600				

C	-2.19162800	-3.99615000	3.17435400	H	-6.12843000	1.72168400	0.77834400
C	-1.10260600	-2.91575000	3.23507800	H	-5.23603700	1.22383900	3.67071500
C	-1.53704100	-1.63304800	2.50535500	H	-6.12668700	2.62855800	3.09145500
C	-2.41345400	4.31841900	-0.52720300	H	-1.04480600	-2.36569500	0.56456000
C	-2.61367600	-4.27283700	1.72478800	H	-3.95764800	-2.60035200	1.47276700
H	3.76979400	-2.77245800	-3.43892800	H	-3.31864700	-3.23527200	-0.03412900
H	2.47362400	-2.27516600	-4.52253000	H	1.25488500	3.28801100	0.14840400
H	2.96648400	-0.49171200	-2.86284000	H	-2.44692200	2.71860800	-1.96943200
H	1.32641900	-1.06986000	-2.67673100	H	0.24483400	5.15254100	1.42557300
H	3.69685700	-1.95739000	-0.95479900	H	-2.09982900	5.85957300	0.96044800
H	2.02896400	-3.25426000	0.35558100	H	-3.06784900	-3.65716200	3.74708800
H	0.75039900	-2.72918700	-0.73691100	H	-1.84316700	-4.91979200	3.65409100
H	1.52046200	-5.01558100	-1.31631100	H	-0.85365800	-2.68350300	4.27894400
H	3.18200600	-4.45322400	-1.46547400	H	-0.18187500	-3.30179200	2.77218000
H	0.82965800	-3.62201700	-3.24872200	H	-0.73495100	-0.88727900	2.54161600
H	2.17817600	-4.65226400	-3.72273300	H	-2.39523800	-1.20227200	3.03811900
H	5.47277800	1.94228700	-2.40660600	H	-3.42415800	4.64162200	-0.76681900
H	6.89345300	1.10913300	-1.78298100	H	-1.77128200	-4.72760800	1.18212200
H	4.89129800	-0.34434000	-1.70517300	H	-3.43097400	-5.00543300	1.69878400
H	5.51678900	-0.06303100	-0.08721500	<b>8<sub>H</sub><sup>†</sup> [Pd(PH<sub>3</sub>)<sub>2</sub>(Ph··Br)]<sup>‡</sup></b>			
H	3.19818300	1.48137800	-1.36450000	Pd	-0.82604900	-0.31741300	0.02810700
H	2.93725100	2.51769200	0.91319100	Br	0.07766800	2.05664600	-0.67170400
H	4.38034400	1.66949000	1.44467200	P	-0.60521400	-2.37062400	-1.13529400
H	4.93792600	3.99150000	0.77774400	P	-2.94409900	-0.08801300	1.12455000
H	4.26191700	3.71948800	-0.82701600	C	1.22374600	0.30202000	0.04472600
H	6.69650700	2.29609100	0.38276000	C	2.17353400	-0.20466300	-0.86225200
H	6.73134900	3.47564800	-0.92509400	C	3.32751000	-0.80195400	-0.36566900
H	1.57909100	-1.38598500	4.31566700	C	3.56826900	-0.86376800	1.01612800
H	2.00026600	0.16584700	5.03512100	C	2.65225900	-0.30008100	1.90082200
H	1.17274200	0.44561300	2.68056000	C	1.48955300	0.32324400	1.42404300
H	2.82747500	1.00513100	2.86539200	H	1.99238000	-0.14496100	-1.93063200
H	1.96697200	-1.72902600	1.82276200	H	4.04944300	-1.22065600	-1.06270700
H	4.38107900	-2.10383700	1.26613800	H	4.47970300	-1.32135400	1.38961100
H	4.78255800	-0.54860600	1.98446000	H	2.84791400	-0.30604800	2.97022300
H	5.20320100	-2.36814800	3.60867500	H	0.81781300	0.83211600	2.10741500
H	3.54760900	-2.94447600	3.44316600	H	0.03214300	-2.43314600	-2.40349500
H	4.40876000	-0.23578300	4.59681700	H	0.16453400	-3.40728900	-0.54702300
H	3.74582100	-1.58795900	5.50962800	H	-1.70214300	-3.20062300	-1.49129000
H	-3.56535500	-3.18913300	-3.24377000	H	-3.07889300	-0.35374400	2.51274700
H	-2.00007400	-3.26340700	-4.04713300	H	-3.60908300	1.16505100	1.15009400
H	-1.72606400	-2.81260200	-1.62276100	H	-4.08346600	-0.84019300	0.73612800
H	-1.11152200	-1.46680200	-2.57414400	<b>8<sub>H</sub><sup>†</sup> [Pd(PH<sub>3</sub>)<sub>2</sub>(Ph··Cl)]<sup>‡</sup></b>			
H	-3.86325500	-1.54184000	-1.24435700	Pd	0.83114000	0.06682900	-0.05557200
H	-4.06852400	0.81615300	-2.05055400	P	0.50667700	2.37948100	-0.35742800
H	-2.49277100	0.67823800	-2.83365100	P	3.04901900	-0.41488900	0.76075000
H	-4.33207700	0.35031100	-4.47122600	Cl	-0.06872700	-1.98447200	-1.17537200
H	-5.00227900	-0.95925500	-3.50256700	C	-1.21746700	-0.54498600	-0.19067200
H	-2.27436500	-0.95610000	-4.90314200	C	-2.14938200	0.12007000	-1.00781900
H	-3.67741200	-1.91637500	-5.36831000	C	-3.35666100	0.53212800	-0.45210900
H	-4.20782300	3.31717600	1.67552500	C	-3.66638100	0.25271800	0.88759600
H	-3.66560100	3.11897800	3.33687500	C	-2.76143600	-0.46738800	1.66567500
H	-2.06684800	2.09915800	1.70033000	C	-1.54569100	-0.90655000	1.12587800
H	-2.71508100	0.90553600	2.82095000	H	-1.91351100	0.32262700	-2.04752400
H	-3.70349200	1.44949400	-0.01102200	H	-4.06621300	1.07471800	-1.07237800
H	-5.20865500	-0.54158800	0.30154600	H	-4.61762400	0.56953800	1.30493800
H	-4.65055700	-0.68359400	1.96513500				
H	-6.80832500	0.52717500	1.88033000				

H	-3.00544600	-0.72295300	2.69392300
H	-0.87122100	-1.52472500	1.70961200
H	-0.19148700	2.87135700	-1.49241600
H	-0.27246200	3.07887000	0.59921200
H	1.55730500	3.33453200	-0.40873700
H	3.30168400	-0.56435700	2.14978300
H	3.70906200	-1.60619900	0.36306100
H	4.15252900	0.44362300	0.51705800

**8<sub>Ph</sub><sup>‡</sup> [Pd(PPh<sub>3</sub>)<sub>2</sub>(Ph...Br)]<sup>‡</sup>**

Pd	-0.00723900	-0.70713000	-0.23264600
Br	0.32651400	-2.60838000	-2.05496200
P	-2.03178200	0.55287400	-0.02590500
P	2.22762900	0.28887000	0.09049900
C	-0.60608700	-2.72685900	0.00291900
C	0.28946500	-3.19709400	0.97886500
C	-0.20847900	-3.95282200	2.04952100
C	-1.94910700	-3.13782500	0.00489500
C	-1.98912000	2.29757900	-0.65979000
C	-3.50871400	-0.13182100	-0.90910000
C	-2.63438400	0.77268100	1.71420800
C	3.65568200	-0.88300700	-0.06806900
C	2.57557600	1.09415900	1.72006400
C	2.61151200	1.59431300	-1.16882300
C	-0.82765200	3.05798100	-0.44888800
C	-3.06525300	2.89226900	-1.33854100
C	-2.97996000	4.21145000	-1.79022300
C	-1.82144900	4.95767500	-1.56877700
C	-0.74523600	4.37713700	-0.89434500
C	2.10423600	1.40036100	-2.46587700
C	3.34608300	2.75876700	-0.89978400
C	3.57467800	3.70118000	-1.90528500
C	3.08166900	3.49032600	-3.19422200
C	2.34774200	2.33544400	-3.47287800
C	3.93124300	-1.76396900	0.99336300
C	4.40285000	-1.00166600	-1.24849400
C	5.40210300	-1.97171400	-1.36281600
C	5.67133600	-2.83648700	-0.30212000
C	4.93264700	-2.72734200	0.87905500
C	1.48961500	1.41679900	2.54791800
C	3.87584800	1.38877700	2.16765700
C	4.07866400	2.00882400	3.40077900
C	2.98706900	2.33895000	4.20912100
C	1.69315500	2.03899000	3.78233700
C	-3.35215300	1.90109200	2.14213200
C	-2.34367200	-0.23714000	2.64734100
C	-2.77175500	-0.12541400	3.97143600
C	-3.77213900	2.01455900	3.46919100
C	-3.48504100	1.00132300	4.38618300
C	-4.77287200	-0.27885900	-0.32046700
C	-3.32788300	-0.55944400	-2.23669400
C	-4.38858400	-1.10442500	-2.95993400
C	-5.83211200	-0.83619400	-1.04316800
C	-5.64467300	-1.24738400	-2.36309500
C	-2.41763700	-3.90371000	1.06988700
C	-1.55702800	-4.30302100	2.10278600
H	1.35181900	-2.99893500	0.89063200

H	0.47843400	-4.29595700	2.81957200
H	-2.61365100	-2.83714000	-0.79581600
H	0.02269900	2.61231600	0.05721600
H	-3.97300900	2.32516400	-1.51787300
H	-3.82215400	4.65373300	-2.31639000
H	-1.75542100	5.98261800	-1.92434300
H	0.16725600	4.94305200	-0.72752000
H	1.50728800	0.51721600	-2.68046400
H	3.73566700	2.93990100	0.09658700
H	4.14198600	4.60050100	-1.67885700
H	3.26210700	4.22469100	-3.97483400
H	1.95149400	2.16649700	-4.47063900
H	3.36870400	-1.68685700	1.92054900
H	4.21094200	-0.33451600	-2.08248400
H	5.97179300	-2.04622700	-2.28547300
H	6.44907800	-3.58985400	-0.39320800
H	5.13567200	-3.39363100	1.71358400
H	0.48255600	1.16351800	2.22793800
H	4.73208000	1.12133600	1.55510000
H	5.08968800	2.23047500	3.73284000
H	3.14771800	2.81886200	5.17099200
H	0.83912200	2.27785300	4.41040700
H	-3.58019100	2.69645600	1.43918800
H	-1.77714700	-1.10997800	2.33588700
H	-2.53958400	-0.91697400	4.67908200
H	-4.32342800	2.89651800	3.78534500
H	-3.81147500	1.09171400	5.41900900
H	-4.93555800	0.04021900	0.70415000
H	-2.34630600	-0.48188700	-2.69789100
H	-4.22994900	-1.42954300	-3.98470700
H	-6.80470900	-0.94675500	-0.57027900
H	-6.46881200	-1.68192100	-2.92261200
H	-3.46576800	-4.19218700	1.09162600
H	-1.93269500	-4.91176300	2.92053000

**8<sub>Ph</sub><sup>‡</sup> [Pd(PPh<sub>3</sub>)<sub>2</sub>(Ph...Cl)]<sup>‡</sup>**

Pd	-0.03868600	-0.87758400	-0.47145000
P	2.23751400	-0.03484700	-0.01993600
P	-1.87690200	0.58096000	-0.04869100
Cl	0.16472100	-2.61209500	-2.31562800
C	-1.01933600	-2.77110800	-0.58886300
C	-0.38886300	-3.49225600	0.44162300
C	-1.16464500	-4.28685000	1.29607200
C	-2.38487500	-2.97265800	-0.86092000
C	3.64633200	-0.93855600	-0.81849400
C	2.70113200	-0.08048500	1.77336000
C	2.57206400	1.71270400	-0.53037100
C	-1.55981700	2.40703200	-0.12372900
C	-2.70795300	0.42524200	1.60115000
C	-3.25919700	0.37284900	-1.26437700
C	3.55519100	-2.33523900	-0.92909900
C	4.79557200	-0.29847700	-1.30985500
C	5.83152600	-1.04025000	-1.88205700
C	5.73563400	-2.42995300	-1.97166200
C	4.59381000	-3.07584500	-1.49361600
C	-2.53415700	-4.43277300	1.07914100
C	-3.13196800	-3.78160300	-0.01095900

C	1.66774300	-0.07855700	2.72435500	H	4.03467000	4.65088400	0.40072800
C	4.03095300	-0.12994300	2.22296700	H	3.19581100	5.33222000	-1.83932400
C	4.31770600	-0.15811900	3.58885200	H	1.94466500	3.69621700	-3.23744400
C	3.28140300	-0.14003400	4.52555500	<i>t</i> - <b>9</b> <sub>Cy</sub> [Pd(PCy <sub>3</sub> ) <sub>2</sub> (Ph)(Br)] (conformer <b>F</b> )			
C	1.95562100	-0.10181400	4.09063200	Pd	-0.00464900	-0.08026700	-0.12656000
C	-3.41917600	1.48148300	2.19563300	Br	-0.02451500	-2.58295700	-0.85161600
C	-4.02620000	1.31616800	3.44163300	P	-2.44755400	0.03114500	-0.23274700
C	-3.93179600	0.09435700	4.11231700	P	2.39608400	-0.22944700	0.21930400
C	-3.22642800	-0.96059500	3.53129700	C	-2.91482400	0.34563700	-4.42395800
C	-2.61478600	-0.79638800	2.28652900	C	-2.35911800	-0.07237200	-3.05264500
C	-2.90858700	0.18064600	-2.61235900	C	-3.08058500	0.66011900	-1.89879100
C	-3.89180500	0.01628000	-3.58831300	C	-3.00065900	2.18826600	-2.09720200
C	-5.24240000	0.02069600	-3.22927600	C	-3.56027300	2.59763900	-3.47194200
C	-5.60087000	0.19560500	-1.89182300	C	-2.85134200	1.86646100	-4.62021900
C	-4.61725300	0.37462600	-0.91528500	H	-3.96014400	0.01257000	-4.51053800
C	-0.56125000	2.93779600	0.71048700	H	-2.35769700	-0.16787700	-5.21781800
C	-2.26170400	3.27941800	-0.96888800	H	-2.43559700	-1.15891300	-2.93410200
C	-1.97263500	4.64708100	-0.97662400	H	-1.28631400	0.15969700	-3.00219800
C	-0.98562600	5.16279700	-0.13708200	H	-4.14387500	0.38906000	-1.93802000
C	-0.28143500	4.30281400	0.70978400	H	-3.55772600	2.71307600	-1.31385700
C	2.09177900	2.11285900	-1.78906000	H	-1.96238000	2.52155800	-2.01151900
C	3.27082200	2.64296900	0.25228800	H	-4.63638900	2.36975200	-3.50896500
C	3.49120000	3.94080700	-0.21774500	H	-3.46836300	3.68456400	-3.59439300
C	3.02203300	4.32308900	-1.47510900	H	-1.79816900	2.18281200	-4.65613700
C	2.32171700	3.40424800	-2.26094800	H	-3.29561800	2.14756100	-5.58367400
H	0.68744100	-3.44190600	0.56915800	C	-5.14746000	-3.30478500	-0.55536400
H	-0.67749600	-4.81810300	2.11036000	C	-4.73917200	-1.81868200	-0.51766900
H	-2.84802500	-2.48303500	-1.70957800	C	-3.25752700	-1.67632100	-0.10262100
H	2.65728000	-2.84283200	-0.59167000	C	-3.02576600	-2.35094100	1.26788200
H	4.88396300	0.78176800	-1.25014000	C	-3.42778300	-3.83517900	1.22400700
H	6.71366500	-0.52862400	-2.25864300	C	-4.88823200	-4.00699600	0.78391500
H	6.54145200	-3.00510600	-2.42006500	H	-4.57669300	-3.81155400	-1.34681500
H	4.50221000	-4.15571700	-1.57340400	H	-6.20699400	-3.38580000	-0.83192400
H	-3.12748400	-5.07308000	1.72563800	H	-5.38944500	-1.28825700	0.18956400
H	-4.19511100	-3.90640200	-0.20201800	H	-4.92344800	-1.38194600	-1.50490200
H	0.63448500	-0.07752900	2.38656400	H	-2.65673200	-2.24493600	-0.82294300
H	4.84446900	-0.15558400	1.50407400	H	-1.97396900	-2.26150600	1.55794700
H	5.35196000	-0.19859900	3.92093600	H	-3.62780700	-1.85057300	2.03757200
H	3.50711000	-0.16515000	5.58843600	H	-2.76335400	-4.36190100	0.52564600
H	1.14250800	-0.10101700	4.81180500	H	-3.27137600	-4.28824500	2.21176800
H	-3.49334000	2.43798000	1.68699400	H	-5.55186300	-3.57880900	1.55070900
H	-4.57079100	2.14379000	3.88903200	H	-5.14407000	-5.07177900	0.70933600
H	-4.40266200	-0.03189900	5.08384600	C	-3.24299500	2.06356200	3.40814400
H	-3.14546600	-1.91467100	4.04539800	C	-2.84079000	0.89662900	2.48956500
H	-2.06072500	-1.61950300	1.84800900	C	-3.22406000	1.20321800	1.02400900
H	-1.85810800	0.13878700	-2.89103900	C	-4.75049700	1.42687900	0.93906200
H	-3.60174000	-0.13147400	-4.62518700	C	-5.17464700	2.59598200	1.84795200
H	-6.00919700	-0.11946500	-3.98659400	C	-4.74559300	2.36726100	3.30508200
H	-6.64907600	0.19329600	-1.60371200	H	-2.66672400	2.95622700	3.12632600
H	-4.91193500	0.51029600	0.12047300	H	-2.97514800	1.82924700	4.44675300
H	0.00204800	2.27775900	1.36413100	H	-3.35784700	-0.00977700	2.82501100
H	-3.04028200	2.89613100	-1.61977500	H	-1.76908300	0.69404300	2.57572000
H	-2.52689400	5.30781200	-1.63850400	H	-2.73320000	2.15249400	0.76763700
H	-0.76297400	6.22657700	-0.14347500	H	-5.07462200	1.62263600	-0.08890400
H	0.49737400	4.69193000	1.35939700	H	-5.27277400	0.51848800	1.26461900
H	1.52798500	1.40835100	-2.39606500	H	-4.71921800	3.52474800	1.47400000
H	3.64543000	2.35829100	1.23046100				

H	-6.26198100	2.73516800	1.78946700	C	0.14728900	3.93876900	1.58792300
H	-5.31281000	1.51939200	3.71733100	H	-0.05767900	1.94832600	2.34654000
H	-5.00172300	3.24104700	3.91777500	C	0.36397100	4.15844700	-0.79705600
C	2.69975600	-3.10009500	3.36817600	H	0.32222000	2.33641300	-1.92503800
C	2.37380400	-2.52352900	1.97871600	C	0.30355200	4.75351700	0.46507600
C	2.73394100	-1.02519200	1.90057300	H	0.10777300	4.38109400	2.58146100
C	2.01269600	-0.24854300	3.02487400	H	0.49317800	4.77435900	-1.68480700
C	2.33392200	-0.82739900	4.41341200	H	0.38090200	5.83248300	0.57125100
C	1.99831700	-2.32278200	4.49018300	<i>t</i> - <b>9</b> <sub>Cy</sub> [Pd(PCy <sub>3</sub> ) <sub>2</sub> (Ph)(Cl)]			
H	3.78777500	-3.06775000	3.53237500	Pd	-0.00337300	-0.15450800	0.04750600
H	2.41148500	-4.15843000	3.39902200	P	2.40180400	-0.18145900	0.25849200
H	1.30929900	-2.65944300	1.75822200	P	-2.39968700	-0.19637400	-0.24027600
H	2.91683300	-3.09303700	1.21697300	Cl	-0.01339500	-2.61103200	0.12419600
H	3.81660000	-0.94073100	2.06664400	C	3.13434100	-2.36322500	3.85686600
H	2.27386800	0.81614800	2.99787700	C	2.65483700	-2.08037200	2.42178600
H	0.93001500	-0.30736900	2.84637900	C	2.95338900	-0.62249500	2.01160300
H	3.40327200	-0.68267000	4.62914800	C	2.32970400	0.35576700	3.03206300
H	1.78327000	-0.26941900	5.18199600	C	2.80538500	0.06728700	4.46607700
H	0.91017800	-2.45395300	4.39584900	C	2.52210400	-1.38570200	4.86901200
H	2.27960500	-2.72723700	5.47098600	H	4.23161100	-2.28593100	3.89967300
C	4.19323600	3.44737400	-0.95855200	H	2.88435600	-3.39736100	4.12578800
C	3.64611700	2.01465800	-1.07405700	H	3.14341100	-2.78179800	1.73671300
C	3.34646500	1.41416400	0.31869300	H	1.57989900	-2.27462400	2.33912400
C	4.62840700	1.44112400	1.18300200	H	4.04413800	-0.49176300	2.03370200
C	5.18895600	2.87202800	1.29283400	H	2.55621400	1.39611500	2.76873200
C	5.45261800	3.49673600	-0.08355100	H	1.23680800	0.25386200	2.98488600
H	3.41664000	4.09446900	-0.52812800	H	3.88632500	0.26121900	4.53731600
H	4.41023200	3.83908400	-1.96105200	H	2.31800900	0.76208000	5.16244900
H	4.39330100	1.39624000	-1.58696200	H	1.43428500	-1.54315800	4.91188900
H	2.74618700	2.01112500	-1.69609500	H	2.90853100	-1.58479900	5.87689100
H	2.61754200	2.07848800	0.79937200	C	5.08557500	-2.99943600	-1.51401500
H	4.43109200	1.06840100	2.19263600	C	4.66328600	-1.71318000	-0.77886500
H	5.39393200	0.78600900	0.74816900	C	3.12938100	-1.54899800	-0.80773900
H	4.46767600	3.49615900	1.84052700	C	2.60200000	-1.54855000	-2.26018300
H	6.10933000	2.85915600	1.89118400	C	3.02761600	-2.83582000	-2.98721500
H	6.26373300	2.94551000	-0.58279800	C	4.55043400	-3.03242200	-2.95352000
H	5.80147000	4.53131200	0.02890500	H	4.69945600	-3.86962600	-0.96351400
C	5.31670200	-2.66924900	-1.72774000	H	6.18005400	-3.08612600	-1.51002800
C	4.78287900	-1.56004100	-0.80175200	H	5.14318900	-0.85371800	-1.26613400
C	3.26502100	-1.36547000	-1.00581000	H	5.03696100	-1.74004200	0.25210800
C	2.94074600	-1.05266700	-2.48445800	H	2.68086100	-2.43272000	-0.33666300
C	3.47929100	-2.16527600	-3.40030000	H	1.51000500	-1.47115300	-2.25088600
C	4.98563400	-2.38840800	-3.20075500	H	2.98911500	-0.68184100	-2.80991900
H	4.86823400	-3.62884200	-1.43222700	H	2.53525200	-3.69300100	-2.50695500
H	6.40108900	-2.77453300	-1.59155000	H	2.67159500	-2.80964800	-4.02540300
H	5.31573000	-0.62583800	-1.02268500	H	5.03272100	-2.23287100	-3.53624300
H	5.01072900	-1.81299700	0.24099700	H	4.82456200	-3.97894900	-3.43687300
H	2.76946900	-2.32070400	-0.79491100	C	3.89634300	3.20618500	-1.83374400
H	1.85689700	-0.96535200	-2.60928600	C	3.38120700	1.77641600	-1.59601700
H	3.38729300	-0.09698700	-2.78350200	C	3.29740900	1.45465100	-0.08655400
H	2.93704100	-3.09641600	-3.18381200	C	4.68266900	1.65329700	0.56861300
H	3.26765800	-1.91529800	-4.44804400	C	5.21297000	3.07859800	0.32100800
H	5.53315200	-1.49193500	-3.52949800	C	5.26355100	3.42527700	-1.17277900
H	5.33641300	-3.21592900	-3.83078900	H	3.16810200	3.92135400	-1.42666400
C	0.09182600	1.92654500	0.18668500	H	3.95912800	3.39981300	-2.91262000
C	0.04636200	2.54836000	1.44762900	H	4.06758100	1.07172800	-2.08301200
C	0.26209000	2.76857900	-0.92892200				

H	2.40310600	1.65130900	-2.07046200
H	2.61539300	2.19120700	0.35867000
H	4.63368700	1.48410500	1.64856200
H	5.39878100	0.92529400	0.16606700
H	4.55805200	3.79642900	0.83639700
H	6.20787900	3.18276800	0.77331500
H	6.01237800	2.78866200	-1.66771800
H	5.59498200	4.46241900	-1.31116700
C	-3.03411600	-2.57172900	-3.73611100
C	-2.59245300	-2.21526700	-2.30508600
C	-2.89070200	-0.73524800	-1.98387300
C	-2.22913000	0.18122500	-3.03676500
C	-2.67066800	-0.17896200	-4.46511800
C	-2.38861100	-1.65341000	-4.78256300
H	-4.12930600	-2.49140400	-3.81249300
H	-2.78391300	-3.62013600	-3.94224700
H	-1.52206200	-2.41192600	-2.18026800
H	-3.10645300	-2.87461700	-1.59765300
H	-3.97906400	-0.59739700	-2.04622600
H	-2.45166300	1.23598000	-2.83525500
H	-1.13894600	0.07126500	-2.95579200
H	-3.74786800	0.01810400	-4.57373200
H	-2.16027100	0.47422400	-5.18485700
H	-1.30119200	-1.81954100	-4.78804200
H	-2.75014200	-1.90410300	-5.78813500
C	-3.90051500	3.33039400	1.58634300
C	-3.40508300	1.88066900	1.45450900
C	-3.29452000	1.46113900	-0.02810500
C	-4.66304700	1.63280900	-0.72616800
C	-5.17349800	3.07999100	-0.58604800
C	-5.24879900	3.52711000	0.88020400
H	-3.15072300	4.00572200	1.15132000
H	-3.98483600	3.59578500	2.64837000
H	-4.11291800	1.21933300	1.97052000
H	-2.43812200	1.77199700	1.95524400
H	-2.59509300	2.16185500	-0.50253800
H	-4.59506900	1.38729300	-1.79080300
H	-5.39959200	0.94570800	-0.29007700
H	-4.49562800	3.75105300	-1.13371200
H	-6.15701000	3.16961700	-1.06555700
H	-6.01952300	2.93786100	1.39962800
H	-5.56452400	4.57652900	0.94112900
C	-5.18252600	-2.87782700	1.59210000
C	-4.71446400	-1.64554000	0.79489200
C	-3.18112500	-1.49331000	0.87669000
C	-2.71341900	-1.40769800	2.34737300
C	-3.18537800	-2.64158500	3.13580300
C	-4.70788000	-2.82321500	3.05184600
H	-4.78433100	-3.78524400	1.11517300
H	-6.27687200	-2.95426000	1.54727100
H	-5.20320900	-0.75153000	1.20515400
H	-5.04603500	-1.73477900	-0.24703500
H	-2.72337400	-2.40786600	0.47899800
H	-1.62116200	-1.34326700	2.37983200
H	-3.11103400	-0.50437200	2.82636500
H	-2.68553800	-3.53342700	2.73230100
H	-2.87115600	-2.55270600	4.18397900

H	-5.20246000	-1.98188900	3.56077000
H	-5.01466000	-3.73307100	3.58362000
C	0.00049000	1.87282500	-0.00571000
C	-0.01218100	2.58422800	-1.22087200
C	0.01854800	2.63660600	1.17716800
C	-0.00665000	3.98417400	-1.25486500
H	-0.02987000	2.04244100	-2.16287800
C	0.02224900	4.03667600	1.15029400
H	0.03232300	2.13654400	2.14224500
C	0.01023000	4.71979400	-0.06782600
H	-0.01616100	4.49818300	-2.21412700
H	0.03452000	4.59192700	2.08621900
H	0.01391500	5.80653100	-0.09164300

*c*-**9<sub>H</sub>** [Pd(PH<sub>3</sub>)<sub>2</sub>(Ph)(Br)]

Pd	0.60195400	0.43210200	0.00019400
Br	0.98043100	-2.03936600	-0.00017200
P	-0.03434000	2.61794000	-0.00052300
P	3.01630900	0.55305900	0.00022100
C	-1.41519800	0.10388000	0.00013100
C	-2.11097500	-0.02918800	-1.20868400
C	-2.11117600	-0.02875300	1.20891900
C	-3.48301000	-0.30460600	-1.20629100
H	-1.58685300	0.05593900	-2.15759300
C	-3.48317200	-0.30417700	1.20642600
H	-1.58714700	0.05675400	2.15784800
C	-4.17207700	-0.44160500	0.00002700
H	-4.00861800	-0.41717600	-2.15178700
H	-4.00897400	-0.41639600	2.15185500
H	-5.23721800	-0.65770600	0.00001500
H	0.91120900	3.67353900	0.00035600
H	-0.84159000	3.05871900	1.06917400
H	-0.83933800	3.05844000	-1.07202300
H	3.78856500	1.74655100	0.00009300
H	3.66454600	-0.09800700	-1.06919100
H	3.66458700	-0.09784200	1.06971300

*c*-**9<sub>H</sub>** [Pd(PH<sub>3</sub>)<sub>2</sub>(Ph)(Cl)]

Pd	-0.73796500	0.08268000	-0.00001900
P	-0.35918200	2.31705500	0.00025100
P	-3.15212000	-0.10326500	-0.00013300
Cl	-0.84865300	-2.28159200	-0.00031900
C	1.29952800	-0.01684200	0.00006100
C	2.00426900	-0.08089000	1.20897000
C	2.00440500	-0.08005900	-1.20880900
C	3.39675000	-0.21908600	1.20656400
H	1.47337900	-0.04786100	2.15738100
C	3.39688300	-0.21826000	-1.20633800
H	1.47362200	-0.04637900	-2.15725700
C	4.09581700	-0.28654600	0.00013000
H	3.93131600	-0.27874500	2.15188200
H	3.93155300	-0.27727800	-2.15163700
H	5.17726600	-0.39502600	0.00015400
H	-1.42264800	3.25340200	0.00072600
H	0.38837300	2.85179200	-1.07005700
H	0.38889700	2.85137600	1.07041200
H	-4.09263300	0.96221100	-0.00009300



H	-3.69603300	-0.84333000	1.06942400	C	-2.28345100	1.75803900	-0.07960300
H	-3.69594200	-0.84315800	-1.06985800	C	-2.84189100	-0.46969000	1.64838000
<i>t</i> - <b>9<sub>H</sub></b> [Pd(PH <sub>3</sub> ) <sub>2</sub> (Ph)(Br)]				C	-3.12657200	-0.71873600	-1.27200400
Pd	-0.32653100	0.00003300	-0.00006400	C	4.30035400	0.11283900	0.58650100
Br	-2.88757500	-0.00007500	0.00001000	C	4.01392200	1.13427500	-1.58418500
P	-0.39049700	2.31731200	0.00007800	C	5.38610400	1.01084300	-1.81851300
P	-0.39034700	-2.31726000	0.00002500	C	6.21579000	0.43999300	-0.85475000
C	1.70702700	0.00001200	-0.00004500	C	5.66758800	-0.00835600	0.34954200
C	2.42436500	-0.00007000	1.20643300	C	0.84543500	1.15486300	2.65170300
C	2.42444900	0.00008500	-1.20647000	C	2.51061500	2.73142900	1.88613500
C	3.82425900	-0.00007200	1.20547800	C	2.52145100	3.32973300	3.14595600
H	1.89594200	-0.00013900	2.15771100	C	1.69633900	2.84133700	4.16286500
C	3.82434300	0.00007300	-1.20541600	C	0.86411100	1.74904400	3.91635200
H	1.89609000	0.00015300	-2.15778400	C	-3.91525300	0.29707200	2.13708700
C	4.52833900	-0.00000300	0.00005600	C	-4.53333900	-0.02999600	3.34469400
H	4.36154300	-0.00013000	2.15129200	C	-4.08828100	-1.12547500	4.08752600
H	4.36169400	0.00012300	-2.15119100	C	-3.02438600	-1.89331100	3.61298700
H	5.61512900	-0.00000400	0.00009300	C	-2.40443700	-1.57043600	2.40348400
H	-1.07581800	2.92140500	-1.07320000	C	-2.57159600	-1.09777400	-2.50317500
H	0.78559600	3.10024800	-0.00046900	C	-3.39045000	-1.52811300	-3.54815500
H	-1.07454400	2.92106200	1.07436600	C	-4.77292500	-1.60164600	-3.36952400
H	-1.07479200	-2.92122800	-1.07388700	C	-5.33270800	-1.24124400	-2.14220300
H	-1.07514900	-2.92123500	1.07369700	C	-4.51575400	-0.79944000	-1.10050800
H	0.78581900	-3.10008700	0.00020000	C	-1.97130300	2.59370400	1.00710800
<i>t</i> - <b>9<sub>H</sub></b> [Pd(PH <sub>3</sub> ) <sub>2</sub> (Ph)(Cl)]				C	-2.78542900	2.34755600	-1.24955400
Pd	-0.70931500	0.00000000	-0.00003700	C	-2.98365900	3.72817400	-1.32470900
P	-0.78832600	2.31619000	0.00016500	C	-2.68583700	4.54453300	-0.23373600
P	-0.78832700	-2.31619000	-0.00001300	C	-2.17484100	3.97139900	0.93278200
Cl	-3.13043100	0.00000000	-0.00008500	C	0.75837300	1.51323400	-2.55801200
C	1.31905100	0.00000000	-0.00000500	C	1.00210400	3.40449600	-1.07399200
C	2.03810700	-0.00005100	1.20592800	C	0.64075400	4.26033400	-2.11670500
C	2.03811800	0.00005100	-1.20593100	C	0.35326600	3.74905900	-3.38269600
C	3.43790600	-0.00005100	1.20529000	C	0.41004300	2.37107800	-3.60146000
H	1.50979600	-0.00009300	2.15731900	C	2.00672700	-2.23917100	-0.02835600
C	3.43791700	0.00005000	-1.20528000	C	2.44867200	-2.75312300	1.19799500
H	1.50981500	0.00009200	-2.15732800	C	2.71364400	-2.56668800	-1.19116000
C	4.14222100	-0.00000100	0.00000800	C	3.58339500	-3.57024000	1.26012800
H	3.97515800	-0.00009100	2.15116400	C	3.84538400	-3.38618800	-1.12882500
H	3.97517800	0.00009000	-2.15115000	C	4.28752500	-3.88745100	0.09718200
H	5.22904700	-0.00000100	0.00001300	H	3.88944400	-0.25418300	1.52059700
H	-1.48329100	2.90912300	-1.07334000	H	3.38746500	1.58661300	-2.34477500
H	0.37450500	3.11814300	0.00003400	H	5.80203500	1.36672700	-2.75745100
H	-1.48286200	2.90888500	1.07408200	H	7.28230700	0.34284200	-1.03929600
H	-1.48299200	-2.90903600	-1.07376300	H	6.30331900	-0.46179500	1.10481600
H	-1.48316700	-2.90897000	1.07365900	H	0.20634800	0.29594900	2.46663600
H	0.37450200	-3.11814400	0.00010200	H	3.18236800	3.09709900	1.11514800
<i>c</i> - <b>9<sub>Ph</sub></b> [Pd(PPh <sub>3</sub> ) <sub>2</sub> (Ph)(Br)]				H	3.18387200	4.16969200	3.33716400
Pd	0.30756100	-1.12249500	-0.08137700	H	1.71364400	3.30305300	5.14643700
Br	-0.83421100	-3.35896500	-0.34477700	H	0.23288200	1.35135100	4.70629400
P	1.64049000	0.79995300	-0.02138100	H	-4.26485400	1.16189600	1.58263600
P	-1.99752600	-0.07644600	0.04315600	H	-5.36213900	0.57431300	3.70440900
C	3.45540500	0.68583500	-0.37913100	H	-4.56906400	-1.37832600	5.02894900
C	1.65664700	1.64670000	1.61863800	H	-2.67326400	-2.75205200	4.17886900
C	1.07347000	2.02162900	-1.28578100	H	-1.59873500	-2.19292700	2.02962200
				H	-1.49409400	-1.08633200	-2.63346400
				H	-2.94429300	-1.82659700	-4.49295700
				H	-5.41010200	-1.94852900	-4.17872800

H	-6.40697800	-1.30762800	-1.99134900
H	-4.96457500	-0.53124100	-0.14969200
H	-1.58685300	2.16806300	1.92774200
H	-3.03809300	1.72819300	-2.10334500
H	-3.38142100	4.16145200	-2.23867100
H	-2.85163000	5.61722800	-0.29006000
H	-1.93841100	4.59477500	1.79135100
H	0.79155500	0.44003400	-2.73012800
H	1.21407400	3.81959900	-0.09504000
H	0.58269500	5.32999700	-1.93484200
H	0.07784100	4.41928200	-4.19252000
H	0.17810200	1.96157700	-4.58097500
H	1.89984900	-2.53931400	2.11249400
H	2.38072500	-2.19704300	-2.15809400
H	3.90730100	-3.96675100	2.22036300
H	4.37786100	-3.63547200	-2.04421100
H	5.16588900	-4.52631600	0.14416500

*c*-**9**<sub>Ph</sub> [Pd(PPh<sub>3</sub>)<sub>2</sub>(Ph)(Cl)]

Pd	0.32425100	-1.25009200	-0.16012600
P	1.57574500	0.70230200	0.01225100
P	-2.02749500	-0.30955200	0.00170200
Cl	-0.71487700	-3.37282400	-0.48468500
C	3.39669300	0.67488200	-0.33238500
C	1.54786400	1.46045300	1.69502900
C	0.97418800	1.97040900	-1.18898200
C	-2.39560900	1.51216800	-0.03483600
C	-2.86050400	-0.83479500	1.57475800
C	-3.11526500	-0.94236300	-1.35138000
C	4.25229700	0.06299200	0.59947700
C	3.94995700	1.22927700	-1.49469600
C	5.32786300	1.17043400	-1.72149700
C	6.16804700	0.55944500	-0.79216200
C	5.62490800	0.00591600	0.37007000
C	0.73672300	0.89291100	2.68849000
C	2.36659100	2.55286100	2.03153100
C	2.34298900	3.08432800	3.32085400
C	1.51797400	2.52080600	4.29819500
C	0.72065000	1.42032700	3.98237500
C	-3.94728900	-0.12989800	2.12300300
C	-4.55490500	-0.56271700	3.30257500
C	-4.08719000	-1.70486200	3.95559300
C	-3.01183100	-2.41353500	3.41884100
C	-2.40079600	-1.98500200	2.23821600
C	-2.52889000	-1.30992000	-2.57091100
C	-3.32156200	-1.73141800	-3.63974800
C	-4.70787600	-1.80525600	-3.49707500
C	-5.29925100	-1.45574200	-2.28113500
C	-4.50878200	-1.02503400	-1.21507900
C	-2.12514400	2.30983600	1.09101200
C	-2.90917700	2.13404800	-1.18304600
C	-3.15956300	3.50805200	-1.19892600
C	-2.90368200	4.28538300	-0.06942400
C	-2.38195500	3.68062600	1.07613100
C	0.67539400	1.52008300	-2.48660700
C	0.85939000	3.33704900	-0.90448100
C	0.47165500	4.23524700	-1.90109600

C	0.20217900	3.78287500	-3.19318500
C	0.30203100	2.42076400	-3.48435500
C	2.05338500	-2.31395100	-0.17480300
C	2.50417400	-2.90701600	1.01166700
C	2.76449800	-2.54465400	-1.35774500
C	3.65503000	-3.70358800	1.01615000
C	3.91151700	-3.34525300	-1.35355200
C	4.36438900	-3.92309400	-0.16600100
H	3.84591000	-0.38461100	1.49994500
H	3.31420500	1.71371000	-2.22732000
H	5.73961900	1.60761400	-2.62735400
H	7.23891900	0.51208900	-0.97094000
H	6.26920400	-0.47944400	1.09777400
H	0.12603200	0.02693900	2.44912800
H	3.03803500	2.97675800	1.29076000
H	2.97875700	3.93096900	3.56565000
H	1.50851500	2.93068800	5.30458400
H	0.09015700	0.96414700	4.74067400
H	-4.31640600	0.76765400	1.63765200
H	-5.39401400	-0.00458400	3.70997300
H	-4.56027400	-2.04023100	4.87491700
H	-2.64461200	-3.30853800	3.91397900
H	-1.58639200	-2.56138100	1.81219600
H	-1.44856100	-1.29744000	-2.67168700
H	-2.85183900	-2.02173500	-4.57562700
H	-5.32447000	-2.14392600	-4.32554500
H	-6.37719900	-1.52204800	-2.15897600
H	-4.98113600	-0.76424100	-0.27323000
H	-1.73108900	1.85817700	1.99510900
H	-3.12883300	1.54442500	-2.06659300
H	-3.56453800	3.96673900	-2.09719600
H	-3.10994100	5.35247300	-0.08006200
H	-2.17776400	4.27361100	1.96399200
H	0.73808000	0.45837800	-2.71249000
H	1.05790300	3.70624200	0.09545400
H	0.37964000	5.29142700	-1.66305100
H	-0.09332200	4.48605200	-3.96721000
H	0.08305600	2.05655500	-4.48450700
H	1.95140100	-2.76898900	1.93820200
H	2.42524600	-2.11124100	-2.29561900
H	3.98802200	-4.16058400	1.94593300
H	4.44872200	-3.51774600	-2.28378300
H	5.25587500	-4.54535500	-0.16375200

*t*-**9**<sub>Ph</sub> [Pd(PPh<sub>3</sub>)<sub>2</sub>(Ph)(Br)]

Pd	-0.00001300	-0.09400400	-0.00004800
Br	0.00005500	-2.68567000	-0.00003900
P	2.39586600	-0.10525900	-0.02580300
P	-2.39587800	-0.10532600	0.02577300
C	3.29912400	1.44892900	0.41387700
C	3.08424000	-0.53264600	-1.68682400
C	3.12033100	-1.33805400	1.13906600
C	-3.08414400	-0.53261500	1.68685600
C	-3.12044200	-1.33816900	-1.13899000
C	-3.29909000	1.44886700	-0.41397000
C	3.25876500	2.54574800	-0.46394800
C	3.99380800	1.58114000	1.62506400

C	4.63197100	2.78102700	1.95042700	H	-4.48774100	-1.52849800	5.18421700
C	4.58881900	3.86158600	1.07056500	H	-2.23839700	-2.31709800	4.46683900
C	3.90074000	3.73897500	-0.13933500	H	1.56362800	-1.01923700	2.59853100
C	2.32834200	-1.33590500	-2.55609300	H	4.78636900	-1.91507400	-0.11010300
C	4.35623200	-0.09746400	-2.09703300	H	5.73633300	-3.48439800	1.54045100
C	4.85740800	-0.45609900	-3.34948400	H	4.62743800	-3.80914100	3.74261100
C	4.09730500	-1.25244200	-4.20820800	H	2.54006800	-2.56059500	4.26959700
C	2.83485700	-1.69241100	-3.80716800	H	-0.26856500	2.12761700	-2.13874900
C	-4.29423100	-2.04548700	-0.84803300	H	0.26828300	2.12744700	2.13882800
C	-4.83142000	-2.93373700	-1.78207700	H	-0.25613100	4.59103800	-2.13614200
C	-4.20864200	-3.11655300	-3.01749600	H	0.25555900	4.59086800	2.13645100
C	-3.03865500	-2.41396700	-3.31507200	H	-0.00035900	5.84713700	0.00021400
C	-2.49231100	-1.53799600	-2.37757900	<i>t</i> - <b>9</b> <sub>Ph</sub> [Pd(PPh <sub>3</sub> ) <sub>2</sub> (Ph)(Cl)]			
C	-3.25913700	2.54557000	0.46401900	Pd	0.00000200	0.18689500	0.00007900
C	-3.90098200	3.73883300	0.13927600	P	-2.39154000	0.22097000	-0.02696600
C	-4.58851500	3.86160100	-1.07091600	P	2.39154000	0.22115100	0.02699100
C	-4.63124200	2.78116400	-1.95095000	Cl	0.00006500	2.63484100	0.00075800
C	-3.99320900	1.58124300	-1.62546300	C	-3.31612000	-1.32397400	0.39323000
C	-2.32813800	-1.33575300	2.55614200	C	-3.07379500	0.70027700	-1.67719100
C	-4.35615600	-0.09751600	2.09709200	C	-3.09060800	1.45170800	1.15394200
C	-4.85724300	-0.45611000	3.34958900	C	3.07393900	0.69965200	1.67737300
C	-4.09703400	-1.25233400	4.20833100	C	3.09040200	1.45239500	-1.15351800
C	-2.83456700	-1.69222200	3.80726300	C	3.31608300	-1.32363200	-0.39390200
C	2.49225700	-1.53762400	2.37772500	C	-3.25792800	-2.42554600	-0.47781200
C	4.29399000	-2.04558800	0.84811500	C	-4.04309900	-1.44623400	1.58649100
C	4.83110300	-2.93381100	1.78223100	C	-4.69706400	-2.64067700	1.90015500
C	4.20838100	-3.11637700	3.01771400	C	-4.63775300	-3.72525900	1.02613300
C	3.03852700	-2.41356600	3.31528700	C	-3.91656400	-3.61298000	-0.16538900
C	-0.00011200	1.93231200	0.00002700	C	-2.34864400	1.60220700	-2.47436000
C	-0.14499000	2.65496600	-1.19493500	C	-4.30673600	0.21677000	-2.14602600
C	0.14466600	2.65487000	1.19505900	C	-4.79919900	0.62085300	-3.38856800
C	-0.14109300	4.05432400	-1.19661900	C	-4.07026700	1.51290500	-4.17660500
C	0.14059600	4.05422800	1.19687600	C	-2.84800200	2.00420200	-3.71409100
C	-0.00028900	4.75993000	0.00016200	C	4.29110900	2.12893700	-0.89862300
H	2.71751000	2.47249000	-1.40096900	C	4.81597900	3.01295200	-1.84312800
H	4.04714200	0.74791200	2.31738400	C	4.15225600	3.22347500	-3.05288800
H	5.16777900	2.86345300	2.89247100	C	2.95546000	2.55276600	-3.31367600
H	5.08649900	4.79391000	1.32404200	C	2.42256900	1.67908000	-2.36590800
H	3.85474200	4.57642300	-0.82998800	C	3.25823200	-2.42541700	0.47688600
H	1.35693800	-1.70156800	-2.23968300	C	3.91677800	-3.61276100	0.16393800
H	4.95501900	0.52851700	-1.44353800	C	4.63756000	-3.72473400	-1.02786500
H	5.84222300	-0.11040800	-3.65258000	C	4.69653700	-2.63992600	-1.90163500
H	4.48807900	-1.52863700	-5.18405900	C	4.04264300	-1.44558100	-1.58744600
H	2.23876800	-2.31737700	-4.46673300	C	2.34855300	1.60056400	2.47545500
H	-4.78665500	-1.91478900	0.11013700	C	4.30728300	0.21642400	2.14548700
H	-5.73675200	-3.48415400	-1.54029000	C	4.79988800	0.61979600	3.38819600
H	-4.62775900	-3.80934000	-3.74233600	C	4.07070100	1.51085400	4.17714100
H	-2.54015200	-2.56119400	-4.26932800	C	2.84805500	2.00186700	3.71536100
H	-1.56358000	-1.01979200	-2.59838000	C	-2.42295200	1.67801900	2.36649600
H	-2.71828900	2.47220400	1.40126800	C	-4.29142400	2.12812300	0.89919300
H	-3.85530800	4.57618700	0.83006500	C	-4.81653300	3.01169700	1.84397700
H	-5.08609800	4.79395000	-1.32448800	C	-4.15295800	3.22188000	3.05388000
H	-5.16661800	2.86371300	-2.89322900	C	-2.95608500	2.55126700	3.31453600
H	-4.04622100	0.74811100	-2.31792400	C	0.00011700	-1.83415900	-0.00017900
H	-1.35671800	-1.70135300	2.23971100	C	0.15989100	-2.55821600	-1.19295300
H	-4.95502500	0.52837600	1.44358600	C	-0.15951100	-2.55841400	1.19249000
H	-5.84207400	-0.11048300	3.65270800				

C	0.15580500	-3.95752200	-1.19512900	H	0.00280200	4.54358200	-2.15181100
C	-0.15515100	-3.95771600	1.19447100	C	-3.38109900	-2.91796800	-0.64601600
C	0.00039900	-4.66356700	-0.00037400	H	-3.61857200	-3.61462700	-1.46151000
H	-2.68897500	-2.36051500	-1.39892200	H	-2.39531100	-3.18026800	-0.27162900
H	-4.10721400	-0.60982600	2.27399900	H	-4.12506600	-3.08327400	0.13669500
H	-5.25715800	-2.71611400	2.82853400	C	-2.51478300	-1.44793900	-2.46783700
H	-5.14766000	-4.65339600	1.27056100	H	-2.86322300	-2.19545600	-3.19331800
H	-3.85680200	-4.45428300	-0.85025500	H	-2.51562100	-0.47720800	-2.97018700
H	-1.40953700	2.00590900	-2.10870600	H	-1.48821800	-1.70031500	-2.19370100
H	-4.88286800	-0.48039900	-1.54694500	C	-3.47449700	1.80582600	-1.99234200
H	-5.75366100	0.23599100	-3.73817600	H	-3.87399500	2.79950200	-2.23523400
H	-4.45411100	1.82452600	-5.14454900	H	-2.40900600	1.81679300	-2.23721300
H	-2.27745500	2.70499400	-4.31779000	H	-3.97301100	1.09087600	-2.64652800
H	4.81481200	1.97450000	0.03957400	C	-3.16395700	2.80735600	0.22830600
H	5.74330400	3.53821300	-1.63035300	H	-3.84204700	3.63616700	-0.01821500
H	4.56148600	3.91329900	-3.78623300	H	-3.13694100	2.72623800	1.31253900
H	2.42640700	2.72194800	-4.24763300	H	-2.17681800	3.08398000	-0.12090500
H	1.47503100	1.18409400	-2.55681900	C	-5.22516400	1.53556900	-0.18402900
H	2.68960500	-2.36062600	1.39821900	H	-5.41866500	1.68069800	0.88282300
H	3.85727400	-4.45422800	0.84861600	H	-5.75470000	0.64347400	-0.50771800
H	5.14738800	-4.65279800	-1.27270800	H	-5.67708000	2.39124500	-0.70403600
H	5.25631000	-2.71511000	-2.83023200	C	-4.90650800	-1.31507900	-1.69797600
H	4.10649100	-0.60900000	-2.27477900	H	-5.61819000	-1.39151000	-0.87090700
H	1.40917300	2.00412000	2.11035300	H	-5.12761000	-2.14344700	-2.38397900
H	4.88358700	-0.48001300	1.54572900	H	-5.10414700	-0.39349800	-2.24497600
H	5.75464300	0.23516200	3.73724500	C	-3.11662000	0.65679300	2.75935500
H	4.45466300	1.82193200	5.14521300	H	-3.19232200	0.31520200	3.79993000
H	2.27731900	2.70189800	4.31975600	H	-2.13014200	1.11329500	2.63320200
H	-1.47536200	1.18310200	2.55732300	H	-3.87968100	1.42585500	2.61960300
H	-4.81502700	1.97393000	-0.03909900	C	-2.40800500	-1.67991300	2.37828300
H	-5.74393800	3.53686600	1.63131700	H	-2.69949000	-1.88489300	3.41771600
H	-4.56237100	3.91136300	3.78744500	H	-2.48161300	-2.61159100	1.81933100
H	-2.42715100	2.72019600	4.24860800	H	-1.35701300	-1.38114100	2.36876900
H	0.29572900	-2.03081500	-2.13503800	C	-4.78997500	-1.02116700	1.97104300
H	-0.29546600	-2.03117600	2.13465500	H	-4.99993000	-1.93812600	1.41867800
H	0.28248100	-4.49402500	-2.13330800	H	-4.98447000	-1.23346300	3.03123500
H	-0.28172400	-4.49436900	2.13257400	H	-5.50586800	-0.26135300	1.65652200
H	0.00050900	-5.75079400	-0.00044600	C	3.70542900	1.54811300	0.48124900
<i>t</i> - <b>9</b> <sub>tBu</sub> [Pd(P <sup><i>i</i></sup> Bu <sub>3</sub> ) <sub>2</sub> (Ph)(Br)]				C	3.32157600	-0.56624700	-1.83240000
Pd	0.00095600	-0.11252600	-0.00006600	C	3.44186300	-1.48499800	1.23306600
Br	-0.00004200	-2.71176300	0.00005700	C	5.22475700	1.53568300	0.17994400
P	2.74892300	-0.11261200	-0.02073500	H	5.67713600	2.39185800	0.69871800
P	-2.74937700	-0.11258100	0.02062100	H	5.75415600	0.64383900	0.50451500
C	-3.44243000	-1.48751600	-1.23028500	H	5.41784200	1.67945800	-0.88716300
C	-3.32199400	-0.56253800	1.83316900	C	3.47493800	1.80954000	1.98852600
C	-3.70571800	1.54715500	-0.48470000	H	2.40957200	1.82115200	2.23386200
C	-0.00056800	4.71289200	-0.00006500	H	3.97363300	1.09572000	2.64380200
C	-0.00221100	4.00624000	1.20560800	H	3.87471100	2.80359900	2.22939100
C	-0.00073900	2.60624900	1.20348600	C	3.16369000	2.80722600	-0.23375200
C	0.00060400	1.88121400	-0.00006600	H	2.17720700	3.08535900	0.11612900
C	0.00125100	2.60625500	-1.20361600	H	3.84271900	3.63602200	0.01021800
C	0.00158000	4.00624500	-1.20573900	H	3.13523500	2.72387900	-1.31777400
H	-0.00099100	5.79965600	-0.00006300	C	4.90631000	-1.31228600	1.69952700
H	-0.00392900	4.54357400	2.15168000	H	5.61749100	-1.39138900	0.87227900
H	-0.00296300	2.07929100	2.15512200	H	5.10491800	-0.38943600	2.24402100
H	0.00381500	2.07929700	-2.15525000	H	5.12720100	-2.13902600	2.38755600
				C	2.51489000	-1.44201600	2.47100200

H	2.51638000	-0.47007200	2.97099700	H	-5.70943000	0.40344700	-0.51184500
H	1.48808200	-1.69463200	2.19799200	H	-5.68142300	2.15650200	-0.67218400
H	2.86339800	-2.18792300	3.19810300	C	-4.79233800	-1.52972800	-1.70962900
C	3.37953800	-2.91678900	0.65218600	H	-5.49857900	-1.63776600	-0.88138800
H	2.39347600	-3.17947300	0.27880200	H	-4.98845900	-2.35746900	-2.40388700
H	4.12313600	-3.08431900	-0.13040200	H	-5.02156700	-0.60902400	-2.24576800
H	3.61695800	-3.61163600	1.46924000	C	-3.08187400	0.45140500	2.76521100
C	4.78925900	-1.02617900	-1.96916500	H	-3.14457600	0.09556200	3.80193800
H	4.99844400	-1.94227300	-1.41508100	H	-2.11156500	0.94266200	2.64290000
H	4.98371600	-1.24059900	-3.02893400	H	-3.87086300	1.19557800	2.63491900
H	5.50569600	-0.26632500	-1.65599700	C	-2.29825800	-1.85678500	2.36425700
C	2.40700600	-1.68397500	-2.37579200	H	-2.61140700	-2.10359400	3.38827200
H	2.69853200	-1.89080400	-3.41484600	H	-2.31149900	-2.77271500	1.77617400
H	2.48003400	-2.61478100	-1.81530800	H	-1.26280200	-1.50962600	2.39668700
H	1.35618400	-1.38459900	-2.36691600	C	-4.69792100	-1.27190200	1.95049400
C	3.11721300	0.65160700	-2.76074300	H	-4.86940000	-2.19720600	1.39864700
H	2.13105400	1.10903200	-2.63547800	H	-4.89488100	-1.48853000	3.00936600
H	3.88081900	1.42035700	-2.62227400	H	-5.43807300	-0.53940700	1.62724400
H	3.19275300	0.30812700	-3.80070600	C	3.68723100	1.36274200	0.46634500
<i>t</i> - <b>9</b> <sub>tBu</sub> [Pd(P <sup><i>i</i></sup> Bu <sub>3</sub> ) <sub>2</sub> (Ph)(Cl)]				C	3.24437800	-0.76412100	-1.82494300
Pd	0.00111000	-0.20055600	0.00000400	C	3.32221800	-1.65720100	1.24636400
P	2.68270300	-0.27205500	-0.02054500	C	5.20554800	1.30384800	0.16729400
P	-2.68331400	-0.27202900	0.02051700	H	5.68093500	2.15646700	0.67113100
Cl	0.00025300	-2.64277200	0.00039700	H	5.70867200	0.40344600	0.51048800
C	-3.32248100	-1.65771400	-1.24589700	H	5.40460400	1.42199400	-0.90173000
C	-3.24513700	-0.76349800	1.82498800	C	3.46604900	1.64455400	1.97159500
C	-3.68789900	1.36236700	-0.46716700	H	2.40195700	1.69378500	2.21746500
C	-0.00054800	4.62899800	0.00032800	H	3.94186300	0.92002300	2.63237000
C	0.00479700	3.92171000	1.20557700	H	3.89838100	2.62700000	2.20360400
C	0.00554800	2.52198400	1.20267500	C	3.17856000	2.62948100	-0.26053800
C	0.00068000	1.79408400	0.00000100	H	2.19736000	2.93441500	0.08341400
C	-0.00488100	2.52229400	-1.20248400	H	3.87763300	3.44306200	-0.02213300
C	-0.00536100	3.92201900	-1.20508800	H	3.15019800	2.53718300	-1.34400500
H	-0.00101400	5.71582000	0.00046100	C	4.79210900	-1.52873200	1.70989500
H	0.00806300	4.45878100	2.15188900	H	5.49828600	-1.63729300	0.88167100
H	0.00639200	1.99583600	2.15495900	H	5.02134900	-0.60767600	2.24541500
H	-0.00529500	1.99634500	-2.15488400	H	4.98831900	-2.35601300	2.40466700
H	-0.00909400	4.45930300	-2.15127500	C	2.39605700	-1.57109800	2.48292600
C	-3.20832900	-3.09395900	-0.68151300	H	2.41357400	-0.58947900	2.96312000
H	-3.42777300	-3.78592700	-1.50617000	H	1.36585700	-1.81121300	2.21157700
H	-2.21138500	-3.32391500	-0.31566100	H	2.73137500	-2.30791600	3.22552000
H	-3.94276700	-3.29583400	0.10187500	C	3.20836900	-3.09367100	0.68249000
C	-2.39622300	-1.57180500	-2.48239900	H	2.21137700	-3.32405300	0.31704000
H	-2.73123700	-2.30898600	-3.22477400	H	3.94258100	-3.29560400	-0.10108200
H	-2.41396700	-0.59036800	-2.96295300	H	3.42832600	-3.78527400	1.50731500
H	-1.36597400	-1.81150800	-2.21086300	C	4.69723700	-1.27237400	-1.95033600
C	-3.46642700	1.64368700	-1.97249000	H	4.86895400	-2.19744700	-1.39818000
H	-3.89895500	2.62593000	-2.20498100	H	4.89411800	-1.48936600	-3.00914400
H	-2.40227000	1.69308600	-2.21812500	H	5.43730300	-0.53964000	-1.62745500
H	-3.94189400	0.91876900	-2.63310800	C	2.29765100	-1.85770500	-2.36387400
C	-3.17909300	2.62928200	0.25930700	H	2.61107900	-2.10497700	-3.38769000
H	-3.87765300	3.44306100	0.02013400	H	2.31068900	-2.77333200	-1.77532700
H	-3.15128000	2.53756900	1.34284300	H	1.26221500	-1.51052300	-2.39676400
H	-2.19760300	2.93354700	-0.08440600	C	3.08097400	0.45045900	-2.76555800
C	-5.20624300	1.30372900	-0.16839700	H	2.11062500	0.94164900	-2.64338700
H	-5.40553900	1.42171200	0.90060500	H	3.86990900	1.19474100	-2.63552900
				H	3.14369000	0.09426500	-3.80216100

$\alpha$ - <b>10</b> <sub>Cy</sub> [( $\mu$ -Br) <sub>2</sub> Pd <sub>2</sub> (PCy <sub>3</sub> ) <sub>2</sub> (Ph) <sub>2</sub> ] (conformer <b>F</b> )				H	-5.93138800	-0.90912300	-1.30069100
Pd	-1.86021000	0.54458000	-0.18606400	H	-6.35313200	1.44110600	-0.66489700
Pd	1.86017700	-0.54456200	-0.18603900	H	-5.00092400	1.97634300	-1.65123600
Br	0.45096000	1.68116700	-0.36328800	H	-7.54047400	0.56870100	-2.64815300
Br	-0.45098600	-1.68114400	-0.36329300	H	-7.13356000	2.26782900	-2.87251600
P	3.97950100	0.41540200	0.04721700	H	-5.18740000	1.65504400	-4.28789100
P	-3.97951000	-0.41542200	0.04726200	H	-6.64719600	0.91281700	-4.93809700
C	3.06918100	-4.38434300	-1.60849500	C	-4.90940600	1.16701800	3.87306300
C	2.69647100	-3.04013200	-1.50282300	C	-4.15518600	0.33372500	2.82264300
C	2.63576800	-2.40154500	-0.25198500	C	-4.94877200	0.28855000	1.49643700
C	2.94602500	-3.15486500	0.88893400	C	-6.35174400	-0.30879000	1.73954400
C	3.32005700	-4.50088000	0.78365200	C	-7.11364700	0.50943400	2.79908500
C	3.38936000	-5.11994600	-0.46473600	C	-6.32473200	0.61878000	4.11226200
H	3.10194000	-4.85600300	-2.58838400	H	-4.97418300	2.21017500	3.53056600
H	2.43339300	-2.49505400	-2.40595600	H	-4.34286100	1.17915200	4.81292800
H	2.87443100	-2.71037400	1.87687400	H	-4.01624800	-0.68020200	3.21293800
H	3.54796800	-5.06489400	1.68586200	H	-3.15199500	0.73968700	2.65453100
H	3.67752200	-6.16491700	-0.54561800	H	-5.07911000	1.33321000	1.17998600
C	-3.38942000	5.11993000	-0.46512600	H	-6.93571400	-0.34277300	0.81243300
C	-3.32010100	4.50096800	0.78331200	H	-6.25400000	-1.34520200	2.08887300
C	-2.94607000	3.15496100	0.88870400	H	-6.25400000	1.51785000	2.40311400
C	-2.63583500	2.40154200	-0.25215700	H	-8.09602800	0.05489300	2.98109200
C	-2.69654700	3.04002800	-1.50304700	H	-6.25147200	-0.37779700	4.57262400
C	-3.06925400	4.38423200	-1.60882800	H	-6.86483200	1.25329500	4.82630500
H	-3.67758000	6.16489400	-0.54609200	C	4.77270500	4.64567400	-0.15689700
H	-3.54799900	5.06505900	1.68547900	C	5.10283000	3.13959400	-0.17115700
H	-2.87445800	2.71055600	1.87668200	C	3.85617500	2.30422000	0.20142800
H	-2.43347300	2.49487700	-2.40613600	C	3.31537300	2.75363600	1.57715200
H	-3.10201900	4.85581100	-2.58875500	C	2.97052800	4.25184200	1.57373200
C	-4.77250900	-4.64576300	-0.15610800	C	4.18664300	5.10294500	1.18568400
C	-5.10272700	-3.13970500	-0.17058100	H	4.04896500	4.85730400	-0.95745900
C	-3.85610000	-2.30420400	0.20180600	H	5.67858400	5.21796700	-0.39605700
C	-3.31519900	-2.75336800	1.57757400	H	5.91992500	2.94008400	0.53458600
C	-2.97025500	-4.25155100	1.57436100	H	5.47251300	2.87631800	-1.16730000
C	-4.18633700	-5.10279100	1.18650900	H	3.07823700	2.53950300	-0.53667600
H	-4.04880300	-4.85747100	-0.95668000	H	2.43049700	2.17072600	1.85042100
H	-5.67836800	-5.21814600	-0.39512700	H	4.08130600	2.57395000	2.34313900
H	-5.91979200	-2.94013500	0.53517700	H	2.14805300	4.42824800	0.86701400
H	-5.47247800	-2.87660100	-1.16674500	H	2.59990200	4.54431700	2.56453500
H	-3.07818900	-2.53958000	-0.53629900	H	4.95664600	5.01394100	1.96708800
H	-2.43035200	-2.17035300	1.85071200	H	3.91336100	6.16462800	1.13634400
H	-4.08111000	-2.57362300	2.34356800	C	4.90902100	-1.16632500	3.87340500
H	-2.14780900	-4.42801000	0.86762100	C	4.15488400	-0.33330300	2.82271100
H	-2.59955300	-4.54385100	2.56518600	C	4.94863000	-0.28833200	1.49659300
H	-4.95630000	-5.01371800	1.96794500	C	6.35156400	0.30908700	1.73974100
H	-3.91299200	-6.16446400	1.13731600	C	7.11335900	-0.50886700	2.79956700
C	-5.29057500	-0.48110100	-3.96522800	C	6.32427900	-0.61794600	4.11266500
C	-4.36639100	-0.55785200	-2.73822400	H	4.97390800	-2.20955300	3.53114400
C	-5.11624900	-0.18654000	-1.43821000	H	4.34235600	-1.17828900	4.81320000
C	-5.77195700	1.20514200	-1.56365900	H	4.01580400	0.68069500	3.21277600
C	-6.69895300	1.26343600	-2.79196500	H	3.15175000	-0.73938500	2.65454600
C	-5.95716000	0.89628700	-4.08482100	H	5.07902300	-1.33303700	1.18031100
H	-6.06844500	-1.25524500	-3.88361200	H	6.93564800	0.34284900	0.81269300
H	-4.71660700	-0.71018100	-4.87208200	H	6.25376300	1.34558600	2.08879900
H	-3.52087500	0.13007200	-2.86913800	H	7.30365600	-1.51736500	2.40384900
H	-3.93311200	-1.56284200	-2.66369100	H	8.09569900	-0.05424700	2.98159900
				H	6.25089600	0.37873600	4.57277700

H	6.86432300	-1.25225800	4.82693200	H	5.33164200	-3.09169200	0.66160500
C	5.29087200	0.48023500	-3.96518700	H	2.90780000	-2.58568200	0.19419400
C	4.36658400	0.55722400	-2.73827500	H	2.20055800	-1.81265800	-2.06716800
C	5.11634500	0.18619200	-1.43812600	H	3.80713400	-2.20685600	-2.69322500
C	5.77206100	-1.20551400	-1.56323900	H	1.84065900	-4.17532400	-1.42645400
C	6.69917700	-1.26404100	-2.79144300	H	2.23165900	-4.05926000	-3.13960900
C	5.95749500	-0.89716400	-4.08444200	H	4.57830700	-4.72225400	-2.71036800
H	6.06872000	1.25441100	-3.88366900	H	3.50292000	-5.93216300	-2.01616000
H	4.71697400	0.70911600	-4.87213500	C	4.71806800	-1.33776000	4.00780100
H	3.52109300	-0.13074300	-2.86911600	C	3.94295600	-1.17822500	2.68889400
H	3.93328400	1.56222200	-2.66398400	C	4.82329500	-0.54424800	1.58784900
H	5.93147600	0.90880200	-1.30070300	C	5.40047100	0.80390200	2.06863600
H	6.35314500	-1.44130500	-0.66437200	C	6.17707800	0.63388900	3.38685900
H	5.00103600	-1.97672800	-1.65075500	C	5.31047000	-0.00366200	4.48163500
H	7.54067100	-0.56926100	-2.64769200	H	5.53110600	-2.06564300	3.86548700
H	7.13380800	-2.26844200	-2.87175100	H	4.05451800	-1.75741700	4.77441300
H	5.18776900	-1.65597700	-4.28742900	H	3.06351500	-0.54096100	2.85191500
H	6.64761000	-0.91385100	-4.93765100	H	3.55867500	-2.15332600	2.36778200
<b><math>\alpha</math>-10<sub>Cy</sub> [(μ-Cl)<sub>2</sub>Pd<sub>2</sub>(PCy<sub>3</sub>)<sub>2</sub>(Ph)<sub>2</sub>] (conformer F)</b>				H	5.67360600	-1.21597800	1.40638000
Pd	1.78481900	0.55090200	0.16957100	H	6.06457100	1.23734300	1.31213500
Pd	-1.76755600	-0.53784300	0.15420900	H	4.58686900	1.52162800	2.21160200
P	-3.86843200	0.44200200	-0.02375400	H	7.06090000	0.00191500	3.21063800
P	3.87942000	-0.44577600	-0.03968300	H	6.55343900	1.61050700	3.71678800
Cl	-0.43453700	1.58512600	0.34552800	H	4.49209400	0.68372200	4.74213600
Cl	0.45349900	-1.58463900	0.24829400	H	5.89890600	-0.15090500	5.39628500
C	-2.96527300	-4.39581200	1.50626700	C	5.37086900	1.59762900	-3.43953700
C	-2.58461100	-3.05247300	1.42355400	C	4.50010300	0.61104800	-2.64310400
C	-2.54871200	-2.38479900	0.18722000	C	5.05704300	0.43475000	-1.21253000
C	-2.88956400	-3.10886900	-0.96388400	C	6.50488900	-0.09798000	-1.28582000
C	-3.27089100	-4.45428600	-0.88161300	C	7.39480100	0.87023800	-2.08867200
C	-3.31736700	-5.10170000	0.35335900	C	6.83380800	1.13127300	-3.49466200
H	-2.98175200	-4.89001800	2.47542600	H	5.31780800	2.58843700	-2.96623400
H	-2.29922700	-2.52904200	2.33277400	H	4.97046500	1.71086100	-4.45516900
H	-2.83907900	-2.64068300	-1.94216300	H	4.50085000	-0.35455700	-3.16159000
H	-3.52429200	-4.99525100	-1.79112500	H	3.45918000	0.94872600	-2.61567000
H	-3.61372000	-6.14563700	0.41651100	H	5.09087600	1.43826500	-0.76560200
C	3.32707400	5.09994400	0.61665300	H	6.93069200	-0.24265800	-0.28690400
C	3.24328000	4.52999600	-0.65422400	H	6.51156200	-1.07985900	-1.77654900
C	2.86360900	3.19032700	-0.80730300	H	7.47002200	1.82216500	-1.54289900
C	2.56261800	2.39442400	0.30716700	H	8.41356100	0.46682500	-2.15419700
C	2.62937600	2.98638400	1.57980100	H	6.89331200	0.20389100	-4.08365500
C	3.01053400	4.32345800	1.73359900	H	7.45193100	1.87242500	-4.01701300
H	3.62304100	6.13915500	0.73537100	C	-4.55898000	4.67567000	0.34139200
H	3.46561900	5.12732500	-1.53615100	C	-4.92864800	3.17946000	0.29447200
H	2.78284700	2.78217100	-1.80991700	C	-3.70273400	2.32952400	-0.11220000
H	2.36405100	2.40970100	2.46261600	C	-3.15371400	2.81740000	-1.47172700
H	3.05280700	4.75777200	2.73027500	C	-2.76773500	4.30405300	-1.40714500
C	4.48635500	-4.66528600	-0.55084400	C	-3.95991600	5.17148200	-0.98177500
C	4.89518800	-3.19465200	-0.33741300	H	-3.83047100	4.83515600	1.14953300
C	3.67506900	-2.26377100	-0.52176100	H	-5.44949600	5.26181200	0.60373900
C	3.06553500	-2.46769700	-1.92721600	H	-5.75012500	3.03053700	-0.41911800
C	2.64732200	-3.93364300	-2.13160000	H	-5.30690000	2.88532600	1.27883100
C	3.83040300	-4.88908100	-1.92020900	H	-2.91558300	2.51892200	0.62884100
H	3.78085600	-4.95634900	0.24091300	H	-2.28558800	2.22221700	-1.76950000
H	5.36765800	-5.31012700	-0.43767700	H	-3.92597900	2.69052100	-2.24216500
H	5.68246200	-2.93246800	-1.05608300	H	-1.94017200	4.42679400	-0.69549800
				H	-2.39042000	4.62762600	-2.38567100

H	-4.73235800	5.13675200	-1.76516200
H	-3.65740900	6.22229100	-0.88847400
C	-4.83474800	-0.98682600	-3.89849300
C	-4.06348000	-0.20891100	-2.81861900
C	-4.85388300	-0.19771700	-1.48979200
C	-6.24736100	0.43138300	-1.70665000
C	-7.02494400	-0.33165400	-2.79546400
C	-6.23967400	-0.40328800	-4.11344500
H	-4.91929200	-2.04095800	-3.59612800
H	-4.26978700	-0.97382300	-4.83925500
H	-3.90412400	0.81619400	-3.16983900
H	-3.06855000	-0.64064800	-2.66647800
H	-4.99999000	-1.25047600	-1.20889300
H	-6.82916400	0.43876800	-0.77748500
H	-6.13277200	1.47885700	-2.01549000
H	-7.23178900	-1.35139400	-2.43879700
H	-7.99962300	0.14640500	-2.95753300
H	-6.14850800	0.60924100	-4.53414600
H	-6.79225700	-0.99889100	-4.85109400
C	-5.16307000	0.40241100	3.99448500
C	-4.24372100	0.51044800	2.76603700
C	-5.00101500	0.18239100	1.45878300
C	-5.66693700	-1.20734700	1.54645000
C	-6.58913400	-1.29588600	2.77647200
C	-5.83838900	-0.97346100	4.07592600
H	-5.93604000	1.18377500	3.93991800
H	-4.58351500	0.60044100	4.90510100
H	-3.40177300	-0.18600500	2.87265400
H	-3.80556300	1.51494600	2.71952800
H	-5.81028800	0.91577700	1.34436700
H	-6.25368700	-1.41217900	0.64369300
H	-4.90117200	-1.98645300	1.60812700
H	-7.42607300	-0.59103100	2.65747900
H	-7.03069100	-2.29912200	2.82868500
H	-5.07284300	-1.74322900	4.25146900
H	-6.52397500	-1.01131700	4.93211800

$\alpha$ -**10<sub>H</sub>** [( $\mu$ -Br)<sub>2</sub>Pd<sub>2</sub>(PH<sub>3</sub>)<sub>2</sub>(Ph)<sub>2</sub>]

Pd	1.69591000	-0.71538900	-0.05713400
Pd	-1.69592200	0.71539700	-0.05697800
Br	0.75084700	1.64103700	-0.30584600
Br	-0.75087700	-1.64101900	-0.30585300
P	2.68431000	-2.73102400	0.18641900
P	-2.68431200	2.73102500	0.18668300
C	-5.31367600	-1.00534900	1.48612100
C	-4.05711000	-0.39803600	1.37936700
C	-3.55415800	-0.03816500	0.12199900
C	-4.32803400	-0.27342900	-1.02225100
C	-5.58382800	-0.88105000	-0.90900900
C	-6.07939700	-1.24716000	0.34389700
H	-5.68955900	-1.29002600	2.46617300
H	-3.46724100	-0.22811400	2.27682900
H	-3.95031200	-0.00527700	-2.00593500
H	-6.17092200	-1.06865400	-1.80504600
H	-7.05484400	-1.71863600	0.42950700
C	6.07945700	1.24712100	0.34318200
C	5.58373400	0.88098500	-0.90965600

C	4.32791800	0.27337800	-1.02273300
C	3.55417400	0.03815600	0.12161600
C	4.05728100	0.39805300	1.37891400
C	5.31386800	1.00535200	1.48550300
H	7.05492100	1.71858500	0.42866300
H	6.17072400	1.06855700	-1.80576700
H	3.95007600	0.00520500	-2.00636500
H	3.46751500	0.22816400	2.27645100
H	5.68987100	1.29005000	2.46550300
H	-1.87962700	3.89137500	0.15092300
H	-3.67515800	3.10711600	-0.74514900
H	-3.40263100	2.98432700	1.37484300
H	1.87960400	-3.89136400	0.15081300
H	3.67500400	-3.10715200	-0.74556100
H	3.40281400	-2.98430800	1.37447200

*s*-**10<sub>H</sub>** [( $\mu$ -Br)<sub>2</sub>Pd<sub>2</sub>(PH<sub>3</sub>)<sub>2</sub>(Ph)<sub>2</sub>]

Pd	-1.83796400	-0.55004500	-0.02505000
Pd	1.83640200	-0.54976900	-0.01305300
Br	-0.00028400	-2.44136900	-0.12261000
Br	0.00024700	1.17765300	-0.32671500
P	3.58503800	-1.95325700	0.28021700
P	-3.58862900	-1.95331900	0.25639900
C	4.44153300	2.60027700	1.29420700
C	3.54610800	1.52491400	1.26733300
C	3.20957800	0.91979400	0.04904000
C	3.79024400	1.38923000	-1.13680100
C	4.68503100	2.46503200	-1.10312800
C	5.01313900	3.07171000	0.11079100
H	4.68735600	3.06888700	2.24432400
H	3.09951100	1.17754200	2.19579200
H	3.53587500	0.93486600	-2.09124400
H	5.12146100	2.82766300	-2.03089400
H	5.70778200	3.90715800	0.13415600
C	-5.00738300	3.07630500	0.13782700
C	-4.68617100	2.47827400	-1.08219300
C	-3.79388200	1.40084100	-1.12814700
C	-3.20872000	0.92116500	0.05134000
C	-3.53836600	1.51759500	1.27579400
C	-4.43138800	2.59456700	1.31496700
H	-5.70009500	3.91303100	0.17081300
H	-5.12606800	2.84892700	-2.00514000
H	-3.54491400	0.95314800	-2.08716000
H	-3.08817000	1.16233100	2.19951400
H	-4.67185000	3.05640300	2.26976000
H	4.62156500	-1.94006800	-0.67771000
H	4.37121900	-1.81137000	1.44396500
H	3.33684500	-3.34261100	0.33546200
H	-4.37098700	-1.82231300	1.42397700
H	-4.62793000	-1.92798500	-0.69827000
H	-3.34298900	-3.34365300	0.29634900

$\alpha$ -**10<sub>H</sub>** [( $\mu$ -Cl)<sub>2</sub>Pd<sub>2</sub>(PH<sub>3</sub>)<sub>2</sub>(Ph)<sub>2</sub>]

Pd	1.65390000	-0.66405300	-0.07427200
Pd	-1.65391200	0.66407900	-0.07442000
P	2.65144200	-2.67150600	0.09451700
P	-2.65155200	2.67149900	0.09417000



Cl	0.68101500	1.55600900	-0.23183800
Cl	-0.68098600	-1.55589800	-0.23273300
C	-5.27943400	-1.09930200	1.37085100
C	-4.02959100	-0.47422600	1.29562900
C	-3.50254400	-0.10283100	0.05157300
C	-4.24629100	-0.34384800	-1.11119700
C	-5.49575500	-0.96910900	-1.02943800
C	-6.01503200	-1.34688900	0.21021100
H	-5.67448500	-1.39244600	2.34081100
H	-3.46350700	-0.29770900	2.20697000
H	-3.85014200	-0.06458900	-2.08448200
H	-6.06002700	-1.16007000	-1.93932900
H	-6.98596600	-1.83135900	0.27146200
C	6.01511800	1.34677800	0.20977800
C	5.49569300	0.96879100	-1.02974700
C	4.24619600	0.34356300	-1.11125400
C	3.50255900	0.10280400	0.05164800
C	4.02975000	0.47441200	1.29557100
C	5.27963400	1.09943900	1.37054100
H	6.98608100	1.83121500	0.27083700
H	6.05987900	1.15955600	-1.93973200
H	3.84994300	0.06412400	-2.08444500
H	3.46374400	0.29810500	2.20700000
H	5.67480000	1.39274700	2.34040500
H	-1.83150800	3.82071700	0.07058000
H	-3.60065600	3.03898000	-0.88328800
H	-3.41416800	2.95024200	1.24827000
H	1.83140800	-3.82071800	0.07028500
H	3.60126500	-3.03894400	-0.88225500
H	3.41320400	-2.95031600	1.24916900

***s*-10<sub>H</sub> [(μ-Cl)<sub>2</sub>Pd<sub>2</sub>(PH<sub>3</sub>)<sub>2</sub>(Ph)<sub>2</sub>]**

Pd	-1.78131000	-0.62956700	-0.01620300
Pd	1.78131000	-0.62956800	-0.01619500
P	3.51143400	-2.06420100	0.07046900
P	-3.51143700	-2.06420300	0.07038100
Cl	0.00000000	1.01279400	-0.09874600
Cl	-0.00000100	-2.39409800	-0.04653000
C	4.50366000	2.43542500	1.22600400
C	3.59911900	1.36757700	1.21958800
C	3.17031900	0.81637100	0.00481000
C	3.66886000	1.33080900	-1.19945000
C	4.57311000	2.39878400	-1.18626500
C	4.99328500	2.95188800	0.02486500
H	4.82222500	2.86201600	2.17430600
H	3.21845000	0.98284800	2.16256200
H	3.34309900	0.91665900	-2.15048100
H	4.94614600	2.79661700	-2.12717300
H	5.69632700	3.78061400	0.03251400
C	-4.99328300	2.95189000	0.02492000
C	-4.57309500	2.39882300	-1.18622200
C	-3.66884600	1.33084800	-1.19943100
C	-3.17031800	0.81637200	0.00481900
C	-3.59913100	1.36754100	1.21960900
C	-4.50367100	2.43538900	1.22604800
H	-5.69632400	3.78061600	0.03258700
H	-4.94612000	2.79668600	-2.12712200

H	-3.34307300	0.91672700	-2.15047100
H	-3.21847400	0.98278100	2.16257500
H	-4.82224600	2.86195100	2.17436000
H	4.47919400	-2.02470000	-0.95595700
H	4.37865600	-2.00903300	1.18248800
H	3.22051500	-3.44596400	0.06757000
H	-4.37871400	-2.00905500	1.18235800
H	-4.47914600	-2.02468600	-0.95609200
H	-3.22051500	-3.44596500	0.06747200

***a*-10<sub>Ph</sub> [(μ-Br)<sub>2</sub>Pd<sub>2</sub>(PPh<sub>3</sub>)<sub>2</sub>(Ph)<sub>2</sub>]**

Pd	1.81705600	0.52613200	-0.22836800
Pd	-1.80540000	-0.54534200	-0.11013900
Br	-0.44623300	1.68756500	-0.52535600
Br	0.44932900	-1.73498000	-0.36259000
P	-3.87113200	0.49777000	0.01453500
P	3.88029600	-0.49189600	0.04263400
C	-3.35171900	-4.18494000	1.55899900
C	-2.87063700	-2.87980200	1.40715400
C	-2.64556300	-2.35025300	0.13003700
C	-2.91348400	-3.14617600	-0.99279300
C	-3.40052300	-4.44964500	-0.83785500
C	-3.62223900	-4.97257700	0.43804600
H	-3.51614500	-4.58292800	2.55806400
H	-2.66885000	-2.28150900	2.29233400
H	-2.72952800	-2.76156500	-1.99308300
H	-3.59801200	-5.05659700	-1.71899400
H	-3.99711400	-5.98597500	0.55760800
C	3.58353700	4.98655800	0.19116200
C	3.56449000	4.35756600	-1.05543800
C	3.09944100	3.04350100	-1.17835100
C	2.63963600	2.34577200	-0.05425600
C	2.65494000	2.98288400	1.19479600
C	3.12586100	4.29578800	1.31539900
H	3.94610700	6.00714600	0.28477500
H	3.91160000	4.88792800	-1.93956200
H	3.09156800	2.57189400	-2.15789700
H	2.28678500	2.46625500	2.07809000
H	3.12721900	4.77797500	2.29083400
C	-3.57045700	4.50288500	2.35793700
C	-4.37457400	4.43670500	1.21897800
C	-4.47164200	3.24661700	0.49497200
C	-3.75640000	2.11129100	0.90141000
C	-2.93923200	2.18992300	2.04035800
C	-2.85459300	3.37618500	2.76914300
H	-3.49383800	5.43107900	2.91777400
H	-4.92636300	5.31256400	0.88840100
H	-5.09819600	3.20903700	-0.39028500
H	-2.35251300	1.32679600	2.34217100
H	-2.21558000	3.42414100	3.64652300
C	-7.43558900	-1.68466900	2.07020800
C	-6.87852400	-0.55525900	2.66891700
C	-5.81530500	0.11388400	2.05709000
C	-5.29372200	-0.34411400	0.83862100
C	-5.85700200	-1.48766500	0.24629500
C	-6.92172400	-2.14805400	0.85617400
H	-8.26355800	-2.20342800	2.54604000

H	-7.27180300	-0.18536200	3.61212600	C	2.88015200	-2.90554000	-1.33895900
H	-5.40012600	0.99671900	2.53080900	C	2.60235700	-2.33559700	-0.09010400
H	-5.45649400	-1.87105100	-0.68603200	C	2.82337000	-3.09363500	1.06848300
H	-7.34310300	-3.03180000	0.38528700	C	3.31851400	-4.39972800	0.97656200
C	-5.44308300	1.58534600	-4.22719600	C	3.59392800	-4.96306200	-0.27134700
C	-6.34888200	1.44263000	-3.17393100	H	3.57457600	-4.64389300	-2.40559200
C	-5.89412800	1.10430200	-1.89841300	H	2.71667300	-2.33517200	-2.25000100
C	-4.52348300	0.90541800	-1.66230800	H	2.59992200	-2.67514200	2.04696400
C	-3.62022800	1.04700500	-2.72809900	H	3.48283000	-4.97658600	1.88434100
C	-4.07963700	1.38777100	-4.00159100	H	3.97633500	-5.97827400	-0.34191200
H	-5.79959300	1.84582400	-5.22022200	C	-3.53983500	4.96970700	-0.06537000
H	-7.41204000	1.59078700	-3.34371700	C	-3.49349100	4.30184200	1.16009700
H	-6.60819700	0.98651700	-1.08934100	C	-3.02465700	2.98551800	1.23166700
H	-2.55867300	0.89423800	-2.55820900	C	-2.58845100	2.32511800	0.07635200
H	-3.36879800	1.49441700	-4.81635000	C	-2.63079700	3.00089100	-1.15134600
C	7.73909700	1.91018000	-0.97794400	C	-3.10555300	4.31588000	-1.22044700
C	7.35451500	0.84149300	-1.78693200	H	-3.90690900	5.99159200	-0.11898100
C	6.20637100	0.10563700	-1.48270400	H	-3.82441400	4.80300100	2.06717400
C	5.42524200	0.43550900	-0.36567700	H	-2.99931100	2.48117900	2.19443400
C	5.81735500	1.51848000	0.44009600	H	-2.28274800	2.51102900	-2.05784100
C	6.96745100	2.24506100	0.13769700	H	-3.12939200	4.82840500	-2.17996800
H	8.63312000	2.48089400	-1.21470900	C	3.59748000	4.49456000	-2.36518200
H	7.94852700	0.57127200	-2.65597300	C	4.41760600	4.41083900	-1.23847400
H	5.92630400	-0.72825700	-2.11690700	C	4.47907800	3.22722300	-0.50139500
H	5.21773000	1.80428300	1.29748200	C	3.71379300	2.11559400	-0.88319000
H	7.25360000	3.08070600	0.77024200	C	2.88322500	2.21123700	-2.01023100
C	4.48422600	-1.97269100	4.41227600	C	2.83196200	3.39239000	-2.75092000
C	5.60074300	-1.67968300	3.62676100	H	3.54781900	5.41848100	-2.93514300
C	5.43786200	-1.22475500	2.31700500	H	5.00915400	5.26810900	-0.92845700
C	4.15160900	-1.05629300	1.77813300	H	5.11802800	3.17468500	0.37447700
C	3.03412000	-1.35265200	2.57567100	H	2.26180400	1.36689700	-2.29364700
C	3.20227700	-1.81058200	3.88347800	H	2.18033700	3.45536900	-3.61796600
H	4.61324400	-2.32392500	5.43260100	C	7.45017600	-1.66270200	-1.89213800
H	6.60158400	-1.80179100	4.03236600	C	6.91168300	-0.53548800	-2.51166100
H	6.31330400	-0.99282400	1.71888700	C	5.82491800	0.13064600	-1.93958100
H	2.03484100	-1.23191400	2.16843100	C	5.26000800	-0.32869000	-0.74076200
H	2.32827300	-2.03681000	4.48808000	C	5.80437000	-1.47081100	-0.12799400
C	4.22263900	-4.26546200	-2.65304100	C	6.89353400	-2.12742600	-0.69777400
C	4.75064700	-4.29716600	-1.36114500	H	8.29654000	-2.17913500	-2.33715000
C	4.64917500	-3.17813500	-0.53234500	H	7.33758600	-0.16536900	-3.44047600
C	4.00995400	-2.01627400	-0.98803200	H	5.42387200	1.01110600	-2.42960300
C	3.46999900	-1.99653600	-2.28422400	H	5.36981900	-1.85648200	0.78801500
C	3.58418200	-3.11201900	-3.11430600	H	7.29958000	-3.01010600	-0.21168400
H	4.30034200	-5.13882000	-3.29495200	C	5.13931400	1.68634000	4.31736300
H	5.24054000	-5.19476200	-0.99344100	C	6.10867100	1.42999000	3.34596300
H	5.06134800	-3.21625900	0.47086100	C	5.72794900	1.06384000	2.05348800
H	2.94370200	-1.11352300	-2.63598600	C	4.36864600	0.94830100	1.71998300
H	3.15877200	-3.08421500	-4.11363000	C	3.39953800	1.20644100	2.70376000
$\alpha$ -10 <sub>Ph</sub> [(μ-Cl) <sub>2</sub> Pd <sub>2</sub> (PPh <sub>3</sub> ) <sub>2</sub> (Ph) <sub>2</sub> ]				C	3.78572300	1.57605600	3.99272900
Pd	-1.75310700	0.51373200	0.16606000	H	5.43783900	1.96847200	5.32353400
Pd	1.74808000	-0.53671200	0.06556900	H	7.16407900	1.51196900	3.59195000
P	3.80223400	0.51024300	0.01965500	H	6.49106000	0.85992400	1.30920300
P	-3.80920900	-0.51168400	-0.01920700	H	2.34527600	1.12476500	2.45644600
Cl	0.42879000	1.58626000	0.37156300	H	3.02535800	1.77336200	4.74338700
Cl	-0.43137100	-1.63405300	0.18004400	C	-7.63590400	1.89219800	1.10178900
C	3.36825500	-4.21370200	-1.42790600	C	-7.22029700	0.83415400	1.90944700
				C	-6.08165700	0.09725800	1.57361800

C	-5.34181600	0.41585900	0.42572700	H	5.85619400	-3.19415500	1.17846300
C	-5.76353300	1.48942000	-0.37739300	H	4.89663800	-3.63495000	2.58801300
C	-6.90424400	2.21682100	-0.04349000	H	6.19328000	0.07100700	-2.23193200
H	-8.52251100	2.46369500	1.36328900	H	4.53407700	0.63887500	-2.52292600
H	-7.78229900	0.57367400	2.80240200	H	5.25113200	-0.59925900	-3.56074100
H	-5.77507100	-0.72768800	2.20749700	H	6.62469700	-2.23012000	-1.17667800
H	-5.19326100	1.76768000	-1.25708700	H	5.89332400	-2.80472200	-2.67358200
H	-7.21414800	3.04527600	-0.67429400	H	5.31826000	-3.42081500	-1.12944300
C	-4.52296500	-2.09375300	-4.33647200	H	2.87211800	-2.71888800	-1.84036400
C	-5.61812100	-1.72208600	-3.55469400	H	3.64721700	-2.25615800	-3.35789200
C	-5.42442000	-1.23590000	-2.26017800	H	2.62106900	-1.10060100	-2.48807000
C	-4.12788900	-1.11379900	-1.73438100	H	5.07466800	2.42112900	0.37226000
C	-3.03110100	-1.49021900	-2.52765600	H	5.87742900	1.65928300	-0.99773700
C	-3.23108100	-1.97970200	-3.81902100	H	6.81043300	2.12161800	0.42236700
H	-4.67597700	-2.46921100	-5.34480800	H	7.03370300	-1.41108200	1.01488100
H	-6.62658600	-1.80745700	-3.95078200	H	7.77612500	0.17431600	1.20800800
H	-6.28381600	-0.94362800	-1.66549400	H	7.36107300	-0.40217300	-0.40041000
H	-2.02422400	-1.40875300	-2.12923900	H	4.46175200	1.17459900	2.42127900
H	-2.37341500	-2.26796600	-4.42062900	H	6.20534300	1.37139800	2.60513100
C	-4.05673300	-4.24013900	2.74516200	H	5.47041600	-0.19402800	2.93618800
C	-4.73963000	-4.24142300	1.52707200	C	-5.66822300	-0.34153500	0.78825700
C	-4.66221800	-3.13659800	0.67817500	C	-5.84694400	-1.71252900	0.08897200
C	-3.89518600	-2.01896300	1.03969700	H	-5.07530400	-2.42128900	0.37342300
C	-3.20392100	-2.02914700	2.26073100	H	-5.87631300	-1.65920500	-0.99745300
C	-3.29038000	-3.13217600	3.11117700	H	-6.81095500	-2.12081200	0.42181400
H	-4.11478700	-5.10353400	3.40256200	C	-5.42274400	-0.67389800	2.27789000
H	-5.33126400	-5.10441400	1.23348800	H	-4.46135900	-1.17424000	2.42149700
H	-5.19396200	-3.14957500	-0.26814200	H	-6.20490800	-1.37130700	2.60544700
H	-2.58242900	-1.18164400	2.53442200	H	-5.47019500	0.19422600	2.93651200
H	-2.74447700	-3.13050500	4.05049500	C	-7.02418200	0.38991000	0.64028600
$\alpha$ -10 <sub>t</sub> Bu [(μ-Br) <sub>2</sub> Pd <sub>2</sub> (P <sup>t</sup> Bu <sub>3</sub> ) <sub>2</sub> (Ph) <sub>2</sub> ]				H	-7.36109700	0.40231300	-0.39988600
Pd	1.96272900	0.42133600	-0.13999200	H	-7.03328900	1.41150100	1.01510400
Pd	-1.96271600	-0.42144800	-0.13990000	H	-7.77584600	-0.17377900	1.20875200
Br	-0.27403600	1.65584100	-0.44121000	C	-3.89378200	2.19397500	1.34742500
Br	0.27411900	-1.65626800	-0.43945300	C	-3.14987000	3.37636000	0.68698200
P	-4.13286500	0.68498300	0.10207600	H	-3.76006600	3.90406400	-0.04883000
P	4.13300200	-0.68490300	0.10198700	H	-2.20789700	3.08634800	0.22652200
C	3.89430000	-2.19393400	1.34737800	H	-2.90786300	4.09850400	1.47795900
C	4.63411400	-1.38440000	-1.64910700	C	-5.18647800	2.79363000	1.94539600
C	5.66838600	0.34175600	0.78794100	H	-5.85528300	3.19499500	1.17881900
C	2.99401500	-1.68494800	2.49927500	H	-4.89571600	3.63470100	2.58872000
C	3.15047400	-3.37643500	0.68704500	H	-5.74979500	2.10011800	2.57055600
C	5.18715700	-2.79342900	1.94517000	C	-2.99340100	1.68489600	2.49921100
C	5.18783800	-0.23873400	-2.52579700	H	-3.42815300	0.84738600	3.04825800
C	5.67830200	-2.52236000	-1.63402100	H	-2.84060200	2.50561200	3.21305100
C	3.36118500	-1.89540000	-2.36051600	H	-2.01211400	1.37828500	2.12762800
C	5.84696800	1.71275600	0.08865300	C	-4.63425600	1.38461300	-1.64887200
C	7.02439300	-0.38957900	0.63983600	C	-3.36141900	1.89561200	-2.36044100
C	5.42305200	0.67411900	2.27759800	H	-2.62140000	1.10076400	-2.48824800
H	2.01259800	-1.37860300	2.12782500	H	-2.87217200	2.71896600	-1.84024800
H	3.42867000	-0.84728300	3.04815800	H	-3.64760000	2.25655400	-3.35770600
H	2.84153900	-2.50562900	3.21322500	C	-5.67834600	2.52265500	-1.63343700
H	2.20838700	-3.08657300	0.22673500	H	-6.62490700	2.23023300	-1.17655100
H	2.90869800	-4.09861800	1.47805800	H	-5.89302600	2.80565900	-2.67289400
H	3.76064600	-3.90403100	-0.04885900	H	-5.31836800	3.42077100	-1.12820800
H	5.75015500	-2.10003500	2.57075100	C	-5.18820700	0.23906600	-2.52557700
				H	-4.53460700	-0.63865900	-2.52272900

H	-5.25142800	0.59961400	-3.56051700	H	-7.86995200	-0.57747600	-0.03094600
H	-6.19371000	-0.07049600	-2.23171400	H	-6.99294200	-1.24651100	1.33735700
C	-3.03420700	-4.30253600	1.29519600	H	-5.64235800	0.91792900	1.84937500
C	-2.69339100	-2.94662700	1.22450200	H	-6.96407600	1.39637700	0.78869500
C	-2.67896900	-2.27983800	-0.00844900	H	-5.32190500	1.94213900	0.45318000
C	-2.97634700	-3.00223300	-1.17201100	H	-2.40983500	-1.09776500	-2.54041900
C	-3.31505500	-4.35782400	-1.09948300	H	-4.07318500	-0.72688400	-3.02060200
C	-3.35403200	-5.01124200	0.13483400	H	-3.32364200	-2.23926600	-3.53941600
H	-3.04241100	-4.80383800	2.26076100	H	-5.60965700	-3.59732500	-0.95925700
H	-2.42409500	-2.41911200	2.13606700	H	-5.02371300	-3.70812000	-2.61714200
H	-2.93561000	-2.51669300	-2.14370700	H	-6.01447300	-2.33710400	-2.13962600
H	-3.54377000	-4.90285200	-2.01279900	H	-1.88031500	-3.02630100	-0.94636400
H	-3.61840800	-6.06404900	0.19018400	H	-2.78006500	-4.00556400	-2.09740000
C	3.35315800	5.01128800	0.13675600	H	-3.18582200	-4.09538300	-0.38819000
C	3.31424200	4.35849500	-1.09789400	C	5.59115200	-0.22133900	0.90715500
C	2.97579800	3.00287400	-1.17110100	C	6.03431100	1.04224500	0.12804600
C	2.67864800	2.27981400	-0.00789400	H	5.37286400	1.88566600	0.30158500
C	2.69299600	2.94598000	1.22539800	H	6.12257100	0.89501200	-0.94638500
C	3.03353600	4.30192400	1.29677000	H	7.02971500	1.31922900	0.50157500
H	3.61733300	6.06411800	0.19263300	C	5.31369000	0.26198300	2.34892600
H	3.54279600	4.90403700	-2.01094300	H	4.42999100	0.90406200	2.39166800
H	2.93509000	2.51782900	-2.14304500	H	6.17066800	0.86298700	2.68020600
H	2.42386000	2.41794500	2.13671100	H	5.19430600	-0.54962900	3.06775500
H	3.04169500	4.80273100	2.26259400	C	6.81333600	-1.17086600	0.90718100
<i>s</i> - <b>10</b> <sub>tBu</sub> [(μ-Br) <sub>2</sub> Pd <sub>2</sub> (P <sup><i>i</i></sup> Bu <sub>3</sub> ) <sub>2</sub> (Ph) <sub>2</sub> ]				H	7.21130700	-1.31123000	-0.10163000
Pd	-1.98982300	0.42368600	-0.15256300	H	6.62695200	-2.15152600	1.34074200
Pd	2.00282700	0.40093500	-0.21473100	H	7.60963600	-0.69790000	1.49725400
Br	-0.01341600	-1.37929600	-0.59455500	C	3.38400400	-2.38454900	1.51221600
Br	0.01136000	1.98729100	-0.45934900	C	2.48772700	-3.46897300	0.87331900
P	-3.98604400	-0.98626200	0.02103800	H	3.03145400	-4.12567000	0.19079000
P	3.94823100	-1.03492400	0.18910900	H	1.62591000	-3.05022200	0.35600800
C	-3.91930100	-1.94996700	1.71427100	H	2.10319500	-4.10096900	1.68530400
C	-5.76093900	-0.13946400	-0.10781700	C	4.51933600	-3.14075100	2.23675000
C	-3.90120100	-2.28995200	-1.45467200	H	5.14702500	-3.71390200	1.54859700
C	-2.45315500	-2.34806500	1.99699000	H	4.05498100	-3.86205000	2.92219100
C	-4.33873200	-1.00766500	2.86428200	H	5.16231700	-2.49925600	2.84055400
C	-4.79623300	-3.21866300	1.79118700	C	2.51514200	-1.65328100	2.56305300
C	-5.95671900	0.39242600	-1.54667800	H	3.05972900	-0.88175100	3.11073700
C	-6.93633400	-1.07807900	0.25837600	H	2.15963100	-2.39035600	3.29572700
C	-5.90645900	1.09972300	0.80964700	H	1.63914100	-1.19037200	2.10013400
C	-3.40148900	-1.52802300	-2.70609400	C	4.42114300	-1.94449600	-1.46966700
C	-5.22580100	-3.00724000	-1.79641000	C	3.12066500	-2.29908500	-2.22563500
C	-2.87216200	-3.41019700	-1.17912700	H	2.53592000	-1.40632200	-2.46364700
H	-1.80145300	-1.47217800	2.05778100	H	2.47046800	-2.98080500	-1.67828100
H	-2.03235900	-3.01727200	1.24744700	H	3.39524400	-2.78695100	-3.17090400
H	-2.41894100	-2.86581400	2.96551200	C	5.26248500	-3.22900600	-1.30326200
H	-3.81454700	-0.04798400	2.82440900	H	6.22020700	-3.05320200	-0.81103300
H	-4.07567900	-1.48867100	3.81547200	H	5.47945200	-3.62957100	-2.30287900
H	-5.41456700	-0.82068800	2.88687700	H	4.73570200	-4.01205500	-0.75473700
H	-4.48512700	-3.99103900	1.08531600	C	5.20107800	-0.97793600	-2.38815900
H	-5.85608300	-3.01637700	1.63035400	H	4.70029400	-0.01037200	-2.49110000
H	-4.69608700	-3.64660300	2.79792500	H	5.25917400	-1.42714000	-3.38816000
H	-6.08702000	-0.39215800	-2.29351800	H	6.22669100	-0.80986500	-2.05217200
H	-5.12697200	1.03503900	-1.85308200	C	3.69776300	4.17758900	0.89090700
H	-6.86669800	1.00653900	-1.56265600	C	3.11805800	2.90479600	0.94514400
H	-6.92135000	-2.04648500	-0.23860100	C	3.01885800	2.11951700	-0.21189200
				C	3.47209600	2.64590500	-1.42947800

C	4.04871300	3.91978200	-1.48124800	H	-5.77017400	1.59243500	1.08967500
C	4.17251500	4.68645000	-0.32019100	H	-6.72474800	2.06474900	-0.31300500
H	3.76782600	4.77334100	1.79841400	H	-6.89610800	-1.46393700	-0.95678200
H	2.73009200	2.53804400	1.89174800	H	-7.66744400	0.11100100	-1.12048800
H	3.37212700	2.07138300	-2.34696900	H	-7.22608900	-0.48033600	0.47552500
H	4.39687700	4.31227100	-2.43418700	H	-4.38435700	1.18856200	-2.35038300
H	4.62002000	5.67603600	-0.36135200	H	-6.13300700	1.35532100	-2.51510900
C	-3.94379300	4.70597900	0.81267000	H	-5.37192400	-0.19094900	-2.87679100
C	-3.86786300	4.25504000	-0.50689700	C	5.55867200	-0.30889100	-0.71938700
C	-3.35588400	2.98337500	-0.79188700	C	5.75166500	-1.66553800	0.00338000
C	-2.92314100	2.14333600	0.24358200	H	4.99279100	-2.39006300	-0.27588200
C	-2.97498100	2.61284000	1.56339800	H	5.77016600	-1.59281700	1.08901400
C	-3.48695500	3.88350400	1.84541500	H	6.72463300	-2.06489200	-0.31381800
H	-4.34059000	5.69354300	1.03288000	C	5.33449600	-0.66772900	-2.20612000
H	-4.19975400	4.89396200	-1.32235200	H	4.38415900	-1.18827600	-2.35082800
H	-3.28445600	2.65881600	-1.82672900	H	6.13279200	-1.35498200	-2.51575000
H	-2.60925400	1.99522000	2.37987600	H	5.37165800	0.19134500	-2.87707500
H	-3.52322700	4.23053300	2.87582800	C	6.90039700	0.44746000	-0.56816700
$\alpha$ -10 <sub>t</sub> Bu [(μ-Cl) <sub>2</sub> Pd <sub>2</sub> (P <sup>t</sup> Bu <sub>3</sub> ) <sub>2</sub> (Ph) <sub>2</sub> ]				H	7.22617400	0.48007000	0.47511300
Pd	-1.86510600	0.42703700	0.16648800	H	6.89610500	1.46391100	-0.95701900
Pd	1.86508800	-0.42700600	0.16628800	H	7.66735600	-0.11103800	-1.12103100
P	-4.00000700	-0.69895100	-0.06299400	C	3.73937500	2.18503500	-1.33124900
P	4.00003800	0.69891300	-0.06310100	C	2.96184100	3.36267700	-0.69986400
Cl	0.28803600	1.56361900	0.42306100	H	3.54781200	3.91149000	0.04059900
Cl	-0.28800900	-1.56354000	0.42340100	H	2.01534100	3.06167500	-0.25627000
C	-3.73926100	-2.18477300	-1.33148600	H	2.72712000	4.07061300	-1.50593600
C	-4.46701700	-1.43316600	1.68182600	C	5.02747700	2.79964300	-1.92379600
C	-5.55872900	0.30888800	-0.71899500	H	5.68051000	3.22254000	-1.15526500
C	-2.86150800	-1.64034700	-2.48491500	H	4.72893000	3.62688000	-2.58119800
C	-2.96160000	-3.36250300	-0.70041900	H	5.61009400	2.10837800	-2.53376800
C	-5.02732100	-2.79934100	-1.92416900	C	2.86155300	1.64093900	-2.48478100
C	-5.03245300	-0.31294700	2.58314800	H	3.31665600	0.80297900	-3.01645300
C	-5.48908700	-2.59079300	1.65713700	H	2.70245100	2.44768500	-3.21306700
C	-3.17658800	-1.93194700	2.37095000	H	1.88189200	1.32280600	-2.11849900
C	-5.75174100	1.66538200	0.00405200	C	4.46708500	1.43279500	1.68185600
C	-6.90040800	-0.44754800	-0.56777900	C	3.17668800	1.93157000	2.37103700
C	-5.33468800	0.66800200	-2.20568200	H	2.45163700	1.12445600	2.50709700
H	-1.88186400	-1.32220900	-2.11858200	H	2.67536500	2.73372500	1.83043200
H	-3.31668900	-0.80230700	-3.01639300	H	3.44703200	2.31666600	3.36376000
H	-2.70235100	-2.44691700	-3.21338200	C	5.48922300	2.59036500	1.65735600
H	-2.01508500	-3.06152900	-0.25683600	H	6.44792700	2.30721800	1.22021000
H	-2.72689400	-4.07024000	-1.50667200	H	5.68329700	2.89929800	2.69342000
H	-3.54747100	-3.91152800	0.03996500	H	5.11881600	3.46998300	1.12774400
H	-5.60998000	-2.10798600	-2.53399800	C	5.03242800	0.31240600	2.58302500
H	-5.68032800	-3.22244600	-1.15573200	H	4.39504100	-0.57725300	2.58654100
H	-4.72871200	-3.62641500	-2.58174900	H	5.07672700	0.69041000	3.61267700
H	-6.04698000	-0.01764800	2.30590500	H	6.04697800	0.01714700	2.30582200
H	-4.39507400	0.57671800	2.58687400	C	2.96292800	-4.30862000	-1.22811600
H	-5.07683800	-0.69112800	3.61273000	C	2.61941800	-2.95271500	-1.17290900
H	-6.44782000	-2.30761700	1.22007100	C	2.59059600	-2.27526300	0.05384100
H	-5.68311600	-2.89992800	2.69314900	C	2.87417000	-2.98785400	1.22686600
H	-5.11864800	-3.47029200	1.12735500	C	3.21600400	-4.34307200	1.16977400
H	-2.67521100	-2.73400700	1.83025600	C	3.27115000	-5.00657200	-0.05840400
H	-3.44690700	-2.31717800	3.36362600	H	2.98448200	-4.81791800	-2.18931700
H	-2.45158700	-1.12480300	2.50710900	H	2.36365900	-2.43227700	-2.09248900
H	-4.99292300	2.39000100	-0.27511300	H	2.82412300	-2.49278200	2.19335800
				H	3.43717900	-4.87978100	2.08989600

H	3.54058300	-6.05870300	-0.10200300
C	-3.27129000	5.00658200	-0.05781800
C	-3.21595000	4.34301200	1.17031300
C	-2.87408200	2.98779400	1.22727300
C	-2.59065900	2.27528300	0.05416300
C	-2.61966900	2.95280800	-1.17254000
C	-2.96322300	4.30870500	-1.22761700
H	-3.54075400	6.05870800	-0.10131500
H	-3.43700400	4.87966000	2.09049800
H	-2.82389200	2.49266200	2.19372800
H	-2.36402500	2.43243100	-2.09218600
H	-2.98492600	4.81805900	-2.18878500

**$\alpha$ -10<sub>tBu</sub> [( $\mu$ -I)<sub>2</sub>Pd<sub>2</sub>(P'<sup>t</sup>Bu<sub>3</sub>)<sub>2</sub>(Ph)<sub>2</sub>]**

Pd	-2.11002200	-0.41788600	-0.12739900
Pd	2.11001600	0.41781300	-0.12750100
I	0.25376000	-1.78621800	-0.49055400
I	-0.25374300	1.78597200	-0.49141200
P	-4.31357800	0.69080300	0.16124800
P	4.31361100	-0.69070900	0.16141000
C	-4.08001700	2.19607500	1.41367600
C	-4.85753600	1.39490000	-1.57777600
C	-5.83243800	-0.35226100	0.86617900
C	-3.15669700	1.69115400	2.54903000
C	-3.36455700	3.39237500	0.74897900
C	-5.37010500	2.77796300	2.03514600
C	-5.41082500	0.24565100	-2.45011300
C	-5.91576700	2.51924800	-1.53991100
C	-3.60564300	1.92633400	-2.30964600
C	-6.00967700	-1.72403200	0.16751000
C	-7.19646500	0.36801400	0.73667600
C	-5.56801700	-0.68616600	2.35236400
H	-2.17932200	1.38941400	2.16258600
H	-3.57812400	0.85019200	3.10311300
H	-2.99630200	2.51088700	3.26232100
H	-2.42706500	3.11859600	0.27040100
H	-3.11675700	4.11401100	1.53847800
H	-3.99329900	3.91478000	0.02527800
H	-5.91881200	2.07387100	2.66101100
H	-6.05266400	3.18023700	1.28124700
H	-5.07823200	3.61569600	2.68240000
H	-6.40464600	-0.08232800	-2.13761400
H	-4.74303500	-0.62122700	-2.46643900
H	-5.50127500	0.61096700	-3.48136300
H	-6.85188700	2.21217900	-1.07159900
H	-6.14881200	2.80630600	-2.57431700
H	-5.55997000	3.41878100	-1.03409600
H	-3.12919300	2.76511500	-1.80167000
H	-3.91078500	2.27488800	-3.30559500
H	-2.85132300	1.14582900	-2.44204000
H	-5.24292900	-2.43427300	0.46081600
H	-6.02890800	-1.67445800	-0.91910200
H	-6.97747200	-2.12910100	0.49328100
H	-7.20746800	1.39193000	1.10456200
H	-7.93372900	-0.19782300	1.32171500
H	-7.55153000	0.37046200	-0.29749000
H	-4.60143600	-1.17907200	2.48550000

H	-6.34087800	-1.39126600	2.68558300
H	-5.61645000	0.17908700	3.01455300
C	5.83242600	0.35256600	0.86612600
C	6.00948000	1.72427100	0.16727300
H	5.24289700	2.43458000	0.46085600
H	6.02822400	1.67462200	-0.91934200
H	6.97743900	2.12930300	0.49259900
C	5.56811000	0.68664000	2.35229100
H	4.60151500	1.17950900	2.48545100
H	6.34095900	1.39183100	2.68534900
H	5.61665200	-0.17852300	3.01458800
C	7.19649200	-0.36763600	0.73660900
H	7.55148400	-0.37019200	-0.29758100
H	7.20758100	-1.39150800	1.10462100
H	7.93376300	0.19831800	1.32152600
C	4.08018000	-2.19581300	1.41406100
C	3.36477000	-3.39225300	0.74956200
H	3.99351700	-3.91473500	0.02592200
H	2.42725000	-3.11859500	0.27096900
H	3.11702900	-4.11378400	1.53917600
C	5.37033100	-2.77752800	2.03556300
H	6.05280600	-3.18000600	1.28169600
H	5.07852600	-3.61508100	2.68308100
H	5.91910900	-2.07326300	2.66116600
C	3.15686200	-1.69078300	2.54937000
H	3.57830400	-0.84979500	3.10340100
H	2.99643200	-2.51046100	3.26271700
H	2.17950000	-1.38904300	2.16289100
C	4.85757500	-1.39504900	-1.57751100
C	3.60568200	-1.92662700	-2.30927700
H	2.85130400	-1.14618100	-2.44169800
H	3.12931600	-2.76539700	-1.80120400
H	3.91079700	-2.27524300	-3.30521300
C	5.91583600	-2.51936400	-1.53947500
H	6.85193400	-2.21221100	-1.07117300
H	6.14892000	-2.80654700	-2.57383800
H	5.56004800	-3.41884200	-1.03355700
C	5.41082000	-0.24592200	-2.45003700
H	4.74297300	0.62090900	-2.46653300
H	5.50131300	-0.61141800	-3.48121900
H	6.40461300	0.08217800	-2.13757500
C	3.24033400	4.28160900	1.34260300
C	2.85671700	2.93804200	1.25794500
C	2.84166100	2.27845100	0.02103500
C	3.18258100	2.99729400	-1.13281800
C	3.56338800	4.34086500	-1.04662400
C	3.60178200	4.98627600	0.19193700
H	3.24808200	4.77700500	2.31119800
H	2.55301800	2.41515800	2.16132600
H	3.14257000	2.51896200	-2.10807300
H	3.82475800	4.88306700	-1.95281400
H	3.89739100	6.03009100	0.25780300
C	-3.60205200	-4.98624200	0.19232500
C	-3.56354300	-4.34091700	-1.04627800
C	-3.18265200	-2.99737300	-1.13253900
C	-2.84176800	-2.27847100	0.02128800
C	-2.85694800	-2.93797600	1.25824300

C	-3.24064400	-4.28151600	1.34296700	H	-5.36020200	1.45266800	-3.11103200
H	-3.89772300	-6.03003600	0.25824300	H	-6.47926500	0.71172600	-1.97502700
H	-3.82488300	-4.88316600	-1.95244700	C	-4.02476300	4.43413500	-0.50567300
H	-3.14255700	-2.51910800	-2.10782200	H	-4.87904800	5.12230400	-0.45206000
H	-2.55328300	-2.41504700	2.16161100	H	-3.46823000	4.54615500	0.43595500
H	-3.24848600	-4.77684500	2.31159500	C	-3.95525700	-3.14943700	0.81676200
<i>s</i> - <b>10</b> <sub>SP</sub> [(μ-Br) <sub>2</sub> Pd <sub>2</sub> (SPhos) <sub>2</sub> (Ph) <sub>2</sub> ]				H	-3.96744500	-2.50367400	1.68920400
Pd	-1.92634300	-1.22721500	-0.22732900	C	-3.55028500	-0.61218400	-3.34479400
Pd	1.92743400	-1.22733100	0.22560900	H	-3.13834600	0.33955300	-3.69943500
Br	0.00233100	0.59588300	-0.01452100	H	-2.70705500	-1.20024900	-2.96845400
Br	0.00031400	-2.91865100	0.00150300	C	-2.48754400	2.35968900	-1.94203900
P	-3.76108200	0.16986900	-0.59406000	H	-1.64743400	1.66823000	-2.04611800
P	3.76015700	0.17148800	0.59555300	H	-3.10325700	2.27701100	-2.84751500
C	-1.77355900	2.67957100	3.92717300	C	-4.72765400	-5.16464400	-0.29429700
H	-0.96960300	3.22141000	4.41826500	H	-5.32105500	-6.07559700	-0.29105800
C	-1.63318500	1.31585800	3.69400100	C	-4.71864100	-4.32338800	0.81938300
H	-0.73334400	0.80275800	4.00747000	H	-5.30967100	-4.57429200	1.69784300
O	-2.65245300	-0.72905200	2.86403100	C	-3.95728000	-4.82872600	-1.40993400
C	-3.34372700	2.00749800	-0.70535600	H	-3.94049700	-5.48247400	-2.27957200
H	-2.70992500	2.15528100	0.17867400	C	-3.11008600	4.81053400	-1.68044800
C	-5.09932700	0.02931800	0.70541100	H	-2.71237300	5.82482700	-1.54434100
C	-4.57575700	-0.36198200	-2.21253700	H	-3.70325100	4.82992700	-2.60734000
H	-4.96106600	-1.35619900	-1.95170500	C	-4.22399400	-1.33874300	-4.52171500
C	-7.29761100	-0.90567600	1.27842200	H	-3.49284800	-1.49750400	-5.32524100
H	-8.17225800	-1.47161100	0.96971700	H	-4.54580300	-2.33571100	-4.18805700
C	-2.66976600	0.61724400	3.05650400	C	-5.43672500	-0.55985200	-5.05508400
C	-3.96300000	2.65468800	2.92764600	H	-5.08990300	0.37921400	-5.51189800
C	-3.83000000	1.28496000	2.61185000	H	-5.93520700	-1.12799600	-5.85082000
C	-2.93312200	3.36120200	3.56091400	C	-6.43161700	-0.23279600	-3.93173800
H	-3.03098800	4.41780400	3.77717300	H	-6.88876800	-1.16422000	-3.56600800
C	-6.26126600	-0.69319000	0.37253300	H	-7.25172900	0.38663100	-4.31732200
H	-6.36868900	-1.12360700	-0.61337900	C	1.78131000	2.67562600	-3.93588000
C	-3.18108700	-2.80183200	-0.29973600	H	0.97867100	3.21578400	-4.43097800
O	-5.16037900	3.22695100	2.58893100	C	1.64251900	1.31170700	-3.70326600
C	-7.19548600	-0.39824700	2.56983400	H	0.74510600	0.79686700	-4.02087400
H	-7.99059500	-0.55276600	3.29429200	O	2.66137000	-0.73106500	-2.86756600
C	-1.53498200	-1.47663400	3.34185600	C	3.33899800	2.00824200	0.70592500
H	-0.61211000	-1.17282700	2.83815100	H	2.71105600	2.15559200	-0.18236200
H	-1.74805400	-2.51514700	3.08891600	C	5.10183500	0.03332600	-0.70054900
H	-1.43195800	-1.36923200	4.42958200	C	4.57163900	-0.35992600	2.21590500
C	-5.42037100	4.55725900	3.00741200	H	4.96017800	-1.35284400	1.95487600
H	-5.33371600	4.65842500	4.09696500	C	7.30354400	-0.89718700	-1.26781700
H	-6.44758100	4.76791800	2.70368300	H	8.17892200	-1.46060100	-0.95657500
H	-4.74732300	5.27571000	2.52267900	C	2.67729400	0.61510500	-3.06054200
C	-1.96315700	3.80195400	-1.83651100	C	3.96606000	2.65523400	-2.92596300
H	-1.36262900	4.04048600	-2.72410200	C	3.83438500	1.28515400	-2.61113000
H	-1.28526900	3.87039100	-0.97410200	C	2.93768200	3.35966500	-3.56402600
C	-4.98955700	0.52742500	2.03280900	H	3.03440800	4.41645900	-3.77987000
C	-4.53613500	2.98511500	-0.61056700	C	6.26485100	-0.68595600	-0.36432300
H	-5.16869500	2.75803900	0.24929200	H	6.37137900	-1.11476900	0.62239900
H	-5.16220300	2.89346800	-1.50630400	C	3.18391000	-2.80053700	0.29985400
C	-3.18817000	-3.65935800	-1.41221200	O	5.16071400	3.22986700	-2.58162100
H	-2.57240600	-3.43792900	-2.27951800	C	7.20280700	-0.39172200	-2.56010400
C	-6.05006000	0.30476600	2.92804100	H	7.99969600	-0.54538000	-3.28279100
H	-5.95505000	0.69838800	3.93570700	C	1.54478000	-1.48012000	-3.34501400
C	-5.74562200	0.48813600	-2.75655800	H	0.62103000	-1.17477600	-2.84384100
				H	1.75756400	-2.51781200	-3.08855300

H	1.44363500	-1.37604600	-4.43319300	Cl	0.000000	0.000000	-0.395262
C	5.41951500	4.56105100	-2.99797900	O	2.434028	2.885267	0.850758
H	5.33856200	4.66253600	-4.08795800	C	-1.087350	3.045717	-1.937578
H	6.44448000	4.77423900	-2.68851100	H	-0.106343	2.566051	-2.045797
H	4.74192400	5.27750900	-2.51663300	C	0.000000	5.028379	0.026046
C	1.94644500	3.79820700	1.82922500	C	-2.824970	4.109900	0.359832
H	1.33902800	4.03436700	2.71274800	H	-2.651144	4.546606	1.351959
H	1.27457200	3.86602300	0.96207900	C	0.243024	7.299425	0.928624
C	4.99373400	0.52986500	-2.02865700	H	-0.195300	8.132681	1.470969
C	4.52981100	2.98853700	0.61999500	C	2.661976	2.926314	-0.488641
H	5.16793800	2.76374100	-0.23638700	C	2.415816	4.182147	-2.539323
H	5.15052000	2.89714700	1.51944400	C	2.086677	4.015572	-1.176228
C	3.18982900	-3.65950600	1.41124600	C	3.204900	3.246598	-3.219727
H	2.57180300	-3.44012300	2.27745200	H	3.436149	3.369515	-4.270535
C	6.05658300	0.30840000	-2.92143300	C	-0.506601	6.144628	0.718833
H	5.96279500	0.70069400	-3.92973800	H	-1.507997	6.121425	1.126040
C	5.73764200	0.49250600	2.76468500	C	-0.783420	3.031795	2.867909
H	5.34847500	1.45525300	3.11995800	O	1.925892	5.315610	-3.131378
H	6.47279300	0.71976100	1.98566500	C	1.547028	7.367956	0.448263
C	4.01590100	4.43659300	0.51360800	H	2.151467	8.257945	0.601499
H	4.86898100	5.12674100	0.46666300	C	3.069266	1.867963	1.624241
H	3.46555000	4.54859700	-0.43164500	H	2.733783	0.871238	1.321401
C	3.96112100	-3.14552300	-0.81533000	H	2.758758	2.045608	2.653575
H	3.97428700	-2.49869600	-1.68696500	H	4.161346	1.944901	1.541916
C	3.54368300	-0.61420600	3.34500900	C	2.328060	5.619733	-4.457307
H	3.12867300	0.33608100	3.69995400	H	3.420196	5.696037	-4.537681
H	2.70281900	-1.20366800	2.96556900	H	1.878793	6.587539	-4.688086
C	2.47341900	2.35712300	1.93688700	H	1.963624	4.873668	-5.174792
H	1.63427900	1.66350900	2.03421700	C	-1.921230	1.456592	-3.722246
H	3.08299600	2.27492200	2.84654900	H	-2.687983	0.710078	-3.966367
C	4.73394500	-5.16112500	0.29481900	H	-0.955846	0.931954	-3.751443
H	5.32870600	-6.07119100	0.29171900	C	1.339772	5.094519	-0.445908
C	4.72620700	-4.31838700	-0.81774100	C	-1.159682	4.214693	-2.945529
H	5.31964600	-4.56718400	-1.69517100	H	-0.421974	4.985271	-2.714043
C	3.96059700	-4.82778000	1.40916600	H	-2.147929	4.687065	-2.895974
H	3.94275500	-5.48271000	2.27789600	C	-1.904062	2.877028	3.699807
C	3.09220200	4.80945300	1.68252400	H	-2.666995	2.141719	3.458836
H	2.69331500	5.82307900	1.54491700	C	2.075052	6.272186	-0.226396
H	3.67882300	4.82892700	2.61357700	H	3.094350	6.311675	-0.598930
C	4.21588700	-1.34104900	4.52261000	C	-3.498861	5.173577	-0.532704
H	3.48291200	-1.50287100	5.32386500	H	-3.764291	4.724015	-1.497916
H	4.54094900	-2.33669900	4.18819400	H	-2.818390	6.003388	-0.749374
C	5.42528900	-0.56017500	5.06059100	C	-0.928768	3.693351	-4.376260
H	5.07497700	0.37724700	5.51812000	H	-0.992919	4.528292	-5.086851
H	5.92301100	-1.12850600	5.85666700	H	0.093138	3.294070	-4.447106
C	6.42236300	-0.22865800	3.94047800	C	0.200078	3.960994	3.236749
H	6.88291300	-1.15827100	3.57441300	H	1.073947	4.102555	2.608333
H	7.23983900	0.39222700	4.32930600	C	-3.806593	2.938817	0.604074
<i>s</i> -10 <sub>SP</sub> [(μ-Cl) <sub>2</sub> Pd <sub>2</sub> (SPhos) <sub>2</sub> (Ph) <sub>2</sub> ]				H	-4.066161	2.458316	-0.346290
C	3.707815	2.151626	-2.518984	H	-3.330764	2.174329	1.226347
H	4.322370	1.422590	-3.040401	C	-2.154324	1.987360	-2.297256
C	3.454667	1.984079	-1.162033	H	-2.138170	1.155334	-1.588917
H	3.873447	1.137835	-0.633437	H	-3.151298	2.446261	-2.255764
P	-1.094202	3.519109	-0.111154	C	-1.056921	4.562148	5.224503
Pd	-0.496445	1.792092	1.315271	H	-1.160969	5.150295	6.132941
Cl	0.000000	0.000000	2.920259	C	0.065414	4.715235	4.408779
				H	0.842769	5.427303	4.678327



C	-2.041169	3.638462	4.865711
H	-2.915084	3.497689	5.498489
C	-1.927722	2.590806	-4.756847
H	-1.700134	2.199052	-5.757007
H	-2.938313	3.023188	-4.813531
C	-5.092303	3.452786	1.275472
H	-5.788992	2.618196	1.428179
H	-4.842722	3.840742	2.273488
C	-5.763919	4.559018	0.447534
H	-6.128620	4.130529	-0.498154
H	-6.644595	4.948304	0.974029
C	-4.783648	5.699374	0.134612
H	-4.519790	6.220497	1.066861
H	-5.260224	6.444349	-0.515602
C	-3.707815	-2.151626	-2.518984
H	-4.322370	-1.422590	-3.040401
C	-3.454667	-1.984079	-1.162033
H	-3.873447	-1.137835	-0.633437
P	1.094202	-3.519109	-0.111154
Pd	0.496445	-1.792092	1.315271
O	-2.434028	-2.885267	0.850758
C	1.087350	-3.045717	-1.937578
H	0.106343	-2.566051	-2.045797
C	0.000000	-5.028379	0.026046
C	2.824970	-4.109900	0.359832
H	2.651144	-4.546606	1.351959
C	-0.243024	-7.299425	0.928624
H	0.195300	-8.132681	1.470969
C	-2.661976	-2.926314	-0.488641
C	-2.415816	-4.182147	-2.539323
C	-2.086677	-4.015572	-1.176228
C	-3.204900	-3.246598	-3.219727
H	-3.436149	-3.369515	-4.270535
C	0.506601	-6.144628	0.718833
H	1.507997	-6.121425	1.126040
C	0.783420	-3.031795	2.867909
O	-1.925892	-5.315610	-3.131378
C	-1.547028	-7.367956	0.448263
H	-2.151467	-8.257945	0.601499
C	-3.069266	-1.867963	1.624241
H	-2.733783	-0.871238	1.321401
H	-2.758758	-2.045608	2.653575
H	-4.161346	-1.944901	1.541916
C	-2.328060	-5.619733	-4.457307
H	-3.420196	-5.696037	-4.537681
H	-1.878793	-6.587539	-4.688086
H	-1.963624	-4.873668	-5.174792
C	1.921230	-1.456592	-3.722246
H	2.687983	-0.710078	-3.966367
H	0.955846	-0.931954	-3.751443
C	-1.339772	-5.094519	-0.445908
C	1.159682	-4.214693	-2.945529
H	0.421974	-4.985271	-2.714043
H	2.147929	-4.687065	-2.895974
C	1.904062	-2.877028	3.699807
H	2.666995	-2.141719	3.458836
C	-2.075052	-6.272186	-0.226396

H	-3.094350	-6.311675	-0.598930
C	3.498861	-5.173577	-0.532704
H	3.764291	-4.724015	-1.497916
H	2.818390	-6.003388	-0.749374
C	0.928768	-3.693351	-4.376260
H	0.992919	-4.528292	-5.086851
H	-0.093138	-3.294070	-4.447106
C	-0.200078	-3.960994	3.236749
H	-1.073947	-4.102555	2.608333
C	3.806593	-2.938817	0.604074
H	4.066161	-2.458316	-0.346290
H	3.330764	-2.174329	1.226347
C	2.154324	-1.987360	-2.297256
H	2.138170	-1.155334	-1.588917
H	3.151298	-2.446261	-2.255764
C	1.056921	-4.562148	5.224503
H	1.160969	-5.150295	6.132941
C	-0.065414	-4.715235	4.408779
H	-0.842769	-5.427303	4.678327
C	2.041169	-3.638462	4.865711
H	2.915084	-3.497689	5.498489
C	1.927722	-2.590806	-4.756847
H	1.700134	-2.199052	-5.757007
H	2.938313	-3.023188	-4.813531
C	5.092303	-3.452786	1.275472
H	5.788992	-2.618196	1.428179
H	4.842722	-3.840742	2.273488
C	5.763919	-4.559018	0.447534
H	6.128620	-4.130529	-0.498154
H	6.644595	-4.948304	0.974029
C	4.783648	-5.699374	0.134612
H	4.519790	-6.220497	1.066861
H	5.260224	-6.444349	-0.515602

**11<sub>Cy</sub> [Pd(PCy<sub>3</sub>)<sub>3</sub>] (conformer F)**

Pd	0.03885100	-0.00534600	0.08012000
P	1.81376200	-1.65380100	-0.17078200
P	0.62184500	2.35151500	0.21084300
P	-2.33264800	-0.68605100	0.07295200
C	1.80710800	-2.62014800	-1.81020600
C	1.71347900	-3.06360800	1.10514900
C	3.64381700	-1.05694400	-0.16481400
C	4.74018400	-1.92548100	-0.82623400
C	6.09209700	-1.18558100	-0.86892200
C	6.54466000	-0.72491900	0.52309800
C	5.45568600	0.11591100	1.20279900
C	4.11350600	-0.63463500	1.24331900
C	2.79451500	-4.16454000	1.09859600
C	2.43668400	-5.30593200	2.06934400
C	2.21259600	-4.78301700	3.49553100
C	1.15065600	-3.67331800	3.51834400
C	1.49253000	-2.53461400	2.54131400
C	1.94827800	-1.65519300	-3.00842200
C	1.99570600	-2.40584300	-4.35058300
C	0.76841300	-3.30817400	-4.53777000
C	0.59823900	-4.25918000	-3.34505300
C	0.55555400	-3.49454300	-2.00968800

C	0.95195600	3.02149700	1.96311400	H	0.69466500	-1.78152600	2.53664200
C	-3.35749700	-0.07656800	1.56554300	H	2.39716600	-2.02719600	2.89795600
C	-0.68236000	3.61287700	-0.40638400	H	1.09248400	-0.96579100	-3.00356500
C	2.26260500	2.80299100	-0.65573000	H	2.84521900	-1.03325200	-2.90843100
C	-2.66256100	-2.56585400	-0.00655500	H	2.90732600	-3.02111200	-4.39003100
C	-3.16230600	0.05885800	-1.47238000	H	2.06993500	-1.68646100	-5.17679700
C	2.11794900	2.29364000	2.66151700	H	-0.13030700	-2.68018700	-4.62978300
C	-0.57861900	5.10090300	-0.00139100	H	0.84994500	-3.87726700	-5.47298600
C	-0.92986200	3.50787500	-1.92623300	H	1.43572200	-4.97259200	-3.32779200
C	2.75033200	4.26639600	-0.63075200	H	-0.31651700	-4.85581200	-3.46011400
C	2.34526700	2.25054500	-2.09534900	H	0.44324600	-4.21181000	-1.18827300
C	-1.84302200	5.87754300	-0.41670400	H	-0.33055200	-2.84837000	-1.98938000
C	-2.12204900	5.75237800	-1.92057300	H	1.22675500	4.08200900	1.87603600
C	-2.19248000	4.27933800	-2.34885200	H	-2.69598900	-0.34379700	2.40477800
C	3.76707300	2.37800400	-2.67071300	H	-1.58928200	3.22152400	0.07520400
C	4.27799100	3.82527900	-2.61348600	H	2.97868400	2.21283300	-0.06382800
C	4.18017200	4.39025500	-1.18959100	H	-1.90886700	-2.88021700	-0.73988100
C	2.37335900	2.83481600	4.07953800	H	-2.82594600	1.10363000	-1.40578900
C	1.11228100	2.76128100	4.95018400	H	3.03892200	2.38071200	2.07416800
C	-0.06221100	3.47359100	4.26754900	H	1.87813500	1.22335100	2.71687000
C	-0.30828800	2.93031400	2.84911700	H	-0.43589000	5.20887800	1.07863400
C	-3.44989500	1.46339500	1.55165700	H	0.29244800	5.56462100	-0.47865400
C	-4.74684000	-0.67923800	1.88034500	H	-1.01047700	2.45545700	-2.22480400
C	-4.01008900	-3.13364200	-0.50627100	H	-0.07167100	3.92591600	-2.46887000
C	-2.25600200	-3.21860900	1.33455200	H	2.08382700	4.88594200	-1.24459300
C	-4.69977000	0.09995700	-1.62522100	H	2.71786100	4.67900000	0.38404700
C	-2.50340500	-0.52962100	-2.74183700	H	1.65603700	2.80082100	-2.74782100
C	-4.01842700	2.02360200	2.86473300	H	2.01738700	1.20584200	-2.10721300
C	-5.39037200	1.41613700	3.18721500	H	-2.70568700	5.48907700	0.14546900
C	-5.31847800	-0.11638600	3.19658000	H	-1.73915100	6.93387200	-0.13501700
C	-2.23615600	-4.75383300	1.24882000	H	-1.31659100	6.25198900	-2.47965200
C	-3.58341400	-5.30592200	0.76507000	H	-3.05253400	6.27287300	-2.18213000
C	-3.98084700	-4.67365500	-0.57552500	H	-2.33046700	4.20464100	-3.43580700
C	-2.93490500	0.21446300	-4.01654300	H	-3.07464800	3.80972900	-1.88826600
C	-4.46267100	0.25386600	-4.15917800	H	3.78568100	2.00829100	-3.70461700
C	-5.11405900	0.85248000	-2.90508700	H	4.45054200	1.73447200	-2.09691600
H	2.67663800	-3.29096900	-1.80859900	H	5.31214500	3.88122200	-2.97751900
H	0.76820900	-3.54337400	0.81322000	H	3.67406500	4.44870200	-3.28983300
H	3.56934500	-0.13621500	-0.76124000	H	4.87411800	3.84459000	-0.53264600
H	4.86453900	-2.86392100	-0.27216900	H	4.49779300	5.44133600	-1.17339500
H	4.46468100	-2.20199900	-1.84854500	H	3.19394800	2.27430000	4.54663600
H	5.99908200	-0.30840700	-1.52680200	H	2.70800600	3.88115000	4.01417500
H	6.85348500	-1.83383800	-1.32288400	H	1.30298500	3.19618800	5.93992800
H	6.75852400	-1.60765700	1.14431600	H	0.84832400	1.70594300	5.11579500
H	7.48224400	-0.15821200	0.45265100	H	-0.97577900	3.36778400	4.86740200
H	5.32903100	1.06078300	0.65339200	H	0.15090400	4.55182900	4.21150500
H	5.76233300	0.38651500	2.22206500	H	-0.61850400	1.87809800	2.90945800
H	3.35295900	-0.01663000	1.72863800	H	-1.14341000	3.47618300	2.39670300
H	4.24145800	-1.52824700	1.86878200	H	-2.45878400	1.88097900	1.36220900
H	3.76019800	-3.74014300	1.40181000	H	-4.09518100	1.78786700	0.72351700
H	2.93327200	-4.57080300	0.08919700	H	-4.69317700	-1.76790000	1.96207100
H	1.52191400	-5.80604100	1.71788100	H	-5.44721500	-0.46186000	1.06482600
H	3.23006600	-6.06510700	2.06112200	H	-4.83339400	-2.82046600	0.14518300
H	3.16118200	-4.38457200	3.88593100	H	-4.23695300	-2.74527500	-1.50332500
H	1.92142200	-5.60503700	4.16238000	H	-2.96001800	-2.92639500	2.12501500
H	0.17566000	-4.10390200	3.24772000	H	-1.27345600	-2.84366900	1.64018900
H	1.04225400	-3.27164100	4.53473500	H	-5.11326500	-0.91365200	-1.66170800

H	-5.15956100	0.59170900	-0.76228600	C	1.27570600	3.86199800	-0.06687700
H	-2.77706600	-1.58984900	-2.84392900	C	2.04571600	4.96859900	-0.42009900
H	-1.41251500	-0.49407100	-2.63458900	H	2.15678500	6.76032500	-1.62059300
H	-3.32073800	1.79987600	3.68536000	H	-0.10559800	6.43864800	-2.60518500
H	-4.08938300	3.11789600	2.80405300	H	-1.47929600	4.49684700	-1.95758200
H	-6.11772800	1.74047100	2.42776700	H	1.67964500	3.13127700	0.62831300
H	-5.75926900	1.78782400	4.15203800	H	3.03717600	5.09156500	0.00710200
H	-6.31308700	-0.54474600	3.37854300	C	-2.33697400	3.33912800	4.24136100
H	-4.68189200	-0.44252000	4.03290800	C	-2.04567100	4.34862400	3.32110300
H	-1.97769400	-5.17897200	2.22781100	C	-1.62947000	4.02376700	2.02826400
H	-1.44566500	-5.07005400	0.55174300	C	-1.50044000	2.68202100	1.63275800
H	-3.54043900	-6.39903600	0.67386700	C	-1.78373100	1.67685500	2.57262800
H	-4.35682700	-5.08431000	1.51591000	C	-2.20372900	2.00149100	3.86416000
H	-3.25959800	-4.98507300	-1.34621900	H	-2.65829500	3.59425500	5.24793900
H	-4.96161600	-5.04644800	-0.89951900	H	-2.13941600	5.39267400	3.60942900
H	-2.54910000	1.24398000	-3.98126400	H	-1.39674200	4.81875800	1.32601000
H	-2.47991000	-0.25975100	-4.89642600	H	-1.65958000	0.63514700	2.28773000
H	-4.83989500	-0.76873700	-4.31142200	H	-2.41723600	1.20794600	4.57572900
H	-4.74970300	0.82816600	-5.04965400	C	4.06328500	0.25372300	4.25752200
H	-6.20794700	0.84347000	-3.00073100	C	4.77033100	-0.52495100	3.33863900
H	-4.81759900	1.90836100	-2.81516100	C	4.28764700	-0.69235600	2.03878200
<b>11<sub>H</sub> [Pd(PH<sub>3</sub>)<sub>3</sub>]</b>				C	3.08852200	-0.08166500	1.63551000
Pd	0.00535700	-0.00488600	-0.00130500	C	2.38117000	0.68875500	2.57376800
P	-1.62871200	-1.67398500	-0.00615700	C	2.86636400	0.86024100	3.87172600
P	-0.65627700	2.23404600	0.00031900	H	4.43968800	0.38079300	5.26932300
P	2.27801200	-0.55287100	0.00477800	H	5.69971000	-1.00609500	3.63309700
H	-1.41604300	-2.98804700	-0.50924100	H	4.84415200	-1.30721000	1.33772800
H	-2.12988400	-2.10736100	1.25096000	H	1.43760400	1.14312700	2.28297100
H	-2.91185600	-1.53744600	-0.60620800	H	2.30254300	1.46009000	4.58161200
H	0.21967100	3.35659500	0.00071300	C	4.63772100	2.90153200	-2.67040300
H	-1.48056200	2.73746700	-1.04280500	C	5.16854800	2.54796000	-1.42878300
H	-1.47178200	2.73035600	1.05351000	C	4.51844100	1.60569500	-0.62699900
H	3.04370000	-0.28096700	-1.16130300	C	3.32117100	1.01114700	-1.05244200
H	3.19304000	0.06595800	0.90034200	C	2.78918100	1.38814100	-2.29662500
H	2.81194200	-1.85962500	0.18995800	C	3.44546500	2.31662300	-3.10405700
<b>11<sub>Ph</sub> [Pd(PPh<sub>3</sub>)<sub>3</sub>]</b>				H	5.14503100	3.63383900	-3.29310800
Pd	0.01692600	-0.00151600	-0.09855200	H	6.09367800	3.00206500	-1.08198200
P	-0.96070500	2.16479200	-0.06964600	H	4.94696000	1.33558800	0.33329100
P	2.37587100	-0.25247100	-0.07364200	H	1.84276100	0.96077100	-2.61993500
P	-1.40055800	-1.90688900	-0.06176000	H	3.01732400	2.59633800	-4.06306900
C	-4.78017200	2.50516500	-2.73520100	C	4.32513500	-4.29105000	-1.40820800
C	-4.75309700	3.17560000	-1.51112900	C	4.86323600	-3.09282200	-1.87778700
C	-3.62554700	3.09724700	-0.68939700	C	4.30488100	-1.86992800	-1.49373200
C	-2.51095500	2.33854600	-1.07700800	C	3.19267500	-1.82801700	-0.63923200
C	-2.55708100	1.65750900	-2.30447500	C	2.65349200	-3.04292100	-0.18451600
C	-3.67644100	1.74665900	-3.13173000	C	3.21770700	-4.26201400	-0.55665200
H	-5.65822600	2.56698000	-3.37286100	H	4.76032300	-5.24104800	-1.70773100
H	-5.60984500	3.76489200	-1.19324900	H	5.72330000	-3.10405800	-2.54295600
H	-3.61856400	3.62799000	0.25764600	H	4.74204700	-0.94752100	-1.86167900
H	-1.71239200	1.03921900	-2.59913400	H	1.77779700	-3.03311500	0.45780500
H	-3.69335100	1.21054800	-4.07703300	H	2.77997800	-5.18876800	-0.19590400
C	1.55352500	5.90187500	-1.33646100	C	0.06071800	-5.35593800	-2.85342100
C	0.28622000	5.71985700	-1.88953700	C	-0.48078900	-5.68159900	-1.60866600
C	-0.49158900	4.61662100	-1.52463800	C	-0.92994000	-4.67455900	-0.75010900
C	-0.00818300	3.67290800	-0.60582500	C	-0.83351100	-3.32465500	-1.11999800
				C	-0.27255600	-3.01022700	-2.36905300
				C	0.16115000	-4.01550200	-3.23312600

H	0.40870300	-6.14043500	-3.52039700	C	-4.43789700	0.09717800	2.27814600
H	-0.55899900	-6.72228000	-1.30342500	H	-6.31390000	0.89632800	2.96722700
H	-1.35320700	-4.94527100	0.21229300	H	-4.91182400	-0.73973600	1.77668300
H	-0.16236400	-1.96650900	-2.65394900	C	-2.06754000	2.82823800	-1.44706600
H	0.59169000	-3.75139700	-4.19553300	C	0.23447900	2.25441700	-3.03592600
C	-5.91385300	-1.47470000	-1.22193700	C	0.70013200	2.97184300	2.24619700
C	-5.13927300	-2.44117700	-1.86247000	C	2.97578000	2.24029700	0.68828100
C	-3.79096400	-2.60159300	-1.52773500	C	2.25137900	0.68632700	2.97269100
C	-3.19473400	-1.79064400	-0.55070000	C	2.81635200	-1.45801200	-2.08311900
C	-3.98459500	-0.81252900	0.07806700	C	0.52792800	-3.16068500	-2.03198900
C	-5.33110100	-0.66090600	-0.24643000	C	2.26057500	-3.03293900	0.23569800
H	-6.96186400	-1.35138400	-1.48265400	C	-2.46881900	1.33252200	2.91371000
H	-5.58177300	-3.07929600	-2.62359600	H	-1.39535700	1.47825000	2.88356700
H	-3.20727600	-3.36646500	-2.02915500	C	-1.61383300	-0.70968600	-3.64259200
H	-3.53996300	-0.15939200	0.82380900	H	-0.69928200	-1.15327400	-3.26537400
H	-5.92109000	0.10403100	0.25110800	C	-2.35503100	-1.39564800	-4.60506500
C	-1.66049500	-3.78736100	4.21069500	H	-1.99989900	-2.35640300	-4.96671500
C	-2.70179100	-4.00595000	3.30564700	C	-3.99689500	0.37182400	-4.58900400
C	-2.64810200	-3.45269700	2.02471600	H	-4.92726900	0.80157200	-4.95232300
C	-1.54971700	-2.67248700	1.62608900	C	-3.24567500	1.06424000	-3.63477400
C	-0.51494700	-2.45144900	2.55004300	H	-3.60178400	2.02365400	-3.27558600
C	-0.56669200	-3.00804300	3.82982900	C	4.87514800	-0.72998000	-3.87000900
H	-1.70547400	-4.21645900	5.20839300	H	5.66952100	-0.44977900	-4.55722300
H	-3.56000500	-4.60652700	3.59672000	C	3.64432400	-3.24164100	2.23165300
H	-3.46828500	-3.62344600	1.33389000	H	4.16248700	-2.76411200	3.05836900
H	0.32862200	-1.82883900	2.26329900	C	2.94717000	-2.45466400	1.31490300
H	0.24438700	-2.82319100	4.52950300	H	2.92635700	-1.37977600	1.45134200
<b>12<sub>H</sub> [Pd(PH<sub>3</sub>)<sub>4</sub>]</b>				C	2.28232600	-4.43186500	0.10855100
Pd	0.00014100	0.00109200	-0.00534400	H	1.76685200	-4.91166100	-0.71628700
P	1.17731600	2.01675800	0.44188500	C	2.96812600	-5.22333600	1.03462200
P	-0.80117800	-0.91571800	2.03355200	H	2.96994600	-6.30431800	0.91726700
P	-1.84788200	0.44735100	-1.42701300	C	3.65460500	-4.63191100	2.09653300
P	1.47197700	-1.54991100	-1.03843300	H	4.19080400	-5.24864500	2.81341500
H	1.31812900	2.53288900	1.76132300	C	4.08643700	-2.05110400	-1.99640200
H	2.55428400	2.17544800	0.11755600	H	4.28419400	-2.80438900	-1.24152400
H	0.79011000	3.26604300	-0.12041000	C	5.10750100	-1.68509500	-2.87854400
H	-0.59581300	-0.27322700	3.28737600	H	6.08369800	-2.15616700	-2.79202000
H	-2.18484300	-1.16005400	2.26435600	C	3.61513700	-0.13557500	-3.96944400
H	-0.38823600	-2.19559100	2.50097000	H	3.41900900	0.61900900	-4.72590100
H	-2.17240400	1.76094500	-1.87027500	C	2.60191300	-0.49210700	-3.07927000
H	-1.98195800	-0.13518000	-2.71929600	H	1.63888900	-0.00089900	-3.15327900
H	-3.17938900	0.13544100	-1.03117000	C	1.05605100	-3.65315800	-3.23678700
H	1.72178900	-2.83671700	-0.48287700	H	2.01306700	-3.29350000	-3.59873200
H	1.25952800	-2.03963200	-2.35844300	C	0.36299100	-4.61193400	-3.98135900
H	2.84879600	-1.25781000	-1.25315500	H	0.78973900	-4.97764100	-4.91218800
<b>12<sub>Ph</sub> [Pd(PPh<sub>3</sub>)<sub>4</sub>]</b>				C	-0.71023500	-3.65986200	-1.59681100
Pd	0.00080100	-0.00365000	0.00055100	H	-1.15157500	-3.28032500	-0.68220000
P	-0.95933800	1.39008800	-1.88769900	C	-5.09746500	-3.54447600	-0.86181100
P	-1.89513800	-0.95973800	1.38411800	H	-5.84411400	-4.12662000	-1.39607700
P	1.46667200	1.45798100	1.46308000	C	-3.66235800	-1.60355600	-0.71033300
P	1.38726500	-1.89392300	-0.96127800	H	-3.28906400	-0.68659600	-1.15064900
C	-2.04133400	0.53193900	-3.14585600	C	-2.83597900	5.12981000	-1.66307500
C	-3.15879700	-2.03645400	0.52646100	H	-2.73696300	6.10760900	-2.12832600
C	-3.04088700	0.23851100	2.24584600	C	-1.96430200	4.10105600	-2.03211300
C	-5.23409800	1.02434100	2.95666400	H	-1.20524300	4.29591000	-2.78195200
				C	-3.06848500	2.61939300	-0.48491900
				H	-3.15444800	1.65428200	0.00091700

C	-0.69661300	4.94963900	1.95962600	C	-4.62682800	-2.34244000	-1.39568400
H	-1.32558400	5.55930800	1.31714200	H	-4.99376000	-1.98269000	-2.35280500
C	-0.11566500	3.78947200	1.44711300	C	-3.26050400	2.25149900	3.60332800
H	-0.31103200	3.51299400	0.41739200	H	-2.78815800	3.09060300	4.10604100
C	-0.48614000	5.30840600	3.29316000	C	-4.64902900	2.10180400	3.62463800
H	-0.94312300	6.20800800	3.69772000	H	-5.26988400	2.81962500	4.15479100
C	0.31473000	4.50135600	4.10280500	C	-3.64343300	-3.24436800	1.05449900
H	0.48821800	4.77116300	5.14176100	H	-3.27953700	-3.60495100	2.01046000
C	0.90823200	3.34703600	3.58335500	C	-4.59966700	-3.99374800	0.36260200
H	1.53864600	2.74195500	4.22601400	H	-4.95956600	-4.92686400	0.78933700
C	3.28692500	-0.50449400	5.31199700	C	1.33864700	2.90883800	-2.46722000
H	3.68730300	-0.96330500	6.21253500	H	1.49473200	2.86411200	-1.39573800
C	1.95050000	-0.69968600	4.95609100	C	2.25294400	3.60332600	-3.26010300
H	1.30117100	-1.31880200	5.56864400	H	3.09930200	4.09642100	-2.79051500
C	1.44407700	-0.11628200	3.79444800				
H	0.41190900	-0.29988300	3.51898500				
C	3.59257500	0.87798700	3.34389600				
H	4.24361900	1.49589100	2.73538600				
C	4.10583200	0.28229500	4.49989200				
H	5.14749100	0.44302500	4.76715300				
C	5.30942800	3.27460900	-0.51434700				
H	6.20786200	3.67458600	-0.97761200				
C	4.95025800	1.93924300	-0.71042100				
H	5.55784500	1.29018300	-1.33463700				
C	-0.73323600	-3.84038000	4.89502600				
H	-0.45329700	-4.52187500	5.69441200				
C	-1.69620900	-2.85434700	5.11688500				
H	-2.17343600	-2.76603000	6.08992200				
C	-2.06220100	-1.98014300	4.08939100				
H	-2.82195200	-1.23016100	4.28009100				
C	-0.13068100	-3.94234200	3.63900900				
H	0.62974100	-4.69509000	3.45127000				
C	-0.48676900	-3.05928900	2.61923300				
H	0.00951800	-3.13299500	1.65889900				
C	-0.86304600	-5.10487300	-3.53059200				
H	-1.39838700	-5.85333200	-4.10940400				
C	-1.39681200	-4.62697600	-2.33147200				
H	-2.35512800	-4.98963500	-1.97068800				
C	-1.46028300	-2.06868900	2.82316600				
C	4.50351800	4.09284700	0.27971800				
H	4.77345600	5.13368700	0.44140700				
C	3.35050500	3.57994400	0.88132900				
H	2.74637800	4.22949500	1.50511800				
C	3.79123200	1.43356600	-0.12114900				
H	3.51244100	0.40242300	-0.30585200				
C	2.08879900	3.64235400	-4.64663400				
H	2.80294300	4.17636300	-5.26845300				
C	1.00172800	2.98764900	-5.22854600				
H	0.86297100	3.01192600	-6.30670900				
C	0.07861600	2.30503100	-4.43121700				
H	-0.76591900	1.81460700	-4.90322700				
C	-3.55334200	-0.85746200	-5.08036600				
H	-4.13728700	-1.39218100	-5.82528800				
C	-3.94844900	3.64050800	-0.12575600				
H	-4.70992000	3.44866000	0.62491300				
C	-3.83325200	4.90296800	-0.71288500				
H	-4.51284300	5.70311100	-0.43055200				

SI only:

Table SI2c – Jaguar optimization of PCy<sub>3</sub> ligand in different coordination environments.

PCy<sub>3</sub>

Conformer A

P1	-3.2574170903	2.2783635060	10.1373892104
C4	-0.0063605452	1.3181065668	7.5834871162
C5	-0.9326974843	2.0838555331	8.5444367810
C6	-2.2271303780	1.2960482872	8.8605609559
C7	-2.9472615855	0.9788880307	7.5321259506
C8	-2.0346584024	0.1986987210	6.5666470368
C9	-0.7283213265	0.9521363026	6.2788697023
H10	0.3466231795	0.3986933432	8.0746248076
H11	0.8874918433	1.9188111233	7.3699485749
H12	-0.3887252061	2.3316249509	9.4611738151
H13	-1.2155763422	3.0446186778	8.0903893842
H14	-1.9536470211	0.3313619822	9.3154462097
H15	-3.8590071896	0.3977249834	7.7071365542
H16	-3.2553181600	1.9171913415	7.0483337093
H17	-1.7998830419	-0.7816071247	7.0077977626
H18	-2.5735104089	-0.0024875354	5.6313157122
H19	-0.9581281536	1.8734432136	5.7231812347
H20	-0.0751261943	0.3519498095	5.6322454026
C21	-2.6272911726	1.9529328357	14.3230425898
C22	-3.0385914233	2.5025282929	12.9457938800
C23	-2.6129411095	1.5640465624	11.7905765557
C24	-1.0855020002	1.3505773550	11.8684350646
C25	-0.6621163887	0.7863486651	13.2381367058
C26	-1.1167731852	1.6881859183	14.3943268219
H27	-3.1708528462	1.0159978746	14.5174952700
H28	-2.9291533218	2.6561443558	15.1103225879
H29	-2.5639954002	3.4817454976	12.7872962618
H30	-4.1177018086	2.6837042429	12.9288701356
H31	-3.0837291169	0.5800648214	11.9411418205
H32	-0.7418393340	0.6697997218	11.0824097250
H33	-0.5722770702	2.3095339960	11.7060593752
H34	-1.0992466166	-0.2154965278	13.3643781991
H35	0.4277999772	0.6550928626	13.2622210531
H36	-0.5795235094	2.6465879099	14.3371025278
H37	-0.8497646427	1.2373639616	15.3589372352
C38	-7.1743345810	1.5144850934	8.6920326316
C39	-5.8085037655	2.1824271484	8.9287837481
C40	-4.9652706860	1.4318306771	9.9879421549
C41	-5.7781701590	1.3502451459	11.2983382320
C42	-7.1426233056	0.6700648434	11.0763413045
C43	-7.9701757323	1.3842185517	9.9983895041
H44	-7.0197212318	0.5148997312	8.2584400427
H45	-7.7465259812	2.0889377101	7.9517345007
H46	-5.9624800814	3.2136134305	9.2784004730
H47	-5.2686358830	2.2624493184	7.9801975110
H48	-4.8030360696	0.3980970720	9.6449256085
H49	-5.2285844988	0.7998713277	12.0694258991
H50	-5.9465907237	2.3641589877	11.6895231465
H51	-6.9778999361	-0.3754246107	10.7754929526
H52	-7.6966689799	0.6371073002	12.0237745085
H53	-8.2409987604	2.3882436006	10.3575990017

H54 -8.9130643364 0.8500017961 9.8235681144

Conformer B

P1	-3.0325148996	2.2068339318	10.3318354146
C4	-1.4085398983	2.2424180899	6.4414797387
C5	-2.2381407344	2.6124831118	7.6832002670
C6	-2.1376862307	1.5423070624	8.7966448288
C7	-2.5232456477	0.1584184417	8.2300088362
C8	-1.6823967890	-0.2112554211	6.9918768122
C9	-1.7864723623	0.8578011453	5.8952254082
H10	-0.3410340075	2.2465835902	6.7087185729
H11	-1.5376671768	3.0086614431	5.6659184155
H12	-1.9214159992	3.5861108041	8.0746129728
H13	-3.2933735537	2.7277155226	7.3900724727
H14	-1.0825465698	1.5000653732	9.1121415508
H15	-2.4127707994	-0.6191819919	8.9919113990
H16	-3.5839254033	0.1691549972	7.9414704545
H17	-0.6293800872	-0.3219914900	7.2913961798
H18	-1.9997637793	-1.1888604140	6.6049791680
H19	-2.8191271470	0.8868672924	5.5160415912
H20	-1.1480765919	0.5946901246	5.0419119458
C21	-0.5389300319	1.6012487657	13.6785017800
C22	-1.1197583982	2.1723084593	12.3732137525
C23	-2.2651915364	1.2976445855	11.8102656647
C24	-1.7772324174	-0.1578902705	11.6402458786
C25	-1.2047873301	-0.7293020816	12.9525904529
C26	-0.0738814177	0.1477325244	13.5076016108
H27	-1.3092117527	1.6444768554	14.4632239231
H28	0.2915741616	2.2310390996	14.0234060237
H29	-0.3177855239	2.2420483911	11.6217990928
H30	-1.4787925683	3.1954316791	12.5336468884
H31	-3.0728459811	1.3012844111	12.5603037303
H32	-2.5873111043	-0.8017210420	11.2847488662
H33	-0.9902898298	-0.1882289824	10.8732129241
H34	-2.0110858949	-0.7960987095	13.6983879909
H35	-0.8480331014	-1.7548911834	12.7881296542
H36	0.7789796290	0.1191541771	12.8127791377
H37	0.2884902928	-0.2538485357	14.4627821163
C38	-7.2246356249	2.1963801108	10.7829558607
C39	-5.7360312083	2.5373921848	10.9688161748
C40	-4.8120739967	1.5602948772	10.2033583552
C41	-5.1296450674	0.1065983155	10.6175009043
C42	-6.6197093531	-0.2338365861	10.4192007872
C43	-7.5298915082	0.7436175733	11.1753866890
H44	-7.4994253801	2.3512736746	9.7287029440
H45	-7.8415236902	2.8894007242	11.3699079105
H46	-5.4886808665	2.5001634826	12.0412186586
H47	-5.5394202231	3.5658419209	10.6446892345
H48	-5.0469837579	1.6678210034	9.1319362323
H49	-4.5154724212	-0.6026732584	10.0546936334
H50	-4.8777929187	-0.0301928548	11.6787208854
H51	-6.8583489575	-0.1954677232	9.3457194477
H52	-6.8125715255	-1.2651861652	10.7436784744
H53	-7.3720062011	0.6197027407	12.2573839168
H54	-8.5852492209	0.5088893937	10.9856848212

Conformer C

P1 -3.3746198672 2.0579945812 10.0496616395  
C4 -0.0817779886 0.7650186797 7.6966123898  
C5 -0.8851841177 1.3872011849 8.8535865750  
C6 -2.4061434234 1.1701829065 8.6862115429  
C7 -2.8570830803 1.7024185989 7.3055154374  
C8 -2.0603442082 1.0710625778 6.1504782184  
C9 -0.5504772087 1.2839153480 6.3297689492  
H10 -0.1963332934 -0.3289234283 7.7267039726  
H11 0.9878164541 0.9694169682 7.8368786572  
H12 -0.5360265741 0.9610435077 9.8013155573  
H13 -0.6775282391 2.4668320614 8.9007667918  
H14 -2.6012585664 0.0889057842 8.7204372177  
H15 -3.9283769310 1.5242919407 7.1535211665  
H16 -2.7213971709 2.7935918812 7.2856332590  
H17 -2.2732352372 -0.0076509010 6.1079837655  
H18 -2.3948968336 1.4924989979 5.1934761913  
H19 -0.3253983862 2.3581406585 6.2530590296  
H20 0.0054336937 0.7893643779 5.5227273367  
C21 -1.9253432409 -0.5985543234 13.1381734394  
C22 -2.6436776736 -0.1895221993 11.8379494408  
C23 -2.6353828243 1.3398939685 11.6414917415  
C24 -3.2496419534 2.0431886527 12.8736831887  
C25 -2.5410672779 1.6313729639 14.1768909753  
C26 -2.5314590503 0.1060884188 14.3613461189  
H27 -0.8593896418 -0.3373225371 13.0594449825  
H28 -1.9702453884 -1.6884016810 13.2648082001  
H29 -3.6823532191 -0.5453319552 11.8838055241  
H30 -2.1768371182 -0.6934249011 10.9824047953  
H31 -1.5846056972 1.6644356923 11.5923774595  
H32 -3.2032021650 3.1317867022 12.7459396282  
H33 -4.3161120565 1.7842369582 12.9538878995  
H34 -1.5047549304 2.0000705054 14.1538580817  
H35 -3.0247519421 2.1159805194 15.0351366956  
H36 -3.5635714978 -0.2473028542 14.5061822664  
H37 -1.9791568234 -0.1646349966 15.2704990574  
C38 -6.7154035642 -0.6397556763 9.4681208693  
C39 -5.2653393034 -0.1291984261 9.3635507909  
C40 -5.1110596934 1.2727074545 9.9919192931  
C41 -6.1147364789 2.2593428686 9.3486194930  
C42 -7.5629680319 1.7477435128 9.4405410954  
C43 -7.7095106095 0.3442705824 8.8335283775  
H44 -6.9728424925 -0.7825400416 10.5284496698  
H45 -6.7985282919 -1.6260623067 8.9924672080  
H46 -4.9844818552 -0.0912039258 8.3021869958  
H47 -4.5867663210 -0.8463796036 9.8379230464  
H48 -5.3891017960 1.1875666081 11.0542232992  
H49 -6.0292233066 3.2422336136 9.8271950814  
H50 -5.8515691679 2.4113310425 8.2912408853  
H51 -7.8667769437 1.7172516218 10.4979156141  
H52 -8.2420948906 2.4521340404 8.9424825337  
H53 -7.5232916751 0.3968458792 7.7502273843  
H54 -8.7378276600 -0.0199470020 8.9556527518

#### Conformer D

P1 -3.3068046427 2.1710874949 10.0913229291  
C4 -0.1755493830 0.4331696354 7.6948829705  
C5 -0.8834835259 1.0234209883 8.9296952292

C6 -2.3662417345 1.3464597840 8.6448522098  
C7 -2.4528367536 2.2813031062 7.4126728190  
C8 -1.7604385286 1.6859325919 6.1752100120  
C9 -0.2920485655 1.3478320991 6.4677579364  
H10 -0.6228596469 -0.5445045112 7.4606987813  
H11 0.8797136924 0.2428138782 7.9312816292  
H12 -0.7912951700 0.3146383294 9.7596357210  
H13 -0.3608858573 1.9415369473 9.2389979820  
H14 -2.8699384764 0.3983868485 8.3998024915  
H15 -3.4960792065 2.5193209334 7.1775610716  
H16 -1.9764994361 3.2383721807 7.6702634462  
H17 -2.2899252279 0.7727871330 5.8637318334  
H18 -1.8309200722 2.3884194305 5.3343812949  
H19 0.2623548059 2.2794316755 6.6557637642  
H20 0.1766718636 0.8757656362 5.5945858426  
C21 -1.8506310159 -0.5113654631 13.1486417792  
C22 -2.6970707059 -0.0466367533 11.9482180062  
C23 -2.4636568708 1.4447939183 11.6329528761  
C24 -2.7222158534 2.3179048967 12.8841390276  
C25 -1.8749642200 1.8482234793 14.0803949362  
C26 -2.1040344062 0.3601754515 14.3885324194  
H27 -0.7845071200 -0.4593155410 12.8811253566  
H28 -2.0641356238 -1.5650017773 13.3725671827  
H29 -3.7579034232 -0.2134773932 12.1806055502  
H30 -2.4717819688 -0.6669082243 11.0710275001  
H31 -1.3955573465 1.5692316972 11.4045505323  
H32 -2.5051981269 3.3682410748 12.6546272595  
H33 -3.7833899844 2.2773375614 13.1637204261  
H34 -0.8103777517 2.0107353949 13.8538752146  
H35 -2.1017564005 2.4596560538 14.9636736547  
H36 -3.1419454796 0.2162632670 14.7248620062  
H37 -1.4607082741 0.0385486588 15.2177722226  
C38 -7.0406578980 0.7806526581 8.5749447318  
C39 -5.6631198999 1.4651475578 8.6428194165  
C40 -4.9621826932 1.2389643670 10.0016062157  
C41 -5.8992750371 1.6768141365 11.1499720998  
C42 -7.2769289796 0.9936355812 11.0788444185  
C43 -7.9558868572 1.2270898053 9.7227524630  
H44 -6.9047222459 -0.3101809585 8.6238231458  
H45 -7.5100647381 0.9924096586 7.6052602024  
H46 -5.7880606681 2.5454717087 8.4759598961  
H47 -5.0403778586 1.0908201943 7.8228660315  
H48 -4.7687126282 0.1603022531 10.1012342243  
H49 -5.4427152742 1.4611242283 12.1217261692  
H50 -6.0318773395 2.7678291258 11.1053661906  
H51 -7.1542382192 -0.0878423474 11.2408162632  
H52 -7.9136325086 1.3599085599 11.8948631675  
H53 -8.1839812111 2.2975438063 9.6103065895  
H54 -8.9153922163 0.6958478562 9.6769271707

#### Conformer E

P1 -3.2428978097 2.0218127661 10.0039265920  
C4 -0.0160019013 1.1267896809 7.3985588197  
C5 -0.8097106448 1.6658813417 8.6022159382  
C6 -2.2957444589 1.2382030338 8.5628447428  
C7 -2.9146566021 1.6785995537 7.2154474282  
C8 -2.1268108893 1.1381963866 6.0084285207

C9 -0.6493259360 1.5504888275 6.0661380578  
H10 0.0190309416 0.0282629652 7.4508082134  
H11 1.0239139080 1.4743535758 7.4557116285  
H12 -0.3330543036 1.3276735992 9.5285000053  
H13 -0.7553777160 2.7645419601 8.6094680012  
H14 -2.3436754547 0.1412675363 8.6250196002  
H15 -3.9574470199 1.3516475450 7.1419426473  
H16 -2.9313341575 2.7777373350 7.1747299147  
H17 -2.1969459490 0.0402484876 5.9921589333  
H18 -2.5868988722 1.4932806897 5.0769344179  
H19 -0.5740651909 2.6430369952 5.9606340078  
H20 -0.0964020404 1.1158149847 5.2233555428  
C21 -1.0087250456 1.6457185402 13.5946707514  
C22 -1.4641038912 2.1569612113 12.2165808735  
C23 -2.5188147737 1.2233288830 11.5755414799  
C24 -1.9890546321 -0.2250253814 11.5073018755  
C25 -1.5302670452 -0.7300665118 12.8891501862  
C26 -0.4857744826 0.2033768132 13.5187992023  
H27 -1.8584488439 1.6855688459 14.2929109590  
H28 -0.2377955966 2.3111336670 14.0049656663  
H29 -0.5880838882 2.2361543045 11.5575485182  
H30 -1.8730667720 3.1706604678 12.3040737211  
H31 -3.3851271219 1.2220308732 12.2568244792  
H32 -2.7553737493 -0.8995963568 11.1102755268  
H33 -1.1395579657 -0.2777775148 10.8128559214  
H34 -2.4031925110 -0.7974821899 13.5556638232  
H35 -1.1284572686 -1.7481239074 12.7991626063  
H36 0.4317830516 0.1822251506 12.9115858435  
H37 -0.2067467491 -0.1560533980 14.5177498925  
C38 -6.5805871794 -0.7165816203 9.5583874623  
C39 -5.1300725989 -0.2140746875 9.4258493483  
C40 -4.9743406894 1.2257887044 9.9600733729  
C41 -5.9817496894 2.1725075257 9.2641211683  
C42 -7.4282845651 1.6650873727 9.3949640042  
C43 -7.5742636813 0.2295114878 8.8689225936  
H44 -6.8380978783 -0.7974217917 10.6251320112  
H45 -6.6638852705 -1.7288135226 9.1407471891  
H46 -4.8398619839 -0.2507844451 8.3669993134  
H47 -4.4577496250 -0.8988008579 9.9542239997  
H48 -5.2510309516 1.2081931836 11.0266628195  
H49 -5.8940124684 3.1807442267 9.6861957504  
H50 -5.7296245348 2.2639493005 8.1980512384  
H51 -7.7260682750 1.6939536846 10.4540214942  
H52 -8.1114988920 2.3388626182 8.8613840578  
H53 -7.3884543883 0.2207534625 7.7842533249  
H54 -8.6023450590 -0.1278311433 9.0113858422

#### Conformer F

P1 -3.3729228310 2.1626085597 10.2146282600  
C4 -0.1987679424 0.8436849475 7.7295598944  
C5 -0.9659721929 1.5384585475 8.8682796276  
C6 -2.4774947685 1.2125302130 8.8390682512  
C7 -3.0577925887 1.5641357290 7.4498456282  
C8 -2.2915179030 0.8697564494 6.3096281400  
C9 -0.7909205881 1.1889410263 6.3563467696  
H10 -0.2380379655 -0.2458642436 7.8784666358  
H11 0.8616850277 1.1251005144 7.7707599679

H12 -0.5256461199 1.2485632121 9.8294386847  
H13 -0.8348794100 2.6274265327 8.7825381053  
H14 -2.5965816070 0.1295601867 8.9907651650  
H15 -4.1162326250 1.2852603910 7.3899658223  
H16 -3.0135249125 2.6540604316 7.3068310030  
H17 -2.4331611910 -0.2184944518 6.3896018749  
H18 -2.7160181841 1.1682084411 5.3420719395  
H19 -0.6423364503 2.2608054088 6.1573701598  
H20 -0.2597429551 0.6473603311 5.5629096194  
C21 -1.4261820640 -0.3705961774 13.1440148336  
C22 -2.2901068302 -0.0580109066 11.9066926481  
C23 -2.5418141751 1.4594908058 11.7741890630  
C24 -3.1957269663 2.0041109630 13.0640425812  
C25 -2.3374727530 1.6938978591 14.3035902139  
C26 -2.0528257871 0.1892672074 14.4303399302  
H27 -0.4267256850 0.0688980153 13.0063020922  
H28 -1.2790803707 -1.4551299620 13.2329009058  
H29 -3.2459934526 -0.5883219963 11.9974532158  
H30 -1.7990460669 -0.4538046323 11.0102539528  
H31 -1.5522752931 1.9412274420 11.7112839279  
H32 -3.3611075156 3.0856498224 12.9796905242  
H33 -4.1846659271 1.5437559360 13.1965752265  
H34 -1.3851523027 2.2395222875 14.2272122715  
H35 -2.8373003828 2.0643678597 15.2082508504  
H36 -2.9961863217 -0.3404592272 14.6316455327  
H37 -1.3976785140 -0.0043410800 15.2895997401  
C38 -7.5871148485 1.9309895374 10.6297479088  
C39 -6.1264734510 2.2881194267 10.9583268370  
C40 -5.1398693752 1.4811649332 10.0825755869  
C41 -5.3992188887 -0.0305276616 10.2415389491  
C42 -6.8585032138 -0.3875020043 9.9012753028  
C43 -7.8470976490 0.4216786204 10.7548008849  
H44 -7.8130940786 2.2532530849 9.6021541014  
H45 -8.2664466729 2.4895757655 11.2869533389  
H46 -5.9400385817 2.0787364018 12.0203358763  
H47 -5.9594272502 3.3632286385 10.8187227964  
H48 -5.3854941888 1.7423488906 9.0408494359  
H49 -4.7164098517 -0.6127994469 9.6107140119  
H50 -5.1991470552 -0.3282375905 11.2794514451  
H51 -7.0427929335 -0.1811700165 8.8362126328  
H52 -7.0241754802 -1.4637131751 10.0431568515  
H53 -7.7408115854 0.1229031702 11.8086277653  
H54 -8.8803659855 0.1874965350 10.4675602055

#### Conformer G

P1 -3.0368929221 2.2868326457 10.1490392312  
C4 -1.0179959205 2.3951463001 6.4356824706  
C5 -1.9661309939 2.7742445153 7.5867002156  
C6 -2.0919163001 1.6380101858 8.6318932610  
C7 -2.5260555262 0.3293419931 7.9370139905  
C8 -1.5676592338 -0.0507617831 6.7913373638  
C9 -1.4378063270 1.0806508252 5.7612377417  
H10 0.0029892510 2.2876194179 6.8321963982  
H11 -0.9809082487 3.2081116085 5.6986564063  
H12 -1.6192884480 3.6922481785 8.0752267936  
H13 -2.9603520768 3.0017688116 7.1749239758  
H14 -1.0802928666 1.4754728937 9.0398215498



H15	-2.5843006529	-0.4938591088	8.6554671611
H16	-3.5348232727	0.4564878319	7.5212896862
H17	-0.5754832513	-0.2758132199	7.2108298850
H18	-1.9155226343	-0.9720487263	6.3053182415
H19	-2.4063429806	1.2242726726	5.2589172718
H20	-0.7187657157	0.8049823875	4.9789398704
C21	-0.7516248767	1.3430315684	13.5758724710
C22	-1.2373260285	2.0286779697	12.2871291946
C23	-2.3877851039	1.2497617114	11.6041048183
C24	-1.9548198467	-0.2117581555	11.3574108887
C25	-1.4808522441	-0.8973126974	12.6537384135
C26	-0.3427459300	-0.1157730139	13.3251739717
H27	-1.5600986078	1.3684141044	14.3220788576
H28	0.0862910912	1.9069757212	14.0063396894
H29	-0.3935923253	2.1132235872	11.5844181422
H30	-1.5592842247	3.0542648443	12.5019222110
H31	-3.2356409046	1.2370347591	12.3083095328
H32	-2.7710180133	-0.7918852408	10.9148592269
H33	-1.1293799050	-0.2282934025	10.6316351805
H34	-2.3283424214	-0.9756327957	13.3512939989
H35	-1.1621573088	-1.9252645257	12.4352427192
H36	0.5437787916	-0.1373102735	12.6735407022
H37	-0.0499913113	-0.5990363236	14.2663001997
C38	-6.8254781065	0.1618542627	10.1725629708
C39	-5.2909677761	0.3008978300	10.1250658253
C40	-4.8633174255	1.7821479419	10.0402523145
C41	-5.5455903295	2.4805240458	8.8413452742
C42	-7.0765035709	2.3309768806	8.8882211753
C43	-7.4977391127	0.8565108861	8.9790626084
H44	-7.1991592393	0.6071481307	11.1069060317
H45	-7.1023333071	-0.9003580870	10.2021151095
H46	-4.9091231543	-0.2518336850	9.2582984433
H47	-4.8594024024	-0.1703314950	11.0154096857
H48	-5.2548750079	2.2723910796	10.9480246028
H49	-5.2716581115	3.5428405627	8.8206112599
H50	-5.1757011694	2.0437643617	7.9027805074
H51	-7.4641398289	2.8734495130	9.7633773597
H52	-7.5256397248	2.8033705994	8.0047330100
H53	-7.2107604546	0.3398433664	8.0507355506
H54	-8.5897486585	0.7754379407	9.0559921549

#### [AuCl(PCy<sub>3</sub>)]

##### Conformer A

P1	-3.2621072308	2.1897166790	10.1526791723
Au2	-3.2311957131	4.4841969398	9.9508515126
Cl3	-3.1915173916	6.8105502914	9.7564759190
C4	-0.0032194628	1.3305294968	7.5769670004
C5	-0.9177271937	2.0969397889	8.5491270404
C6	-2.2176834392	1.3099582668	8.8452404656
C7	-2.9496758268	1.0197656547	7.5155056296
C8	-2.0410464459	0.2464761363	6.5404629529
C9	-0.7285331459	0.9941388903	6.2667846952
H10	0.3416256866	0.4011022592	8.0552416576
H11	0.8943370262	1.9280401661	7.3741612095
H12	-0.3740646660	2.3251937126	9.4697731464
H13	-1.1928076780	3.0650183126	8.1089094924
H14	-1.9529417013	0.3388774339	9.2924624289

H15	-3.8633933244	0.4410389157	7.6860190967
H16	-3.2497599954	1.9693832529	7.0511509082
H17	-1.8179194339	-0.7442411591	6.9645978937
H18	-2.5826808687	0.0682979523	5.6027595402
H19	-0.9487601633	1.9260486576	5.7259709607
H20	-0.0805534382	0.3972265664	5.6126642091
C21	-2.6098771303	1.9725289839	14.3358971869
C22	-3.0387542946	2.5203791068	12.9627202694
C23	-2.6040285876	1.5763304042	11.8143921298
C24	-1.0741542547	1.3708441004	11.8727840621
C25	-0.6418194066	0.8168130424	13.2432495501
C26	-1.0962820691	1.7230473656	14.3958930660
H27	-3.1453514769	1.0321891408	14.5375401166
H28	-2.9131011045	2.6779015804	15.1195726460
H29	-2.5746961728	3.5020379978	12.7971223641
H30	-4.1192076793	2.6898604656	12.9497723818
H31	-3.0732196114	0.5914710650	11.9642739231
H32	-0.7380729140	0.6853699997	11.0873366824
H33	-0.5711699702	2.3322820285	11.7002226151
H34	-1.0699418386	-0.1883384456	13.3762752018
H35	0.4487378084	0.6948009022	13.2578293679
H36	-0.5684830394	2.6855978013	14.3305900645
H37	-0.8187726397	1.2773131818	15.3593618309
C38	-7.1745656354	1.5127138450	8.6761050196
C39	-5.8129978062	2.1893478532	8.9111152040
C40	-4.9910661439	1.4454615677	9.9922396344
C41	-5.8068113744	1.4001691393	11.3041775637
C42	-7.1702422998	0.7169817316	11.0789463674
C43	-7.9847533121	1.4076382379	9.9755466829
H44	-7.0140149018	0.5064744930	8.2599843680
H45	-7.7364342367	2.0759831293	7.9205931791
H46	-5.9687610346	3.2225517993	9.2499462737
H47	-5.2632749173	2.2585100561	7.9686037301
H48	-4.8283581011	0.4059768024	9.6674209445
H49	-5.2636826971	0.8627503708	12.0900217793
H50	-5.9705492769	2.4245782032	11.6673266397
H51	-7.0033113730	-0.3362629066	10.8072637565
H52	-7.7321079781	0.7109469968	12.0214694684
H53	-8.2627980500	2.4178079798	10.3096079015
H54	-8.9227952415	0.8664055464	9.7983942424

##### Conformer B

P1	-3.0377119766	2.1701536429	10.3190273242
Au2	-2.9216485065	4.4775747245	10.5050518955
Cl3	-2.8096711332	6.7998252192	10.6973781834
C4	-1.4262487217	2.2317873608	6.4012939645
C5	-2.2732499475	2.6211703390	7.6257460473
C6	-2.1338213116	1.5851065063	8.7688774228
C7	-2.4958496959	0.1755241515	8.2462261322
C8	-1.6321502931	-0.2086300171	7.0291846866
C9	-1.7577597377	0.8200732383	5.8971344770
H10	-0.3613842560	2.2806951523	6.6730184474
H11	-1.5777283322	2.9707035397	5.6049254204
H12	-1.9815763391	3.6156506128	7.9794485812
H13	-3.3303286831	2.6944362342	7.3295846531
H14	-1.0788870466	1.5788295836	9.0842984875
H15	-2.3783203606	-0.5801470220	9.0281256097

H16	-3.5526233576	0.1632821221	7.9453458608
H17	-0.5800639283	-0.2817715023	7.3422288712
H18	-1.9226484025	-1.2067465883	6.6771843948
H19	-2.7860136593	0.8046068320	5.5063066846
H20	-1.1013261388	0.5485228644	5.0609985858
C21	-0.4981429670	1.5963053576	13.6607141746
C22	-1.0542851821	2.1760880753	12.3482453526
C23	-2.2509686747	1.3450813797	11.8224115392
C24	-1.8324228564	-0.1343704619	11.6607150446
C25	-1.2907952976	-0.7084060447	12.9840865410
C26	-0.1130494949	0.1172667853	13.5189918549
H27	-1.2588493171	1.7009029546	14.4484948279
H28	0.3662719636	2.1896607767	13.9829709080
H29	-0.2585064939	2.1889958381	11.5886245390
H30	-1.3547677357	3.2181554426	12.4996447533
H31	-3.0489222651	1.3976853852	12.5797825964
H32	-2.6685268804	-0.7478086466	11.3132799707
H33	-1.0447737603	-0.2047297724	10.8977623966
H34	-2.0992047374	-0.7202549418	13.7301541963
H35	-0.9911991169	-1.7533089596	12.8327477470
H36	0.7363798217	0.0266154348	12.8257530980
H37	0.2263139940	-0.2831909967	14.4824866802
C38	-7.2354422168	2.1717417428	10.8639609272
C39	-5.7501332513	2.5281937151	11.0517592756
C40	-4.8330459156	1.6069470507	10.2104294941
C41	-5.1157892222	0.1273047908	10.5589450745
C42	-6.6023491295	-0.2221356543	10.3530057234
C43	-7.5187699050	0.6949783200	11.1747565342
H44	-7.5260752741	2.3871631465	9.8251003750
H45	-7.8473780528	2.8237494845	11.4992307215
H46	-5.4835764960	2.4324780438	12.1148790311
H47	-5.5814515069	3.5765137275	10.7835331812
H48	-5.0821280934	1.7688432514	9.1499967334
H49	-4.4976285135	-0.5469607937	9.9590578062
H50	-4.8556055565	-0.0512497322	11.6114391141
H51	-6.8507140812	-0.1268665638	9.2855604539
H52	-6.7691995287	-1.2737678048	10.6191584520
H53	-7.3504133400	0.5088924850	12.2458937500
H54	-8.5717519116	0.4575212667	10.9780052708

#### Conformer C

P1	-3.3810099893	1.9890534321	10.0629077579
Au2	-3.2560637686	4.2912089290	9.9923770185
Cl3	-3.1028024626	6.6171083403	9.9244854771
C4	-0.0859888076	0.7927032772	7.6976773486
C5	-0.8846158103	1.4257186198	8.8519525577
C6	-2.4033483549	1.1968122552	8.6754442268
C7	-2.8681164609	1.7278599772	7.2989125108
C8	-2.0689631674	1.0864931774	6.1508672767
C9	-0.5590245905	1.3022291231	6.3286907035
H10	-0.1983827508	-0.3011721795	7.7382824675
H11	0.9818962629	1.0021466132	7.8371742947
H12	-0.5361035913	1.0082747545	9.8039415050
H13	-0.6852883110	2.5060944117	8.8874542111
H14	-2.5980541469	0.1156856288	8.7171006499
H15	-3.9388516944	1.5446009741	7.1519437754
H16	-2.7325847312	2.8179454800	7.2753347329

H17	-2.2832178973	0.0077090263	6.1146904989
H18	-2.4061773187	1.5044800010	5.1942019695
H19	-0.3346295365	2.3752209248	6.2433700770
H20	-0.0046155035	0.8009690270	5.5253565633
C21	-1.8599269347	-0.5716048105	13.1309513446
C22	-2.6017602948	-0.1802995396	11.8383801939
C23	-2.6383295725	1.3538913481	11.6677941972
C24	-3.2869301529	2.0248672038	12.9003085428
C25	-2.5531597817	1.6260001167	14.1933411786
C26	-2.4835208524	0.1003115678	14.3643514489
H27	-0.8049228046	-0.2724734708	13.0454340979
H28	-1.8670021058	-1.6632443337	13.2431254722
H29	-3.6278400839	-0.5689672305	11.8900372064
H30	-2.1228213227	-0.6603453333	10.9759313298
H31	-1.6014202991	1.7159457778	11.6169157095
H32	-3.2792029216	3.1148403098	12.7835047098
H33	-4.3407868202	1.7208119299	12.9786159936
H34	-1.5337630674	2.0377409351	14.1677222877
H35	-3.0528506572	2.0860694555	15.0547874999
H36	-3.4991552548	-0.2949617753	14.5158868766
H37	-1.9118383947	-0.1557718957	15.2651037046
C38	-6.7454829993	-0.5919856771	9.5024705415
C39	-5.2888746049	-0.1003227379	9.4025932604
C40	-5.1440954532	1.3236015015	9.9882054627
C41	-6.1135204013	2.3008937871	9.2831132041
C42	-7.5661959169	1.8017165985	9.3716256148
C43	-7.7184995140	0.3778307043	8.8152378139
H44	-7.0197660643	-0.6951744716	10.5628379784
H45	-6.8243113576	-1.5936630521	9.0608796106
H46	-4.9907967154	-0.0945493774	8.3458044587
H47	-4.6244934083	-0.8068262349	9.9121956006
H48	-5.4394002475	1.2832086693	11.0473586720
H49	-6.0298787928	3.2990007742	9.7271096821
H50	-5.8276177985	2.4075790762	8.2274987698
H51	-7.8885042745	1.8176251419	10.4234616102
H52	-8.2238207196	2.4962570513	8.8345405714
H53	-7.5164817658	0.3867908198	7.7338249267
H54	-8.7515842885	0.0287331292	8.9369346109

#### Conformer D

P1	-3.2996259897	2.0783624294	10.1010948410
Au2	-3.3523974068	4.3816380604	10.0472817783
Cl3	-3.3819768174	6.7135251816	10.0015763515
C4	-0.1090560388	0.5179909292	7.7141163224
C5	-0.8353093015	1.1145181381	8.9356707072
C6	-2.3377168623	1.3386250323	8.6475442742
C7	-2.4952720823	2.2227211725	7.3841108065
C8	-1.7832863281	1.6081930297	6.1667338014
C9	-0.2941019102	1.3728054859	6.4530692232
H10	-0.4981651546	-0.4942325486	7.5273681996
H11	0.9571328552	0.4032331523	7.9476248479
H12	-0.6951028843	0.4416610800	9.7886171078
H13	-0.3700700218	2.0745393902	9.2033870551
H14	-2.7949908520	0.3565525415	8.4503314683
H15	-3.5503273459	2.3961050476	7.1528367358
H16	-2.0655683381	3.2111173819	7.5961426047
H17	-2.2626620469	0.6533819534	5.9022530467

H18	-1.9070816737	2.2702490360	5.3006588959
H19	0.2045619910	2.3428818764	6.5936301240
H20	0.1913395537	0.8913262080	5.5947869256
C21	-1.7772471300	-0.5252079988	13.1164507623
C22	-2.6401894465	-0.0642434999	11.9261144368
C23	-2.4579971964	1.4464724626	11.6635333804
C24	-2.7733992502	2.2730294046	12.9330201645
C25	-1.9060661309	1.8036765143	14.1150074161
C26	-2.0693882016	0.2989056127	14.3796588195
H27	-0.7143517656	-0.4214283715	12.8525413991
H28	-1.9493070198	-1.5925956792	13.3056143507
H29	-3.6956395176	-0.2731066456	12.1490097512
H30	-2.3864566546	-0.6506691822	11.0331329918
H31	-1.3958025374	1.6252067577	11.4481909029
H32	-2.6040619768	3.3383588508	12.7397196499
H33	-3.8313759791	2.1690657633	13.2029268815
H34	-0.8503014868	2.0246322382	13.8982233270
H35	-2.1664410065	2.3792719677	15.0119590284
H36	-3.0990951623	0.0986255761	14.7114476198
H37	-1.4106114795	-0.0182226154	15.1979612216
C38	-7.0629680730	0.7877462487	8.5923632543
C39	-5.6718495676	1.4473452975	8.6353846175
C40	-4.9978690385	1.2693311416	10.0153228223
C41	-5.9295807098	1.7852964267	11.1373884340
C42	-7.3201003498	1.1269270862	11.0805574783
C43	-7.9789804850	1.3097879085	9.7069466634
H44	-6.9487560510	-0.3019541217	8.6950914002
H45	-7.5158421298	0.9624159638	7.6082037665
H46	-5.7692012754	2.5198593812	8.4151973438
H47	-5.0494675836	1.0134745070	7.8453600825
H48	-4.8246140382	0.1935680315	10.1704843730
H49	-5.4857639344	1.6040994329	12.1211057980
H50	-6.0343245453	2.8747316453	11.0377491932
H51	-7.2230571322	0.0524665211	11.2984106214
H52	-7.9545207715	1.5489592346	11.8701419815
H53	-8.1832497577	2.3774269028	9.5408210313
H54	-8.9478673710	0.7953953474	9.6756391699

#### Conformer E

P1	-3.2439855580	1.9644431422	10.0051465304
Au2	-3.2521128180	4.2734057632	10.0320827623
Cl3	-3.2567448764	6.6059636886	10.0534870539
C4	-0.0237047623	1.1563744527	7.3787189767
C5	-0.8033680060	1.7012915366	8.5894692704
C6	-2.2911708960	1.2804430584	8.5422318967
C7	-2.9236606193	1.7317725793	7.2039515973
C8	-2.1411676650	1.1842295262	5.9966397243
C9	-0.6610455715	1.5876755613	6.0504125740
H10	0.0044776945	0.0573989913	7.4304763564
H11	1.0174875294	1.4983248763	7.4337125906
H12	-0.3293353719	1.3515444194	9.5126839367
H13	-0.7439992586	2.7987381631	8.6015649010
H14	-2.3479855694	0.1841564833	8.6058441753
H15	-3.9678277900	1.4081536889	7.1372627926
H16	-2.9330389623	2.8302071922	7.1678785594
H17	-2.2209722554	0.0867029553	5.9794666009
H18	-2.6041098913	1.5455767633	5.0697295825

H19	-0.5785287707	2.6792034516	5.9455887346
H20	-0.1154415379	1.1482414405	5.2058669867
C21	-0.9874773611	1.6545855051	13.5983062553
C22	-1.4232903049	2.1699347360	12.2152720563
C23	-2.5102560967	1.2576798000	11.5976522779
C24	-2.0189957708	-0.2061779406	11.5276402801
C25	-1.5785711380	-0.7108001870	12.9155235601
C26	-0.5083652444	0.1965959959	13.5393213182
H27	-1.8353302274	1.7318816054	14.2952903386
H28	-0.1972870774	2.3028689512	13.9969651094
H29	-0.5487221684	2.2115857962	11.5527044367
H30	-1.7986343124	3.1960564120	12.2971867724
H31	-3.3739993143	1.2888400312	12.2803006602
H32	-2.8000071167	-0.8655280607	11.1344273313
H33	-1.1688229550	-0.2776408205	10.8358311538
H34	-2.4556831061	-0.7489667963	13.5786023944
H35	-1.2079863878	-1.7403028761	12.8290054383
H36	0.4112827632	0.1396484562	12.9379261227
H37	-0.2476973608	-0.1607286232	14.5435292643
C38	-6.5757034003	-0.7063081019	9.5803143334
C39	-5.1287750750	-0.1950724364	9.4394826073
C40	-4.9966296562	1.2551674041	9.9593387433
C41	-6.0003471903	2.1849790992	9.2349622887
C42	-7.4417589086	1.6630789540	9.3724319612
C43	-7.5770046909	0.2174359796	8.8720967289
H44	-6.8319658174	-0.7719310577	10.6482503076
H45	-6.6429435760	-1.7261408344	9.1801128532
H46	-4.8396749457	-0.2354982791	8.3808265978
H47	-4.4525210738	-0.8697791123	9.9749216400
H48	-5.2757054075	1.2548418119	11.0246928893
H49	-5.9283113350	3.2009730369	9.6386196168
H50	-5.7413001905	2.2558925974	8.1701443042
H51	-7.7436593278	1.7124073253	10.4293472306
H52	-8.1232287392	2.3247503365	8.8234108544
H53	-7.3931601747	0.1884628139	7.7876491656
H54	-8.6011606930	-0.1455636631	9.0251569405

#### Conformer F

P1	-3.3734826959	2.0635407525	10.2163861496
Au2	-3.2150817163	4.3586730345	10.0671885649
Cl3	-3.0269602435	6.6786655846	9.9217436052
C4	-0.1925827242	0.8559960451	7.7091671049
C5	-0.9553133316	1.5388608829	8.8584968313
C6	-2.4655609574	1.2069996007	8.8149570410
C7	-3.0578754134	1.5755466455	7.4344515403
C8	-2.2847984060	0.8957123047	6.2893754099
C9	-0.7854120302	1.2214156733	6.3410153190
H10	-0.2311689082	-0.2353787142	7.8445784051
H11	0.8660784448	1.1395066426	7.7572515715
H12	-0.5181805529	1.2354468092	9.8172013907
H13	-0.8289605004	2.6281279728	8.7862916150
H14	-2.5868047399	0.1241540638	8.9645957545
H15	-4.1137843387	1.2875188757	7.3744840134
H16	-3.0190843027	2.6664735287	7.3069116413
H17	-2.4238739186	-0.1938396115	6.3557185636
H18	-2.7125079856	1.2068000359	5.3282281726
H19	-0.6400629515	2.2956612657	6.1572915573

H20	-0.2534713498	0.6908596861	5.5414378136
C21	-1.4192101261	-0.35297778311	13.1654283173
C22	-2.2736051903	-0.0537279160	11.9179874330
C23	-2.5341066572	1.4636772605	11.7896031511
C24	-3.2061400161	2.0145856994	13.0677658950
C25	-2.3489452301	1.7116900215	14.3094998970
C26	-2.0598679195	0.2086613138	14.4440018591
H27	-0.4216555299	0.0906292745	13.0320009285
H28	-1.2692970155	-1.4361735609	13.2564541159
H29	-3.2263409182	-0.5913733430	11.9995818057
H30	-1.7682248591	-0.4430498662	11.0262889843
H31	-1.5559667357	1.9608406017	11.7099289158
H32	-3.3706549675	3.0949401971	12.9760465853
H33	-4.1917887758	1.5473980312	13.1948501669
H34	-1.4009980452	2.2638789010	14.2349887846
H35	-2.8575289006	2.0849536540	15.2070120165
H36	-3.0017153048	-0.3251427814	14.6407968599
H37	-1.4091223804	0.0213655596	15.3072893178
C38	-7.5909219433	1.9512213048	10.6336649730
C39	-6.1304063692	2.3062325501	10.9668659100
C40	-5.1574578521	1.4919492142	10.0824815695
C41	-5.4085091072	-0.0226723750	10.2446064329
C42	-6.8711993257	-0.3711045521	9.9074568383
C43	-7.8558264715	0.4430137214	10.7612780652
H44	-7.8145087517	2.2762104568	9.6070008006
H45	-8.2643127816	2.5140679938	11.2917098380
H46	-5.9419187287	2.0920494552	12.0263389517
H47	-5.9604058379	3.3798589755	10.8257733547
H48	-5.3913572892	1.7600871880	9.0417713910
H49	-4.7302469308	-0.6061306156	9.6098885343
H50	-5.2051831155	-0.3173244237	11.2821312123
H51	-7.0548317121	-0.1669179516	8.8423624168
H52	-7.0363522444	-1.4462103151	10.0519965524
H53	-7.7520719967	0.1440685750	11.8150818566
H54	-8.8888016761	0.2124679849	10.4723111147

#### Conformer G

P1	-3.0694984766	2.2220856361	10.1620644116
Au2	-2.9351552008	4.5026805952	10.5375458355
Cl3	-2.8310291802	6.7986770544	10.9353351069
C4	-1.0381022175	2.4385511655	6.4430790203
C5	-2.0021191630	2.8196738011	7.5803210422
C6	-2.0873927186	1.6945914457	8.6406461406
C7	-2.5036012185	0.3637007775	7.9716917459
C8	-1.5275837912	-0.0146929676	6.8416456637
C9	-1.4180300366	1.1005152463	5.7921979735
H10	-0.0166913205	2.3706156432	6.8460306204
H11	-1.0235396590	3.2392175232	5.6933863981
H12	-1.6789647683	3.7557870933	8.0481889893
H13	-3.0013743179	3.0082479786	7.1644203675
H14	-1.0745352193	1.5644569877	9.0539809347
H15	-2.5547965612	-0.4495922749	8.7011492720
H16	-3.5098593319	0.4728153893	7.5462393390
H17	-0.5348035016	-0.2115210236	7.2728853927
H18	-1.8554927077	-0.9519303753	6.3740312189
H19	-2.3845052994	1.2080536312	5.2776177430
H20	-0.6842303459	0.8280595911	5.0233252860

C21	-0.6593840980	1.3214406302	13.5250124848
C22	-1.1557712662	2.0098200734	12.2417386322
C23	-2.3702855286	1.2674019391	11.6304800314
C24	-2.0070105282	-0.2146784294	11.3810461660
C25	-1.5271350548	-0.8978703495	12.6758015268
C26	-0.3315750209	-0.1600631013	13.2935496797
H27	-1.4360275135	1.4065771506	14.2993326620
H28	0.2198072345	1.8547648231	13.9068312757
H29	-0.3395420868	2.0392294089	11.5044295355
H30	-1.4181298898	3.0513874401	12.4550264255
H31	-3.1893015602	1.3053934959	12.3659277945
H32	-2.8550620052	-0.7690325866	10.9678183567
H33	-1.2001771608	-0.2678192485	10.6370913546
H34	-2.3555992051	-0.9245136040	13.3990215241
H35	-1.2663294045	-1.9421460609	12.4616318219
H36	0.5318468719	-0.2409575600	12.6165202563
H37	-0.0349549263	-0.6372574704	14.2359096836
C38	-6.8500926425	0.1660031123	10.1672920754
C39	-5.3145617044	0.2998065666	10.1456572192
C40	-4.8968738199	1.7825578871	10.0356630988
C41	-5.5470861712	2.4574522807	8.8048681476
C42	-7.0784076403	2.3077407587	8.8344021825
C43	-7.5014566334	0.8354124411	8.9480640455
H44	-7.2374340371	0.6299258942	11.0862396805
H45	-7.1225097827	-0.8959793063	10.2150957675
H46	-4.9157118646	-0.2711042996	9.2984467475
H47	-4.9031109856	-0.1482554847	11.0568056944
H48	-5.2891464453	2.2968112766	10.9268676716
H49	-5.2746635515	3.5190782259	8.7703173328
H50	-5.1605967901	1.9969701144	7.8850767683
H51	-7.4779688855	2.8711449848	9.6899235908
H52	-7.5077391075	2.7630388895	7.9333249225
H53	-7.2014461242	0.2989403436	8.0353162616
H54	-8.5938814189	0.7563613159	9.0114919485

#### [PdCl<sub>3</sub>(PCy<sub>3</sub>)]<sup>-</sup>

##### Conformer A, $\tau_1$

P1	-0.2337132352	0.1676683730	0.0714302330
Pd1	-0.0225274647	0.0751322013	2.4471358697
C4	-0.1970464065	4.3587988089	-0.8459243437
C5	0.0064042017	3.0474023031	-0.0678318469
C6	-0.6348125624	1.8399386550	-0.7858020215
C7	-2.1321213476	2.1305946378	-1.0343434274
C8	-2.3382456957	3.4503707306	-1.8045358461
C9	-1.6820684778	4.6442945757	-1.1006555942
H10	0.3306931654	4.3016921984	-1.8116804888
H11	0.2637879529	5.1850880304	-0.2886430496
H12	1.0675957100	2.8806682007	0.1113451880
H13	-0.4367502953	3.1385311037	0.9315871179
H14	-0.1712243606	1.7355635012	-1.7796071579
H15	-2.5954877941	1.3261774182	-1.6116588086
H16	-2.6614987524	2.1879525892	-0.0732924949
H17	-1.9084209054	3.3464467033	-2.8132745722
H18	-3.4144111841	3.6251407862	-1.9422773679
H19	-2.1861053642	4.8206923079	-0.1388860344
H20	-1.8100513275	5.5588525803	-1.6968169653
C21	3.3891315145	-1.9390879259	-0.6233314978

C22	2.1538246071	-1.3800417513	0.1049530324
C23	1.4109023575	-0.3340335931	-0.7607757277
C24	2.3893044764	0.8061412085	-1.1221510866
C25	3.6229407129	0.2540151464	-1.8632501044
C26	4.3525951801	-0.8177325267	-1.0399257476
H27	3.0702135549	-2.4959435459	-1.5193928722
H28	3.9030187787	-2.6610652675	0.0253730445
H29	2.4593924716	-0.8918365908	1.0377298080
H30	1.4886980718	-2.1991884557	0.3948109699
H31	1.1062581888	-0.8074374027	-1.7080644383
H32	1.9076231326	1.5591278660	-1.7564805384
H33	2.7046755841	1.3066906185	-0.2004830842
H34	3.3078803817	-0.1798812999	-2.8260692285
H35	4.3057573860	1.0809565770	-2.1034984914
H36	4.7715188871	-0.3518762788	-0.1367217435
H37	5.1998019082	-1.2267850464	-1.6088186927
C38	-3.8377889394	-1.8319867579	-1.1275656097
C39	-2.8912114230	-0.9754904261	-0.2673186095
C40	-1.4447869467	-1.0099907378	-0.8213916434
C41	-0.9664761160	-2.4824582163	-0.8573165442
C42	-1.9138030600	-3.3616118093	-1.6963816052
C43	-3.3634884784	-3.2901266229	-1.1975481122
H44	-3.8994866298	-1.4180414114	-2.1479136203
H45	-4.8528326954	-1.7840463793	-0.7100592321
H46	-2.8761946403	-1.3610742155	0.7556780456
H47	-3.2794334936	0.0422703360	-0.2053890228
H48	-1.4589058466	-0.6364067503	-1.8609317592
H49	0.0390888933	-2.5628926252	-1.2815896825
H50	-0.9223795032	-2.8580547731	0.1717604525
H51	-1.8775650283	-3.0334594590	-2.7478792160
H52	-1.5543270317	-4.3999263763	-1.6823143253
H53	-3.4228900789	-3.7331103016	-0.1936616953
H54	-4.0218668835	-3.8829058896	-1.8486495058

#### Conformer A, $\tau_2$

Pd1	-0.2374135785	0.0542683030	2.4648490980
Cl2	-0.4488848483	-0.1291644777	4.8276199866
Cl3	0.4211852368	-2.2518764486	2.4311058816
Cl4	-1.3188404662	2.1813816499	2.6254620228
P1	0.0501324500	0.1787356507	0.1005535940
C4	0.2160805585	4.2974965479	-1.0623373182
C5	0.3916290447	3.0456692728	-0.1847186886
C6	-0.3175171629	1.8178854516	-0.8096004695
C7	-1.8204450022	2.1495197329	-0.9727793147
C8	-2.0202848093	3.4109217038	-1.8358482218
C9	-1.2694196263	4.6251070629	-1.2713631390
H10	0.6966364358	4.1423322238	-2.0427719610
H11	0.7304363422	5.1481270074	-0.5946235840
H12	1.4552127243	2.8608935358	-0.0199320460
H13	-0.0454332088	3.2183742735	0.8041799437
H14	0.0901612585	1.6499281775	-1.8220534324
H15	-2.3617521366	1.3226898133	-1.4436467977
H16	-2.2535564700	2.3038748729	0.0221108020
H17	-1.6643397820	3.2098155216	-2.8593809115
H18	-3.0938658949	3.6306615237	-1.9180887540
H19	-1.7120016451	4.9040644938	-0.3049753338
H20	-1.3863490994	5.4913229718	-1.9383690417

C21	3.6930225311	-1.9243426885	-0.7990304075
C22	2.4500869578	-1.4626783510	-0.0179353518
C23	1.7229755424	-0.2979514713	-0.7238614942
C24	2.7227712380	0.8628015620	-0.9334245056
C25	3.9760370731	0.4052372629	-1.7064176733
C26	4.6816731987	-0.7743407947	-1.0267480843
H27	3.3854626257	-2.3354055785	-1.7742295718
H28	4.1778387086	-2.7457418368	-0.2548796903
H29	2.7452034275	-1.1377345159	0.9868836472
H30	1.7804081550	-2.3050677405	0.1471557366
H31	1.4175693189	-0.6331722373	-1.7286109402
H32	2.2641564816	1.6832733708	-1.4908865344
H33	3.0279083232	1.2646441152	0.0426829866
H34	3.6786929865	0.1094932270	-2.7248348384
H35	4.6634413763	1.2553490248	-1.8186621537
H36	5.0832876429	-0.4464350478	-0.0565317376
H37	5.5399715141	-1.1065736784	-1.6278204904
C38	-3.5678765748	-1.8959513052	-0.6704127577
C39	-2.4890004199	-1.0791187109	0.0623009054
C40	-1.1791644106	-0.9996888492	-0.7580630931
C41	-0.6767871103	-2.4321200042	-1.0473122685
C42	-1.7500491110	-3.2516523450	-1.7901889277
C43	-3.0703640822	-3.3090148067	-1.0080988477
H44	-3.8550345175	-1.3793696114	-1.6006167571
H45	-4.4730975555	-1.9483453769	-0.0508985817
H46	-2.2572671343	-1.5485380226	1.0262299176
H47	-2.8700621420	-0.0811285939	0.2979207057
H48	-1.3937031937	-0.5283256186	-1.7307669042
H49	0.2344423643	-2.4158634417	-1.6560334589
H50	-0.4277435714	-2.9196226955	-0.0980414101
H51	-1.9339734206	-2.8020917392	-2.7794459035
H52	-1.3722028485	-4.2668763104	-1.9753808632
H53	-2.9093891709	-3.8648567711	-0.0734396726
H54	-3.8303691003	-3.8608944772	-1.5794381478

#### Conformer A, $\tau_3$

Pd1	-0.0943182107	0.2896767971	2.4631551060
Cl2	-0.1880281754	0.6940977698	4.8058877287
Cl3	-2.4213516220	0.8535602006	2.3636812921
Cl4	2.2794914114	0.1183444228	2.6951251421
P1	-0.0646149408	-0.0758012037	0.1030459701
C4	-0.0356823373	4.0869736310	-0.7188588923
C5	0.1171990140	2.7546781329	0.0362490011
C6	-0.4495583680	1.5694887878	-0.7814964258
C7	-1.9352554535	1.8445943181	-1.1060017909
C8	-2.0944351726	3.1735189627	-1.8698773512
C9	-1.5009494821	4.3569204922	-1.0914464211
H10	0.5748521440	4.0647925794	-1.6361724305
H11	0.3581086389	4.9058708229	-0.1022418896
H12	1.1669505387	2.5898469974	0.2971607508
H13	-0.4258780128	2.8020962753	0.9881217629
H14	0.0881039652	1.5094695935	-1.7416189049
H15	-2.3641148816	1.0388078574	-1.7126322150
H16	-2.5014050823	1.8852195262	-0.1685895202
H17	-1.5928101592	3.0950333289	-2.8480006233
H18	-3.1586735649	3.3500567244	-2.0794311273
H19	-2.0823261264	4.5083090705	-0.1709033808

H20	-1.5871929031	5.2827825479	-1.6779345998
C21	3.4612196734	-2.2699885531	-0.9449632578
C22	2.2575454986	-1.8016675522	-0.1083393971
C23	1.5655690630	-0.5762651762	-0.7564763028
C24	2.6026081998	0.5643479738	-0.8918351178
C25	3.8248052785	0.1094217884	-1.7133787740
C26	4.4879939018	-1.1418419986	-1.1206558009
H27	3.1218656553	-2.6120004872	-1.9369184115
H28	3.9293032981	-3.1372893746	-0.4596245332
H29	2.5918720201	-1.5095709656	0.8906648016
H30	1.5639395837	-2.6331465159	0.0321607794
H31	1.2465527561	-0.8483302708	-1.7779607272
H32	2.1657746141	1.4410568620	-1.3813506340
H33	2.9194922105	0.8699770837	0.1118556633
H34	3.5083074803	-0.1044951746	-2.7472210839
H35	4.5497666504	0.9329499691	-1.7746363009
H36	4.9141761456	-0.8919933521	-0.1390402309
H37	5.3220412276	-1.4708518603	-1.7569970173
C38	-3.6813140445	-2.1841668390	-0.8751465055
C39	-2.6770126563	-1.3383764559	-0.0728810489
C40	-1.2897667004	-1.2921844625	-0.7484701718
C41	-0.7803403298	-2.7379065655	-0.9475617439
C42	-1.7856667331	-3.5920521365	-1.7456858360
C43	-3.1741780457	-3.6146926876	-1.0952441869
H44	-3.8641002072	-1.7109219035	-1.8534200816
H45	-4.6459048081	-2.1949126549	-0.3505388799
H46	-2.5649695835	-1.7551806101	0.9354301450
H47	-3.0745970780	-0.3366698130	0.0824357986
H48	-1.4064712399	-0.8608036048	-1.7557661306
H49	0.1732938669	-2.7515710534	-1.4812904793
H50	-0.6100918266	-3.2048392972	0.0324929638
H51	-1.8710713062	-3.1841206020	-2.7651521546
H52	-1.3909036428	-4.6121977311	-1.8517369911
H53	-3.1113296901	-4.1287686613	-0.1246543778
H54	-3.8780428213	-4.1907224544	-1.7124924476

#### Conformer B, $\tau_2$

P1	0.000000	0.000000	0.000000
Pd1	0.000000	0.000000	2.354868
C4	4.196101	0.000000	-0.581032
C5	2.821713	-0.161040	0.091348
C6	1.678957	0.368638	-0.811827
C7	1.951881	1.847947	-1.169387
C8	3.327409	2.011000	-1.844073
C9	4.463626	1.461669	-0.968899
H10	4.244565	-0.630761	-1.483531
H11	4.980236	-0.364243	0.096344
H12	2.656362	-1.211411	0.351986
H13	2.799025	0.399074	1.033085
H14	1.684869	-0.208554	-1.749541
H15	1.180562	2.239480	-1.840892
H16	1.914266	2.443251	-0.251082
H17	3.327155	1.480692	-2.810300
H18	3.500167	3.072166	-2.071538
H19	4.537577	2.067019	-0.054474
H20	5.427182	1.552906	-1.490367
C21	-0.063513	-4.134230	-0.913508

C22	0.450701	-2.768547	-0.429945
C23	-0.527411	-1.629170	-0.807022
C24	-0.757676	-1.630879	-2.333946
C25	-1.264945	-3.002197	-2.824755
C26	-0.320336	-4.144475	-2.426658
H27	-0.993615	-4.369978	-0.377360
H28	0.659310	-4.915876	-0.643009
H29	1.434162	-2.583534	-0.886274
H30	0.573669	-2.794571	0.656729
H31	-1.475776	-1.851191	-0.300372
H32	-1.480654	-0.866682	-2.626468
H33	0.180738	-1.390499	-2.855997
H34	-2.258342	-3.188964	-2.390132
H35	-1.400431	-2.976171	-3.915400
H36	0.636210	-4.024130	-2.959078
H37	-0.735873	-5.111242	-2.744127
C38	-3.348748	2.546399	0.221973
C39	-2.524233	1.250566	0.328089
C40	-1.206648	1.376014	-0.474656
C41	-1.539560	1.686559	-1.950309
C42	-2.314240	3.014790	-2.051451
C43	-3.616430	2.954564	-1.236025
H44	-2.799194	3.351323	0.730738
H45	-4.297347	2.426828	0.762211
H46	-3.112656	0.402154	-0.052966
H47	-2.304748	1.035534	1.378958
H48	-0.668212	2.237612	-0.054468
H49	-0.642296	1.721251	-2.577948
H50	-2.178927	0.895041	-2.360551
H51	-1.682150	3.833630	-1.677460
H52	-2.533829	3.241278	-3.104577
H53	-4.291462	2.218912	-1.700650
H54	-4.136053	3.922169	-1.274273

#### Conformer C, $\tau_1$

Pd1	-0.2755037115	0.4293312556	2.3196700834
Cl2	-0.3817243969	0.8428094505	4.6637777093
Cl3	1.7021300734	-0.8772716983	2.6429021374
Cl4	-2.1719873762	1.8626741404	1.9745897151
P1	-0.1375264524	0.0791147602	0.0076732790
C4	3.2153116719	2.4511685614	-1.0834976103
C5	2.3801906967	1.3201579192	-0.4552347159
C6	0.8738787928	1.4731269652	-0.7816806804
C7	0.3953754108	2.8687487249	-0.3166129432
C8	1.2224048336	3.9956040056	-0.9591947759
C9	2.7193701416	3.8394477194	-0.6567562224
H10	3.1656475713	2.3722808498	-2.1815556745
H11	4.2709882584	2.3195638267	-0.8092671115
H12	2.7666565873	0.3598996811	-0.8114335627
H13	2.5098648702	1.3164544946	0.6342680477
H14	0.7465923092	1.3983089650	-1.8735180050
H15	-0.6651723157	3.0156052145	-0.5307695498
H16	0.4826944963	2.9218442827	0.7753381635
H17	1.0699486450	3.9920638407	-2.0507678678
H18	0.8580280127	4.9661073963	-0.5966499204
H19	2.8819257493	3.9637731576	0.4235295883
H20	3.3017126123	4.6256468121	-1.1578251799

C21	2.0314455230	-2.8162613729	-2.2840517111
C22	1.1204696243	-1.6011635087	-2.0185988285
C23	0.8045332157	-1.4724417153	-0.5123074113
C24	0.1460009608	-2.7693988680	0.0056641619
C25	1.0595944825	-3.9814375906	-0.2488318636
C26	1.4203697224	-4.1156022825	-1.7368293137
H27	3.0057130865	-2.6436109128	-1.8033992833
H28	2.2253283805	-2.9096061350	-3.3621309206
H29	0.1901033173	-1.7282013018	-2.5913168772
H30	1.6018858520	-0.6953393948	-2.4052927618
H31	1.7438169578	-1.3704717267	0.0424022165
H32	-0.0580177835	-2.6748457526	1.0767607022
H33	-0.8121678914	-2.9375787965	-0.5068672283
H34	1.9763582149	-3.8628532811	0.3453937592
H35	0.5709513259	-4.8987508098	0.1068791310
H36	0.5097231827	-4.3522041939	-2.3094328289
H37	2.1126968420	-4.9547534848	-1.8927353696
C38	-3.5697477218	0.8949183984	-2.4493420280
C39	-2.3295214214	1.1962250064	-1.5867745039
C40	-1.7481959017	-0.1007724413	-0.9832215723
C41	-2.8363191520	-0.8299126854	-0.1587981167
C42	-4.0679807310	-1.1404919901	-1.0278258137
C43	-4.6449309103	0.1380986879	-1.6544240249
H44	-3.2712355295	0.2919912435	-3.3220275109
H45	-3.9786963707	1.8348477197	-2.8454439601
H46	-2.6044613018	1.8736780543	-0.7706970507
H47	-1.5799412402	1.7068088756	-2.2037839837
H48	-1.4737346771	-0.7550130743	-1.8244797059
H49	-2.4414232333	-1.7533289803	0.2772470011
H50	-3.1238365650	-0.1841593351	0.6765516860
H51	-3.7929639540	-1.8467755433	-1.8278482589
H52	-4.8318983296	-1.6405759830	-0.4174072722
H53	-5.0235290665	0.7884089725	-0.8531823221
H54	-5.5008075827	-0.1003143736	-2.3018486444

#### Conformer C, $\tau_2$

Pd1	-0.2150919156	-0.0103711875	2.4077358844
Cl2	-0.3489608572	-0.3963241165	4.7530013459
Cl3	-1.9920978770	-1.5999561147	2.0809783247
Cl4	1.5821286235	1.5107980754	2.7992551744
P1	-0.0873018452	0.2498423661	0.0607887509
C4	2.9149886840	2.9883159155	-1.2904909557
C5	2.3013642079	1.7426121273	-0.6241523432
C6	0.7571009451	1.7609838490	-0.7134071007
C7	0.1962676016	3.0768268778	-0.1240242836
C8	0.8245736986	4.3129993535	-0.7912332926
C9	2.3564160489	4.2880409249	-0.6937149422
H10	2.7061150481	2.9694784954	-2.3727853738
H11	4.0080580213	2.9578194855	-1.1837253493
H12	2.7064391079	0.8482457505	-1.1116273935
H13	2.5943242806	1.7004470432	0.4297344142
H14	0.4889987081	1.7281244004	-1.7802646794
H15	-0.8920427064	3.1167812941	-0.2447866582
H16	0.4021947469	3.0905483305	0.9519773333
H17	0.5298373282	4.3514258422	-1.8526448060
H18	0.4263022028	5.2238079027	-0.3236780946
H19	2.6506435304	4.3548937272	0.3628813977

H20	2.7886518406	5.1609698664	-1.2033768854
C21	2.1088557683	-2.3638201939	-2.5570011346
C22	1.0755949348	-1.2900890829	-2.1649653753
C23	0.9274683125	-1.1953431218	-0.6299347716
C24	0.5143280627	-2.5702313239	-0.0606910431
C25	1.5298649812	-3.6572377916	-0.4573365975
C26	1.7350329516	-3.7368299539	-1.9779094185
H27	3.0993374183	-2.0660178641	-2.1808829986
H28	2.1931731227	-2.4180976262	-3.6516761708
H29	0.1079570439	-1.5661260952	-2.6050638351
H30	1.3607150543	-0.3261394029	-2.6029537320
H31	1.9186103016	-0.9691110975	-0.2097729544
H32	0.4223230603	-2.5179178945	1.0265331347
H33	-0.4821550643	-2.8442888963	-0.4329741055
H34	2.4943729030	-3.4403884338	0.0263567282
H35	1.1986212642	-4.6284648434	-0.0665587453
H36	0.8032381011	-4.0829397304	-2.4513266987
H37	2.5065034418	-4.4790641292	-2.2264584893
C38	-3.2636386749	0.3298338689	-2.8403666034
C39	-1.8638299037	0.6161577195	-2.2611933991
C40	-1.7919168546	0.2030459743	-0.7734541706
C41	-2.8655273437	0.9870134092	0.0208037004
C42	-4.2695059558	0.7071603154	-0.5430460235
C43	-4.3658892473	1.0406055257	-2.0400984321
H44	-3.4430323688	-0.7557062883	-2.8220824509
H45	-3.2989877310	0.6352124954	-3.8959698297
H46	-1.6601322544	1.6925474280	-2.3547232794
H47	-1.1096940039	0.1033162627	-2.8651367229
H48	-2.0582550774	-0.8587676464	-0.6867321036
H49	-2.8271022010	0.7048384535	1.0746188479
H50	-2.6635153031	2.0654396134	-0.0429590835
H51	-4.5065113154	-0.3545798530	-0.3837010653
H52	-5.0165296089	1.2809807560	0.0218247589
H53	-4.2603880313	2.1282554408	-2.1760399923
H54	-5.3558469218	0.7715081293	-2.4346996828

#### Conformer C, $\tau_3$

Pd1	-0.1469378082	0.4241210017	2.3262967397
Cl2	-0.2458272155	0.8443073240	4.6701909889
Cl3	-2.0091322395	1.9027356269	1.9898358404
Cl4	1.8084391982	-0.9177014990	2.6488854775
P1	-0.0197489069	0.0546650123	0.0119227354
C4	3.3597900339	2.3691663025	-1.1240912565
C5	2.5149358541	1.2518965212	-0.4840511138
C6	1.0074426359	1.4283215764	-0.7914942414
C7	0.5556555630	2.8320288828	-0.3235633878
C8	1.3916545377	3.9438612069	-0.9804226336
C9	2.8893882641	3.7661909300	-0.6954628961
H10	3.2973300318	2.2885365186	-2.2213791075
H11	4.4163028405	2.2225806436	-0.8608437502
H12	2.8819361341	0.2850006840	-0.8426420327
H13	2.6576877652	1.2481321624	0.6041156567
H14	0.8636527375	1.3557486608	-1.8814732427
H15	-0.5053059232	2.9939768992	-0.5253297078
H16	0.6575944400	2.8868022427	0.7666650240
H17	1.2257811257	3.9383931659	-2.0701030286
H18	1.0465788780	4.9211219872	-0.6173307579

H19	3.0667606146	3.8910957698	0.3824116335
H20	3.4770343881	4.5425526384	-1.2058277599
C21	2.1082174618	-2.8952011066	-2.2493476977
C22	1.2117214407	-1.6667272874	-1.9970699342
C23	0.8975908549	-1.5179496011	-0.4918192597
C24	0.2213108360	-2.8009041538	0.0381454531
C25	1.1188851776	-4.0272246557	-0.2048192162
C26	1.4805394009	-4.1820585950	-1.6908737020
H27	3.0835079981	-2.7300849689	-1.7679979850
H28	2.3033227500	-3.0000970540	-3.3261444933
H29	0.2796853204	-1.7903208386	-2.5674888723
H30	1.7026254814	-0.7707829354	-2.3950358641
H31	1.8388544639	-1.4260189736	0.0617642875
H32	0.0195082330	-2.6945031452	1.1083491925
H33	-0.7395235209	-2.9590327765	-0.4728241136
H34	2.0362011458	-3.9152981904	0.3899681655
H35	0.6172917481	-4.9340363663	0.1596884936
H36	0.5680953711	-4.4132327675	-2.2627500113
H37	2.1631443495	-5.0309942740	-1.8365142857
C38	-3.4377005219	0.9173806822	-2.4495287322
C39	-2.1908894692	1.2008501810	-1.5906427687
C40	-1.6339171106	-0.1035467651	-0.9794714058
C41	-2.7356620549	-0.8067345999	-0.1502847826
C42	-3.9812048097	-1.0910403526	-1.0087235285
C43	-4.5298016002	0.1943309398	-1.6469974008
H44	-3.1527592488	0.2961640680	-3.3140037308
H45	-3.8257960370	1.8607298326	-2.8584412790
H46	-2.4504551217	1.8878410291	-0.7780002848
H47	-1.4332806488	1.6930602093	-2.2124307598
H48	-1.3709149156	-0.7632707715	-1.8203292552
H49	-2.3622445740	-1.7418826971	0.2799350623
H50	-2.9984152070	-0.1599046600	0.6931554921
H51	-3.7297439217	-1.8115199894	-1.8040972854
H52	-4.7534030919	-1.5670512589	-0.3893992631
H53	-4.8927243722	0.8614947208	-0.8524476868
H54	-5.3912777886	-0.0314421562	-2.2916551464

Conformer D,  $\tau_1$

Pd1	-0.0468355899	0.1607319399	2.4072383678
Cl2	0.2575423411	0.2783741142	4.7665048826
Cl3	2.2973387590	0.5983434321	2.0834810804
Cl4	-2.3704210870	-0.2473666695	2.7521872161
P1	-0.1941180496	0.0854621019	0.0593306396
C4	1.7743801852	3.4230033296	-1.8094258922
C5	1.6172599298	2.0317513520	-1.1661206601
C6	0.1560296247	1.7810858834	-0.7321739421
C7	-0.3014345208	2.9073655143	0.2263219152
C8	-0.1472729137	4.2967335583	-0.4159506865
C9	1.2970641830	4.5448736470	-0.8753873089
H10	1.1935669727	3.4604322505	-2.7452036451
H11	2.8253165159	3.5803437864	-2.0892628552
H12	1.9474915800	1.2720970880	-1.8841805964
H13	2.2672049397	1.9496921397	-0.2874055197
H14	-0.4709741351	1.8170781846	-1.6373359821
H15	-1.3385907459	2.7525167978	0.5421202877
H16	0.3049937501	2.8495054638	1.1386154062
H17	-0.8238229185	4.3812680936	-1.2817323511

H18	-0.4585234859	5.0693658711	0.2996620627
H19	1.9524502288	4.5813784755	0.0064633542
H20	1.3816708698	5.5203565624	-1.3750348659
C21	2.1736002889	-2.2160097492	-2.6655527498
C22	0.9633309617	-1.4058214613	-2.1622914834
C23	1.1043695054	-1.0818223414	-0.6600900230
C24	1.2751866746	-2.3762308655	0.1677511622
C25	2.4811533042	-3.1865741625	-0.3408269275
C26	2.3737084669	-3.4984945855	-1.8424234802
H27	3.0783606979	-1.5940212362	-2.5931468053
H28	2.0446522430	-2.4595914544	-3.7297781551
H29	0.0509020131	-1.9934479220	-2.3345104629
H30	0.8589645753	-0.4889369701	-2.7568552695
H31	2.0274468175	-0.5093443666	-0.5097059326
H32	1.4139025976	-2.1158385457	1.2212100742
H33	0.3709855299	-2.9965190428	0.1049862745
H34	3.3997355817	-2.6120851450	-0.1519855265
H35	2.5718459639	-4.1177394334	0.2343377681
H36	1.5183079708	-4.1705606568	-2.0130580475
H37	3.2671180415	-4.0361676313	-2.1896438825
C38	-4.1928187484	0.2544776260	-1.4239462032
C39	-2.9248766959	0.6527928621	-0.6461763852
C40	-1.7964090119	-0.3887674121	-0.8320253225
C41	-2.2931229844	-1.8029583295	-0.4560927375
C42	-3.5676398675	-2.1835868822	-1.2313373502
C43	-4.6825234367	-1.1470408258	-1.0323650930
H44	-3.9843237071	0.2747927896	-2.5061411978
H45	-4.9802935743	0.9991637992	-1.2441482391
H46	-3.1546164698	0.7369006145	0.4215284435
H47	-2.5957971004	1.6404474595	-0.9898174199
H48	-1.5240889788	-0.3936179855	-1.9003101151
H49	-1.5164046545	-2.5485277713	-0.6592231542
H50	-2.4914974728	-1.8285462688	0.6210374376
H51	-3.3366075556	-2.2635581351	-2.3061457080
H52	-3.9074739178	-3.1778963588	-0.9107495568
H53	-4.9845233864	-1.1410615969	0.0241164558
H54	-5.5711840737	-1.4210680881	-1.6186431357

Conformer D,  $\tau_2$

Pd1	-0.0501381643	0.1644832961	2.4221421648
Cl2	0.2617270192	0.2839515188	4.7818053489
Cl3	-2.3456507582	-0.3731776651	2.7768563133
Cl4	2.2721196695	0.6982845572	2.0829960704
P1	-0.2050004962	0.0895866229	0.0749352666
C4	1.6911491074	3.4446499357	-1.8450512376
C5	1.5637647345	2.0536924808	-1.1943781548
C6	0.1150437796	1.7884755139	-0.7270591512
C7	-0.3312465483	2.9138548387	0.2362479264
C8	-0.2098346622	4.3024952041	-0.4141307538
C9	1.2215185267	4.5649816960	-0.9050295507
H10	1.0895883695	3.4717166429	-2.7679458846
H11	2.7338768346	3.6131044455	-2.1482985794
H12	1.8870491846	1.2960216557	-1.9175878990
H13	2.2326194415	1.9813567064	-0.3291853409
H14	-0.5308994027	1.8162921993	-1.6190843887
H15	-1.3572266396	2.7461638624	0.5797369699
H16	0.3002365064	2.8677835871	1.1317614702



H17	-0.9085345351	4.3765669567	-1.2633201273
H18	-0.5116620398	5.0742463004	0.3065247900
H19	1.8951412833	4.6124455432	-0.0375149655
H20	1.2845158656	5.5392721751	-1.4101618577
C21	2.1891365820	-2.1850350887	-2.6501440453
C22	0.9681232426	-1.3928682684	-2.1442048425
C23	1.1127253667	-1.0552507920	-0.6450978194
C24	1.3157923182	-2.3391687228	0.1914840367
C25	2.5321337670	-3.1315849899	-0.3210189772
C26	2.4178159725	-3.4574741916	-1.8191529260
H27	3.0830897172	-1.5465401631	-2.5885406494
H28	2.0572008002	-2.4388800035	-3.7116103223
H29	0.0653538152	-1.9978592415	-2.3058733712
H30	0.8432260289	-0.4823078564	-2.7442872762
H31	2.0249944849	-0.4637766180	-0.5030825321
H32	1.4588074162	-2.0669155239	1.2413894032
H33	0.4226731299	-2.9765988441	0.1431347744
H34	3.4419445112	-2.5395497224	-0.1443174627
H35	2.6441798242	-4.0564960584	0.2604960937
H36	1.5723610973	-4.1450218708	-1.9773140483
H37	3.3171632386	-3.9828539076	-2.1698575158
C38	-4.2091422510	0.1894386692	-1.3906687738
C39	-2.9525079196	0.5953146711	-0.5993784886
C40	-1.7998206729	-0.4126651609	-0.8152433821
C41	-2.2631665449	-1.8464735927	-0.4713810898
C42	-3.5235539877	-2.2377964870	-1.2638311514
C43	-4.6639050771	-1.2345151121	-1.0421495489
H44	-4.0003320183	0.2473103697	-2.4714235225
H45	-5.0155376329	0.9080821611	-1.1899067521
H46	-3.1838699224	0.6397350615	0.4704987909
H47	-2.6483628895	1.6012676348	-0.9104960305
H48	-1.5346802290	-0.3853800941	-1.8850511746
H49	-1.4685705000	-2.5690804145	-0.6878396380
H50	-2.4649155301	-1.9003279004	0.6039723611
H51	-3.2858120177	-2.2844920288	-2.3392439296
H52	-3.8417658147	-3.2477052047	-0.9709757924
H53	-4.9701515534	-1.2660298999	0.0126751102
H54	-5.5435878606	-1.5137366268	-1.6395822575

#### Conformer D, $\tau_3$

Pd1	-0.0567793036	0.1354558407	2.4087730523
Cl2	0.2522707815	0.2134338713	4.7701341842
Cl3	-2.3909423319	-0.2225452994	2.7430619217
Cl4	2.2928139120	0.5468475629	2.0836609145
P1	-0.2045587145	0.0677410760	0.0616671337
C4	1.8314536245	3.3628386522	-1.8086164772
C5	1.6458512660	1.9764381211	-1.1625009175
C6	0.1782990595	1.7535581015	-0.7348423633
C7	-0.2647897262	2.8908348100	0.2174502964
C8	-0.0815895065	4.2754522246	-0.4276847618
C9	1.3695911954	4.4956945585	-0.8800292225
H10	1.2563772323	3.4084125075	-2.7475989599
H11	2.8865196227	3.5007122495	-2.0832597627
H12	1.9654024380	1.2085634533	-1.8770626257
H13	2.2899284064	1.8837341817	-0.2805728705
H14	-0.4434327526	1.7977809029	-1.6430658146
H15	-1.3063211940	2.7557594580	0.5279240150

H16	0.3354444427	2.8239996689	1.1332467347
H17	-0.7518484754	4.3701004405	-1.2972995579
H18	-0.3822737552	5.0557949012	0.2841355965
H19	2.0208609439	4.5225421434	0.0052246789
H20	1.4747565600	5.4681581452	-1.3817436412
C21	2.1412305975	-2.2717970009	-2.6514778474
C22	0.9390030136	-1.4462961641	-2.1539754363
C23	1.0789554970	-1.1207149943	-0.6521851549
C24	1.2326556548	-2.4141804577	0.1800428753
C25	2.4304011307	-3.2399933206	-0.3231952943
C26	2.3233085140	-3.5545425301	-1.8243161714
H27	3.0530442903	-1.6603599230	-2.5775612486
H28	2.0128693152	-2.5164960201	-3.7155272775
H29	0.0205412040	-2.0239908493	-2.3279898406
H30	0.8474077262	-0.5293450765	-2.7507419993
H31	2.0089334023	-0.5599286422	-0.5004015053
H32	1.3723803155	-2.1524034069	1.2329457254
H33	0.3216402110	-3.0242821377	0.1177217595
H34	3.3550988458	-2.6756450108	-0.1336552473
H35	2.5087853986	-4.1705127482	0.2547946600
H36	1.4603352129	-4.2166406370	-1.9958014443
H37	3.2111665428	-4.1039782675	-2.1673460631
C38	-4.1972596111	0.2929240435	-1.4320314843
C39	-2.9273318141	0.6723306199	-0.6481855997
C40	-1.8119723280	-0.3830804103	-0.8330582805
C41	-2.3291084812	-1.7912669752	-0.4605097776
C42	-3.6051539187	-2.1533738740	-1.2423648237
C43	-4.7072000408	-1.1027393229	-1.0460973407
H44	-3.9837884030	0.3129960699	-2.5132753626
H45	-4.9756490753	1.0475177055	-1.2537838295
H46	-3.1595887887	0.7545092235	0.4191828866
H47	-2.5848727142	1.6570385856	-0.9870219447
H48	-1.5375035493	-0.3888934019	-1.9006961098
H49	-1.5613827556	-2.5465779098	-0.6620901185
H50	-2.5315270318	-1.8149796749	0.6159374005
H51	-3.3705621744	-2.2343490270	-2.3163719398
H52	-3.9599329104	-3.1436022043	-0.9253239253
H53	-5.0135013536	-1.0954133797	0.0091311084
H54	-5.5969674636	-1.3634264631	-1.6368504157

#### Conformer E, $\tau_1$

Pd1	-0.3114693764	0.1491062542	2.3825710954
Cl2	-0.8821795907	0.1786260642	4.6956223583
Cl3	1.9996834644	0.0673746815	2.9630546729
Cl4	-2.6496686954	0.2295475213	1.7887570064
P1	0.0741591358	0.1196507326	0.0628361042
C4	3.9627800268	-1.2725353663	-0.9696426683
C5	2.5703957464	-1.2319064128	-0.3134755006
C6	1.8052824249	0.0593139311	-0.6878082052
C7	2.6499041524	1.3035535879	-0.3247599732
C8	4.0417687798	1.2517015075	-0.9810461729
C9	4.7954326526	-0.0336255783	-0.6103106590
H10	3.8536263404	-1.3295486670	-2.0650497849
H11	4.4864180948	-2.1875435047	-0.6604145881
H12	2.0055144558	-2.1182602371	-0.6216597433
H13	2.6698978552	-1.2747046692	0.7767953034
H14	1.6494357665	0.0588555898	-1.7787227471

H15	2.1410598636	2.2209505525	-0.6395643803
H16	2.7525699095	1.3487593397	0.7651200528
H17	3.9360503917	1.3055598777	-2.0769354225
H18	4.6216507766	2.1348935951	-0.6798623439
H19	4.9940667098	-0.0349400009	0.4703766728
H20	5.7710470073	-0.0665191413	-1.1160603037
C21	-1.7162327242	-3.7130104198	-0.2612065921
C22	-0.7820034153	-2.5982703670	0.2393166688
C23	-0.8583997362	-1.3548412621	-0.6788922858
C24	-0.5446416043	-1.7383975491	-2.1413262154
C25	-1.4814103762	-2.8591435127	-2.6339259936
C26	-1.4228098799	-4.0924454073	-1.7206428659
H27	-2.7577106719	-3.3705520206	-0.1747415983
H28	-1.6222538284	-4.5939328386	0.3878335853
H29	0.2471571772	-2.9804780684	0.2786416927
H30	-1.0527349511	-2.3112987108	1.2597267768
H31	-1.8962814550	-1.0000214046	-0.6261828394
H32	-0.6413877985	-0.8741255469	-2.8071287737
H33	0.4948355324	-2.0839687480	-2.2272105295
H34	-2.5132267042	-2.4777608671	-2.6597344825
H35	-1.2222568606	-3.1326191320	-3.6667540706
H36	-0.4187601757	-4.5400833456	-1.7847383659
H37	-2.1288742013	-4.8582950095	-2.0712919313
C38	-1.2871088825	3.1296284087	-2.7051246525
C39	-0.4179591566	1.9687447836	-2.1818696135
C40	-0.7661308947	1.6312193542	-0.7156429825
C41	-0.6255474616	2.8867898597	0.1781577355
C42	-1.4913663157	4.0424984386	-0.3520859801
C43	-1.1672601476	4.3766874847	-1.8163473590
H44	-2.3383043054	2.8054665446	-2.7324832998
H45	-1.0051859659	3.3667767283	-3.7409619962
H46	0.6395322242	2.2556999542	-2.2626691249
H47	-0.5545061626	1.0986978909	-2.8330612228
H48	-1.8232554618	1.3381608156	-0.6668058151
H49	-0.9198399521	2.6370099534	1.2017080640
H50	0.4236755520	3.2099950429	0.2179144022
H51	-2.5509978077	3.7604591870	-0.2674645698
H52	-1.3528933908	4.9291548699	0.2809370594
H53	-0.1397653433	4.7671982862	-1.8812274644
H54	-1.8282305250	5.1724766608	-2.1875539511

#### Conformer E, $\tau_2$

Pd1	-0.3022762449	0.1431643225	2.3759942718
Cl2	-0.8689923743	0.1595712214	4.6895496717
Cl3	-2.6417632079	0.0931482390	1.7845996254
Cl4	2.0084412174	0.2623744617	2.9511165612
P1	0.0800652012	0.1102625848	0.0545721691
C4	3.9897553507	-1.2426267355	-0.9203182440
C5	2.6000516777	-1.1880994374	-0.2605604829
C6	1.8115846144	0.0692446954	-0.6991939155
C7	2.6353519011	1.3448065267	-0.4066023818
C8	4.0277026745	1.2786246700	-1.0618091183
C9	4.8028275699	0.0264510288	-0.6275149310
H10	3.8784994935	-1.3578629514	-2.0109208036
H11	4.5289078659	-2.1318371890	-0.5659534322
H12	2.0468218950	-2.0992678126	-0.5134949308
H13	2.7058974211	-1.1684911217	0.8297495475

H14	1.6535540499	0.0117875066	-1.7880096644
H15	2.1123362653	2.2337347576	-0.7749860543
H16	2.7376129803	1.4544234135	0.6786512252
H17	3.9190794237	1.2734553983	-2.1587429012
H18	4.5943672385	2.1853331842	-0.8091289793
H19	5.0036355254	0.0834282340	0.4512757322
H20	5.7778120330	-0.0160630350	-1.1337259843
C21	-1.7176250887	-3.7187473597	-0.3173770969
C22	-0.7998219831	-2.6058849481	0.2168747837
C23	-0.8223286007	-1.3717389788	-0.7165994277
C24	-0.4287066464	-1.7796254957	-2.1535678271
C25	-1.3548767451	-2.8912037984	-2.6846928210
C26	-1.3598112465	-4.1157722139	-1.7575955679
H27	-2.7588103223	-3.3663834933	-0.2826001925
H28	-1.6624603069	-4.5940639603	0.3435617966
H29	0.2248290824	-2.9928719694	0.3078687470
H30	-1.1181521384	-2.3061821066	1.2190435976
H31	-1.8607508039	-1.0153303535	-0.7304840973
H32	-0.4647789857	-0.9248104952	-2.8373119195
H33	0.6065072948	-2.1468508687	-2.1695825050
H34	-2.3784334427	-2.4960234605	-2.7686659995
H35	-1.0458399528	-3.1791478759	-3.6997498377
H36	-0.3605344948	-4.5781618473	-1.7688873319
H37	-2.0591797515	-4.8749555227	-2.1351396437
C38	-1.4123750857	3.0843977495	-2.6801242233
C39	-0.5300160545	1.9204426546	-2.1870990526
C40	-0.7963906050	1.6097673605	-0.6989663404
C41	-0.6143490297	2.8755304430	0.1730740775
C42	-1.5002970327	4.0270746132	-0.3317640183
C43	-1.2388169045	4.3398534149	-1.8129354849
H44	-2.4664756341	2.7701355199	-2.6519363014
H45	-1.1795949626	3.3070626366	-3.7312614368
H46	0.5255413841	2.1875413511	-2.3359365337
H47	-0.7214411409	1.0414077908	-2.8117797693
H48	-1.8479360611	1.3120389672	-0.5895753654
H49	-0.8629672763	2.6359141062	1.2117451047
H50	0.4348079314	3.1996983016	0.1656768238
H51	-2.5563744598	3.7507641800	-0.1980474661
H52	-1.3309370040	4.9214366323	0.2826003380
H53	-0.2113034125	4.7186722082	-1.9283815823
H54	-1.9072198006	5.1385795166	-2.1639143641

#### Conformer E, $\tau_3$

Pd1	-0.2637242763	0.1875268085	2.4336294604
Cl2	-0.8086942466	0.1075779325	4.7495263382
Cl3	-2.5685163515	0.6443517899	1.9222610120
Cl4	1.9902825629	-0.3932231002	2.9552456637
P1	0.0788295431	0.1832650432	0.0880681690
C4	3.9429785895	-1.2112347260	-1.1398621869
C5	2.5435387534	-1.2462607575	-0.4949367262
C6	1.8149245436	0.1048149691	-0.6639429666
C7	2.6870315622	1.2644086331	-0.1191433336
C8	4.0808651437	1.2829779056	-0.7693733373
C9	4.7989710092	-0.0621517976	-0.5889447737
H10	3.8429667345	-1.0937905295	-2.2315091066
H11	4.4457316313	-2.1742385510	-0.9756031823
H12	1.9614541589	-2.0496892772	-0.9599041147

H13	2.6266341000	-1.4766010064	0.5722070861
H14	1.6725599489	0.2626107171	-1.7437443666
H15	2.1953065386	2.2288356151	-0.2873323026
H16	2.7880780587	1.1438200534	0.9652046993
H17	3.9874016647	1.5034435725	-1.8452698318
H18	4.6775870888	2.0962061270	-0.3340747647
H19	4.9822099284	-0.2304961898	0.4813521915
H20	5.7803363663	-0.0441545860	-1.0841330756
C21	-1.6495829155	-3.6974686409	-0.1869363913
C22	-0.6628919130	-2.5941594825	0.2362755891
C23	-0.9155717197	-1.2915073052	-0.5607868782
C24	-0.8551723605	-1.5516947033	-2.0810176780
C25	-1.8298910432	-2.6724185941	-2.4951149456
C26	-1.5898249723	-3.9627126009	-1.6986864715
H27	-2.6698225018	-3.3952420506	0.0911188094
H28	-1.4349566460	-4.6204679917	0.3680607810
H29	0.3618178064	-2.9518605523	0.0792187562
H30	-0.7625941553	-2.3887810104	1.3074306035
H31	-1.9324181530	-0.9670764906	-0.2995030222
H32	-1.1027975206	-0.6429607390	-2.6409330045
H33	0.1659048485	-1.8366444454	-2.3742086633
H34	-2.8608446744	-2.3292939119	-2.3225965841
H35	-1.7406891206	-2.8656356254	-3.5738203452
H36	-0.5989396943	-4.3677898097	-1.9570173564
H37	-2.3244345993	-4.7277191858	-1.9871313324
C38	-1.0294044238	3.1382782737	-2.8668738642
C39	-0.1761583231	2.0284086620	-2.2191865163
C40	-0.7231533882	1.6614037671	-0.8214113362
C41	-0.7755040695	2.9162833455	0.0785459037
C42	-1.6003594504	4.0403084494	-0.5765690887
C43	-1.0929562022	4.3918595579	-1.9832808061
H44	-2.0490613215	2.7587469589	-3.0329480095
H45	-0.6224826937	3.3892261817	-3.8567195154
H46	0.8580748114	2.3886075288	-2.1383094176
H47	-0.1510091348	1.1560960721	-2.8820330268
H48	-1.7628554605	1.3277587379	-0.9430083657
H49	-1.2568051080	2.6779850605	1.0439751479
H50	0.2396842621	3.2817168759	0.2858443911
H51	-2.6503245763	3.7184059724	-0.6412631472
H52	-1.5891734037	4.9332985809	0.0623811167
H53	-0.0850418043	4.8279784925	-1.9045033122
H54	-1.7294749971	5.1554974837	-2.4526773528

#### Conformer F, $\tau_1$

Pd1	-0.0420110260	0.1077329135	2.4274465275
Cl2	-0.0566077282	0.2870336599	4.8037115421
Cl3	2.1159202988	-0.9206078094	2.5232520962
Cl4	-2.1486937793	1.2568298872	2.3326166839
P1	-0.0468609356	-0.0216932237	0.0801888057
C4	2.6295617034	3.1484888258	-0.7557516215
C5	2.0490711317	1.8524709730	-0.1639836045
C6	0.6187843408	1.5721745259	-0.6822784218
C7	-0.2982085286	2.7870704979	-0.4177210163
C8	0.2947974809	4.0790945792	-1.0079545988
C9	1.7129126737	4.3501267646	-0.4857733861
H10	2.7617214152	3.0312947098	-1.8434792930
H11	3.6292600718	3.3264535767	-0.3371879994

H12	2.7158941698	1.0131083478	-0.3922849963
H13	2.0212671208	1.9234726017	0.9306269252
H14	0.6699224792	1.4182220396	-1.7710834006
H15	-1.2923929178	2.6193635107	-0.8478973676
H16	-0.4519037886	2.8998236939	0.6616330098
H17	0.3251836836	4.0015765116	-2.1069477662
H18	-0.3665670451	4.9241614733	-0.7736383597
H19	1.6696639613	4.5336804317	0.5974105800
H20	2.1241786782	5.2597839029	-0.9458364201
C21	2.6129104194	-2.3014808441	-2.4083527366
C22	1.5127170069	-1.2672697887	-2.0951698767
C23	1.1029617244	-1.3490900346	-0.6091202643
C24	0.6344827538	-2.7762396373	-0.2517726383
C25	1.7356469875	-3.8046821845	-0.5629619009
C26	2.1817199797	-3.7278880736	-2.0317750715
H27	3.5201867180	-2.0388328410	-1.8447471253
H28	2.8787182677	-2.2504291221	-3.4738828946
H29	0.6499865404	-1.4588480644	-2.7462779469
H30	1.8805286014	-0.2660858566	-2.3481076002
H31	1.9980869818	-1.1712645862	0.0005745711
H32	0.3735166472	-2.8232966966	0.8105336985
H33	-0.2645989537	-3.0341182510	-0.8290585734
H34	2.5934319612	-3.6114282256	0.0959021863
H35	1.3782294978	-4.8163147262	-0.3264251500
H36	1.3459767155	-4.0339225679	-2.6808464368
H37	3.0006894305	-4.4351035215	-2.2238818496
C38	-4.0618865802	-1.2648939297	-0.4642664512
C39	-2.5925544212	-1.3465827084	-0.0150380465
C40	-1.7712673689	-0.2058929854	-0.6563520979
C41	-1.8769876037	-0.2571248101	-2.1943780531
C42	-3.3493796222	-0.1719576299	-2.6416042137
C43	-4.1981477438	-1.2787310049	-1.9954639993
H44	-4.5008046035	-0.3400808583	-0.0637504839
H45	-4.6312844854	-2.0958737287	-0.0261976810
H46	-2.1828860126	-2.3239352224	-0.3021666291
H47	-2.5326467568	-1.2662431880	1.0740895991
H48	-2.2435398831	0.7206318219	-0.3066042779
H49	-1.3026558362	0.5541056548	-2.6594828405
H50	-1.4523534048	-1.1992812960	-2.5668600770
H51	-3.7549664899	0.8098551177	-2.3554597165
H52	-3.4121776421	-0.2307964391	-3.7376049582
H53	-3.8655250054	-2.2555035609	-2.3806111957
H54	-5.2515081931	-1.1700138255	-2.2896009446

#### Conformer F, $\tau_2$

Pd1	-0.1199858544	0.1659032772	2.3765413413
Cl2	-0.0979698019	0.3800784459	4.7491742699
Cl3	1.9650296156	-1.0080510215	2.4796048986
Cl4	-2.1503251245	1.4361760357	2.2811362505
P1	-0.1217187697	0.0381323357	0.0275426971
C4	2.6522171264	3.1292790144	-0.7692144503
C5	2.0167861309	1.8662535483	-0.1624423855
C6	0.6018717861	1.6073328557	-0.7314974152
C7	-0.2945665609	2.8485817965	-0.5288823381
C8	0.3511142922	4.1097163676	-1.1317630654
C9	1.7574268110	4.3609912745	-0.5690012308
H10	2.8205436216	2.9760212387	-1.8474633343

H11	3.6401838396	3.2959227808	-0.3194865564
H12	2.6705668013	1.0037776839	-0.3349431029
H13	1.9435939074	1.9736612964	0.9272896592
H14	0.6911127189	1.4332580409	-1.8147368086
H15	-1.2758831132	2.6935179754	-0.9923626086
H16	-0.4838898853	2.9924687151	0.5412127151
H17	0.4163513439	4.0006181575	-2.2265796395
H18	-0.2960756578	4.9771940064	-0.9438379756
H19	1.6820757435	4.5803585344	0.5057078510
H20	2.2072836910	5.2451101073	-1.0426023932
C21	2.4619358231	-2.3263916456	-2.4645203428
C22	1.3976115457	-1.2550459064	-2.1517643099
C23	0.9819111715	-1.3258083458	-0.6662316636
C24	0.4622185094	-2.7370880781	-0.3148057254
C25	1.5293162880	-3.8013139116	-0.6239952531
C26	1.9822244212	-3.7375899759	-2.0910534317
H27	3.3766907474	-2.0953748490	-1.8990497389
H28	2.7314280538	-2.2832289301	-3.5295126852
H29	0.5297434774	-1.4144782086	-2.8049223347
H30	1.8023001757	-0.2679174370	-2.4026606178
H31	1.8822341493	-1.1840473294	-0.0550373303
H32	0.1963442248	-2.7774136589	0.7462226635
H33	-0.4428147676	-2.9605677450	-0.8972427656
H34	2.3902840430	-3.6373585018	0.0385945698
H35	1.1384358290	-4.8012920180	-0.3908628622
H36	1.1388420908	-4.0149389266	-2.7431641173
H37	2.7781981588	-4.4709200603	-2.2816103721
C38	-4.1809125999	-1.0504121859	-0.5206221802
C39	-2.7158243885	-1.1881182970	-0.0709444156
C40	-1.8508046632	-0.0784480255	-0.7101860209
C41	-1.9588370147	-0.1215591122	-2.2484889816
C42	-3.4269086054	0.0184119789	-2.6958431647
C43	-4.3163323934	-1.0570543180	-2.0519441187
H44	-4.5843386233	-0.1101695890	-0.1188963290
H45	-4.7820336407	-1.8597791791	-0.0843769804
H46	-2.3429982003	-2.1798339944	-0.3596477632
H47	-2.6531015389	-1.1143222791	1.0185179925
H48	-2.2858246679	0.8653127863	-0.3572445986
H49	-1.3547215534	0.6688998325	-2.7117191417
H50	-1.5681646008	-1.0776302249	-2.6227068173
H51	-3.7961376777	1.0140950407	-2.4083540146
H52	-3.4916795525	-0.0366268527	-3.7919267833
H53	-4.0197845751	-2.0450698228	-2.4379734575
H54	-5.3646381171	-0.9089400829	-2.3468825071

#### Conformer F, $\tau_3$

Pd1	-0.1175973952	0.1723037657	2.3761720803
Cl2	-0.1330441251	0.3466409277	4.7533467691
Cl3	-2.2183062338	1.3265462011	2.2877336814
Cl4	2.0375631711	-0.8647473895	2.4785821477
P1	-0.1110380582	0.0371527664	0.0282764297
C4	2.6127912452	3.1624579058	-0.8269004647
C5	2.0212219185	1.8732905612	-0.2300633886
C6	0.5809633253	1.6192589150	-0.7324217597
C7	-0.3139170631	2.8478459057	-0.4514187769
C8	0.2893253953	4.1330029123	-1.0467570872
C9	1.7191865712	4.3787097987	-0.5436398695

H10	2.7283764460	3.0448063576	-1.9164691950
H11	3.6206775432	3.3247721748	-0.4219014873
H12	2.6714997623	1.0247725226	-0.4716809209
H13	2.0089207154	1.9401294323	0.8649291254
H14	0.6182110932	1.4701687153	-1.8223824004
H15	-1.3172424064	2.6960731040	-0.8658561026
H16	-0.4482839370	2.9601366138	0.6309423933
H17	0.3023071092	4.0580293146	-2.1461796877
H18	-0.3551092684	4.9876358160	-0.8001743631
H19	1.6931913455	4.5618527710	0.5401812382
H20	2.1398653077	5.2817839849	-1.0080687530
C21	2.4949652128	-2.2931833120	-2.4668192754
C22	1.3934271011	-1.2608238878	-2.1524030879
C23	1.0225287390	-1.3070593278	-0.6546912591
C24	0.5697701400	-2.7280738037	-0.2533343979
C25	1.6720316452	-3.7555279728	-0.5637473471
C26	2.0854265262	-3.7128283980	-2.0434446181
H27	3.4135550997	-2.0084198215	-1.9329963328
H28	2.7339867098	-2.2677443662	-3.5396202242
H29	0.5146760253	-1.4803782255	-2.7730118818
H30	1.7425809350	-0.2632922941	-2.4437493962
H31	1.9318041780	-1.1127382891	-0.0718524835
H32	0.3319903903	-2.7513264043	0.8147258705
H33	-0.3388790855	-3.0050827694	-0.8060040485
H34	2.5418907590	-3.5394497063	0.0716962622
H35	1.3283199155	-4.7637921306	-0.2948413662
H36	1.2387234773	-4.0429205442	-2.6659775334
H37	2.9066648604	-4.4175088904	-2.2352613372
C38	-4.1300818705	-1.1692462281	-0.5515578175
C39	-2.6570667751	-1.2795330357	-0.1208798080
C40	-1.8356311103	-0.1129265771	-0.7138248581
C41	-1.9517441849	-0.0955585635	-2.2519410522
C42	-3.4273219828	0.0176307780	-2.6828730966
C43	-4.2786076198	-1.1116909238	-2.0805492239
H44	-4.5594243963	-0.2618259905	-0.1041404741
H45	-4.7003963664	-2.0169380661	-0.1478597560
H46	-2.2555126344	-2.2426653885	-0.4628586813
H47	-2.5867634943	-1.2580075709	0.9704839839
H48	-2.3024484479	0.7991500196	-0.3208246793
H49	-1.3771405633	0.7326880725	-2.6852645110
H50	-1.5345739358	-1.0217652704	-2.6699372541
H51	-3.8245504244	0.9879980451	-2.3499816366
H52	-3.4989904410	0.0080575521	-3.7798739783
H53	-3.9560741700	-2.0721777226	-2.5125028174
H54	-5.3334669660	-0.9825897712	-2.3606963472

#### Conformer G, $\tau_1$

Pd1	-0.1175973952	0.1723037657	2.3761720803
Cl2	-0.1330441251	0.3466409277	4.7533467691
Cl3	-2.2183062338	1.3265462011	2.2877336814
Cl4	2.0375631711	-0.8647473895	2.4785821477
P1	-0.1110380582	0.0371527664	0.0282764297
C4	2.6127912452	3.1624579058	-0.8269004647
C5	2.0212219185	1.8732905612	-0.2300633886
C6	0.5809633253	1.6192589150	-0.7324217597
C7	-0.3139170631	2.8478459057	-0.4514187769
C8	0.2893253953	4.1330029123	-1.0467570872

C9	1.7191865712	4.3787097987	-0.5436398695
H10	2.7283764460	3.0448063576	-1.9164691950
H11	3.6206775432	3.3247721748	-0.4219014873
H12	2.6714997623	1.0247725226	-0.4716809209
H13	2.0089207154	1.9401294323	0.8649291254
H14	0.6182110932	1.4701687153	-1.8223824004
H15	-1.3172424064	2.6960731040	-0.8658561026
H16	-0.4482839370	2.9601366138	0.6309423933
H17	0.3023071092	4.0580293146	-2.1461796877
H18	-0.3551092684	4.9876358160	-0.8001743631
H19	1.6931913455	4.5618527710	0.5401812382
H20	2.1398653077	5.2817839849	-1.0080687530
C21	2.4949652128	-2.2931833120	-2.4668192754
C22	1.3934271011	-1.2608238878	-2.1524030879
C23	1.0225287390	-1.3070593278	-0.6546912591
C24	0.5697701400	-2.7280738037	-0.2533343979
C25	1.6720316452	-3.7555279728	-0.5637473471
C26	2.0854265262	-3.7128283980	-2.0434446181
H27	3.4135550997	-2.0084198215	-1.9329963328
H28	2.7339867098	-2.2677443662	-3.5396202242
H29	0.5146760253	-1.4803782255	-2.7730118818
H30	1.7425809350	-0.2632922941	-2.4437493962
H31	1.9318041780	-1.1127382891	-0.0718524835
H32	0.3319903903	-2.7513264043	0.8147258705
H33	-0.3388790855	-3.0050827694	-0.8060040485
H34	2.5418907590	-3.5394497063	0.0716962622
H35	1.3283199155	-4.7637921306	-0.2948413662
H36	1.2387234773	-4.0429205442	-2.6659775334
H37	2.9066648604	-4.4175088904	-2.2352613372
C38	-4.1300818705	-1.1692462281	-0.5515578175
C39	-2.6570667751	-1.2795330357	-0.1208798080
C40	-1.8356311103	-0.1129265771	-0.7138248581
C41	-1.9517441849	-0.0955585635	-2.2519410522
C42	-3.4273219828	0.0176307780	-2.6828730966
C43	-4.2786076198	-1.1116909238	-2.0805492239
H44	-4.5594243963	-0.2618259905	-0.1041404741
H45	-4.7003963664	-2.0169380661	-0.1478597560
H46	-2.2555126344	-2.2426653885	-0.4628586813
H47	-2.5867634943	-1.2580075709	0.9704839839
H48	-2.3024484479	0.7991500196	-0.3208246793
H49	-1.3771405633	0.7326880725	-2.6852645110
H50	-1.5345739358	-1.0217652704	-2.6699372541
H51	-3.8245504244	0.9879980451	-2.3499816366
H52	-3.4989904410	0.0080575521	-3.7798739783
H53	-3.9560741700	-2.0721777226	-2.5125028174
H54	-5.3334669660	-0.9825897712	-2.3606963472

#### Conformer G, $\tau_2$

Pd1	0.1405589811	0.1680897506	2.3815304684
Cl2	0.7236377655	0.3735903998	4.6763964075
Cl3	-1.2222718379	-1.6953735002	2.9585485991
Cl4	1.8414791656	1.7910235470	1.8562443893
P1	-0.3016946105	0.0842601822	0.0324973956
C4	-4.1484842358	-1.7431761522	-0.5451863011
C5	-2.7783174442	-1.4832525248	0.1053237993
C6	-1.9175524695	-0.5482016771	-0.7671119054
C7	-1.7643615815	-1.1501338936	-2.1849411428

C8	-3.1360527537	-1.4118731864	-2.8363137273
C9	-4.0157802483	-2.3169409395	-1.9627228099
H10	-4.7152809644	-0.7995388433	-0.5906480470
H11	-4.7306411143	-2.4239441202	0.0899479123
H12	-2.9046363046	-1.0633515609	1.1039916460
H13	-2.2562581859	-2.4354308618	0.2587266599
H14	-2.4874734381	0.3881717975	-0.8716349916
H15	-1.1752154103	-0.4991405527	-2.8357837125
H16	-1.2219941249	-2.1016484095	-2.1146184131
H17	-3.6489585496	-0.4504959563	-2.9948786312
H18	-2.9935488788	-1.8561738975	-3.8315809001
H19	-3.5588340214	-3.3166435062	-1.9061751761
H20	-5.0044701162	-2.4499457289	-2.4241628390
C21	-0.8722464447	4.2544650515	-0.2881936353
C22	-1.0634096383	2.7911249572	0.1393658435
C23	-0.1894169586	1.8299172040	-0.7016878384
C24	-0.4932541976	2.0272702505	-2.2030425430
C25	-0.2709805031	3.4930084056	-2.6235735134
C26	-1.1291999042	4.4542470994	-1.7881485720
H27	0.1556433656	4.5579976792	-0.0437151063
H28	-1.5375711787	4.9000135622	0.3011810169
H29	-2.1265589091	2.5202420122	0.0335736643
H30	-0.7976323294	2.6827992024	1.1950482202
H31	0.8528497320	2.1057040308	-0.5085954958
H32	0.1288884401	1.3752995390	-2.8245592527
H33	-1.5388788665	1.7650462292	-2.4167435002
H34	0.7908547270	3.7488762000	-2.4928362084
H35	-0.4930077075	3.6080572430	-3.6940700466
H36	-2.1927006191	4.2673232980	-2.0055150537
H37	-0.9295588253	5.4953857647	-2.0775411413
C38	3.0438583333	-1.5395113551	-2.1739522451
C39	1.7091669028	-0.7845187822	-2.0099418063
C40	1.1924998849	-0.9108884196	-0.5610381152
C41	1.0569699546	-2.3942098896	-0.1412997432
C42	2.3905056727	-3.1404819450	-0.3200574489
C43	2.9243222120	-3.0133373768	-1.7556602686
H44	3.8081483221	-1.0494803621	-1.5533697141
H45	3.3880494413	-1.4631453351	-3.2151305036
H46	0.9799825507	-1.1926195014	-2.7213600442
H47	1.8612743909	0.2688869077	-2.2710113093
H48	1.9594391191	-0.4646339596	0.0878640046
H49	0.7217131842	-2.4620558029	0.8995964060
H50	0.2897468455	-2.8889981662	-0.7544418296
H51	3.1280311557	-2.7268649709	0.3826645781
H52	2.2624327096	-4.1979080147	-0.0519865384
H53	2.2376445875	-3.5301807247	-2.4446384465
H54	3.8976947472	-3.5143893201	-1.8508081676

#### Conformer G, $\tau_3$

Pd1	-0.2552812227	0.2092978599	2.3853647031
Cl2	-0.4619594635	0.4593799127	4.7476211995
Cl3	-2.5457873469	0.9048043994	2.1078987568
Cl4	2.0624078864	-0.3208388711	2.6515526032
P1	-0.0999717823	-0.0026259347	0.0448351269
C4	-3.6263027183	-2.3092076508	-0.3385656126
C5	-2.2231910289	-1.8995100969	0.1405665318
C6	-1.6675913982	-0.7357097859	-0.7193512022

C7	-1.6279096199	-1.1728898413	-2.2013795373
C8	-3.0328342395	-1.5771078876	-2.6909745917
C9	-3.6377453767	-2.6926510404	-1.8260954825
H10	-4.3149254896	-1.4695021692	-0.1672547303
H11	-3.9956512556	-3.1444687909	0.2715843732
H12	-2.2669249761	-1.5961511441	1.1884005966
H13	-1.5504587885	-2.7655044348	0.0724547531
H14	-2.3792499954	0.0944658608	-0.6131754691
H15	-1.2354991279	-0.3848206423	-2.8485912484
H16	-0.9559939402	-2.0352933885	-2.3107611996
H17	-3.6900025308	-0.6950232239	-2.6585799491
H18	-2.9828467644	-1.8916449426	-3.7433521380
H19	-3.0495651321	-3.6128575202	-1.9675708787
H20	-4.6596397639	-2.9214694470	-2.1601912641
C21	0.1360085764	4.2343994421	-0.2761816939
C22	-0.2802756054	2.8468432392	0.2398176387
C23	0.2116603633	1.7200936177	-0.6989006185
C24	-0.2910734554	1.9731475671	-2.1373247001
C25	0.1222978966	3.3670245454	-2.6485030010
C26	-0.3550956441	4.4831062743	-1.7095125017
H27	1.2334938010	4.3213392312	-0.2510970517
H28	-0.2528602144	5.0066177605	0.4004080735
H29	-1.3710971277	2.7943333935	0.3387156914
H30	0.1128637074	2.6846477101	1.2484600518
H31	1.3122109721	1.7674568446	-0.7102951674
H32	0.0879599485	1.2141988285	-2.8291849310
H33	-1.3876968632	1.9010363444	-2.1538981810
H34	1.2193997908	3.4078775656	-2.7313117510
H35	-0.2726139494	3.5192342529	-3.6631147761
H36	-1.4552374816	4.5128120882	-1.7153614046
H37	-0.0125460954	5.4615277704	-2.0748888121
C38	3.2268854419	-1.5765283325	-2.1770445237
C39	1.8787757406	-0.8542398742	-1.9784065454
C40	1.4006355104	-0.9933141707	-0.5171370226
C41	1.3009517942	-2.4798688045	-0.1102218731
C42	2.6486326275	-3.1936418310	-0.3125509039
C43	3.1538816500	-3.0527215925	-1.7567419529
H44	3.9944599459	-1.0686072082	-1.5748537142
H45	3.5431561629	-1.4917278091	-3.2265454242
H46	1.1403663450	-1.2783150214	-2.6717232137
H47	1.9998302198	0.2007350584	-2.2497837847
H48	2.1714554763	-0.5554476082	0.1314108052
H49	1.0010757476	-2.5523594506	0.9398162594
H50	0.5341633301	-2.9864906491	-0.7140642921
H51	3.3812217609	-2.7591183512	0.3813556717
H52	2.5522440668	-4.2548958588	-0.0451689059
H53	2.4696745799	-3.5868496985	-2.4349455754
H54	4.1384676506	-3.5279302041	-1.8688636985

Table SI4a

**3<sub>tBu</sub>,[Pd(PhI)L], $\eta^2$ -meta-para**

Pd	0.349329	-1.050091	-0.268000
P	2.278054	0.239273	0.027285
C	2.087685	1.450608	1.542459
C	3.822994	-0.907517	0.355495

C	2.639656	1.306818	-1.565417
C	-1.254372	-2.632136	-0.048232
C	-1.963223	-2.334576	1.141880
C	-2.949309	-1.355625	1.160357
C	-3.222046	-0.637782	-0.016640
C	-2.530307	-0.878990	-1.193828
C	-1.540838	-1.894463	-1.222666
H	-0.634851	-3.524092	-0.094104
H	-1.757508	-2.905444	2.043350
H	-3.500868	-1.151593	2.071484
H	-2.756785	-0.327699	-2.099856
H	-1.139902	-2.205879	-2.183945
C	2.164453	0.643003	2.857272
H	1.859256	1.297461	3.684418
H	1.482983	-0.214020	2.845356
H	3.172426	0.288860	3.085378
C	3.105569	2.606033	1.621676
H	4.140577	2.256082	1.655945
H	2.923551	3.179582	2.540914
H	3.010547	3.304739	0.786947
C	0.655882	2.038460	1.501773
H	0.494981	2.635863	2.409762
H	0.478650	2.691210	0.646991
H	-0.094342	1.241334	1.476128
C	3.385881	-2.027725	1.330404
H	4.204029	-2.755529	1.420627
H	3.160158	-1.663778	2.332740
H	2.499112	-2.548474	0.953699
C	5.079693	-0.214968	0.922191
H	4.917613	0.193305	1.923311
H	5.445713	0.592179	0.282521
H	5.887186	-0.955453	1.006871
C	4.209780	-1.625968	-0.955955
H	4.944901	-2.407328	-0.721479
H	3.344753	-2.111931	-1.419556
H	4.672394	-0.959941	-1.687549
C	4.056902	1.905458	-1.676002
H	4.114515	2.517171	-2.586992
H	4.310004	2.554402	-0.833591
H	4.831099	1.138417	-1.759496
C	1.614234	2.459618	-1.653563
H	1.699559	2.924903	-2.644509
H	0.587405	2.095278	-1.545819
H	1.786642	3.247021	-0.916093
C	2.370222	0.420707	-2.806085
H	2.459133	1.041880	-3.707972
H	3.071681	-0.407246	-2.909742
H	1.359041	0.001805	-2.773511
I	-4.747372	0.862760	0.016335

**3<sub>tBu</sub>,[Pd(PhI)L], $\eta^2$ -ortho-meta**

Pd	0.069455	-0.909625	-0.505010
P	2.048548	0.206657	0.045797
C	2.649342	-0.273123	1.839452
C	3.458707	-0.271172	-1.213477
C	1.800085	2.140746	-0.018115
C	-1.540067	-2.347742	-1.081753
C	-1.723002	-3.209711	0.028577

C	-2.532276	-2.824133	1.088612
C	-3.171511	-1.569700	1.084336
C	-2.967513	-0.709943	0.015881
C	-2.155105	-1.067476	-1.085362
H	-1.090232	-2.732886	-1.994804
H	-1.256038	-4.190453	0.022703
H	-2.688822	-3.494754	1.929170
H	-2.162455	-0.462454	-1.985970
C	3.195842	-1.718230	1.822537
H	3.346213	-2.045613	2.859909
H	2.487530	-2.411685	1.356822
H	4.159870	-1.807091	1.316693
C	3.715228	0.645286	2.470309
H	4.625225	0.712656	1.868578
H	4.000802	0.239711	3.450810
H	3.346003	1.659610	2.641806
C	1.405944	-0.312489	2.761184
H	1.709425	-0.696616	3.744971
H	0.952775	0.666394	2.918626
H	0.637347	-0.977266	2.353029
C	3.357608	-1.791368	-1.489917
H	4.069016	-2.052652	-2.285583
H	3.596314	-2.408760	-0.623567
H	2.350143	-2.058951	-1.826787
C	4.901018	0.065797	-0.784031
H	5.218396	-0.496911	0.097556
H	5.044083	1.129327	-0.576876
H	5.587914	-0.202763	-1.598586
C	3.179957	0.412762	-2.570136
H	3.864066	-0.006802	-3.319784
H	2.156960	0.224796	-2.912358
H	3.350900	1.491045	-2.548061
C	3.087831	2.988187	-0.072221
H	2.814588	4.052079	-0.044335
H	3.753218	2.801871	0.774367
H	3.656446	2.830779	-0.992465
C	0.970389	2.587810	1.206134
H	0.671292	3.633967	1.059111
H	0.055910	1.995661	1.313220
H	1.531211	2.544033	2.142518
C	0.926242	2.472119	-1.252487
H	0.694389	3.545952	-1.239019
H	1.414935	2.255598	-2.202762
H	-0.016988	1.917268	-1.223704
H	-3.814017	-1.284084	1.910155
I	-3.949847	1.189928	-0.006397

**3<sub>tBu</sub>,[Pd(PhI)L],ipso**

Pd	0.5223738719	0.195650641	-0.0107399179
P	-1.8176880524	0.3872286617	0.003051137
C	-2.6211117034	-1.2331990796	-0.7249152935
C	-2.4714055331	0.6299965635	1.8235243052
C	-2.4182502666	1.9034023119	-1.0669615558
C	3.5614895651	2.6635666565	-0.1103180242
C	3.3342422377	2.0431862479	1.1216333631
C	2.8617092113	0.7279738134	1.182125486
C	2.6036358334	0.0252410983	-0.0226074028

C	2.8134079759	0.6634146934	-1.2717418977
C	3.2872631483	1.9804177304	-1.2978474021
H	3.9512548713	3.6769604971	-0.1442499814
H	3.5390812088	2.5746918881	2.0474500981
H	2.7504069098	0.2271210368	2.1375886028
H	2.6701624549	0.1131651898	-2.1951859641
H	3.4567775669	2.4621880972	-2.2574318754
C	-2.4571001686	-2.3874902087	0.2894131849
H	-2.7351731426	-3.326478733	-0.2072538977
H	-1.419773107	-2.4881158981	0.6249642182
H	-3.1027157881	-2.2866857391	1.1648837394
C	-4.1085317668	-1.1366846883	-1.1194700343
H	-4.7499365048	-0.8401945791	-0.2855793026
H	-4.4515926494	-2.1230287391	-1.46100234
H	-4.2777926267	-0.4384460359	-1.9429361199
C	-1.7965630738	-1.656121467	-1.9657371459
H	-2.1689086015	-2.6268113025	-2.3209196714
H	-1.872181428	-0.9548421066	-2.796877114
H	-0.736789128	-1.7699558205	-1.7143528286
C	-1.6490491281	-0.2994883616	2.7490328636
H	-1.9376056939	-0.1041787585	3.7910718733
H	-1.8137473981	-1.3598199852	2.5572935292
H	-0.5764385127	-0.1018508404	2.6483000692
C	-3.973533269	0.3616094536	2.0494715374
H	-4.2444489849	-0.68164396	1.8677658131
H	-4.6153765414	0.9916232673	1.4280918993
H	-4.2211179213	0.5782983017	3.0978031427
C	-2.154554588	2.0666709587	2.2949139137
H	-2.3411980134	2.1268516521	3.3753502447
H	-1.1039912438	2.3248089452	2.1254580668
H	-2.7831569858	2.823255933	1.8195417055
C	-3.8761813342	2.3564529913	-0.8467647665
H	-4.1029700925	3.1791579737	-1.5390059644
H	-4.6007050233	1.5610955655	-1.0392767937
H	-4.0481549154	2.7350572205	0.1639966423
C	-2.2284155799	1.5781670495	-2.5653123501
H	-2.3821664343	2.4991675091	-3.143099624
H	-1.2147335352	1.221412266	-2.7760898809
H	-2.9446929656	0.8430072126	-2.9390143903
C	-1.4707707793	3.0937104351	-0.7795251067
H	-1.7191701976	3.9140613479	-1.4669085194
H	-1.5582092199	3.4816645657	0.2353510924
H	-0.4254444075	2.81181968	-0.9428607753
I	2.5584706801	-2.1912579671	0.0396588949

**3<sub>tBu</sub>,[Pd(PhI)L],via I**

P	-2.205643	0.182870	0.006251
C	-2.590811	1.498964	-1.384624
C	-3.336211	-1.377425	-0.304724
C	-2.699714	0.958151	1.729665
C	-2.559633	0.803186	-2.763240
H	-2.573104	1.575206	-3.544253
H	-1.646619	0.213031	-2.894528
H	-3.423559	0.157541	-2.936404
C	-3.922069	2.266369	-1.254418
H	-4.793036	1.605668	-1.240354
H	-4.035032	2.934028	-2.120070

H	-3.958623	2.895633	-0.361359
C	-1.422268	2.514112	-1.409214
H	-1.567677	3.199523	-2.255906
H	-1.355416	3.119713	-0.505374
H	-0.464937	1.998689	-1.542866
C	-2.680823	-2.226367	-1.421170
H	-3.239241	-3.167549	-1.521687
H	-2.686074	-1.737529	-2.395613
H	-1.641406	-2.463605	-1.170922
C	-4.800790	-1.086538	-0.689900
H	-4.886947	-0.575073	-1.652165
H	-5.325534	-0.489328	0.059993
H	-5.341025	-2.038732	-0.784968
C	-3.328905	-2.271901	0.955050
H	-3.797849	-3.232083	0.702217
H	-2.309091	-2.479592	1.295366
H	-3.897298	-1.847418	1.785869
C	-4.210089	1.049418	2.027410
H	-4.355022	1.554127	2.992716
H	-4.755652	1.624265	1.274905
H	-4.679811	0.065671	2.109528
C	-2.089788	2.372507	1.841945
H	-2.204953	2.720897	2.876940
H	-1.018999	2.366203	1.611998
H	-2.583471	3.106118	1.200605
C	-2.016126	0.123518	2.839876
H	-2.176203	0.623500	3.805317
H	-2.413756	-0.887875	2.925985
H	-0.938181	0.046409	2.662491
Pd	0.016054	-0.413986	-0.024653
C	3.870539	0.209128	-0.000629
C	3.393957	1.517658	-0.060107
C	5.234505	-0.072718	0.066093
C	4.315812	2.568508	-0.052086
H	2.326865	1.711098	-0.110085
C	6.141782	0.990726	0.073020
H	5.592318	-1.096672	0.111992
C	5.685855	2.308917	0.014142
H	3.954812	3.592556	-0.097925
H	7.206914	0.781457	0.124913
H	6.396156	3.130826	0.019899
I	2.472194	-1.426107	-0.011859

**5<sub>tBu</sub>[Pd(Ph)(I)L],*trans* halide**

Pd	0.664963	-0.418604	-0.027780
P	-1.696760	-0.082029	-0.014058
C	-2.261081	-1.627611	-1.061258
C	-2.332263	-0.304384	1.812779
C	-2.481668	1.525594	-0.769861
C	2.397331	4.045373	-0.019667
C	1.955075	3.476912	1.175145
C	1.437300	2.175178	1.196623
C	1.350807	1.444210	0.008690
C	1.818185	1.998380	-1.189107
C	2.332240	3.300119	-1.198378
H	2.802030	5.053705	-0.030109
H	2.018870	4.037285	2.105047

H	1.120481	1.745458	2.140025
H	1.801957	1.421278	-2.108202
H	2.694974	3.720794	-2.133180
C	-1.287953	-2.789635	-0.738304
H	-1.510164	-3.632305	-1.406445
H	-0.240270	-2.513782	-0.931712
H	-1.361605	-3.157643	0.284312
C	-2.076287	-1.331188	-2.566165
H	-2.221482	-2.267182	-3.120576
H	-2.803937	-0.614166	-2.951666
H	-1.068056	-0.969795	-2.792738
C	-1.691537	1.923784	-2.038517
H	-2.105995	2.868377	-2.415234
H	-0.635353	2.088181	-1.819341
H	-1.767168	1.194211	-2.844461
C	-2.320617	2.700575	0.221835
H	-2.645128	3.618526	-0.284799
H	-2.939524	2.593452	1.115344
H	-1.279356	2.845372	0.523999
C	-3.974019	1.391092	-1.140090
H	-4.603135	1.111990	-0.292141
H	-4.140832	0.668578	-1.942895
H	-4.329562	2.363440	-1.506045
C	-3.709505	-2.101762	-0.831243
H	-3.884963	-2.442044	0.191639
H	-3.908336	-2.956029	-1.492329
H	-4.447697	-1.330683	-1.065491
C	-1.505595	0.627173	2.729780
H	-1.877556	0.522188	3.757609
H	-0.451468	0.336555	2.724460
H	-1.570074	1.681407	2.462019
C	-2.030660	-1.737373	2.308180
H	-2.232797	-1.774040	3.386482
H	-2.658982	-2.498046	1.840540
H	-0.979097	-2.008393	2.167767
C	-3.834523	-0.023741	2.023507
H	-4.475037	-0.632164	1.380400
H	-4.092789	-0.264824	3.063202
H	-4.092523	1.026416	1.867825
I	3.057288	-1.500114	0.039090

**5<sub>tBu</sub>[Pd(Ph)(I)L],*trans* aryl**

Pd	-0.712815	0.243561	0.000271
P	1.770622	0.284902	-0.000719
C	2.480103	0.013427	1.785106
C	2.643398	-0.934685	-1.231759
C	2.132105	2.116027	-0.554125
C	-4.998118	2.212388	-0.000987
C	-4.416638	1.822715	-1.210137
C	-3.241019	1.063869	-1.214711
C	-2.623501	0.736579	0.000712
C	-3.233359	1.079112	1.215792
C	-4.408934	1.838047	1.209228
H	-5.919986	2.788035	-0.001686
H	-4.886217	2.091369	-2.153487
H	-2.812404	0.732737	-2.157113
H	-2.798970	0.760043	2.159782



H	-4.872283	2.118900	2.152110
C	1.810748	-1.249401	2.381182
H	2.136086	-1.353362	3.424995
H	0.719781	-1.170269	2.371729
H	2.078904	-2.169666	1.863273
C	2.045282	1.183807	2.695581
H	2.305330	0.930084	3.731259
H	2.549771	2.123459	2.459987
H	0.962520	1.346954	2.663604
C	1.054348	3.010817	0.107831
H	1.159541	4.037964	-0.266637
H	0.038289	2.679527	-0.157843
H	1.120247	3.048610	1.194748
C	1.905874	2.259355	-2.076833
H	1.941852	3.326568	-2.332381
H	2.672678	1.760844	-2.672955
H	0.924655	1.882712	-2.384845
C	3.531145	2.671898	-0.221114
H	4.332883	2.079867	-0.670539
H	3.716728	2.733747	0.853902
H	3.615596	3.692225	-0.619925
C	4.012614	-0.133562	1.877191
H	4.377815	-1.025381	1.361962
H	4.297596	-0.234041	2.933261
H	4.545820	0.732762	1.477135
C	1.768332	-1.031096	-2.505247
H	2.203186	-1.790629	-3.168471
H	0.748207	-1.342714	-2.262461
H	1.718244	-0.099657	-3.069967
C	2.662895	-2.357412	-0.628522
H	3.006923	-3.052052	-1.405885
H	3.351438	-2.455370	0.213765
H	1.666383	-2.683345	-0.316370
C	4.083599	-0.549057	-1.625712
H	4.752672	-0.480793	-0.763846
H	4.486960	-1.323466	-2.291948
H	4.133062	0.397635	-2.169663
I	-1.609366	-2.227879	-0.000340

**5<sub>tBu</sub>\*,[Pd(Ph)(I)L]\*,“Y”**

Pd	-0.6500019723	-0.158480147	-0.0787082551
P	1.8307301948	0.3964636437	0.0864906564
C	2.2616342002	0.7870954935	1.9415366694
C	2.9212683528	-1.0965678968	-0.5214246906
C	2.2181258579	1.9591657395	-1.0023719784
C	-4.4614928886	2.4210346669	0.8955172532
C	-4.0113722941	2.3209818189	-0.4229885677
C	-2.9926991748	1.4216960724	-0.7585699899
C	-2.3986916404	0.6595503992	0.2532736409
C	-2.8781723416	0.7086451542	1.5667802822
C	-3.8982205731	1.6125125557	1.8854377274
H	-5.2630224221	3.1104200279	1.1464285143
H	-4.4640787407	2.9283224549	-1.2030575693
H	-2.6703930837	1.3210475304	-1.7905251296
H	-2.4677810189	0.0562282493	2.331652203
H	-4.2626195836	1.6657522153	2.9085255968
C	1.5415981061	-0.2570114306	2.8302579818

H	1.685653457	0.0213381728	3.8827849062
H	0.4649973486	-0.2767703585	2.6299221186
H	1.9220715937	-1.2706452911	2.7064036432
C	1.6552323953	2.1543047501	2.328569709
H	1.7377799141	2.2743172253	3.4165046896
H	2.1769694185	2.9992216798	1.8736974656
H	0.5921819484	2.2182969601	2.0733203569
C	1.0554021999	2.966375639	-0.8218198389
H	1.1999528141	3.7984248244	-1.5238763926
H	0.0869773093	2.5059488144	-1.0469852644
H	0.9991453856	3.3943513909	0.178947891
C	2.1951320333	1.5611377482	-2.4948890797
H	2.2396524796	2.4779478963	-3.0968721057
H	3.0475189343	0.9445269958	-2.787135596
H	1.2726869074	1.0363915104	-2.7642505824
C	3.553312639	2.670343855	-0.7042488008
H	4.4168808124	2.0112365905	-0.8231478914
H	3.5861554918	3.0961371618	0.3016866026
H	3.6775200709	3.5036354511	-1.4090351515
C	3.7635316758	0.8000854754	2.2907645117
H	4.2298840043	-0.1808770099	2.169505463
H	3.8816876439	1.08366922	3.3453289302
H	4.3282396535	1.5206894503	1.693697708
C	2.2646722684	-1.6873966562	-1.7931094106
H	2.826035441	-2.5841955777	-2.0873297761
H	1.2284433043	-1.9884585357	-1.6089187001
H	2.273022658	-1.0066554269	-2.6443778696
C	2.880836427	-2.2257771759	0.5319923196
H	3.35196159	-3.1163023955	0.0965634527
H	3.4342825122	-1.9836731588	1.4419778857
H	1.8556321596	-2.4993530397	0.801082667
C	4.3947923411	-0.7541019982	-0.8191978269
H	4.9100264865	-0.3207914247	0.0417705188
H	4.9249165217	-1.6776619408	-1.0882425122
H	4.5047773864	-0.068205603	-1.6630894896
I	-2.0693841151	-2.260068438	-0.6847697389

**3<sub>tBu</sub> [Pd(PhBr)L] η<sup>2</sup>-meta-para**

Pd	0.2793144643	0.7811420745	-0.5785832375
Br	-1.8195528879	2.6643853394	2.8611136014
P	0.7683224321	-1.5002784899	-0.5009464473
C	0.1685590781	-2.2847952695	1.1828918862
C	-0.1215845948	-2.4421937388	-1.9613627313
C	2.6894734606	-1.804954942	-0.663373243
C	-1.1119502228	3.0369304571	-1.7806444447
C	-2.4031969348	3.0186353244	-1.266859457
C	-2.6219102533	2.9131855859	0.1183587552
C	-1.5302529382	2.7957432019	0.9654817363
C	-0.2030423784	2.807140954	0.4842408576
C	0.0060775561	2.9586188269	-0.9119772532
H	-0.9483407657	3.153677985	-2.8479974757
H	-3.2572505449	3.0986331464	-1.9336610258
H	-3.6297891102	2.9190172279	0.5190700661
H	0.6233373591	2.8865393777	1.1819706699
H	1.0004308454	3.191703755	-1.2880563682
C	-1.3729931097	-2.384063972	1.177530168
H	-1.7085536336	-2.6323458296	2.1931028158

H	-1.8389826213	-1.4329280917	0.9000055931
H	-1.7489644239	-3.1677555597	0.5156849025
C	0.7472240251	-3.6723343629	1.5263719452
H	0.5445900164	-4.4197130948	0.7550944345
H	0.285961675	-4.0297639438	2.4573241255
H	1.8264039685	-3.6446545614	1.6974031307
C	0.5162125924	-1.2974038719	2.3233380846
H	0.0961349387	-1.6846365735	3.2618347148
H	1.58833685	-1.1693930111	2.4747439412
H	0.0806872915	-0.310760884	2.1357909877
C	-1.5549146112	-1.8710018159	-2.0901571226
H	-2.0251103386	-2.2974101664	-2.9872921955
H	-2.1947063552	-2.1127994769	-1.2414067357
H	-1.5354584611	-0.7811920936	-2.1953621278
C	-0.2037509183	-3.9772455423	-1.8376646485
H	-0.8117544643	-4.2955115272	-0.9871692304
H	0.7786395428	-4.448022706	-1.7490178299
H	-0.6800550152	-4.3830306267	-2.7409301445
C	0.5815714271	-2.0974770143	-3.2930082993
H	-0.0368755926	-2.4711380766	-4.1199839206
H	0.6906740857	-1.0157177097	-3.424873118
H	1.5641046521	-2.5642744259	-3.3938185107
C	3.1226374854	-3.241837211	-1.0162812279
H	4.2202413611	-3.2923639324	-1.0233078643
H	2.7671019871	-3.9797545644	-0.2928188583
H	2.7837929972	-3.5484128179	-2.0090290279
C	3.384860276	-1.3935271228	0.6529443736
H	4.4701348011	-1.3850358203	0.4850196212
H	3.0904849362	-0.3871656407	0.9684297555
H	3.1936789808	-2.0880168483	1.4737825395
C	3.2333935995	-0.8344713144	-1.7403223708
H	4.3298372999	-0.9055594493	-1.7589674096
H	2.8748344838	-1.057970947	-2.7453819618
H	2.9590012598	0.2002229338	-1.5071759561

**3<sub>tBu</sub>** [Pd(PhBr)L]  $\eta^2$ -*ortho-meta*

Pd	-0.31887	-0.77944	-0.51323
P	1.75746	0.13657	0.04427
C	2.27736	-0.36995	1.85532
C	3.13306	-0.49841	-1.18578
C	1.70255	2.0845	-0.05238
C	-2.08453	-2.01131	-1.08868
C	-2.34555	-2.84507	0.0281
C	-3.10034	-2.37335	1.09436
C	-3.60698	-1.06054	1.08941
C	-3.32183	-0.23238	0.01516
C	-2.5599	-0.67351	-1.09016
H	-1.68762	-2.44462	-2.00459
H	-1.98364	-3.86915	0.02273
H	-3.31642	-3.02111	1.93944
H	-2.51253	-0.0672	-1.98849
C	2.67415	-1.86267	1.8706
H	2.768	-2.1881	2.91514
H	1.91048	-2.48817	1.39652
H	3.63512	-2.05481	1.38865
C	3.42167	0.44542	2.4911
H	4.34459	0.40864	1.90644

H	3.64741	0.02963	3.48286
H	3.15541	1.49488	2.63984
C	1.02235	-0.26643	2.75693
H	1.2735	-0.65342	3.75422
H	0.66282	0.75466	2.88416
H	0.19886	-0.8641	2.35206
C	2.88547	-2.00612	-1.4356
H	3.56198	-2.34892	-2.23069
H	3.0719	-2.62639	-0.55856
H	1.85378	-2.18252	-1.75943
C	4.59482	-0.29642	-0.73844
H	4.84249	-0.87211	0.157
H	4.83731	0.75181	-0.54628
H	5.26417	-0.64521	-1.53705
C	2.94315	0.18527	-2.55792
H	3.59243	-0.315	-3.28876
H	1.9118	0.09543	-2.91476
H	3.22222	1.24102	-2.5523
C	3.06924	2.79815	-0.08999
H	2.90469	3.88454	-0.08358
H	3.69498	2.55957	0.77387
H	3.63821	2.56864	-0.99466
C	0.89843	2.63152	1.14758
H	0.70648	3.69943	0.97907
H	-0.07176	2.13379	1.24466
H	1.43499	2.54876	2.09548
C	0.89021	2.48083	-1.30901
H	0.77429	3.57326	-1.32059
H	1.36884	2.1929	-2.24514
H	-0.10722	2.02996	-1.28758
Br	-4.02974	1.55436	-0.01126
H	-4.21059	-0.70032	1.91538

**3<sub>tBu</sub>** [Pd(PhBr)L]  $\eta^2$ -*ipso-ortho*

Pd	-0.68457	0.13647	0.09715
P	1.65473	-0.02993	-0.00793
C	2.46112	1.67095	-0.51914
C	2.40843	-0.57531	1.70605
C	2.13914	-1.36445	-1.34469
C	-2.64699	0.82816	1.2139
C	-2.75399	2.23709	1.21906
C	-3.02948	2.93505	0.04863
C	-3.16225	2.2431	-1.16726
C	-3.06285	0.85571	-1.21172
C	-2.82817	0.13301	-0.01135
H	-2.60378	0.28238	2.15038
H	-2.6504	2.76479	2.16352
H	-3.13711	4.01566	0.07155
C	2.41129	2.64244	0.6815
H	2.69374	3.64342	0.32936
H	1.40324	2.7125	1.10277
H	3.10852	2.37585	1.47913
C	3.91371	1.60665	-1.03409
H	4.60048	1.16004	-0.31052
H	4.26763	2.62791	-1.23207
H	4.00186	1.05236	-1.97218
C	1.56779	2.31384	-1.60815

H	1.94935	3.32115	-1.82534
H	1.5615	1.75901	-2.54671
H	0.53244	2.40384	-1.26331
C	1.67925	0.21469	2.82014
H	2.01938	-0.15857	3.7959
H	1.87729	1.28629	2.79299
H	0.59583	0.0714	2.75445
C	3.93043	-0.38842	1.87046
H	4.23125	0.66163	1.82949
H	4.50766	-0.93565	1.12065
H	4.23233	-0.76934	2.85588
C	2.06517	-2.05967	1.95857
H	2.30437	-2.30047	3.00284
H	0.99864	-2.2579	1.80937
H	2.64149	-2.74457	1.33243
C	3.59316	-1.87521	-1.30068
H	3.74963	-2.57853	-2.13017
H	4.32728	-1.0732	-1.41176
H	3.81746	-2.4165	-0.37815
C	1.86299	-0.79318	-2.75338
H	1.96076	-1.60706	-3.48388
H	0.84624	-0.39478	-2.83631
H	2.57028	-0.01406	-3.04567
C	1.17793	-2.56873	-1.18969
H	1.34516	-3.26116	-2.02617
H	1.33091	-3.13002	-0.26792
H	0.13168	-2.24581	-1.21658
H	-3.35897	2.78919	-2.08626
Br	-3.32372	-1.75765	0.02752
H	-3.21646	0.31487	-2.13963

**3<sub>t</sub>Bu** [Pd(PhBr)L] ipso

Pd	-0.1630513562	0.6792382418	0.075349362
P	0.4745160689	-1.5259499674	-0.3927204973
C	-0.120517688	-2.6923648198	1.0527834239
C	-0.3232801374	-2.1587974901	-2.0553555271
C	2.413411906	-1.6863231781	-0.5473605445
C	-1.6532257385	-2.8704215296	0.9687260288
H	-1.9979537436	-3.3568354827	1.8908854256
H	-2.1699104381	-1.9080545592	0.8914837621
H	-1.9663552597	-3.5050959473	0.1366083002
C	0.5301122877	-4.0885966301	1.1108331668
H	0.3881321455	-4.6614306718	0.1908203568
H	0.070758709	-4.6621961078	1.9275922838
H	1.601741207	-4.0411949172	1.3198018669
C	0.1372547863	-1.9589524693	2.3920915717
H	-0.291802399	-2.5564382817	3.2082263779
H	1.1956377662	-1.8189273902	2.6126606368
H	-0.3420369411	-0.9741700841	2.4008123243
C	-1.7832040186	-1.6468947257	-2.108505074
H	-2.2045478124	-1.8867023448	-3.0944587647
H	-2.4295789782	-2.1036393843	-1.3586669188
H	-1.8215673789	-0.5612495883	-1.9717636352
C	-0.3192635278	-3.6851339802	-2.2759424011
H	-0.9315972052	-4.2159957561	-1.5425629558
H	0.6862046387	-4.112617867	-2.2525694383
H	-0.7442100089	-3.9039707164	-3.2653675671

C	0.3927779859	-1.4907794891	-3.2503031716
H	-0.1864566293	-1.6943308197	-4.1608006394
H	0.4505584911	-0.4040388584	-3.1305900085
H	1.3990648133	-1.8807685709	-3.4190137577
C	2.9443843594	-2.9885449615	-1.1806697445
H	4.0429092687	-2.9723704305	-1.1599676281
H	2.6226191855	-3.8842990934	-0.643205192
H	2.6486521573	-3.0957334369	-2.2273775651
C	3.0472463657	-1.5306811298	0.8530140605
H	4.1340786893	-1.4285946001	0.7339270823
H	2.6847460299	-0.6322799448	1.3636066548
H	2.8763586459	-2.3944712006	1.4994550028
C	2.9280474405	-0.4808035525	-1.3717240794
H	4.0265155228	-0.48067575	-1.3459586068
H	2.6279358652	-0.5133802743	-2.4192910809
H	2.5726242397	0.4647339476	-0.9494828591
C	0.0074750658	3.7860642958	-1.8519881537
C	-1.2745712286	3.2471901204	-1.715036488
C	-1.684030717	2.6688395798	-0.5054575912
C	-0.7833640468	2.643511431	0.5918089417
C	0.5392068093	3.1340699825	0.4316077525
C	0.9149262861	3.7049108906	-0.7921022799
H	0.3020382948	4.2579165961	-2.784871408
H	-1.9785298948	3.290811789	-2.5418846551
H	-2.708156359	2.3393259049	-0.3690327868
H	1.2110340759	3.1580986439	1.2825255276
H	1.9195801222	4.1052134585	-0.8992788469
Br	-1.5081766459	2.4639970875	2.4006844621

**3<sub>t</sub>Bu** [Pd(PhBr)L] via Br

P	1.611640786	1.082256294	0.3379932312
C	1.1710795084	2.1089501747	1.9412852727
C	3.3713521525	0.2772598923	0.5990701792
C	1.7314543742	2.3251522262	-1.1634750239
C	1.4232364889	1.2313315714	3.1868829989
H	0.9909250597	1.734151057	4.0623444426
H	0.9398646923	0.2533180137	3.0922687341
H	2.4845373367	1.0801367599	3.3962656208
C	1.9133179577	3.4477901188	2.1260013693
H	2.9998844315	3.3312532723	2.1521126829
H	1.6112018035	3.8937501865	3.0839794482
H	1.6683576837	4.1739435956	1.3467259287
C	-0.3535435559	2.3761058935	1.9275425066
H	-0.6383142381	2.8477313483	2.8785262411
H	-0.6696323471	3.0426377519	1.1248270512
H	-0.9094103538	1.4376928503	1.8272858878
C	3.1917076455	-0.9910986855	1.4680347297
H	4.1549214079	-1.5170296191	1.5264683973
H	2.8743149294	-0.775010671	2.4882768913
H	2.4531613695	-1.6663079209	1.023281836
C	4.4421313783	1.1801475916	1.2448892254
H	4.1941051172	1.4563247243	2.2731550812
H	4.6197543669	2.0988387348	0.6801626992
H	5.3941172607	0.6326042516	1.2837749387
C	3.9102630197	-0.2247620884	-0.75895159
H	4.7988643007	-0.842712014	-0.5730977016
H	3.1750087659	-0.8482629981	-1.2780556978

H	4.2173173781	0.5852312264	-1.4244358364
C	2.986449505	3.2203049552	-1.2085538335
H	2.9036795061	3.9099695167	-2.0601058561
H	3.1050948169	3.8284241454	-0.3083421371
H	3.9051726344	2.6458132049	-1.3534343426
C	0.4816943737	3.233080661	-1.1725739281
H	0.4597325849	3.7864961635	-2.1207861553
H	-0.4402906827	2.6454525374	-1.1108552668
H	0.4820953843	3.9744187621	-0.3700470862
C	1.6529694002	1.5016612869	-2.4721763339
H	1.5972922211	2.1961356206	-3.3221425025
H	2.5191699945	0.8591085061	-2.6318638639
H	0.7595784378	0.868390388	-2.4803470288
Pd	0.0498215925	-0.5371846765	-0.0665048095
Br	-1.4232580718	-2.5157814291	-0.6162486674
C	-3.2910418362	-2.0063254224	-0.6487143493
C	-3.6563813596	-0.7202365213	-0.2592532256
C	-4.2276295639	-2.9471327097	-1.0718354139
C	-5.0096519703	-0.3734730697	-0.2930929762
H	-2.8964317311	-0.0121489386	0.0572190717
C	-5.5761009706	-2.581421004	-1.0983080194
H	-3.9174008127	-3.9423247097	-1.3739514057
C	-5.9686164192	-1.2987828698	-0.7101427687
H	-5.3094249708	0.6265249307	0.0082346812
H	-6.3172433685	-3.3055000364	-1.4253963092
H	-7.0185162775	-1.0213619139	-0.733795232

$3_{\text{tBu}}^{\dagger}$	$[\text{Pd}(\text{PhBr})\text{L}]^{\dagger}$	<i>meta</i>
Pd	-0.3233358674	-0.7494847824
Br	-4.0610163488	1.4666572436
P	1.7556751014	0.1707761206
C	1.5656198705	2.0300815342
C	2.5883206381	-0.8221516778
C	2.9568483872	0.1152536922
C	-2.2882696797	-2.8906002254
C	-3.0251089988	-2.4952455416
C	-3.5584868414	-1.195735083
C	-3.3179919359	-0.3035077201
C	-2.5766862004	-0.6661766952
C	-2.0736302617	-1.991129041
H	-1.9050425299	-3.904413324
H	-3.205575599	-3.1931613055
H	-4.1476439753	-0.8947836814
H	-2.564360737	-0.0097219978
H	-1.6908302573	-2.3644367691
C	0.9304868135	2.0766989801
H	0.6448003266	3.1143059036
H	0.0234407937	1.4663336371
H	1.6167709917	1.7619531876
C	2.8617138561	2.8649864109
H	3.6287116858	2.4398340096
H	2.6312427782	3.8703549452
H	3.2937797459	2.9908881866
C	0.5410703453	2.7094459297
H	0.3399579132	3.7230742826
H	0.8929747265	2.8042232768
H	-0.4036973033	2.1561917979

C	1.4925028797	-1.1446982787
H	1.9203542999	-1.8118423558
H	1.1144596554	-0.2619189526
H	0.6411494123	-1.6523121296
C	3.768688721	-0.1296715921
H	3.4672131921	0.7863535994
H	4.5872784688	0.1161654684
H	4.1721675016	-0.8078227101
C	3.0725901436	-2.1917252038
H	3.3593235239	-2.8125904592
H	2.2804099201	-2.7207016976
H	3.9491132192	-2.1166631645
C	4.4560723201	0.3210186446
H	5.0110709497	0.327819213
H	4.6609935597	1.2686618978
H	4.8758580875	-0.4843871148
C	2.5149432751	1.1750183826
H	3.0654104543	1.0004707358
H	1.4462596612	1.0977284341
H	2.7338957386	2.1984194542
C	2.7679946565	-1.2515551828
H	3.3551480479	-1.2537563388
H	3.1033871363	-2.0980820828
H	1.7158062688	-1.4163732877

$3_{\text{tBu}}^{\dagger}$	$[\text{Pd}(\text{PhBr})\text{L}]^{\dagger}$	<i>ortho</i>
Pd	-0.62613655	-0.2742197081
P	1.570141002	0.3556750393
C	1.6201485105	2.2654503851
C	2.2116353	-0.6063356686
C	2.7906108474	0.0018004119
C	-2.2233213942	-2.994529376
C	-2.8434777736	-2.864313593
C	-3.3541613907	-1.6184524315
C	-3.2857464141	-0.5141931695
C	-2.6953821164	-0.6521726141
C	-2.1352436253	-1.8963150141
H	-1.8268508435	-3.9548705493
H	-2.9296006482	-3.7234181171
H	-3.8222951641	-1.5105694581
H	-1.8074802242	-2.0472065834
C	0.9615957021	2.5248088096
H	0.8188901636	3.6072269602
H	-0.0233863707	2.0522468998
H	1.5753931279	2.1902741656
C	3.0149154605	2.9225130531
H	3.7012655601	2.4579473061
H	2.9124716582	3.9786499053
H	3.4849594336	2.9034413323
C	0.7212589983	2.9868513965
H	0.6545619096	4.0489396301
H	1.1055576816	2.9344617051
H	-0.2914399248	2.5692879536
C	1.0487909945	-0.6850654428
H	1.3549501333	-1.3341365786
H	0.7792399796	0.2823824964
H	0.1520923976	-1.1133979349

C	3.4547427427	-0.0199181335	2.649003784
H	3.2678236944	0.9687607717	3.0755315888
H	4.320499702	0.0548792204	1.9859311125
H	3.738273481	-0.6787294921	3.4814384932
C	2.5168217475	-2.0692704398	1.5562168915
H	2.6873122783	-2.6469777356	2.4743812302
H	1.675971845	-2.5285422682	1.0264418375
H	3.4159751467	-2.1698306093	0.9441785893
C	4.2941464182	0.0337299616	-0.7605851887
H	4.8726239466	-0.1292699453	-1.68042182
H	4.6131659925	0.991312457	-0.341499758
H	4.5799386401	-0.7548966107	-0.0601893572
C	2.5214232183	1.0140548271	-2.236970364
H	3.0696937775	0.6878575784	-3.1306714987
H	1.4587484936	1.0555667061	-2.4978003916
H	2.8649741331	2.0237784833	-2.0018653235
C	2.4375816538	-1.3849253656	-1.6934084922
H	3.0419144795	-1.5444033144	-2.5970043889
H	2.641828762	-2.2128924581	-1.0142249937
H	1.3801338257	-1.4322906839	-1.9732725973
Br	-3.1665542433	0.6616028707	-1.9475653846
H	-3.7256755599	0.4349936994	0.9925742745

<b>3<sub>tBu</sub><sup>†</sup></b>	<b>[Pd(PhBr)L]<sup>‡</sup> <i>ipso</i></b>		
Pd	-0.6530421319	-0.2257818544	-0.1264649742
P	1.4010207976	0.7460564296	0.4600458569
C	1.2034083415	2.6336586283	0.908191904
C	2.1807862114	-0.1693508885	1.9977256918
C	2.6455027872	0.5979856536	-1.0345452222
C	-2.613766486	-2.1141743222	0.4267692334
C	-3.3563946083	-1.6539152248	1.5116650554
C	-3.9203315516	-0.3678722755	1.50300102
C	-3.7025387111	0.4792588085	0.4213557253
C	-2.9552602761	0.0480667186	-0.695839509
C	-2.429926761	-1.2714275228	-0.7017455871
H	-2.2248938318	-3.1265492236	0.4065285219
H	-3.50875251	-2.3099483286	2.3645241541
H	-4.520783709	-0.0335673267	2.344116492
C	0.5171149181	2.7542866117	2.2868625863
H	0.2315048651	3.802884308	2.4436813279
H	-0.3948435028	2.1504959525	2.3385892867
H	1.171889597	2.4744278189	3.1151635023
C	2.5024908346	3.4641516756	0.9348970593
H	3.2419125861	3.0684213435	1.6355805943
H	2.2652052548	4.4884943883	1.2538135684
H	2.9719762211	3.5379845319	-0.0493460058
C	0.2199612227	3.2688659064	-0.1046451817
H	-0.0078548673	4.2929577628	0.2216341057
H	0.6210976609	3.3313266641	-1.1167552883
H	-0.716328018	2.7031188917	-0.1471342199
C	1.0523844569	-0.4273942365	3.0262798342
H	1.4495690447	-1.0624551512	3.8301997575
H	0.6725654194	0.4837223324	3.488866061
H	0.2066955662	-0.9464553907	2.5632437878
C	3.3471580444	0.5507757741	2.7047197822
H	3.0387103466	1.4905088799	3.1701363007
H	4.1833243768	0.7623889146	2.0334838968

H	3.7285024388	-0.0934556241	3.5090429772
C	2.6657833318	-1.5674356964	1.5542029719
H	2.9173748419	-2.1503052478	2.4501008617
H	1.8860453008	-2.1136219314	1.0126763705
H	3.563566647	-1.5309308278	0.9332614942
C	4.1353161569	0.81504238	-0.7034422064
H	4.7187627843	0.7596140171	-1.6327203575
H	4.3321798422	1.7915270724	-0.253540266
H	4.5305748401	0.0468143284	-0.0340558064
C	2.2371456448	1.6013113897	-2.1360954496
H	2.8127044534	1.3753945804	-3.0434293531
H	1.1752496164	1.5145570762	-2.3887860175
H	2.4521337549	2.6387316812	-1.8705418304
C	2.467877913	-0.80491233	-1.666026786
H	3.0741366712	-0.8576147625	-2.5808776696
H	2.7901524587	-1.6175719201	-1.0146346766
H	1.4224610461	-0.985471199	-1.9383438777
H	-4.1347098905	1.4764441307	0.4078873618
Br	-1.9765407155	-2.1096606812	-2.4096538404
H	-2.9268469745	0.6498486611	-1.5977652086

<b>5<sub>tBu</sub></b>	<b>[Pd(Ph)(Br)L] <i>trans</i> halide</b>		
Pd	-1.0319201598	-0.2446856683	-0.0356557137
Br	-3.4560327351	-0.5121331261	-0.1690216843
P	1.3065342725	-0.6331190747	0.0201780616
C	1.3448644473	-2.3298499284	0.9774053261
C	1.9225853673	-0.9364076656	-1.8034019446
C	2.5024201525	0.6227274236	0.8935169288
C	-1.4067910158	4.5189379531	0.2082906208
C	-1.077565946	3.918390687	-1.00699266
C	-0.9397111188	2.5271694759	-1.1006961627
C	-1.1231357087	1.7348734565	0.0354841749
C	-1.4822450547	2.3285189753	1.2516908207
C	-1.6138400558	3.7193615705	1.3338547709
H	-1.5160958649	5.5979585442	0.2747597092
H	-0.934608709	4.5263513537	-1.8973530529
H	-0.7053299806	2.08114593	-2.060424299
H	-1.6786468396	1.718459006	2.1276748992
H	-1.8955126752	4.170712145	2.2822161346
C	0.0823633971	-3.1284241128	0.5628809064
H	0.0435639777	-4.0547423544	1.1515036748
H	-0.8439226145	-2.580149589	0.791733054
H	0.0625472636	-3.4104652122	-0.4888438456
C	1.2017070008	-2.0817077712	2.4956160725
H	1.0371759788	-3.0495102445	2.9864975327
H	2.0963947903	-1.6436359519	2.9430516417
H	0.3413637015	-1.4460102649	2.7276463164
C	1.819069097	1.1638607237	2.1712476284
H	2.4887445647	1.9056477584	2.6263682895
H	0.8765503574	1.6636810648	1.9421262966
H	1.6296597831	0.3967423512	2.9214910593
C	2.7303886197	1.8488385647	-0.0201365646
H	3.2772214703	2.604618214	0.5581991223
H	3.3361118472	1.622153691	-0.9004407549
H	1.788767082	2.302231459	-0.3421314361
C	3.8746912639	0.0316004562	1.2798599257
H	4.4197307383	-0.3817001431	0.4286030557

H	3.7939187076	-0.74458518	2.0446707358
H	4.4909364439	0.8355262783	1.7036952774
C	2.5956073968	-3.2011028175	0.7428854267
H	2.695029051	-3.5287095843	-0.2943534254
H	2.5127134876	-4.1067649644	1.3587566417
H	3.5207869604	-2.6959183999	1.0312175553
C	1.4433580701	0.2475971493	-2.6750140228
H	1.7902231019	0.0854239613	-3.7041104433
H	0.3510337713	0.2924423544	-2.6930896678
H	1.8208901965	1.2167039041	-2.3491187196
C	1.2320868145	-2.1847789981	-2.398414892
H	1.4666265053	-2.2239544876	-3.4699010966
H	1.5781362855	-3.1239214089	-1.9617352378
H	0.1421278265	-2.1308403721	-2.3085607489
C	3.448547793	-1.0985763649	-1.9626020687
H	3.856703894	-1.9121462297	-1.3576841196
H	3.6673755574	-1.3317319701	-3.0130457659
H	3.9948392098	-0.1841980463	-1.7190132465

<b>5<sub>tBu</sub></b>	[Pd(Ph)(Br)L]	<i>trans</i> aryl	
Pd	-0.8556524742	0.0157110668	-0.0072303534
Br	-1.406852101	-2.3727819754	-0.0000996123
P	1.6193362913	0.2428172459	-0.0032395545
C	2.3109600404	0.086285892	1.8041894581
C	2.5784733234	-0.9724935054	-1.1706259045
C	1.8752344495	2.0682851947	-0.6258741061
C	-5.3420025081	1.477445333	0.0005997657
C	-4.7190540557	1.164305524	-1.2101786275
C	-3.4563995771	0.5608983047	-1.2176554809
C	-2.801592811	0.3161529542	-0.0035180314
C	-3.4449175705	0.5778598501	1.2132464364
C	-4.7075908506	1.1812402679	1.2096075565
H	-6.3292078222	1.9320386479	0.002143567
H	-5.2212658802	1.3715192626	-2.1522212316
H	-2.9904387069	0.2862735911	-2.160721947
H	-2.9702937736	0.3164804032	2.1558052672
H	-5.2006529045	1.4016406493	2.1534964322
C	1.7092786112	-1.1935281145	2.4358361074
H	2.0029851491	-1.2284819053	3.4935842887
H	0.6163956753	-1.1941798893	2.3858968445
H	2.0599017257	-2.1133465334	1.9690838674
C	1.7864615598	1.260878696	2.6603762416
H	2.0469610199	1.0663167924	3.708712207
H	2.2317715185	2.2215340599	2.3926517261
H	0.6958889218	1.3511521014	2.6083665857
C	0.7297895131	2.9155511651	-0.0169332999
H	0.7745409939	3.9329387509	-0.4282987029
H	-0.257955517	2.5093131824	-0.2871122587
H	0.7728961423	2.9973385068	1.0687785738
C	1.6695673792	2.1365259035	-2.1563234324
H	1.6412144214	3.1927419855	-2.4549092529
H	2.4777667064	1.66536885	-2.7191259824
H	0.7208024081	1.6840988557	-2.4639750661
C	3.229862776	2.7219871262	-0.2896665241
H	4.0745403239	2.163435482	-0.7018177696
H	3.3896497705	2.8328814719	0.7856324374
H	3.2602845875	3.7301916527	-0.7249554216

C	3.8473081852	0.0401779015	1.9285206051
H	4.2773560516	-0.8428234652	1.4499750468
H	4.1175156011	-0.0078031817	2.9921492194
H	4.3324000829	0.925381861	1.5087146123
C	1.7289634803	-1.1734277602	-2.4499149583
H	2.2159068376	-1.9361878834	-3.0719024477
H	0.7239418417	-1.5309526094	-2.2069976419
H	1.6377913769	-0.2722146155	-3.0572092435
C	2.6704641513	-2.3649974304	-0.5060184281
H	3.0606712857	-3.07149657	-1.2501093061
H	3.356130994	-2.3874510278	0.3442185139
H	1.6901997694	-2.7312084796	-0.1875126538
C	4.0001555909	-0.5211611436	-1.5620844002
H	4.6526972673	-0.3862755668	-0.6952293999
H	4.4543665413	-1.2950703119	-2.1953903744
H	4.0052604422	0.4073303543	-2.1385423504

<b>5<sub>tBu</sub></b>	[Pd(Ph)(Br)L] <sup>‡</sup>	“Y”	
Pd	-0.7031496447	-0.5390558745	-0.0786722914
Br	-1.3306630624	-2.8446179732	-0.523024911
P	1.5380235303	0.6662411894	0.0698503392
C	2.1504829953	0.7335481659	1.9123555911
C	2.8608056765	-0.2603548576	-1.016218397
C	1.311120249	2.4762043767	-0.5984991258
C	-5.1782889257	0.8115740703	0.4250398417
C	-4.6126681474	0.7506447738	-0.8506827861
C	-3.340205009	0.1974332751	-1.0363216764
C	-2.6275301309	-0.2487502126	0.0804293926
C	-3.202384662	-0.2476445513	1.3546604747
C	-4.4761042703	0.308164573	1.5226528641
H	-6.1718183317	1.2302738801	0.5603163495
H	-5.1657487621	1.1165161063	-1.7123992549
H	-2.9158660771	0.1199363657	-2.0329530871
H	-2.67166808	-0.6683376053	2.2037791403
H	-4.9225381085	0.3284652789	2.5139056597
C	1.8780692875	-0.6499867413	2.5529120002
H	2.1279559445	-0.5956409299	3.6209991038
H	0.8225982107	-0.9285942462	2.4656980994
H	2.4713679821	-1.4548952569	2.1200298275
C	1.2844378001	1.736581148	2.7064880941
H	1.5210283284	1.6274136485	3.7726406338
H	1.4782957185	2.7780644617	2.4404147992
H	0.2142322368	1.5356636574	2.5879091918
C	-0.0334244126	3.0202690629	-0.0555396752
H	-0.2131699653	4.0108890926	-0.4942383333
H	-0.8723329365	2.3754342134	-0.3415587727
H	-0.0527617616	3.1369811832	1.0277563116
C	1.1559932356	2.4447804369	-2.1352623609
H	0.8560421929	3.4459942454	-2.4707447097
H	2.0837598819	2.1969828536	-2.6547642346
H	0.3767679165	1.7446888442	-2.4537534707
C	2.4404326375	3.4643306254	-0.2416046019
H	3.4167003429	3.1363732269	-0.6081908239
H	2.5216550806	3.6380902264	0.8343148753
H	2.2246454142	4.4352174526	-0.7078458274
C	3.6346861054	1.1034258128	2.1088713844
H	4.3113384569	0.3594282692	1.6809385294

H	3.8504021028	1.1515144815	3.1848134416
H	3.8864928451	2.0781497251	1.6822714658
C	2.1746567946	-0.7135055649	-2.3281136108
H	2.8931295888	-1.3103975696	-2.9055670565
H	1.3019368983	-1.3432395913	-2.1281045049
H	1.8576620066	0.1139333616	-2.9628388065
C	3.2923247291	-1.5605727882	-0.3020778328
H	3.9028841666	-2.1468179102	-1.0007309721
H	3.9044124098	-1.3800237493	0.5842863088
H	2.4338358414	-2.1793993802	-0.0218200016
C	4.1220487665	0.5593814322	-1.3554830137
H	4.6499867776	0.9123366487	-0.4658807188
H	4.8179200044	-0.0781144264	-1.9172934055
H	3.9018752457	1.4245566709	-1.9859869284

<b>3<sub>tBu</sub></b>	<b>[Pd(PhCl)L]</b>	<b><math>\eta^2</math>-meta-para</b>
Pd	-0.5337256335	0.9025780153 0.
P	-0.5698270918	-1.4246754784 0.
C	0.3377284993	-2.1096112373 1.6035855533
C	-2.4413532738	-2.0245946444 0.
C	0.3377284993	-2.1096112373 -1.6035855533
C	-0.6992499423	3.0928722296 0.
C	0.0225102051	3.1459391549 1.217803529
C	1.4113370027	3.3258708866 1.2181665208
C	2.0830313856	3.4370798346 0.
C	1.4113370027	3.3258708866 -1.2181665208
C	0.0225102051	3.1459391549 -1.217803529
H	-1.7848025027	3.1720924861 0.
H	-0.5126151433	3.1311493215 2.1623254222
H	1.9599382211	3.3919526787 2.1515724757
H	1.9599382211	3.3919526787 -2.1515724757
H	-0.5126151433	3.1311493215 -2.1623254222
C	-0.3510923738	-1.5006559498 2.8481403566
H	0.313531863	-1.6276624803 3.7125435767
H	-0.5414914088	-0.4292845416 2.7227482231
H	-1.2896211278	-1.9971384887 3.0973463019
C	0.404399834	-3.6371436692 1.7901606861
H	-0.5835686866	-4.0960612855 1.876146685
H	0.9434228957	-3.8569839971 2.7223107
H	0.9440351135	-4.1381408462 0.983151433
C	1.7834057628	-1.5563764832 1.6129401487
H	2.19457293	-1.6713492949 2.6243163963
H	2.4480628043	-2.0989146741 0.9398032612
H	1.8141168015	-0.4924348982 1.3550861698
C	-3.1470725394	-1.4112125853 1.2330973233
H	-4.2327372208	-1.4851287577 1.0876718611
H	-2.9167207623	-1.9394653267 2.1588422643
H	-2.8939258452	-0.3528917108 1.35979917
C	-2.701535808	-3.5425150272 0.
H	-2.2969948383	-4.0394612566 0.8849081956
H	-2.2969948383	-4.0394612566 -0.8849081956
H	-3.7864531158	-3.7183556097 0.
C	-3.1470725394	-1.4112125853 -1.2330973233
H	-4.2327372208	-1.4851287577 -1.0876718611
H	-2.8939258452	-0.3528917108 -1.35979917
H	-2.9167207623	-1.9394653267 -2.1588422643
C	0.404399834	-3.6371436692 -1.7901606861

H	0.9434228957	-3.8569839971	-2.7223107
H	0.9440351135	-4.1381408462	-0.983151433
H	-0.5835686866	-4.0960612855	-1.876146685
C	1.7834057628	-1.5563764832	-1.6129401487
H	2.19457293	-1.6713492949	-2.6243163963
H	1.8141168015	-0.4924348982	-1.3550861698
H	2.4480628043	-2.0989146741	-0.9398032612
C	-0.3510923738	-1.5006559498	-2.8481403566
H	0.313531863	-1.6276624803	-3.7125435767
H	-1.2896211278	-1.9971384887	-3.0973463019
H	-0.5414914088	-0.4292845416	-2.7227482231
Cl	3.8229458285	3.7025095267	0.

<b>3<sub>tBu</sub></b>	<b>[Pd(PhCl)L]</b>	<b><math>\eta^2</math>-ortho-meta</b>
Pd	-0.7431150	-0.5397760 -0.5068890
P	1.4456430	0.0603680 0.0432890
C	1.9226130	-0.6187110 1.8070170
C	2.7044700	-0.6746940 -1.2525130
C	1.6545300	2.0004260 0.0614420
C	-2.6777280	-1.4936570 -1.0836020
C	-3.0738480	-2.2737730 0.0323950
C	-3.7552570	-1.6868810 1.0909250
C	-4.0517760	-0.3120220 1.0785850
C	-3.6341240	0.4602640 0.0055930
C	-2.9414570	-0.0996950 -1.0920210
H	-2.3443310	-1.9863960 -1.9946470
H	-2.8743800	-3.3414360 0.0323200
H	-4.0754590	-2.2905770 1.9355750
H	-2.7977570	0.4929220 -1.9895240
C	2.1142600	-2.1499550 1.7287600
H	2.1861010	-2.5441860 2.7511470
H	1.2625420	-2.6395380 1.2448910
H	3.0294390	-2.4430530 1.2091210
C	3.1778720	-0.0029820 2.4590390
H	4.0748470	-0.1186520 1.8450540
H	3.3692310	-0.5090620 3.4154570
H	3.0534620	1.0599400 2.6810600
C	0.7100530	-0.4010350 2.7455900
H	0.9205190	-0.8847740 3.7094680
H	0.5016880	0.6498960 2.9468670
H	-0.1968450	-0.8479170 2.3248270
C	2.2562750	-2.1187480 -1.5870350
H	2.8829460	-2.5015030 -2.4044860
H	2.3554360	-2.8091080 -0.7492760
H	1.2117030	-2.1362310 -1.9167510
C	4.1871270	-0.6956700 -0.8280340
H	4.3678040	-1.3520300 0.0271070
H	4.5704470	0.2974790 -0.5804070
H	4.7917230	-1.0812700 -1.6606460
C	2.5854670	0.1087970 -2.5785820
H	3.1487630	-0.4295790 -3.3524210
H	1.5450710	0.1772330 -2.9132810
H	3.0033150	1.1163470 -2.5216480
C	3.1038760	2.5269920 0.0289880
H	3.0848650	3.6237110 0.0924770
H	3.7066520	2.1642570 0.8655570
H	3.6215970	2.2715820 -0.8987360

C	0.9527540	2.5802890	1.3097390
H	0.9119570	3.6728360	1.2075740
H	-0.0767620	2.2193390	1.4000530
H	1.4851310	2.3662970	2.2392580
C	0.8813290	2.5758090	-1.1502110
H	0.9004880	3.6726920	-1.0900190
H	1.3089870	2.2939980	-2.1125860
H	-0.1634780	2.2493040	-1.1362350
H	-4.5996490	0.1444660	1.8961520
Cl	-4.0215310	2.1775680	-0.0289520

<b>3<sub>tBu</sub></b> [Pd(PhCl)L] $\eta^2$ - <i>ipso-ortho</i>			
Pd	-0.9476110	-0.1462210	0.0843390
P	1.3842590	0.0264460	-0.0141300
C	1.9353660	1.8300110	-0.5091140
C	2.1896670	-0.4093240	1.7082040
C	2.0894430	-1.2148160	-1.3438540
C	-2.9650530	0.2113280	1.2123990
C	-3.2500860	1.5960980	1.2050260
C	-3.6440540	2.2369660	0.0359570
C	-3.7234780	1.5153950	-1.1673170
C	-3.4508640	0.1513950	-1.1981320
C	-3.0926030	-0.5187840	0.0013610
H	-2.8367040	-0.3154310	2.1521930
H	-3.1884970	2.1460680	2.1402850
H	-3.8849700	3.2959700	0.0502200
C	1.7067150	2.7777110	0.6890600
H	1.8260340	3.8126420	0.3418810
H	0.6937630	2.6780640	1.0925450
H	2.4255210	2.6269220	1.4977040
C	3.3915760	1.9911290	-0.9888610
H	4.1204340	1.6546300	-0.2474350
H	3.5885680	3.0546650	-1.1821660
H	3.5861680	1.4571080	-1.9221080
C	0.9776060	2.3282570	-1.6188710
H	1.1945960	3.3860230	-1.8223490
H	1.0850820	1.7866330	-2.5589390
H	-0.0664160	2.2441820	-1.2993800
C	1.3451070	0.2609670	2.8192640
H	1.7283890	-0.0655340	3.7958490
H	1.3874790	1.3501200	2.7997270
H	0.2943740	-0.0366720	2.7439840
C	3.6665450	-0.0036110	1.8911580
H	3.8075970	1.0804820	1.8804830
H	4.3218170	-0.4387140	1.1326430
H	4.0163200	-0.3611330	2.8695330
C	2.0642030	-1.9291760	1.9576410
H	2.3351890	-2.1333000	3.0020500
H	1.0375710	-2.2795090	1.8078380
H	2.7336430	-2.5241630	1.3323090
C	3.6020520	-1.5080190	-1.2684020
H	3.8775340	-2.1729500	-2.0986300
H	4.2132280	-0.6061120	-1.3576250
H	3.8850130	-2.0195330	-0.3449630
C	1.7671170	-0.6857740	-2.7596010
H	1.9969010	-1.4766690	-3.4858230
H	0.7062810	-0.4369960	-2.8674850

H	2.3623290	0.1866330	-3.0382870
C	1.3105450	-2.5469620	-1.2143040
H	1.6104970	-3.2108460	-2.0367370
H	1.5062950	-3.0755300	-0.2813420
H	0.2301350	-2.3815170	-1.2841950
H	-4.0134160	2.0184600	-2.0857630
H	-3.5628690	-0.4230290	-2.1116390
Cl	-3.2770870	-2.2934250	0.0593120

<b>3<sub>tBu</sub></b> [Pd(PhCl)L] <i>ipso</i>			
Pd	-0.9481140	0.1595320	0.0692380
P	1.3828280	-0.0215400	-0.0140000
C	2.1881280	1.7482010	-0.1574270
C	2.0796620	-0.8791290	1.5927990
C	1.9438950	-1.0760510	-1.5580770
C	2.0723880	2.4769960	1.2001310
H	2.3519470	3.5289440	1.0546700
H	1.0463820	2.4590490	1.5819030
H	2.7403190	2.0718820	1.9636360
C	3.6616690	1.7906210	-0.6088780
H	4.3224030	1.2177080	0.0468180
H	4.0094090	2.8327310	-0.5936970
H	3.7979790	1.4261090	-1.6300840
C	1.3308260	2.5790880	-1.1439400
H	1.6994830	3.6141120	-1.1458380
H	1.3751740	2.2154410	-2.1707880
H	0.2799040	2.5902190	-0.8352540
C	1.3061950	-0.3157750	2.8094200
H	1.6088430	-0.8724020	3.7070970
H	1.5042870	0.7395670	2.9976040
H	0.2266150	-0.4366390	2.6741680
C	3.5932470	-0.7248360	1.8453790
H	3.8842730	0.3124830	2.0293140
H	4.2003950	-1.1071920	1.0210760
H	3.8650880	-1.2967550	2.7434620
C	1.7423900	-2.3863580	1.5498190
H	1.9519430	-2.8180570	2.5376180
H	0.6831020	-2.5561760	1.3309230
H	2.3446920	-2.9402040	0.8259340
C	3.4015780	-1.5792570	-1.5510120
H	3.6001150	-2.1098520	-2.4925510
H	4.1294610	-0.7673080	-1.4759950
H	3.5966910	-2.2870860	-0.7413060
C	1.7198280	-0.2491500	-2.8441540
H	1.8643840	-0.9079850	-3.7106180
H	0.7003300	0.1471740	-2.8984410
H	2.4238890	0.5788650	-2.9513740
C	0.9913660	-2.2909070	-1.6772500
H	1.1964120	-2.8073510	-2.6252390
H	1.1185820	-3.0204870	-0.8770000
H	-0.0559660	-1.9711710	-1.6770840
C	-3.6213700	-2.2484410	0.0424300
C	-3.2393740	-1.5984940	1.2108160
C	-2.9662690	-0.2119240	1.2129470
C	-3.0945910	0.5120600	-0.0016580
C	-3.4383320	-0.1667790	-1.2002480
C	-3.6989770	-1.5336340	-1.1645680



H	-3.8532410	-3.3093700	0.0605070
H	-3.1773790	-2.1438090	2.1487870
H	-2.8431020	0.3204220	2.1502860
H	-3.5519180	0.4024990	-2.1167750
H	-3.9785210	-2.0433990	-2.0825460
Cl	-3.2955720	2.2850180	0.0492150

**3<sub>tBu</sub>** [Pd(PhCl)L] via Cl

P	-1.7202303374	0.105752597	-0.0010838268
C	-2.028582307	1.5045514076	-1.3280135385
C	-2.9411736388	-1.3699131557	-0.3835535538
C	-2.1775258253	0.8289480779	1.7561840171
C	-2.0368708164	0.8734075327	-2.7374381658
H	-2.0070320582	1.6806023529	-3.481631297
H	-1.1586525769	0.2393544042	-2.8979990052
H	-2.9360475074	0.2864564508	-2.9373215238
C	-3.3150870684	2.3380473196	-1.1571683294
H	-4.2200685212	1.7254730915	-1.15697567
H	-3.3984854291	3.0424906717	-1.9965122595
H	-3.3091709261	2.9348205727	-0.2413669433
C	-0.8072315438	2.4553454383	-1.3089608349
H	-0.9172889726	3.1876374189	-2.1211213975
H	-0.7068714468	3.0124142517	-0.3771391724
H	0.1200614348	1.8956587958	-1.4706904018
C	-2.3376682297	-2.2066772721	-1.5383006691
H	-2.9516874386	-3.1073273129	-1.6784075714
H	-2.3132429668	-1.676690685	-2.4909234582
H	-1.3145374469	-2.5165185788	-1.3007270601
C	-4.3874742988	-0.9799505911	-0.7519251073
H	-4.4472645799	-0.4316162205	-1.6959045485
H	-4.8744810556	-0.3793527803	0.0203733026
H	-4.9830235651	-1.8948806761	-0.8775528163
C	-2.9862812349	-2.318547518	0.8351576545
H	-3.5091606853	-3.2384413682	0.5415723639
H	-1.9800620813	-2.5983088907	1.1640467108
H	-3.5302127471	-1.8991652965	1.6846705517
C	-3.6805505636	0.9978713508	2.0576066473
H	-3.7965036649	1.44737255	3.0536783891
H	-4.184730161	1.6552782717	1.3443519907
H	-4.212465647	0.043265651	2.0746052886
C	-1.4859492487	2.1988050838	1.9312642154
H	-1.5807234445	2.5072081659	2.981056994
H	-0.417614003	2.1412029944	1.6974871064
H	-1.9365851413	2.9870777251	1.3241742363
C	-1.5481906113	-0.0918602075	2.8298114415
H	-1.6749116243	0.3777856495	3.8152603425
H	-2.0089088613	-1.0786779236	2.8774909108
H	-0.477672928	-0.2304358676	2.6449589548
Pd	0.4298821218	-0.6257455302	-0.0618526715
C	3.9958046566	-0.434069504	-0.0586190847
C	3.6914049277	0.9078869725	0.1534018438
C	5.3060273523	-0.8852601381	-0.1994544965
C	4.7425598789	1.8248613727	0.2250735815
H	2.6539238295	1.2139956838	0.2564835366
C	6.3432801321	0.0469512864	-0.1246086632
H	5.5110003089	-1.9379505632	-0.3641885615
C	6.0653229081	1.399135228	0.0868115673

H	4.5208048424	2.8756655739	0.3895643867
H	7.3703691608	-0.2901294509	-0.2332162884
H	6.8772484986	2.1183984645	0.1433459702
Cl	2.6803811517	-1.6254928765	-0.1525860878

**5<sub>tBu</sub>** [Pd(Ph)(Cl)L] *trans* halide

Pd	0.7216810	-1.1364220	0.0434070
P	-1.1842480	0.2416610	-0.0220420
C	-2.3830770	-0.9183480	-1.0303160
C	-1.8839070	0.4296660	1.7876320
C	-1.1289640	1.9900400	-0.8657910
C	4.3891380	1.9307320	-0.0496730
C	3.6980750	1.7285030	1.1450110
C	2.6025250	0.8564440	1.1958330
C	2.1909240	0.1926270	0.0374570
C	2.8978680	0.3689250	-1.1579710
C	3.9891730	1.2440700	-1.1975410
H	5.2404420	2.6052180	-0.0828430
H	4.0114650	2.2397240	2.0523780
H	2.0947860	0.6977000	2.1399550
H	2.6190230	-0.1828430	-2.0501080
H	4.5329760	1.3733150	-2.1302980
C	-2.0540980	-2.3820460	-0.6391500
H	-2.6730170	-3.0564160	-1.2460490
H	-1.0087310	-2.6429640	-0.8626250
H	-2.2500030	-2.6140140	0.4068580
C	-2.0721150	-0.8067640	-2.5395560
H	-2.6196260	-1.6014450	-3.0623910
H	-2.3951420	0.1430000	-2.9708980
H	-1.0075830	-0.9477070	-2.7516240
C	-0.2312110	1.9244840	-2.1240410
H	-0.1942480	2.9295470	-2.5648720
H	0.7907410	1.6333030	-1.8757010
H	-0.6060010	1.2481620	-2.8917660
C	-0.4551180	3.0034490	0.0870420
H	-0.2932020	3.9363860	-0.4679310
H	-1.0732220	3.2498530	0.9529400
H	0.5219820	2.6550130	0.4333260
C	-2.5125120	2.5388210	-1.2739980
H	-3.2100860	2.6067490	-0.4366960
H	-2.9813260	1.9454910	-2.0631310
H	-2.3796820	3.5532960	-1.6725250
C	-3.8912980	-0.6684020	-0.8275320
H	-4.2219270	-0.8698760	0.1940730
H	-4.4504780	-1.3484950	-1.4841530
H	-4.1891790	0.3504680	-1.0873230
C	-0.7406990	0.9289350	2.7022800
H	-1.1355620	1.0415660	3.7206870
H	0.0724470	0.1990460	2.7388650
H	-0.3241100	1.8901950	2.4026440
C	-2.2792250	-0.9554410	2.3486940
H	-2.5011220	-0.8383530	3.4170880
H	-3.1728910	-1.3728430	1.8809600
H	-1.4632720	-1.6809660	2.2662550
C	-3.0945200	1.3760000	1.9289180
H	-3.9332690	1.0938420	1.2877190
H	-3.4500870	1.3361260	2.9671670

H	-2.8390380	2.4176240	1.7206570
Cl	2.1652680	-2.9429030	0.1346750

$\mathbf{5_{tBu}}$	$[\text{Pd}(\text{Ph})(\text{Cl})\text{L}] \text{ trans VS}$		
Pd	-0.6584140	-1.1849850	0.0245620
P	0.9871710	0.4340080	0.0124870
C	1.9531160	0.2280720	1.6960960
C	2.1297330	-0.1420600	-1.4727740
C	0.5640990	2.3292410	-0.2357450
C	-4.8886870	0.9179000	-0.0113090
C	-4.1939850	0.7450500	-1.2097940
C	-2.8701650	0.2899420	-1.2022040
C	-2.2373200	-0.0117410	0.0134970
C	-2.9336050	0.1758440	1.2183790
C	-4.2572210	0.6284140	1.2005980
H	-5.9148110	1.2752010	-0.0210160
H	-4.6795110	0.9614680	-2.1585440
H	-2.3498930	0.1496880	-2.1462110
H	-2.4546100	-0.0380260	2.1705830
H	-4.7911440	0.7572620	2.1391880
C	1.9523590	-1.2618770	2.1091070
H	2.4952360	-1.3477470	3.0598710
H	0.9392610	-1.6430250	2.2597010
H	2.4387760	-1.9163130	1.3877170
C	1.2136810	0.9878590	2.8189460
H	1.6632980	0.6999760	3.7775470
H	1.3058680	2.0727880	2.7348230
H	0.1521290	0.7246130	2.8643830
C	-0.5960080	2.7743050	0.6845560
H	-0.7598770	3.8467980	0.5149660
H	-1.5231970	2.2550330	0.4514780
H	-0.3892520	2.6438830	1.7458660
C	0.0719260	2.5628430	-1.6820510
H	-0.2911620	3.5960340	-1.7535740
H	0.8576860	2.4470590	-2.4303520
H	-0.7633120	1.9071360	-1.9392320
C	1.7587410	3.2722500	0.0389600
H	2.6521540	3.0325810	-0.5387860
H	2.0281650	3.3002840	1.0976520
H	1.4555980	4.2904150	-0.2381770
C	3.4154800	0.7233020	1.6496020
H	4.0369540	0.1350610	0.9711040
H	3.8454970	0.6108420	2.6535130
H	3.5075330	1.7758740	1.3755830
C	1.2202870	-0.4472020	-2.6879400
H	1.8575250	-0.7707430	-3.5213700
H	0.5249180	-1.2614200	-2.4634400
H	0.6451710	0.4147600	-3.0293180
C	2.8516620	-1.4645740	-1.1299010
H	3.3536780	-1.8117650	-2.0421640
H	3.6252420	-1.3429070	-0.3685210
H	2.1592490	-2.2506700	-0.8193370
C	3.2028970	0.8863490	-1.8895620
H	3.8765860	1.1534540	-1.0715790
H	3.8163720	0.4325110	-2.6784110
H	2.7809440	1.8037570	-2.3041670
Cl	-0.0449130	-3.4745970	-0.0263340

$\mathbf{5_{tBu}}$	$[\text{Pd}(\text{Ph})(\text{Cl})\text{L}] \text{ trans aryl}$		
Pd	-0.9663490	-0.2113110	0.0518380
P	1.4913240	0.1377790	-0.0236120
C	2.2436160	0.2151270	1.7636330
C	2.4675020	-1.1631090	-1.0767180
C	1.6416500	1.8862390	-0.8556260
C	-5.5668490	0.8441490	-0.1208480
C	-4.9678830	0.2362110	-1.2274900
C	-3.6540340	-0.2375840	-1.1471280
C	-2.9277540	-0.0570300	0.0363100
C	-3.5405320	0.5031870	1.1648130
C	-4.8558170	0.9741420	1.0743000
H	-6.5926120	1.1978280	-0.1839990
H	-5.5273250	0.1146700	-2.1521190
H	-3.2024690	-0.7402850	-1.9982910
H	-3.0032810	0.5764970	2.1080870
H	-5.3269050	1.4248530	1.9446910
C	1.7220800	-1.0112490	2.5538010
H	2.0237880	-0.9004640	3.6039700
H	0.6310330	-1.0826040	2.5172410
H	2.1252910	-1.9585990	2.1980390
C	1.6863560	1.4537670	2.5006000
H	1.9835380	1.3913330	3.5553110
H	2.0762860	2.3982100	2.1144830
H	0.5916560	1.4867360	2.4737320
C	0.4758290	2.7499740	-0.3102740
H	0.4575540	3.7092430	-0.8447110
H	-0.5005760	2.2715070	-0.4906150
H	0.5499460	2.9685420	0.7547730
C	1.3889460	1.7666150	-2.3758290
H	1.3030690	2.7784580	-2.7931120
H	2.2021980	1.2676930	-2.9062210
H	0.4543120	1.2407200	-2.5976040
C	2.9739390	2.6322300	-0.6450730
H	3.8291270	2.0622920	-1.0180020
H	3.1604190	2.8747540	0.4038900
H	2.9472470	3.5825350	-1.1958100
C	3.7832450	0.2524930	1.8394820
H	4.2421600	-0.6565790	1.4432430
H	4.0857210	0.3317510	2.8925350
H	4.2116480	1.1085720	1.3110630
C	1.5882680	-1.5491780	-2.2920860
H	2.0994940	-2.3461130	-2.8484580
H	0.6173050	-1.9355860	-1.9685840
H	1.4204570	-0.7259300	-2.9874670
C	2.6407900	-2.4635480	-0.2584510
H	3.0244270	-3.2400310	-0.9331280
H	3.3642020	-2.3617940	0.5538400
H	1.6895500	-2.8201040	0.1473150
C	3.8549890	-0.7021820	-1.5681500
H	4.5198010	-0.4173860	-0.7481540
H	4.3336170	-1.5332230	-2.1034730
H	3.7995520	0.1366780	-2.2669380
Cl	-1.2490640	-2.5018860	0.3325010

$\mathbf{5_{tBu}^{\ddagger}}$   $[\text{Pd}(\text{Ph})(\text{Cl})\text{L}]^{\ddagger}$  “Y”

Pd	0.9371644533	-0.6124170479	0.046829646
P	-1.4871163349	0.1695056573	-0.0090209036
C	-2.4424679036	-0.7220981105	-1.4488797344
C	-2.380213432	-0.1819851263	1.6797392562
C	-1.471323498	2.0843371437	-0.3354024469
C	5.180769448	1.4115507467	-0.0672378513
C	4.5238860617	1.2270759807	1.1516143978
C	3.3320167345	0.4946847254	1.2092118266
C	2.7898672298	-0.0083805552	0.023532833
C	3.4631265883	0.1185154176	-1.1939812498
C	4.6531155505	0.8543417299	-1.2345450232
H	6.1115806287	1.9710281954	-0.1041848448
H	4.9434822386	1.6369198091	2.067177326
H	2.8389262364	0.324864701	2.1624116308
H	3.0715234744	-0.3442886263	-2.0947537192
H	5.1738765283	0.9743896496	-2.1815123986
C	-2.0440366469	-2.218236593	-1.4196211931
H	-2.5075674317	-2.7186374855	-2.2802135577
H	-0.9594729496	-2.3468488141	-1.4957765335
H	-2.3774752236	-2.7403578657	-0.523542146
C	-1.9454873615	-0.1863406854	-2.8098451381
H	-2.3636134687	-0.822422859	-3.6006684197
H	-2.2700753907	0.8356125831	-3.0173231908
H	-0.854938422	-0.2375559057	-2.8946694659
C	-0.3753799422	2.3811585392	-1.3888654317
H	-0.3416075578	3.4647533516	-1.56415503
H	0.6146441445	2.0727696756	-1.0326810627
H	-0.5497312085	1.8997355795	-2.3506447191
C	-1.0253264456	2.8298910338	0.9428280685
H	-0.8434557547	3.8806239964	0.6818420654
H	-1.7809463014	2.8229363657	1.7316399828
H	-0.0895874788	2.4289234894	1.3460976572
C	-2.8093080353	2.6886170734	-0.8088535862
H	-3.6271075618	2.5050129665	-0.1069210041
H	-3.1141650308	2.3153811478	-1.7896508296
H	-2.6949903698	3.7771047053	-0.9012893934
C	-3.9789760812	-0.595770984	-1.4041259104
H	-4.4114665754	-1.0563537169	-0.5126708645
H	-4.4039650266	-1.1182360275	-2.2717950643
H	-4.3174412522	0.4430208444	-1.4503232967
C	-1.3765366657	0.1155915243	2.8209487393
H	-1.8366928141	-0.1768516396	3.7740499975
H	-0.4564773566	-0.4663445101	2.7009049315
H	-1.105533184	1.1687415526	2.9021471543
C	-2.697753858	-1.6901070529	1.7906021171
H	-3.050889106	-1.8932559952	2.8098815638
H	-3.4869231805	-2.012558148	1.1084449434
H	-1.8107867063	-2.3097229891	1.6215615619
C	-3.6763618174	0.6181199595	1.9178705932
H	-4.4363982773	0.4236525072	1.1565777178
H	-4.1015463817	0.3295299823	2.8884368698
H	-3.497641958	1.6951537399	1.9508714908
Cl	1.8479990198	-2.7308182071	0.1589375817

Table SI4b

Pd(PCy<sub>3</sub>) B3LYP-D2/BS1

Pd 0.0192204277 -0.1057449594 0.0490338517

P	-1.392632701	0.1052559723	-1.6396822682
C	-2.7947461277	1.325082112	-1.3219282643
C	-4.0975564551	1.1231815734	-2.1237699522
C	-5.0972038431	2.2580831553	-1.8401985747
C	-5.4098282144	2.3596041108	-0.3410893552
C	-4.1196146185	2.5481899517	0.4702041662
C	-3.111620686	1.4239566993	0.1851941885
C	-0.5871969278	0.8044857517	-3.188505459
C	-1.3476922612	0.6094539609	-4.5153032361
C	-0.6239437312	1.3162747408	-5.6753324515
C	0.8282856502	0.8369319623	-5.80462122
C	1.5848531912	1.04529811	-4.484647678
C	0.8770127191	0.33 51646507	-3.3206273334
C	-2.2803796594	-1.4431353161	-2.2221073961
C	-3.1279300945	-2.0903974677	-1.0995904302
C	-2.289656089	-2.8391449271	-0.051758123
C	-1.3710166158	-3.8798858731	-0.7079823186
C	-0.4799411967	-3.2256683076	-1.7737482586
C	-1.3355347048	-2.5063727309	-2.8267473218
H	-2.3609337374	2.2909045746	-1.6251625425
H	-4.5574598924	0.1688927665	-1.838493712
H	-3.8977279758	1.0699728164	-3.1982994861
H	-4.6646803835	3.209585183	-2.184038044
H	-6.017982241	2.0947578405	-2.4155415583
H	-5.9057937278	1.4325879811	-0.0157421617
H	-6.1088530061	3.1843298079	-0.1510261536
H	-3.6635896219	3.5126548293	0.1998509894
H	-4.3437390918	2.58678149	1.5441295832
H	-3.5272231928	0.4672723791	0.532058704
H	-2.1790950589	1.5790401917	0.741034786
H	-0.5550496803	1.8852891584	-2.9797298338
H	-2.3684774296	0.9953302041	-4.4350751583
H	-1.4256466087	-0.4611091839	-4.7425049738
H	-1.1710732157	1.1481864338	-6.61229143
H	-0.6274456167	2.4006839944	-5.4886012768
H	1.3322468864	1.3641889114	-6.6249625742
H	0.8328071542	-0.2343753111	-6.0566244751
H	2.6175098423	0.6832704021	-4.5714664323
H	1.6363319821	2.1231249452	-4.2677775033
H	1.3971779631	0.517884516	-2.3721682099
H	0.9060095307	-0.7492343781	-3.4913120947
H	-2.9612507954	-1.1062795385	-3.0133475114
H	-3.8077417976	-2.8089589342	-1.5829351642
H	-3.7573505703	-1.34296572	-0.6051399297
H	-1.6717952971	-2.1159160548	0.4991913048
H	-2.9608133721	-3.3213181091	0.6714145534
H	-1.9866148087	-4.6594531786	-1.1838759228
H	-0.7547915839	-4.3743624871	0.0540704687
H	0.1863384913	-2.4979135468	-1.2885436579
H	0.1484964591	-3.9799788691	-2.2653664405
H	-1.9707911104	-3.2534097881	-3.3278956962
H	-0.6977931838	-2.0688338932	-3.6004213633

Pd(PCy<sub>3</sub>) BP86/BS1

Pd 0.0023597684 -0.115836272 0.0363985424

P -1.4021607162 0.066160232 -1.6430864346

C -2.813420314 1.3178329334 -1.3212605251

C	-4.1218002137	1.149519317	-2.1313153331	C	2.2030463189	-2.7334921754	0.6254119717
C	-5.1002166897	2.3140390404	-1.8570724296	C	3.4058002724	-3.4070657314	1.3164157065
C	-5.4111048649	2.4510405867	-0.3557493993	C	3.2790945735	-4.9384846874	1.2300872506
C	-4.115513623	2.5988285968	0.4646803117	C	3.155477383	-5.4066501909	-0.2282058703
C	-3.1320621956	1.4429852971	0.188982091	C	1.9725148106	-4.7204090863	-0.9285081474
C	-0.5918282772	0.7851800969	-3.2144414538	C	2.0950878434	-3.1918991074	-0.841302946
C	-1.3390539949	0.5983624056	-4.5563403144	C	4.7836021819	-0.6803933118	-0.1899811755
C	-0.6312415992	1.3618484258	-5.6985880879	C	5.7911386738	0.2030733847	-0.9453552717
C	0.8462645831	0.9498219113	-5.832109451	C	5.3779551978	0.3714554212	-2.4161208024
C	1.5900106851	1.1209559505	-4.493887692	C	3.9520953808	0.9331434719	-2.5301849483
C	0.8893119687	0.3560966633	-3.3527591108	C	2.9451195035	0.0606218785	-7650712989
C	-2.2863562856	-1.5262530831	-2.1976550765	C	1.6374874355	-1.2500496032	3.4788953684
C	-3.125331712	-2.1700853171	-1.0583808702	C	1.9964567532	-0.9512905371	4.9425219974
C	-2.2740867368	-2.9105239202	-0.008906545	C	1.9839758483	0.5596013169	5.2127520893
C	-1.3653189163	-3.9684268058	-0.6611546865	C	2.9360858562	1.2871647597	4.252914587
C	-0.4804357999	-3.3255652857	-1.7450038445	C	2.585099472	0.9869290864	2.7865541115
C	-1.3338759975	-2.594481733	-2.7991081301	C	-1.417154701	1.6047585591	-2.4175008519
H	-2.3442204896	2.2766646045	-1.6314794171	C	-2.4965523432	2.4790115883	0.1532771953
H	-4.6149163397	0.19831974	-1.8497155339	C	-3.3207080588	-0.1765679813	-1.0593492154
H	-3.9171576119	1.0890605928	-3.2154474036	C	-0.9200290322	0.4574836522	-3.3201923509
H	-4.6514485576	3.2589972653	-2.2264881334	C	-3.3405093859	3.4850705068	-0.6547061143
H	-6.0323707305	2.1615543806	-2.4344370828	C	-3.2038549478	2.1140095764	1.4726098749
H	-5.9577289074	1.5479056587	-0.0143586559	C	-4.6293214767	0.4753172212	-1.5365994092
H	-6.0834727033	3.3121076425	-0.179028135	C	-3.5810354516	-1.1167997872	0.1358658177
H	-3.6266077414	3.5605685629	0.2046790868	C	-3.6157513269	4.7453088742	0.1841396193
H	-4.3459952558	2.6461837427	1.5460842017	C	-4.3131457227	4.3912474362	1.5064200348
H	-3.5711617192	0.4930816478	0.5558609479	C	-3.4872093229	3.3728186772	2.307098795
H	-2.1869203108	1.5791823238	0.7491792001	C	-4.6252543445	-2.1836508028	-0.2300742699
H	-0.585969635	1.8721855529	-2.9813995121	C	-5.929177058	-1.5410992733	-0.729009474
H	-2.3851692036	0.9443386423	-4.4773421375	C	-5.6627921591	-0.5997860325	-1.913872871
H	-1.3801236276	-0.4781473094	-4.814477744	C	-0.4143189895	0.9764207212	-4.675444688
H	-1.1695644194	1.1918703738	-6.6508430047	C	0.6956974663	2.0193349277	-4.4867213978
H	-0.6890775618	2.4509078869	-5.4942747078	C	0.1999571487	3.178113047	-3.6107072796
H	1.3388236577	1.5400986078	-6.6281825989	C	-0.3076005271	2.6652072088	-2.2545459773
H	0.9013667778	-0.112634301	-6.1471805756	H	3.6083498967	-0.9115811327	2.6490431898
H	2.6384588918	0.7792637228	-4.587472923	H	3.4103442251	0.9352442476	0.1177080596
H	1.6319824262	2.1995198429	-4.2354376359	H	1.2965381212	-3.0915302077	1.1358195831
H	1.4043773114	0.51941298	-2.3860557207	H	4.3380307896	-3.0974971413	0.831867161
H	0.9487725031	-0.7322659981	-3.5545413442	H	3.4711543359	-3.0974676886	2.3655602945
H	-2.9809104164	-1.2008815607	-2.9974731473	H	2.3827734347	-5.2534662285	1.7854779869
H	-3.8182476913	-2.8964063041	-1.534113818	H	4.1423543657	-5.4148912339	1.713315963
H	-3.7636830971	-1.4163376366	-0.5624627929	H	4.0827997026	-5.1527968955	-0.7641468977
H	-1.6371856493	-2.1679101401	0.5207577142	H	3.0466343909	-6.4981955615	-0.2707420625
H	-2.9380079656	-3.3741405951	0.7458209571	H	1.0351590359	-5.0308484177	-0.4432598766
H	-1.9897968511	-4.7654162759	-1.1180738164	H	1.9141667623	-5.0361517077	-1.9785124137
H	-0.7376717931	-4.459880639	0.1064454053	H	1.2371114241	-2.702649404	-1.3202931601
H	0.2027328886	-2.5937265933	-1.2631567244	H	2.9978060939	-2.8778857956	-1.3828028326
H	0.1489378103	-4.0887749678	-2.2415865976	H	4.7844847099	-1.6807268915	-0.6421358877
H	-1.9713986732	-3.340832001	-3.3197171908	H	5.0829457677	-0.797371947	0.8591013344
H	-0.6847010128	-2.1541258868	-3.5771230716	H	5.8288972233	1.1925026524	-0.4654203465
				H	6.7987380138	-0.2281452946	-0.878220452
				H	5.4139146588	-0.6117014189	-2.9096130127
				H	6.090048403	1.0218138843	-2.9405517344
				H	3.9303374955	1.9512440921	-2.1124463023
				H	3.6583414311	1.0128757995	-3.5849123533
				H	1.9369102627	0.4879829663	-1.8129233592
				H	2.8943479454	-0.9292842139	-2.2362399556
Pd(PCy <sub>3</sub> ) <sub>2</sub> B3LYP-D2/BS1							
Pd	-0.0272797332	-0.0488368735	0.1975777537				
P	2.0280112099	-0.8718646289	0.7553134761				
P	-1.8678733018	0.9491721868	-0.7261861748				
C	2.5878762474	-0.5280414927	2.5011679109				
C	3.3680569169	-0.0864286848	-0.2884059455				

H	0.6125749766	-0.9075005564	3.2726787216
H	1.6541638459	-2.3320038798	3.3016023469
H	3.0008288892	-1.3473193978	5.1568318342
H	1.2959370262	-1.4674904009	5.6120519334
H	0.9629091536	0.9406777221	5.0619187752
H	2.2583238054	0.7664349233	6.2554215547
H	3.9669748578	0.9569862443	4.4523191225
H	2.9049288318	2.3705706256	4.4283685399
H	3.2933749315	1.5030676293	2.1271785585
H	1.5839804309	1.3795239101	2.5543155162
H	-2.2944347603	2.0727745089	-2.8880823165
H	-1.5598786133	2.9876278071	0.4261206223
H	-2.950379009	-0.8132076676	-1.8766274829
H	-1.7181540211	-0.2773140584	-3.4820772329
H	-0.1060022241	-0.0610802103	-2.7929975722
H	-2.8271104565	3.7611882614	-1.5822116236
H	-4.2954921515	3.0306598334	-0.9392694321
H	-2.5902799853	1.4029725863	2.0403129918
H	-4.1562003572	1.6154481078	1.2466683816
H	-5.0420325265	1.086814797	-0.7237518632
H	-4.4417525194	1.1460513634	-2.3847967719
H	-3.9458087821	-0.5316738898	0.9904704278
H	-2.6343009986	-1.5783481735	0.4439327515
H	-2.6594963376	5.2435440089	0.4039929138
H	-4.2245765899	5.4544782314	-0.3920946785
H	-5.2992728666	3.9557373264	1.2839195885
H	-4.4872212506	5.2970078708	2.1017340268
H	-4.0079313225	3.1018095078	3.2349208323
H	-2.5294458893	3.8320383758	2.5939961645
H	-4.8245068414	-2.829792044	0.6348956479
H	-4.2152059309	-2.8245459538	-1.02539629
H	-6.6541242241	-2.3152711127	-1.0123067339
H	-6.3791098311	-0.9612442133	0.0911345887
H	-5.2772591214	-1.1862498569	-2.7613371691
H	-6.5968010746	-0.127056816	-2.245389367
H	-0.0533489562	0.1361007778	-5.283187939
H	-1.250430082	1.436610494	-5.2237790974
H	1.0416315642	2.393420639	-5.459275223
H	1.5552117842	1.5423361868	-3.9950416714
H	1.0018280362	3.911729798	-3.4540633583
H	-0.6177470332	3.6989164074	-4.1321396333
H	0.52115745	2.2017992293	-1.6994736519
H	-0.6662566271	3.5046420776	-1.6470491301

Pd(PCy<sub>3</sub>)<sub>2</sub> BP86/BS1

Pd	0.1565271273	0.088976029	-0.1451328876
P	2.1118783429	-0.8187775831	0.6597805508
P	-1.7973400367	1.0095536362	-0.9432487281
C	2.3114486048	-0.7074224699	2.5423102093
C	3.6654527699	0.0570995946	0.0093725398
C	2.2527145515	-2.6938310393	0.3478303057
C	3.3211661674	-3.5018537683	1.120998084
C	3.1517204347	-5.0172642615	0.8727340861
C	3.1916532144	-5.3549407932	-0.6288813915
C	2.1439768363	-4.5386026317	-1.4098228623
C	2.3073263304	-3.0239739235	-1.1625976131
C	5.05069866	-0.5287245574	0.3626259143

C	6.1823570803	0.4259150917	-0.0797209601
C	6.0916873837	0.7498989185	-1.5836613827
C	4.7021361817	1.303765606	-1.9542018252
C	3.5730889534	0.352421512	-1.5076765183
C	1.1463015705	-1.4609877388	3.2300470471
C	1.222031044	-1.37029612	4.7672418911
C	1.2706085046	0.093025255	5.2429136957
C	2.4301655351	0.8493360394	4.5694269203
C	2.3545899279	0.7606506296	3.0305078617
C	-1.7441099025	1.5145816959	-2.7719486704
C	-2.2529658182	2.641166333	-0.0787955428
C	-3.2602799727	-0.1984324832	-0.8791088899
C	-1.4528748129	0.2926915044	-3.6766845645
C	-3.3758701445	3.5231437027	-0.6721142417
C	-2.4610013765	2.4503978551	1.4426562208
C	-4.6626457061	0.3041625494	-1.2895159344
C	-3.3258044614	-0.9527262196	0.4712869831
C	-3.444492076	4.8859789127	0.0531871768
C	-3.6310426452	4.7123857337	1.57233884
C	-2.5335833749	3.8100314163	2.1683210559
C	-4.3337932079	-2.1185053828	0.4066369425
C	-5.7316512858	-1.6374752455	-0.0289975308
C	-5.6675733826	-0.8672047412	-1.3616717688
C	-1.3311302612	0.689772088	-5.1624451086
C	-0.2658447241	1.7808311566	-5.3729131005
C	-0.5516943645	3.00370343	-4.4828670301
C	-0.6719533081	2.6090256101	-2.9963459459
H	3.2676704496	-1.1955542592	2.8252449131
H	3.5797963977	1.0426747238	0.5164511371
H	1.2575333114	-3.0366308599	0.7045148274
H	4.3342254345	-3.1958415041	0.7981971902
H	3.2626160226	-3.3020471645	2.2065162118
H	2.1798318741	-5.3469286721	1.2947428773
H	3.9365652262	-5.5776045171	1.416498152
H	4.2021179905	-5.1254328648	-1.0263515388
H	3.0318374657	-6.4390506933	-0.7845571603
H	1.1272093504	-4.8488998057	-1.0920700472
H	2.2149538782	-4.7539225403	-2.4932890917
H	1.5229344313	-2.4523398983	-1.6945423819
H	3.2823558203	-2.6982861746	-1.5778058987
H	5.1803608784	-1.4980014784	-0.1579690741
H	5.1313128667	-0.7357986773	1.4465532433
H	6.1100251611	1.3676836195	0.502503374
H	7.1675083491	-0.0180135122	0.1613167857
H	6.2796483545	-0.1765098879	-2.1650211669
H	6.8842648069	1.4671387412	-1.8707768985
H	4.559214508	2.289582187	-1.4649644554
H	4.6380580924	1.4819932811	-3.044847248
H	2.577648117	0.7793837899	-1.7371237089
H	3.650134464	-0.5939184662	-2.0787823375
H	0.1924188249	-1.0202639767	2.8726654389
H	1.1334451879	-2.5231604189	2.9218373785
H	2.130032224	-1.9005830535	5.122676768
H	0.356689945	-1.8952506768	5.2156010342
H	0.3131627378	0.5910220114	4.9862150456
H	1.3667537799	0.1401080839	6.3445776835
H	3.3936276215	0.4180285073	4.9124705306

H	2.4332595131	1.9113262968	4.88163275	C	1.1167288752	0.2173416287	5.2646582852
H	3.2192589218	1.2925669499	2.5920477377	C	2.3445232323	0.8904106213	4.6335920951
H	1.4457991133	1.2816420568	2.6653469487	C	2.3039276138	0.7678968215	3.1025730655
H	-2.7335729269	1.9303654347	-3.0560686227	C	-1.4321726928	-1.3943444696	-2.971373263
H	-1.2987091457	3.1994884424	-0.1934159242	C	-0.8092659187	3.3540959845	-1.505259456
H	-2.9416521022	-0.9504554141	-1.633276129	C	-3.1835025096	-0.8492156248	-0.6839008409
H	-2.2454266127	-0.470780142	-3.5677591364	C	-1.232714184	-3.1504902061	-0.6762900303
H	-0.5103755756	-0.181292685	-3.3335895693	C	1.2978565674	3.3793338453	0.6293687897
H	-3.2221634018	3.6886084125	-1.7545260823	C	-1.5733627289	2.6945117919	1.2851733408
H	-4.3515869956	3.0122327743	-0.5662671971	C	-0.0653234608	-1.9274931677	-3.4476053063
H	-1.6418421291	1.8297634633	1.8537588544	C	-4.3566100101	-1.7306355865	-1.1421893051
H	-3.4055182843	1.897633311	1.6218689094	C	-3.3482412647	-0.4987230546	0.8090855393
H	-5.0249207233	1.0349562863	-0.5399420335	C	-2.0049451245	-4.1905000606	-1.5106750839
H	-4.6303869903	0.8342003472	-2.2602578503	C	-1.464820305	-3.3863677944	0.8273058629
H	-3.6321960089	-0.2535954242	1.2745823798	C	-5.6829565445	-0.9739883218	-0.9427169099
H	-2.3135278184	-1.3154727167	0.7359058957	C	-5.8604908511	-0.534735697	0.5209739396
H	-2.5056658096	5.4458137015	-0.1379380608	C	-4.6549518354	0.279848023	1.021024586
H	-4.2655295496	5.4962450626	-0.3700493888	C	-1.0582463672	-4.8109968998	1.2321523392
H	-4.6232367436	4.254560284	1.7661159986	C	-1.8256195897	-5.85254815	0.4037661031
H	-3.6366654828	5.6985473792	2.074810228	C	-1.6153201881	-5.6223225791	-1.1004391276
H	-2.7087299607	3.6528700283	3.2499889654	C	0.0536035963	-1.9217240245	-4.978903254
H	-1.5521880689	4.3197380676	2.077824201	C	-0.1932405926	-0.5151054549	-5.5425525437
H	-4.3897586536	-2.6253056388	1.3891457223	C	-1.5658445983	0.0074815957	-5.0980102985
H	-3.966143989	-2.8747940217	-0.3175932333	C	-1.692446384	0.0006883481	-3.5675101705
H	-6.4277901223	-2.4938613845	-0.1131897872	C	-2.2473609408	2.9011750814	-1.8288631394
H	-6.1465694095	-0.9700640447	0.7545417223	C	-0.7205868872	4.8918228314	-1.5862722982
H	-5.3591033764	-1.5607138523	-2.1710787919	C	1.1313792419	4.7194689472	1.369121157
H	-6.6704575694	-0.4880384044	-1.6376779469	C	2.3432773582	3.4767038393	-0.5015353411
H	-1.0945423292	-0.2052738867	-5.7692755161	C	-2.2097783103	4.0794233778	1.5251243754
H	-2.3119735296	1.0637577879	-5.5230546926	C	-1.1361496718	2.0474773285	2.615251114
H	-0.2220891966	2.0791583671	-6.4378999697	C	-2.6628883818	3.3586329653	-3.2324462798
H	0.7320474716	1.3694859316	-5.1172114416	C	-2.5528644783	4.8864476338	-3.3566210048
H	0.2429457093	3.764952023	-4.6032547326	C	-1.1423539058	5.3723752813	-2.9881625836
H	-1.4972873856	3.4820509593	-4.8128776766	C	3.6863815744	4.0012819919	0.0284299361
H	0.301850273	2.2237110511	-2.6293007706	C	3.5120769892	5.3530566683	0.7352458125
H	-0.8998607398	3.5076990083	-2.3933244176	C	2.490219623	5.2371271973	1.8734854806
Pd(PCy <sub>3</sub> ) <sub>3</sub> B3LYP-D2/BS1				C	-2.2903044474	1.9685340453	3.6230317669
Pd	0.1387162373	0.1159623866	-0.1625075922	C	-2.9249092552	3.3478449616	3.8496071517
P	2.0307412465	-0.8501264211	0.7900786812	C	-3.381736394	3.9585082893	2.5166606314
P	-1.4217420609	-1.3273394595	-1.1002102754	H	3.1322775598	-1.208308794	2.9754683142
P	-0.2081936125	2.4309572549	0.0189553664	H	3.5442475154	0.9497666034	0.5559671127
C	2.2155453047	-0.6976873759	2.6489075842	H	1.2180791563	-3.0763695042	0.8228453634
C	3.5998354072	-0.0667814679	0.1372076723	H	4.2262277604	-3.1569052095	1.351732072
C	2.2311571222	-2.7193242184	0.596362124	H	2.970024279	-3.2492437537	2.5842287818
C	3.1936897267	-3.4752005729	1.5364074328	H	2.0796455408	-5.3256132864	1.6104575818
C	3.0879670336	-4.9960759153	1.3205072529	H	3.7963995266	-5.5171014843	1.9783543631
C	3.3380949533	-5.3810189169	-0.1447681279	H	4.3760511193	-5.1290041794	-0.4101966657
C	2.3870515037	-4.6191605716	-1.0794360736	H	3.2243904115	-6.4647350495	-0.2795898982
C	2.5160566051	-3.1033996732	-0.8675623296	H	1.3535422606	-4.9243742874	-0.8666747227
C	4.9496083151	-0.6704598224	0.5583534056	H	2.5914209929	-4.87468485	-2.1279543356
C	6.1100461713	0.2116388247	0.0669350634	H	1.8411256028	-2.5569631232	-1.5365267584
C	6.0546977061	0.3853912266	-1.4592914335	H	3.5417512856	-2.8074473204	-1.1228173297
C	4.7012869687	0.965415118	-1.9012271573	H	5.0526104735	-1.669178537	0.1113121986
C	3.5375345463	0.0985074758	-1.3967010242	H	4.9941221225	-0.7974073783	1.6476499192
C	1.0023037818	-1.3867545532	3.3103751718	H	6.03 4635857	1.2000598049	0.5449548411
C	1.0328611938	-1.2561062351	4.8405862225	H	7.0732026965	-0.2217590843	0.3679415859
				H	6.1957057124	-0.5979219206	-1.9334592168

H	6.8763531104	1.0287	929705	-1.8003864667
H	4.5985110724	1.9790616569	-1.4927415622	
H	4.6622816715	1.0506614546	-2.9956386338	
H	2.5653879825	0.5270926777	-1.6736111132	
H	3.5952122704	-0.8842072541	-1.8775955147	
H	0.0863619487	-0.9189269797	2.9217854398	
H	0.9611938257	-2.4447118066	3.02327799	
H	1.9103 802284	-1.7927316789	5.2320861158	
H	0.1431389105	-1.7310206597	5.2751640821	
H	0.2097708033	0.7396454672	4.9253898472	
H	1.1516522309	0.300981 7927	6.3587429109	
H	3.2568565666	0.408856605	5.0166015576	
H	2.392022403	1.9493696305	4.9214678794	
H	3.1832636042	1.2535894021	2.6611842273	
H	1.4203362091	1.2945247627	2.7325959237	
H	-2.2202634088	-2.0767691451	-3.3213006526	
H	-0.1653073176	2.953889733	-2.3044175098	
H	-3.2737270151	0.1032642445	-1.2254099142	
H	-0.1637649067	-3.3185824031	-0.8613098089	
H	1.7197356283	2.6771488405	1.3554465736	
H	-2.3743838021	2.0674890443	0.8742908057	
H	0.1047120301	-2.9401503111	-3.0620303375	
H	0.7173038874	-1.286102714	-3.0164230688	
H	-4.2388273986	-2.0275952173	-2.1920531715	
H	-4.3769372783	-2.6502988625	-0.5422635285	
H	-2.4765097039	0.0660824918	1.1557470267	
H	-3.3865243619	-1.4197425068	1.4043825424	
H	-3.0830818656	-4.0600251761	-1.3660548398	
H	-1.8037988579	-4.0487938818	-2.5785826343	
H	-2.5313649492	-3.2541206038	1.0515878154	
H	-0.9120212994	-2.6383596399	1.4102454628	
H	-5.6806442998	-0.0827315759	-1.588438666	
H	-6.5311129638	-1.5973902549	-1.2556854014	
H	-5.9608896516	-1.432797662	1.149180861	
H	-6.7876521263	0.0421568003	0.6344469879	
H	-4.7847465963	0.5353619539	2.0809632223	
H	-4.5970498019	1.2298305643	0.4673378998	
H	-1.2365150096	-4.9668143324	2.3046992546	
H	0.0195838861	-4.9383228738	1.0609678518	
H	-1.516323993	-6.8687003111	0.6815898447	
H	-2.8990291839	-5.7670931319	0.6316456517	
H	-0.5562845407	-5.7888017467	-1.3444290035	
H	-2.1963319914	-6.3502288237	-1.6824254615	
H	1.0447663923	-2.2878273304	-5.2782751294	
H	-0.6891486696	-2.6142873458	-5.4031352048	
H	-0.1187156457	-0.5200057789	-6.6378509014	
H	0.5876313608	0.1625733863	-5.1649810547	
H	-1.7337561243	1.0243099839	-5.4778063082	
H	-2.3503753184	-0.6322222825	-5.5297871131	
H	-0.9673378313	0.7015710637	-3.1309582178	
H	-2.6892120654	0.356303575	-3.2831799799	
H	-2.3178232474	1.8160521566	-1.7361386035	
H	-2.939597478	3.3340929283	-1.0948455766	
H	0.2936434156	5.2402973051	-1.3745987917	
H	-1.3746935385	5.3486609773	-0.8341443276	
H	0.6675773313	5.4692829948	0.717025015	

H	0.4703141292	4.5823780288	2.2299957438
H	1.9895723496	4.1488963929	-1.2932939523
H	2.4776681212	2.4901560007	-0.9545940674
H	-1.478047085	4.7881181456	1.9238901391
H	-2.5760871016	4.4971087822	0.5834938468
H	-0.3150163892	2.6357683863	3.0503820309
H	-0.7390182083	1.0456449975	2.412695364
H	-2.0044885951	2.8793573029	-3.9717094893
H	-3.6875788421	3.0296776926	-3.4528134845
H	-3.2797322795	5.3504506819	-2.6727571261
H	-2.8138264706	5.2108936365	-4.3724923222
H	-1.0911228688	6.4680125412	-3.0416955772
H	-0.4251192147	4.9795277088	-3.7247809426
H	4.4087633808	4.0871214497	-0.7939603468
H	4.0970398441	3.2696047266	0.7413274837
H	4.4753270135	5.7129228346	1.1198098409
H	3.1567459742	6.0957770252	0.0047519796
H	2.877132041	4.5328166733	2.6258798975
H	2.3602879822	6.2052767543	2.3750885438
H	-3.0531913161	1.2809527711	3.2316629989
H	-1.930072756	1.5482592072	4.5720546402
H	-2.1811987888	4.0142070105	4.31272356
H	-3.7699862108	3.2723212076	4.5463728751
H	-3.8353896169	4.9448019692	2.6816972527
H	-4.1568060635	3.3135212968	2.0755901864

Pd(PCy<sub>3</sub>)<sub>3</sub> BP86/BS1

Pd	0.1419629882	0.111485324	-0.0844069225
P	2.1711126408	-0.8996282163	0.6882834182
P	-1.5453443365	-1.2805116779	-1.0487810864
P	-0.2527106105	2.4801934189	0.1967103981
C	2.5065357909	-0.7776386976	2.5644135327
C	3.730531016	-0.0650731435	-0.0356051867
C	2.4454338907	-2.8018606092	0.4595127061
C	3.4534115559	-3.5502257153	1.3698845504
C	3.3916575722	-5.0781293991	1.1391052115
C	3.6261880649	-5.4507414687	-0.335532111
C	2.6449205736	-4.6979324658	-1.251419042
C	2.7177585466	-3.1747912134	-1.0164426368
C	5.1254072672	-0.6361716906	0.3084449713
C	6.2507198765	0.2762477449	-0.2287134765
C	6.1185977945	0.4965463889	-1.747218284
C	4.7289781371	1.0573299916	-2.1064861308
C	3.5944395247	0.1650815646	-1.5618662386
C	1.382467397	-1.4860174594	3.3591800377
C	1.6412863508	-1.4480978597	4.8800082474
C	1.8246377162	-0.0061152604	5.3868543913
C	2.9232374396	0.7217807597	4.5908478546
C	2.6504766466	0.6712956539	3.0721363488
C	-1.4331825854	-1.5433483375	-2.9395569937
C	-0.748770923	3.429622682	-1.3954038062
C	-3.3753927768	-0.705347487	-0.8926536371
C	-1.5081535878	-3.096517382	-0.4363841686
C	1.1973117426	3.5041210261	0.9248411454
C	-1.7155001914	2.7087622563	1.4074267565
C	-0.0939314529	-2.1875590149	-3.3612007566
C	-4.4640703048	-1.3132970021	-1.811132254

C	-3.868046713	-0.7075774365	0.5730656578	H	3.9034005082	0.2462602918	4.8018783341
C	-2.5483308038	-4.1005996992	-0.9833758987	H	3.007441477	1.7747348968	4.9226633436
C	-1.4445667563	-3.1928909159	1.1064145239	H	3.4598906106	1.200799186	2.5354936985
C	-5.798883162	-0.5472290452	-1.6692333082	H	1.7109819199	1.2127470423	2.8467847406
C	-6.2858925324	-0.5162061235	-0.2095251061	H	-2.2498717622	-2.2327150867	-3.2390512022
C	-5.2012039901	0.0555742795	0.722955416	H	0.0068776464	3.0508193618	-2.1176333352
C	-1.1365881427	-4.6312388335	1.5731569546	H	-3.2782234645	0.3623716859	-1.1799388183
C	-2.1474133242	-5.6444674234	1.0031290994	H	-0.5102000732	-3.4189904755	-0.8053243825
C	-2.2268867271	-5.542369644	-0.5309497437	H	1.5652005898	2.8169360304	1.712628609
C	0.0009602392	-2.3837578424	-4.8893794965	H	-2.4594986253	2.0124953142	0.9658172482
C	-0.2073981435	-1.0593462023	-5.644814058	H	0.0460283235	-3.1629385307	-2.8599510002
C	-1.5363828022	-0.4024606353	-5.2333120141	H	0.7315194497	-1.531500744	-3.0186525624
C	-1.6261330965	-0.2130689613	-3.7041827485	H	-4.1500305061	-1.2951493955	-2.8700402513
C	-2.126517147	2.935472534	-1.8923548252	H	-4.6332865677	-2.3750492017	-1.5518706435
C	-0.6980127569	4.9782940484	-1.4508859316	H	-3.0951011554	-0.2688706514	1.2333903057
C	0.9651194377	4.8702589191	1.6154394715	H	-4.0218844162	-1.7517909839	0.9105901012
C	2.3306149213	3.5979821961	-0.1270021461	H	-3.5535890034	-3.8309771905	-0.604192924
C	-2.4253302453	4.0748358533	1.575862014	H	-2.6035466225	-4.0606948887	-2.0868239594
C	-1.3281982346	2.1173577255	2.786432366	H	-2.4126897674	-2.8810533945	1.5430928963
C	-2.4590376342	3.4561807847	-3.3038159659	H	-0.686552585	-2.4832995181	1.4869872749
C	-2.3962476805	4.9931878291	-3.3640768379	H	-5.6602215076	0.4931289298	-2.0301143887
C	-1.0313650349	5.5010505349	-2.8673022347	H	-6.5664352479	-1.0054572767	-2.3227354411
C	3.6317494062	4.1680436173	0.4728885098	H	-6.5334177452	-1.5489249412	0.1126560992
C	3.3899185706	5.5361749243	1.1347717144	H	-7.2198306355	0.0718202855	-0.1248031601
C	2.2810537387	5.4373876513	2.1977869325	H	-5.5408635787	0.0222937953	1.77635197
C	-2.5405326091	2.0197059927	3.734368827	H	-5.0360894906	1.125470793	0.4778907558
C	-3.2433685623	3.3801556724	3.8954213846	H	-1.1269531297	-4.6763539134	2.6794216464
C	-3.640449043	3.9571752353	2.5245341881	H	-0.116753446	-4.9134144236	1.2377414394
H	3.4620070127	-1.3014046096	2.7714132453	H	-1.8793364539	-6.6737767926	1.3094614658
H	3.6678242595	0.9400168934	0.4326177826	H	-3.1499958691	-5.4386855441	1.4319691291
H	1.4370396543	-3.1939238609	0.7092778712	H	-1.2563882431	-5.8536962453	-0.9700488168
H	4.4825441438	-3.1967458711	1.1684924801	H	-2.9889972301	-6.2416803369	-0.9262078365
H	3.2554117377	-3.3485015249	2.4372677992	H	0.9812271615	-2.8279621146	-5.149080437
H	2.3939049364	-5.4492981251	1.4529428451	H	-0.7703400992	-3.1133790221	-5.2127743127
H	4.1317092395	-5.5841866578	1.7890996859	H	-0.1787422796	-1.2272457365	-6.7384943256
H	4.6651352005	-5.1821760205	-0.61831442	H	0.6286744332	-0.3695061987	-5.4076461294
H	3.5336784034	-6.5444901168	-0.4784036901	H	-1.6595367486	0.5748908433	-5.7385192767
H	1.6118259914	-5.0505799466	-1.0505382765	H	-2.3792508254	-1.0399530789	-5.5725255383
H	2.8541481147	-4.9263023293	-2.3145857747	H	-0.8438434957	0.4985937698	-3.3711050934
H	2.0084407341	-2.6527779268	-1.681572268	H	-2.5982106912	0.2485575591	-3.4511821671
H	3.7325694902	-2.8308174098	-1.3001559596	H	-2.1395242296	1.832795893	-1.8767174874
H	5.240829084	-1.6398807049	-0.145043953	H	-2.9167290466	3.2753284753	-1.1930068706
H	5.2394658416	-0.766846756	1.4013018121	H	0.2978041268	5.3539929037	-1.1610027846
H	6.2024377853	1.2565757624	0.2887556933	H	-1.417689924	5.4076016846	-0.7279519567
H	7.2389443607	-0.1598106452	0.0147282295	H	0.5353507948	5.6023535158	0.9077878138
H	6.2667441374	-0.4723172464	-2.2677844142	H	0.2347543275	4.7611185331	2.436035501
H	6.9150938692	1.1740406666	-2.1103186573	H	2.018720984	4.2507579106	-0.9661328503
H	4.6299512599	2.0760272079	-1.6786631428	H	2.5102684265	2.5968611372	-0.5606425724
H	4.6292322592	1.1669610218	-3.2038549045	H	-1.7263282066	4.8286392649	1.9812724943
H	2.6043869243	0.6141534048	-1.7763697492	H	-2.7678885973	4.459579646	0.5987720027
H	3.6181967448	-0.8057267827	-2.0926577975	H	-0.5544865418	2.7559541219	3.2608235125
H	0.422705672	-0.9791714606	3.1308346742	H	-0.8702989109	1.1199952155	2.637938448
H	1.2642050661	-2.5352721001	3.0307361115	H	-1.7334227998	3.0319761205	-4.0280534597
H	2.5556684149	-2.034382072	5.1083145484	H	-3.4598457988	3.0970458932	-3.613019858
H	0.8091947772	-1.9435305807	5.4165347628	H	-3.198177897	5.416229564	-2.7241533417
H	0.8679579278	0.5435699799	5.270987844	H	-2.5919633223	5.3517861867	-4.392803088
H	2.0621385644	-0.002355084	6.4679771842	H	-1.0048382955	6.6079795465	-2.8710164043



H	-0.2411336162	5.1662251261	-3.570986901
H	4.4071484715	4.2493173947	-0.3135178718
H	4.0259258762	3.4614461814	1.2327617334
H	4.3244349095	5.9208159279	1.5862599043
H	3.0891541062	6.2694285595	0.3578655544
H	2.6272976573	4.7757051423	3.0187954186
H	2.0903100666	6.4282217829	2.6537309038
H	-3.2626040703	1.2843919685	3.3235215872
H	-2.2196153025	1.6294081423	4.7196245651
H	-2.557396318	4.0881480652	4.4052826002
H	-4.1338405036	3.2817853009	4.5455313668
H	-4.1183674431	4.948654326	2.6448741322
H	-4.4008398917	3.2956273377	2.0597853797

Table SI4c

Pd(PPh<sub>3</sub>) B3LYP-D2/BS1

Pd	0.097875079	0.0073369964	0.07546926
P	2.2906810077	-0.0066628143	0.0037922146
C	4.2395847065	4.2100252446	-0.0397254036
C	4.9139309675	3.1575455181	0.5848359546
C	4.3432205556	1.8824687013	0.6236110403
C	3.0892873251	1.6518438076	0.03816801
C	2.412588941	2.7166164129	-0.5763456788
C	2.9874125223	3.9875027476	-0.62121633
H	4.6839711591	5.2016443513	-0.0659502056
H	5.8837180357	3.3283305065	1.0453884672
H	4.8681440693	1.067905563	1.1139900069
H	1.4287129467	2.5363973589	-1.0043274456
H	2.4547963757	4.8055260275	-1.0993770377
C	4.3190218437	-2.1518538375	3.5907586862
C	4.9406622098	-2.1866255228	2.3397391374
C	4.3445199152	-1.5602797451	1.2418982503
C	3.1176410269	-0.8956092144	1.3881107194
C	2.4932438381	-0.8759897681	2.6446852952
C	3.0939875358	-1.4947013441	3.7419509583
H	4.783002164	-2.6420330651	4.4427756186
H	5.8890078457	-2.7034811038	2.2162132504
H	4.828306495	-1.5925609689	0.2700799151
H	1.5288898172	-0.3823086835	2.7442477027
H	2.6020582746	-1.4739902852	4.7110009726
C	4.0861594557	-2.1130872297	-3.7275846978
C	4.7719804706	-1.0353940804	-3.1611842475
C	4.2463588117	-0.3762224104	-2.0466465319
C	3.0261850412	-0.7901569826	-1.4913711973
C	2.3369204557	-1.864923678	-2.0737052164
C	2.8673642487	-2.5275796474	-3.1814969055
H	4.495350699	-2.6226472662	-4.5961351256
H	5.7156637105	-0.7046840331	-3.5876302327
H	4.780343617	0.4635195123	-1.6115894293
H	1.3781526155	-2.1629609258	-1.6546597482
H	2.3255102073	-3.3589175218	-3.6250702665

Pd(PPh<sub>3</sub>) BP86/BS1

Pd	0.1219223171	-0.0217291661	0.0722382561
P	2.2985135591	-0.0180550981	0.0023293233
C	4.2006200672	4.2585350732	-0.0183781128
C	4.8503112479	3.2251959001	0.6750673905

C	4.2989919424	1.9327533531	0.6991564994
C	3.0850840737	1.6645965741	0.0315015673
C	2.4326014704	2.7127602379	-0.6542119516
C	2.9908941175	3.998839156	-0.6855938754
H	4.6309028182	5.2663611324	-0.0321968486
H	5.7900842019	3.4232653807	1.2033881924
H	4.8112343155	1.132433592	1.2441191963
H	1.4751867194	2.5081565629	-1.14989478
H	2.4740540664	4.8032750686	-1.2212736965
C	4.3284335964	-2.1801704287	3.6230102064
C	4.8995355268	-2.3043310988	2.3466446088
C	4.3095878216	-1.6674836906	1.2413567343
C	3.1347577019	-0.9030225616	1.4047593871
C	2.5607179904	-0.792892861	2.6906361846
C	3.1581489937	-1.4201838343	3.7932128225
H	4.7888411534	-2.680921145	4.4822526263
H	5.8082387194	-2.9010254593	2.2061464668
H	4.7618199081	-1.7704951197	0.2489411502
H	1.6322336242	-0.2206667341	2.8113451652
H	2.7020633549	-1.326360381	4.7853703562
C	4.0897027938	-2.1162595664	-3.7784025886
C	4.725697143	-0.975009986	-3.2647590298
C	4.2072689584	-0.3247585382	-2.1319056291
C	3.0396414966	-0.8097623262	-1.505557319
C	2.4001163801	-1.9521611865	-2.0355135293
C	2.9263999493	-2.6055601377	-3.1592162954
H	4.4943650838	-2.6192832415	-4.6639942763
H	5.6293242842	-0.5847632012	-3.747140093
H	4.7091231396	0.5655911353	-1.7379943096
H	1.4776089776	-2.3118098932	-1.5624621921
H	2.4202264764	-3.491064891	-3.5602818467

Pd(PPh<sub>3</sub>)<sub>2</sub> B3LYP-D2/BS1

Pd	0.0004457527	0.0128791055	-0.0049884475
P	-2.2795352712	0.0168817647	-0.0059445678
C	-4.154819965	3.7177098109	2.0784242284
C	-4.8572720947	3.1019508867	1.0387033108
C	-4.313778327	1.9925580043	0.385635774
C	-3.060916268	1.4909988914	0.7684433358
C	-2.3542780834	2.1239591615	1.803390363
C	-2.9020971078	3.2275431495	2.45977315
H	-4.5782572354	4.58217 23427	2.5835033158
H	-5.8270324107	3.4869255878	0.7332968694
H	-4.8558672725	1.521905758	-0.4297708241
H	-1.3686658763	1.7493431008	2.0727459206
H	-2.3471342725	3.7117087913	3.2593013376
C	-4.1590556342	-0.0327596719	-4.2512534856
C	-4.8578418146	-0.6286747055	-3.197696732
C	-4.3125475192	-0.6381904305	-1.9110842055
C	-3.0619974225	-0.0511116475	-1.6690229924
C	-2.3586987056	0.5319152845	-2.7351741907
C	-2.9081454562	0.5472456392	-4.0183874876
H	-4.5835290748	-0.0287440493	-5.2519972823
H	-5.8259635225	-1.0895893312	-3.3772267908
H	-4.8520738456	-1.1109586488	-1.0953771452
H	-1.3744252385	0.95647857	-2.546672396

H	-2.3558770731	1.0005249423	-4.837645659
C	-4.1447083878	-3.6337930392	2.1747700251
C	-4.8517584917	-2.4282969296	2.1523749274
C	-4.3115110159	-1.3102053134	1.511625555
C	-3.0575430978	-1.3899487371	0.8880647046
C	-2.3465544721	-2.5998138955	0.9273309478
C	-2.8908821661	-3.7180352182	1.5616039509
H	-4.5651878227	-4.5017362653	2.676321459
H	-5.8223293374	-2.3565209494	2.6369134959
H	-4.8575806454	-0.3709359687	1.5053606156
H	-1.360809729	-2.6450166616	0.4683489122
H	-2.3324017864	-4.650287386	1.5872864366
P	2.2797863776	-0.0028506968	0.0001038645
C	4.1479848269	0.2987996299	4.2397985272
C	4.8559197848	0.8182702446	3.1523470154
C	4.3142790114	0.7504842051	1.8660508315
C	3.0579952098	0.1622552604	1.6583217688
C	2.3458608231	-0.3440008534	2.757291807
C	2.8918371563	-0.2823425341	4.0407070298
H	4.5697725362	0.3549866359	5.2401060855
H	5.8283840766	1.2796656997	3.3051955174
H	4.8609663792	1.1641976016	1.0232932971
H	1.3581354437	-0.7704492243	2.5924627063
H	2.3331040755	-0.676727537	4.8856672235
C	4.1849368811	3.4948679238	-2.3866563576
C	2.9347170369	3.6297976867	-1.7750755452
C	2.3781176287	2.555785979	-1.0782607786
C	3.0735784282	1.3406926519	-0.9737142611
C	4.3239296684	1.2096881404	-1.5956056062
C	4.8762083328	2.2832378023	-2.2993834879
H	4.6148303625	4.3279235792	-2.9370192524
H	2.3886187725	4.5666780179	-1.8506839311
H	1.3944994361	2.6395461566	-0.6200726849
H	4.8574844979	0.2650331748	-1.5382115711
H	5.843830486	2.171724803	-2.7822943527
C	4.1274615688	-3.8400486238	-1.8489487944
C	4.829306928	-3.1723681033	-0.8414234493
C	4.2939113614	-2.0204371576	-0.2589899525
C	3.0494389465	-1.5287153046	-0.6797293817
C	2.3430866461	-2.2132207607	-1.6814955146
C	2.8831501986	-3.3590155939	-2.2681330514
H	4.5446152039	-4.7370956609	-2.2994714084
H	5.7924125075	-3.5492622537	-0.5062969401
H	4.8362554709	-1.508102395	0.530844138
H	1.364201513	-1.8434693446	-1.980478612
H	2.3287624236	-3.8823219014	-3.0430283081

Pd(PPh<sub>3</sub>)<sub>2</sub> BP86/BS1

Pd	0.0000106298	-0.0020613707	0.0017496209
P	2.2842244068	-0.0081439972	-0.0056160341
C	4.1664458811	3.283433341	-2.747603615
C	4.8346039124	2.9206678219	-1.5670897949
C	4.2944672056	1.9363086285	-0.7220401647
C	3.0749670692	1.3071573528	-1.0502984696
C	2.4023319172	1.6883557172	-2.2328934342
C	2.9492261552	2.6640394967	-3.0796285051
H	4.5885107571	4.0537196969	-3.4031988968

H	5.7796850269	3.4068905833	-1.2984330769
H	4.8179698448	1.6646273033	0.2015300472
H	1.4381247868	1.2206047721	-2.4706562979
H	2.4170698315	2.9506951481	-3.993972057
C	4.1828877392	0.7011155765	4.2116302153
C	4.8344911276	-0.1552680273	3.3096573233
C	4.2892866869	-0.3882869707	2.0355506746
C	3.0810116237	0.231893035	1.653908937
C	2.4250208942	1.0813650771	2.5727308245
C	2.9773123923	1.320635742	3.8398287277
H	4.6087062841	0.8785699656	5.205841557
H	5.7705215811	-0.6478933278	3.5975718408
H	4.7996463002	-1.0628788492	1.3391121874
H	1.4694394561	1.5387477771	2.2859315581
H	2.4581435874	1.9816012126	4.5433377694
C	4.1384928482	-4.0353138368	-1.5037433796
C	4.8035867685	-2.8330680271	-1.7932533
C	4.2720880206	-1.6074662602	-1.3570498874
C	3.0642639302	-1.5737846327	-0.6288060723
C	2.3943953878	-2.7871298027	-0.354191715
C	2.9329130284	-4.0099278231	-0.7816604327
H	4.5536709276	-4.9895905184	-1.8477365559
H	5.7395685314	-2.8459720735	-2.3638415278
H	4.7931199979	-0.6730318242	-1.5934274719
H	1.4386387854	-2.7566533659	0.1847214683
H	2.4029362621	-4.9438897577	-0.5619565659
P	-2.2844272793	0.0064332569	0.0084781687
C	-4.1892530961	-0.6530215599	-4.213921624
C	-4.8437649595	0.1862300302	-3.297906786
C	-4.296376211	0.4044225993	-2.0221657678
C	-3.0831237398	-0.2136168446	-1.652835476
C	-2.4243394387	-1.0455695492	-2.5855035736
C	-2.9786572263	-1.2699870188	-3.8545277167
H	-4.6168796174	-0.818989641	-5.2093608295
H	-5.783749005	0.6768939409	-3.5761472029
H	-4.8086167072	1.0662214758	-1.3148382146
H	-1.4651585109	-1.5009477284	-2.3074511922
H	-2.4572609753	-1.9173416682	-4.5689820612
C	-4.1413939009	4.0131945433	1.5564584681
C	-2.9378740215	3.9981990436	0.8307249294
C	-2.3983144171	2.7812684333	0.3881112907
C	-3.0650866919	1.5637276069	0.6512848401
C	-4.2710240243	1.5869560803	1.3830135127
C	-4.8035157418	2.8065640628	1.8343832132
H	-4.5574582956	4.9627814765	1.91205127
H	-2.4102959046	4.935556592	0.6200142325
H	-1.4441653355	2.7585586976	-0.1539274396
H	-4.7897703168	0.6489700206	1.6100793214
H	-5.7380919608	2.8114340008	2.4073376619
C	-4.1624979218	-3.3166793102	2.7153930264
C	-4.8282339117	-2.9463051168	1.5359193957
C	-4.2894318791	-1.9522668607	0.70137382
C	-3.0735754517	-1.3211528946	1.0389899057
C	-2.4032681469	-1.7099129586	2.2205199173
C	-2.9489601569	-2.6951443339	3.0568707191
H	-4.5835560602	-4.0943270795	3.3628948653
H	-5.7705041241	-3.4338643741	1.2599214713

H	-4.8112961195	-1.6743663236	-0.2212334128
H	-1.4417937866	-1.2404093672	2.4657275709
H	-2.4186394762	-2.9875497744	3.9704617085

Pd(PPh<sub>3</sub>)<sub>3</sub> B3LYP-D2/BS1

C	7.1454132485	0.2372894217	5.139439432
C	8.4550614147	0.4656279485	4.7076552378
C	8.7580058648	0.4351662686	3.3437532727
C	7.7533427286	0.1697041036	2.4028492209
C	6.4454866908	-0.0748436105	2.8475146722
C	6.1396690793	-0.0316295478	4.2073044076
H	6.9128318527	0.2525852554	6.201220496
H	9.2409463825	0.6659170556	5.4320627158
H	9.7768592631	0.6070688906	3.006625472
H	5.6825068978	-0.3354467479	2.1173535308
H	5.1280776534	-0.2430460782	4.541566628
C	8.279029198	4.5045510759	-0.8314960944
C	8.225296934	4.24372264	0.5401167091
C	8.1671734445	2.9260617285	1.0054163747
C	8.1556058745	1.855676239	0.0993708921
C	8.2017860308	2.1286782894	-1.2771693617
C	8.2691848495	3.441868084	-1.7412175138
H	8.320473658	5.5300240233	-1.1900790548
H	8.2284330667	5.065976585	1.2516193393
H	8.1284847669	2.7294315475	2.0726584186
H	8.1578348856	1.3041708649	-1.983308107
H	8.291134633	3.6331116843	-2.8107870951
C	12.4635573584	-1.3623433903	0.1899415328
C	12.2066527363	0.0048399217	0.3285935671
C	10.8938033549	0.4649831761	0.4677745924
C	9.8216118881	-0.4395491131	0.472619103
C	10.091121305	-1.8114817	0.3332982593
C	11.4008472683	-2.2717292428	0.1931694974
H	13.4852794894	-1.7153370197	0.0741327347
H	13.0286894148	0.7164234543	0.3226350314
H	10.699291855	1.52983815	0.5587190526
H	9.2657473508	-2.5150848972	0.3032899894
H	11.581652162	-3.3368156112	0.0715195432
P	8.0530671037	0.0797445936	0.5899317389
C	10.2619531062	-3.0221671854	-4.7980215822
C	9.0371890363	-3.3155103792	-5.4059308101
C	7.8442506404	-2.8514329706	-4.8451570363
C	7.8633888293	-2.0839546694	-3.6711632524
C	9.0993443767	-1.7912416765	-3.0707533142
C	10.2910906474	-2.2577572269	-3.627343336
H	11.1871731387	-3.3936005192	-5.2316722111
H	9.0092877218	-3.9134396043	-6.3135852721
H	6.894094496	-3.1081947842	-5.3041485637
H	9.1171563025	-1.2309517297	-2.1408048869
H	11.2331546657	-2.0378697861	-3.1318076937
C	5.3673198691	2.5285640864	-4.9196200431
C	5.7269836532	1.4232407955	-5.70072049
C	6.0101086042	0.2005922442	-5.0913940559
C	5.9392717932	0.0722121752	-3.6951868985
C	5.5815896403	1.1832234238	-2.9210110124
C	5.2940464527	2.408347484	-3.5302662526
H	5.1517227403	3.4817656935	-5.3960288253

H	5.7892540736	1.5179855952	-6.7820136111
H	6.2968790808	-0.6562885759	-5.6951999229
H	5.5647774582	1.0820623617	-1.8383194788
H	5.0330449986	3.2674541318	-2.9181907265
C	3.0707979753	-4.5157887784	-4.1546816309
C	2.8756415771	-3.1541297742	-4.388901905
C	3.8678276604	-2.2297675201	-4.0432253184
C	5.0618960594	-2.6595762957	-3.4496469816
C	5.2429356221	-4.0331864806	-3.2074944708
C	4.2621432066	-4.9536639606	-3.5658022294
H	2.2982673216	-5.2326253607	-4.4208359713
H	1.9530908221	-2.8054857557	-4.8470145112
H	3.7144514601	-1.1728189276	-4.2399289533
H	6.1518133058	-4.3791916349	-2.7233891537
H	4.4143771948	-6.0093775011	-3.3599201415
P	6.3380988533	-1.4935719716	-2.8104855589
Pd	6.7674061948	-1.4604936215	-0.5459992419
C	2.2921877872	-5.3671699913	-0.6192919727
C	3.3003450413	-6.187565411	-0.102895919
C	4.5248335871	-5.6356642	0.2798447516
C	4.7535138515	-4.2594665964	0.140194305
C	3.7402777329	-3.446563526	-0.388491623
C	2.5120011975	-3.9949367362	-0.7591615933
H	1.3425226389	-5.8001857273	-0.9234640363
H	3.1329533442	-7.2569937624	0.0005331517
H	5.3096946262	-6.2751719082	0.6741297616
H	3.9419400845	-2.3886077377	-0.5398564856
H	1.7430552958	-3.3584822665	-1.1873238145
C	6.458532265	-3.3719048158	5.2241152174
C	5.264645413	-3.7017171528	4.5816302575
C	5.2104567478	-3.7678137983	3.1845951711
C	6.3504852489	-3.4929848647	2.4187776643
C	7.5451443965	-3.146630027	3.075667979
C	7.6019259889	-3.0968890362	4.4651410217
H	6.4990461803	-3.3203904899	6.3091779028
H	4.3723751972	-3.9171044093	5.16474055
H	4.2828057351	-4.040409698	2.6899383395
H	8.4296939202	-2.9031828234	2.4927095029
H	8.52937463	-2.8162948284	4.9558224192
C	9.6177892753	-6.5642804535	-0.5182438213
C	8.9259021566	-6.7010387059	0.6899399727
C	7.9341074844	-5.7818075744	1.0405805377
C	7.6168947361	-4.7174352515	0.1824409474
C	8.3206252357	-4.5876222538	-1.024706909
C	9.3145510705	-5.5033300194	-1.3762772286
H	10.3945364427	-7.2772435294	-0.7834037677
H	9.1639955586	-7.5206632451	1.3634512682
H	7.4170891286	-5.8752868519	1.9911885743
H	8.1064685975	-3.7465508305	-1.6740996449
H	9.8532997236	-5.3723437663	-2.3112923521
P	6.3427501319	-3.4411810229	0.578085314

Pd(PPh<sub>3</sub>)<sub>4</sub> B3LYP-D2/BS1

Pd	0.2652589487	0.2600539133	-0.4924367586
P	1.6573730442	1.6511373155	0.8987072613
P	-1.1248558666	1.6534064042	-1.8825327087

C	2.8908798663	2.7378028788	0.0473962557	C	0.3796920024	3.9804595427	4.1138875987
C	-0.2752228988	2.8986510118	-2.9574638039	H	0.6216176432	4.1064814355	5.1666620276
C	-2.3673093078	2.7320409913	-1.0321532093	C	1.1063402662	3.0663598249	3.3440501421
C	-3.4939421211	4.846405688	-0.6196469987	H	1.9024454606	2.4890577632	3.803288091
C	-2.5694224628	4.0854012868	-1.3426220029	C	-0.2264051624	3.64 72768558	1.417899742
H	-3.6360543632	5.8953990716	-0.8680299875	H	-0.4836560313	3.5099806648	0.3762793329
H	-2.0027928683	4.5479142842	-2.1444801769	C	-2.4006794156	1.4576835858	3.8362704257
P	-1.1268516811	-1.1295478179	0.9032530857	H	-1.9320715212	2.256806012	4.4026856723
P	1.6563393786	-1.1287930461	-1.8817556166	C	-1.639320503	0.7397286024	2.9152298354
C	0.8039622129	2.884202949	1.9863541714	H	-0.5969159943	0.99369 72514	2.7802950439
C	2.7473614102	0.8029807242	2.132260349	C	-3.7593379434	1.1665628821	3.9938778448
C	-2.2107150772	-0.2822149582	2.143523582	H	-4.3623634545	1.7321344553	4.7000989393
C	-0.2740021789	-2.3705968592	1.9804461068	C	-4.3403174553	0.1468527278	3.235350 8621
C	-2.3670694428	-2.209773889	0.0528870569	H	-5.3949136115	-0.0898317234	3.355723023
C	2.9057669611	-2.2002809261	-1.0323762028	C	-3.5707561574	-0.578596241	2.3199924552
C	2.7285048664	-0.2766671934	-3.1279578878	H	-4.0322160726	-1.3687997846	1.7366437254
C	0.807521196	-2.3746871437	-2.9574406339	C	-4.220 7699321	-3.7444581275	-1.4044353299
C	-3.1197868877	2.1594894255	0.0029640676	H	-4.9289377507	-4.3421980293	-1.9731238112
H	-2.962906764	1.1227804135	0.2675304843	C	-4.0463409004	-2.3892390249	-1.7005792358
C	3.647345065	2.1708151048	-0.9882013365	H	-4.6009921001	-1.9182363719	-2.506395325
H	3.505624423	1.130295836	-1.249111296	C	-3.1247878779	-1.6341937512	-0.976925663
C	4.5641749078	2.9337943718	-1.7095987162	H	-2.9767601028	-0.5936468162	-1.2319422024
H	5.1191339148	2.4693320936	-2.519015738	C	-2.5597973366	-3.5665506 83	0.3545981512
C	3.9909130573	4.86425724	-0.3731498943	H	-1.9875980144	-4.0312122344	1.1511215291
H	4.1211837038	5.9156011925	-0.1273044175	C	-3.4782021851	-4.3288719332	-0.3746387225
C	3.0778845646	4.0938317494	0.3544724762	H	-3.6124458933	-5.380999804	-0.13434 71732
H	2.5054338759	4.5513292214	1.1550964223	C	1.1863255629	-4.2252384055	3.5119520741
C	4.7681656946	-3.7262032709	0.4246158285	H	1.7565853293	-4.9331246696	4.1085256541
H	5.4786063085	-4.3207947154	0.9937992593	C	1.4763625247	-4.0539357876	2.1548726266
C	-0.9463567486	-4.0535595122	-3.1367489091	H	2.2786 688137	-4.611281879	1.6809346207
H	-1.7526703406	-4.6074803963	-2.6654311494	C	-3.7414927859	-0.6473708088	-4.9840802356
C	-0.2236072254	-3.1306620639	-2.3823060366	H	-4.3403971876	-1.2139179091	-5.6929739588
H	-0.4825535827	-2.9793776285	-1.3432554799	C	-4.3258782094	0.3749849764	-4.231435494
C	1.1073661594	-2.5670348345	-4.3146050679	H	-5.379256992	0.6132096992	-4.3593796414
H	1.9020457895	-1.9929303122	-4.7801112692	C	-3.5616565111	1.1012461365	-3.3121461207
C	0.3783948815	-3.485647941	-5.0769186834	H	-4.0267495284	1.8921127526	-2.7324675857
H	0.6186579541	-3.6195919293	-6.1290807065	C	-2.3850951145	-0.9414150288	-4.8152443377
C	-0.6502323786	-4.2293038762	-4.4919186876	H	-1.9141122201	-1.7437241181	-5.3753936839
H	-1.2189036391	-4.9379879135	-5.0890641914	C	-1.6286638726	-0.2210043256	-3.8919710096
C	3.0886750083	-3.5617525726	-1.3177114927	H	-0.5876833831	-0.4765113684	-3.7499442382
H	2.5047505692	-4.033101918	-2.1017824284	C	4.2522573728	1.1726475832	-4.9982719262
C	4.0111307333	-4.3196737962	-0.5890425374	H	4.8455190669	1.7383327897	-5.7125883857
H	4.1372232845	-5.3754382412	-0.8175340563	C	2.8953800608	1.4620693752	-4.8240955509
C	4.6033243075	-2.366368035	0.7055768932	H	2.4184020977	2.2599440468	-5.3853698555
H	5.1677805962	-1.8882599117	1.5005575779	C	-2.2029935648	0.8041374088	-3.1266909454
C	3.6770365726	-1.6160308507	-0.0171234772	C	0.1617129959	-3.4781494742	4.0997350589
H	3.5366170124	-0.5725738204	0.2300926033	H	-0.0750771293	-3.6100341448	5.1529299187
C	4.0870346673	-0.5699488119	-3.319113705	C	-0.5699485416	-2.5608762003	3.3385275148
H	4.5569488622	-1.3589220925	-2.7407665353	H	-1.3653502167	-1.9885344513	3.8050172437
C	4.8440398314	0.1545932186	-4.2455064092	C	0.7526668282	-3.1305979437	1.4019230447
H	5.8972505435	-0.0814465924	-4.3788876397	H	1.0050778631	-2.9852735661	0.3599577356
C	2.1464869173	0.7433394829	-3.8936016063	C	4.2972892786	-0.6389241976	3.9862292285
H	1.10478412	0.9939149444	-3.7478326142	H	4.9009753641	-1.2013549942	4.6943388182
C	1.1733957252	4.7670265461	-4.4844056666	C	4.8719109843	0.3938079305	3.2399237606
H	1.7386992978	5.4804997484	-5.0790411649	H	5.9220368951	0.6438580024	3.3720861713
C	0.7457555707	3.664602017	-2.3769847142	C	4.1017911729	1.1152657916	2.3217939383
H	0.9987252905	3.5185995585	-1.3357523763	H	4.5588709044	1.9150568705	1.7476199609

C	4.7342184429	4.2881389443	-1.4069262221
H	5.4382993122	4.8917735363	-1.9744552581
C	-0.9472717645	4.5650447389	2.1802135045
H	-1.7529827963	5.1237347074	1.7137068951
C	-0.648414011	4.7305170291	3.5359442042
H	-1.215178385	5.4352237773	4.1395794863
C	1.4643060192	4.5938266197	-3.1276746374
H	2.2632507171	5.1547194908	-2.6520971955
C	-4.0494726093	2.9118943406	0.7188289363
H	-4.6016997655	2.4416232746	1.5268831525
C	-4.2350553762	4.2634848039	0.4121186633
H	-4.9486528585	4.8596870124	0.9756256515
C	-0.5693628602	3.0884345924	-4.3159266464
H	-1.3589316494	2.510188271	-4.7849974262
C	0.1546162897	4.0142188838	-5.0743369654
H	-0.0822885486	4.1467367364	-6.1274539004
C	2.1823297397	-0.2315990182	2.8912207848
H	1.1434587257	-0.495246113	2.7470805174
C	2.9443517949	-0.9468966535	3.8137942009
H	2.4804746513	-1.7557612963	4.3703591047

Table SI4d

Pd(SPhos) B3LYP-D2/BS1

Pd	-0.2694964132	-1.2946808479	-1.456052828
P	0.8973534985	0.161901645	-0.1890509786
O	-3.3549391429	1.1786934988	0.6050673647
O	-1.034107182	-2.8685553565	0.9717921939
C	-1.2180468501	-0.2022118255	1.7336401083
C	0.1214858864	0.2134069983	1.5077042353
C	0.8521028475	0.7124876611	2.5990375838
H	1.87831067	1.0335097258	2.4578796285
C	-1.0315019694	0.432887968	4.0798014738
H	-1.483371738	0.5180669882	5.0647039465
C	-2.0548386984	-0.76808995	0.6394308231
C	-1.7727071863	-0.0728335988	3.012968041
H	-2.8024992026	-0.3836570317	3.1615738608
C	-0.7261408648	2.2955514566	-0.9343766422
H	-1.1965563222	1.5527812681	-1.5925173887
H	-1.2357224462	2.2264297858	0.0343520779
C	-1.7097543038	-2.0489351276	0.1019647809
C	-3.0647010063	-0.0280580217	0.0260775555
C	-3.7007733317	-0.4889922709	-1.1498773541
H	-4.4801685885	0.0952126359	-1.6233921004
C	0.7613043316	1.946343352	-0.7386507898
H	1.2509951433	1.9662568243	-1.7233520967
C	-4.1128964661	2.1104673952	-0.1495376574
H	-3.6465289549	2.2972183349	-1.126429918
H	-4.122464741	3.0329131302	0.4365440795
H	-5.144705961	1.7627271834	-2.996267211
C	2.7098495217	-0.0654383404	0.1663970505
H	3.0659669595	0.7094374706	0.8582691929
C	0.292072283	0.8205598983	3.8729351586
H	0.8880161958	1.2111764673	4.6939218454
C	-3.2953453456	-1.6882835504	-1.7173446861
H	-3.7734714593	-2.0389077988	-2.6280296327
C	1.4475018845	2.9801464703	0.1687243329
H	2.5142745727	2.7462460015	0.2789844228

H	0.9967229517	2.9318864486	1.1686582784
C	-2.2958249857	-2.4939652543	-1.121003465
H	-2.1313903747	-3.5040269258	-1.4781380843
C	2.9440882537	-1.4460381664	0.8068714882
H	2.3872878613	-1.5203956702	1.7486197881
H	2.5383434862	-2.2127679625	0.1303386904
C	-0.4198052139	-4.03102097	0.4348601284
H	-1.1672160239	-4.7371723165	0.0462927257
H	0.121840597	-4.495003959	1.262582375
H	0.2798142755	-3.7527310355	-0.3676176319
C	-0.2078134142	4.7471349093	-0.5858433559
H	-0.7047917659	4.7445857401	0.3959912795
H	-0.3139595947	5.7577325359	-1.0014542605
C	1.2767036231	4.4022177156	-0.3933720884
H	1.755553994	5.1297539616	0.2752407405
H	1.7895321274	4.4692251464	-1.3647566175
C	3.5114360619	0.0754335958	-1.1412960568
H	3.368085184	1.0772485373	-1.5661075848
H	3.1194922796	-0.6460617697	-1.8728790771
C	-0.8946647493	3.7155145358	-1.4934574519
H	-0.4501279383	3.7663152576	-2.4990143949
H	-1.9620975083	3.9521646427	-1.5999530162
C	4.4401009671	-1.7056825483	1.0392658502
H	4.8243807572	-0.9778108737	1.769857725
H	4.5844636584	-2.7039098076	1.4729142943
C	5.2328112143	-1.5695684966	-0.2693439214
H	6.3027609544	-1.7366827953	-0.0895003724
H	4.896330506	-2.3454653046	-0.9733235424
C	5.0072019781	-0.1887625153	-0.9039522922
H	5.5556245837	-0.1077251613	-1.8515042013
H	5.4072276343	0.584997066	-0.2314209114

Pd(SPhos) BP86/BS1

Pd	-1.136382796	-0.4576046883	-0.5841462519
P	-3.0960300957	0.510616582	0.0168952638
O	-3.200333807	-4.0732727736	0.9201764188
O	-2.4143619489	-1.5905604349	-2.9970232022
C	-2.7354557293	-2.6169015054	-0.8753438509
C	-4.1341899965	-2.0919215297	-0.8057653306
C	-4.4294083379	-0.7465101464	-0.4189087013
C	-6.8349665171	-1.2389484371	-0.6078130725
H	-7.8740893758	-0.8993634182	-0.5280950265
C	-6.5412428257	-2.5559842247	-0.9912045353
H	-7.3491182115	-3.2610195237	-1.218370635
C	-5.2065731547	-2.969399786	-1.082204255
H	-4.9718306117	-3.9982445222	-1.3740683789
C	-1.8109629515	-2.0579121164	-1.8385430045
C	-2.262149352	-3.5783869077	0.0382079136
C	-0.3961314131	-2.3247549203	-1.7104859812
H	0.3016856914	-2.0214034388	-2.4966465861
C	-2.8801255512	2.0443025489	2.4507394303
H	-3.1849516384	2.958338729	1.9084928126
H	-1.7803569361	1.9533406936	2.3325160817
C	0.0222761343	-3.2877480973	-0.7446713073
H	1.0869484603	-3.5420354231	-0.6849861596
C	-0.8863860156	-3.9401931056	0.0865316446
H	-0.5281725353	-4.6842704434	0.8015624568

C	-4.1758400581	1.8246559747	-2.3034600643
H	-3.3670748707	1.3285899308	-2.8771104112
H	-5.0236387994	1.1186907283	-2.2928379002
C	-3.2281946054	2.2012623226	3.9469043422
H	-2.7001075568	3.0809951428	4.3621759027
H	-4.3134930285	2.4104391235	4.0457543961
C	-3.6674691595	2.0966205056	-0.8676788789
H	-4.497059266	2.5361624234	-0.2720988845
C	-2.7716076211	-5.04497637	1.8721783495
H	-2.3797443084	-5.9567350223	1.3796383439
H	-3.6695766334	-5.3049773081	2.4533886282
H	-1.9987354999	-4.6403387015	2.5544576172
C	-5.7842869298	-0.3544321067	-0.32465421
H	-6.0275696642	0.6717497813	-0.0220745822
C	-3.5573907061	0.7995960596	1.8377944909
H	-4.658411195	0.9463960485	1.8684342113
C	-2.9058738708	4.4218627246	-1.6287438902
H	-3.6899948293	4.9337847825	-1.0330916487
H	-2.0401394537	5.1106894456	-1.6641036961
C	-2.4982100674	3.1129544454	-0.9201480149
H	-2.1186842154	3.333570761	0.0934162581
H	-1.6558760418	2.6374125347	-1.4632318083
C	-4.5882337187	3.1290971713	-3.0163173516
H	-4.9308190019	2.8994753683	-4.0436003529
H	-5.4580334962	3.57215681	-2.488041221
C	-2.883305545	0.9346626444	4.7514171287
H	-1.783930639	0.785447874	4.7414555409
H	-3.1759785744	1.0602910382	5.8113798733
C	-3.5660833271	-0.3047341398	4.144156686
H	-4.6662681334	-0.2073363538	4.2513049341
H	-3.2766759329	-1.2171272829	4.7001215084
C	-3.2093442678	-0.4683866865	2.6529733076
H	-2.1212855051	-0.6623042464	2.5522209983
H	-3.7226914642	-1.3498991838	2.2271208044
C	-1.5684661165	-0.9445260331	-3.9515613487
H	-1.0320604298	-0.0922908151	-3.4872000839
H	-2.2374120252	-0.5785837379	-4.7452320561
H	-0.8360890121	-1.6498821522	-4.3913732738
C	-3.4401405398	4.1532624503	-3.0477029195
H	-2.6160333286	3.7575651671	-3.6764772951
H	-3.7737390464	5.0963447708	-3.5213101732

Pd(SPhos)<sub>2</sub> B3LYP-D2/BS1

Pd	-0.7295914728	0.5833370613	0.1466056568
P	-0.1737239902	-1.5128428538	0.8489069457
P	-1.4176786014	2.2510582735	-1.2554646086
O	2.8914306482	2.9795040784	-1.5931311271
O	4.1071826035	-1.8126181232	2.2963766371
O	0.4601713303	-4.7413517807	2.539284602
C	3.6121143341	-3.0415512836	1.9583591912
O	-0.3470409076	3.6541441479	1.7375297279
C	1.2994206361	3.3072520157	0.1047443748
C	0.5796190732	4.2542067434	-0.7930517732
C	-0.6415276625	3.9253929347	-1.4164475426
C	1.5340814388	-2.2834187389	3.1491078571
C	-0.6607510092	6.1134212715	-2.5032491105

H	-1.1484899359	6.8261645102	-3.1636579576
C	2.3038670007	-3.3074068246	2.3925063504
C	0.5514607298	6.4329468843	-1.8866644531
H	1.0203083481	7.3976438936	-2.0634470656
C	1.1616164266	5.505858497	-1.044488235
H	2.1096806002	5.7406022963	-0.5690398489
C	-2.2496523872	-2.9461669036	2.1846737762
H	-1.522741981	-3.2753561132	2.9320558067
H	-2.6270375435	-1.9647033128	2.5072522835
C	1.1065261681	-2.2251859339	-0.3123537196
H	1.4942694568	-3.1772323823	0.0558086727
C	0.141407204	-0.4471069971	4.7557856611
H	-0.4111403466	0.2629223539	5.3665087363
C	0.7938424785	2.9934502096	1.3778075037
C	1.7322709785	-4.5538594796	2.0833017894
C	1.9046676089	-2.0620807868	4.485399136
H	2.7431074916	-2.6239199555	4.8874537485
C	0.4797948216	-2.4850230527	-1.6963445431
H	-0.3032010322	-3.2485753541	-1.6219647368
H	0.0063654238	-1.5604376362	-2.052964086
C	2.473306284	2.6675348854	-0.3244279353
C	1.4353010961	2.0544071885	2.1979082357
H	1.0185728025	1.7706506442	3.1546773377
C	-2.5991006975	-2.3582141549	-0.2432449575
H	-2.9713523421	-1.3623865337	0.0323853998
H	-2.1302161004	-2.2366133733	-1.2241206833
C	0.473551219	-1.5432105281	2.5875779798
C	1.2185022509	-1.1573332468	5.2912535895
H	1.5215041987	-1.0085211803	6.3244345468
C	-1.9717842388	0.4525490908	-3.3966087908
H	-3.0402671812	0.6961518289	-3.3625711432
H	-1.7922424813	-0.3296206355	-2.6450024219
C	2.5999026713	1.4391273692	1.7447207207
H	3.0689904943	0.674580466	2.3579193239
C	2.2581121012	-1.2143173997	-0.4380138083
H	2.7033503028	-1.0268499526	0.5399309606
H	1.8352509091	-0.255994451	-0.7648869471
C	3.1351937073	1.7446383793	0.4947660421
H	4.0210480924	1.2287031926	0.1436240259
C	-1.5603543043	-2.78615165	0.8176610824
H	-1.1243340561	-3.7559409494	0.5349695172
C	-3.5523572751	3.7478842283	-0.1496943457
H	-3.1554036718	3.4391248843	0.8275209366
H	-3.0337702627	4.6709437667	-0.4245546303
C	-1.6155597099	-0.0672290627	-4.800998704
H	-2.1989987858	-0.971625449	-5.0196110311
H	-1.9033286578	0.6898580393	-5.5453729424
C	-0.2036569717	-0.6309474084	3.4195468186
H	-1.0013826738	-0.0362734061	2.9827022142
C	-3.2526777347	2.6280980992	-1.1668724496
H	-3.6111943164	2.9435131848	-2.1596299321
C	5.284150748	-1.3663923516	1.6379036455
H	6.1590184118	-1.9606194223	1.9366731383
H	5.4220704763	-0.3278276701	1.9483677417
H	5.1635670226	-1.4166208399	0.5480419501
C	2.4332508796	-5.5025263019	1.3266109813
H	1.9877748474	-6.4578293465	1.0773416862

C	3.7354602086	2.0446820768	-2.2462525517
H	4.7389847865	2.0203675594	-1.7968667205
H	3.8126960203	2.3816113909	-3.2832541712
H	3.3019182589	1.0365286301	-2.2147134537
C	-1.2395007486	4.8670577183	-2.2701253894
H	-2.1774072625	4.6166209901	-2.75994816 41
C	-0.2158633092	-5.928894538	2.1610347682
H	-0.2926467086	-6.0078122699	1.0673440398
H	-1.2149651932	-5.851670252	2.5931385538
H	0.2949048945	-6.8198285725	2.5523273765
C	-3.4292650537	-3.9294820281	2.1055509964
H	-3.0484646951	-4.9285636599	1.8441541706
H	-3.9097606798	-4.015 1926396	3.089361398
C	-1.137025158	1.6890484717	-3.0244190381
H	-1.4117487192	2.5179314205	-3.694134904
C	-4.4499628147	-3.5025466528	1.0410 022805
H	-5.2736715554	-4.2265685935	0.986355401
H	-4.885531092	-2.534222845	1.3298995038
C	-5.5194829914	1.5944622322	-0.6344319626
H	-5.91 66354402	1.8698909052	-1.6235232529
H	-6.0272926947	0.6697562333	-0.3289733966
C	-4.0074347973	1.3474708641	-0.7428026187
H	-3.8004490839	0.5215862347	-1.4288334205
H	-3.6082249065	1.0335108015	0.2323140146
C	-5.0630757169	4.0029378886	-0.0283577083
H	-5.2490435097	4.7974732284	0.7065906078
H	-5.4438319742	4.3641557379	-0.9959207091
C	-3.7672906134	-3.3517458935	-0.3250918503
H	-4.4902604962	-3.0156996843	-1.0803798174
H	-3.3924618499	-4.3344244745	-0.6512719103
C	-0.1131133558	-0.3526374755	-4.9372292068
H	0.1639106754	-1.1606179256	-4.2476019348
H	0.1175244341	-0.6995817238	-5.9533179523
C	4.3269671634	-3.9808164863	1.2012118148
H	5.3298651662	-3.766446459	0.8523114948
C	0.7088943786	0.8973122065	-4.5928783463
H	0.4926964356	1.6880692523	-5.3269956248
H	1.7834043444	0.6786858924	-4.6624684411
C	0.3700862315	1.4012718619	-3.1836347553
H	0.645851043	0.6350450656	-2.4446780626
H	0.9523872109	2.2966289039	-2.9423540001
C	3.3186612884	-1.6776284804	-1.4440171053
H	4.1168850346	-0.9247203375	-1.5167009268
H	3.7805320543	-2.6078961832	-1.0850733666
C	-1.1419283141	3.0636848206	2.7555941771
H	-1.391241718	2.0299838585	2.4777013213
H	-2.0515433129	3.6664891128	2.8134205111
H	-0.6314590116	3.0793330746	3.7292953664
C	3.7238130487	-5.1985699944	0.891796845
H	4.2713053983	-5.928528471	0.3018146302
C	1.5459435954	-2.9444059076	-2.7043827485
H	1.9629486317	-3.906676286	-2.3717496714
H	1.0816297711	-3.112444015	-3.6849662531
C	-5.8189870955	2.7244051328	0.3607093729
H	-5.4941305894	2.4088447358	1.3639904596
H	-6.898585832	2.9171832223	0.41493563

C	2.6847843587	-1.921305374	-2.8205242884
H	2.2760119733	-0.9747722812	-3.2019679827
H	3.4373101625	-2.2667968181	-3.5417636532

Pd(SPhos)<sub>2</sub> BP86/BS1

Pd	-0.5424975536	0.4799297788	-0.3201254249
P	0.0025937312	-1.6010763917	0.5211462344
P	-1.5344433879	2.2371139936	-1.4195160291
O	2.6472384672	3.3234548103	-2.3092902018
O	3.7978840168	-2.2117319064	3.0322489734
O	0.021257453	-5.0090890293	2.6646577271
C	3.3288738935	-3.4593047589	2.6947867903
O	0.0961488154	3.7374589119	1.630246499
C	1.3795756157	3.47338434	-0.3260553204
C	0.4226385147	4.3709933232	-1.0530636719
C	-0.8500676043	3.9840133166	-1.5483386961
C	1.0601539472	-2.4662906685	3.2126585048
C	-1.1984986465	6.279108282	-2.3831665812
H	-1.8392988194	7.0064435396	-2.895243759
C	1.9186153101	-3.6094413782	2.748384224
C	0.0633408908	6.6545545013	-1.8978303162
H	0.4276630669	7.6804077572	-2.0259072711
C	0.8559456005	5.7053628169	-1.244321342
H	1.8426678973	5.9885755336	-0.8611340086
C	-2.366366973	-2.9104735559	1.506395566
H	-1.8386936836	-3.1242776905	2.4504782561
H	-2.7989189997	-1.8930776629	1.6019203115
C	1.5280091222	-2.3939907287	-0.2669606405
H	1.7708961119	-3.3194230202	0.2880389009
C	-0.4218168771	-0.3566985721	4.3978255706
H	-1.0043187361	0.4602665235	4.8403686302
C	1.2337788052	3.2208039177	1.059945155
C	1.3812523488	-4.8963671402	2.4991216028
C	1.0577323373	-2.2538313774	4.6119561061
H	1.6534240026	-2.9295598151	5.2363092741
C	1.2851130335	-2.7685555077	-1.747617502
H	0.4890017757	-3.5312176749	-1.8282697375
H	0.9297007644	-1.8708005202	-2.2950822345
C	2.5587759889	3.0220142859	-0.9679572801
C	2.2256396304	2.5247986424	1.7817904941
H	2.1070696319	2.3167865541	2.8472794634
C	-2.1350325512	-2.6981355854	-1.0030622713
H	-2.5563280694	-1.6730336645	-0.9822267722
H	-1.4477210491	-2.7197239438	-1.8665961917
C	0.3039796552	-1.5888029748	2.3805392056
C	0.3221456967	-1.2241767418	5.2099032578
H	0.337257795	-1.0997773734	6.2989392624
C	-2.6814619347	0.7655913863	-3.6449877681
H	-3.7022113771	0.9837560785	-3.280690523
H	-2.3424291603	-0.1532923505	-3.1250934831
C	3.3761528516	2.0918262936	1.1119365305
H	4.1491911429	1.5532214556	1.6712574621
C	2.7095270664	-1.4033332822	-0.1499425159
H	2.9061183089	-1.1706147988	0.9115655415
H	2.4151820957	-0.4462940137	-0.6270950048
C	3.559386338	2.3289951013	-0.2570483575
H	4.4672116656	1.9799301511	-0.7544967556

C	-1.3698239185	-2.9219000058	0.324006047
H	-0.8662354507	-3.9109834365	0.3047690055
C	-3.3331111368	3.564434519	0.3801046955
H	-2.7150317885	3.1301028003	1.191868781
H	-2.8606838984	4.5250715468	0.1118662888
C	-2.7324152293	0.5159283233	-5.1682213414
H	-3.4042354692	-0.3374775674	-5.3835595449
H	-3.1796945745	1.4008998695	-5.6670770081
C	-0.410589863	-0.5366375602	3.0083292136
H	-0.9613305084	0.1564983769	2.3547578652
C	-3.3148919503	2.5900214636	-0.8227196458
H	-3.8734567017	3.0543172618	-1.664731214
C	5.2117329874	-2.0124407216	3.0342713424
H	5.7191522246	-2.6992225011	3.7396604376
H	5.3617441073	-0.9740205743	3.3658679508
H	5.6438081792	-2.1402903913	2.0230793635
C	2.2084769676	-5.9755047979	2.1217199567
H	1.786863221	-6.9607892336	1.910259591
C	3.8237005947	2.909206227	-3.000502226
H	4.7342829921	3.3719808134	-2.5708918934
H	3.6948474748	3.2531039173	-4.0379482371
H	3.9373215483	1.8075212745	-2.9910054432
C	-1.6361181403	4.9605743591	-2.2080120325
H	-2.625365821	4.6840543637	-2.5918738917
C	-0.5491956537	-6.3145652726	2.5584619273
H	-0.4550567391	-6.7227605374	1.5332527011
H	-1.6145245869	-6.1918531793	2.8028762346
H	-0.0832263888	-7.0181848191	3.2752995852
C	-3.5092555347	-3.9282265572	1.3065393251
H	-3.0874010741	-4.955043934	1.3188938588
H	-4.2130896959	-3.8688370735	2.1594211498
C	-1.7223105307	1.9218526406	-3.2915586038
H	-2.1247784047	2.8559627098	-3.735540826
C	-4.2526773884	-3.7142630113	-0.0231336508
H	-5.0363617657	-4.4844969678	-0.1589979431
H	-4.7718764524	-2.7342578901	0.0032882368
C	-5.4584465895	1.5170508774	0.0870967027
H	-6.0796717856	1.9262365904	-0.7372207432
H	-5.9197699674	0.5531910537	0.3769607608
C	-4.0230958789	1.272000955	-0.4226667339
H	-4.0394915259	0.5595602818	-1.2656172457
H	-3.4138544192	0.7860342653	0.3671423635
C	-4.7654532342	3.8127068261	0.8970429038
H	-4.7342515258	4.4984353084	1.7660115371
H	-5.3516599096	4.3323795177	0.110480156
C	-3.2650321727	-3.728908379	-1.203192474
H	-3.7937260795	-3.5223700689	-2.1538911895
H	-2.8282571917	-4.745067062	-1.3022185862
C	-1.3323378224	0.2622218618	-5.7559179507
H	-0.927392018	-0.6821268309	-5.3373016531
H	-1.3940597968	0.1220144827	-6.8524015387
C	4.1669491063	-4.5303925807	2.3205370981
H	5.2503375453	-4.4037224189	2.2608030809
C	-0.3760246866	1.4179828868	-5.4088509052
H	-0.7195477297	2.3422760021	-5.9184613241
H	0.6405076994	1.2073380664	-5.7941339071
C	-0.3184343852	1.6623741833	-3.8877345567

H	0.1101642845	0.7728950025	-3.3806883019
H	0.3576353393	2.5063794939	-3.6594190341
C	3.9868533572	-1.9483809432	-0.8198986873
H	4.7992950755	-1.1992018255	-0.7409993615
H	4.3303601135	-2.852210792	-0.2747432358
C	-0.0739439503	3.5551295745	3.0357372123
H	-0.1237403806	2.482444971	3.3026276774
H	-1.0291314615	4.0421276632	3.2839065682
H	0.7431575329	4.0369314231	3.6087216033
C	3.5914515535	-5.7740783925	2.0287595633
H	4.2369000617	-6.6086607607	1.7328134887
C	2.568556536	-3.3094707497	-2.4137567105
H	2.854621282	-4.2648850709	-1.9272824299
H	2.3656926575	-3.5445577099	-3.4765983993
C	-5.4771755146	2.5002290912	1.2708131027
H	-4.9573436027	2.0367352424	2.1347973476
H	-6.5163457994	2.6999025343	1.5961760085
C	3.7377691941	-2.316058845	-2.2940898372
H	3.4931338363	-1.3955172995	-2.863515727
H	4.6527279157	-2.7395262273	-2.7519515714

Table SI4e

PhCl/PCy <sub>3</sub>	[4] <sup>‡</sup>	B3LYP-D2/BS1
Pd	0.96129577	-1.986756086 -1.8953394032
Cl	1.9508971298	-3.8093599817 -3.1234507634
P	0.2467938458	-0.1741303573 -0.7357357312
C	2.979839729	-2.1852239084 -2.8221984771
C	1.1461907183	1.3951240676 -1.1770750778
C	2.6637062947	1.170432517 -1.0307130456
C	0.8102966861	1.832731019 -2.6151524638
C	0.4009992752	-0.3051322297 1.1293408259
C	1.4900912902	-1.326941733 1.5188644212
C	0.6281278745	1.0250956559 1.8750417218
C	-1.5506972021	0.2319786203 -1.0154621026
C	-2.4303272897	-1.0046020516 -0.7512756623
C	-3.8942692187	-0.7245797645 -1.1268182918
C	-4.4354278512	0.5080151697 -0.3856823633
C	-3.551240271	1.7374053905 -0.6447061573
C	-2.0911119691	1.4538202646 -0.2531779622
C	3.9809024212	-2.2506889401 -1.8356209381
C	5.0587870134	-1.3689152371 -1.9089115412
C	5.178970834	-0.4692384628 -2.974468951
C	4.206597351	-0.4605663801 -3.9808029485
C	3.1152587468	-1.3278799104 -3.9294813421
C	1.5257856901	-1.544725685 3.0393089935
C	1.7280618634	-0.2186499968 3.787700213
C	0.647525727	0.8002425338 3.3960692663
C	3.461019097	2.4216291744 -1.4276365534
C	3.1122093877	2.867067374 -2.8548321815
C	1.6010465754	3.0924829604 -3.0048166548
H	0.8327203536	2.1926865733 -0.4889640888
H	2.9114767888	0.8781227883 -0.0034464822
H	2.9533613134	0.3347135884 -1.6740774971
H	-0.2652225653	2.0232684302 -2.7172250472
H	1.0663408791	1.0110835751 -3.2997185677
H	-0.5671730446	-0.7138734858 1.4569514682
H	2.4670839278	-0.9550724082 1.1785542202



H	1.3137093101	-2.2701476423	0.9873813033	C	-3.2097600844	0.0888957893	-2.5049664298
H	1.5938447211	1.447515387	1.5694898038	C	-3.8164375147	-0.5005539436	-3.7882908371
H	-0.1394826222	1.7581752568	1.6083737979	C	-2.8180163955	-1.4321057016	-4.4887432739
H	-1.6103288208	0.4451628077	-2.0920651937	C	-3.8161399582	2.5391810749	2.444359978
H	-2.0371869015	-1.8599768271	-1.3160104826	C	-2.725226966	1.597804779	1.9114334826
H	-2.3779672322	-1.2685678944	0.3155848554	C	-3.2895115558	0.68542177	0.8023256033
H	-4.5130666193	-1.6045463563	-0.9092854261	C	-4.5211455174	-0.09458446	1.2940561013
H	-3.9533191278	-0.5466374602	-2.2108896206	C	-5.6046432484	0.868122661	1.8066831933
H	-5.4710739366	0.7116498732	-0.6866252874	C	-5.0496482953	1.7608039423	2.9266697407
H	-4.4470361619	0.3000184256	0.6950045894	C	-1.6716452795	-1.851498269	1.035498679
H	-3.9284721176	2.6057042274	-0.0888242818	C	-2.7239134338	-2.9778293427	0.966235994
H	-3.5916987312	1.9936731867	-1.7137867622	C	-0.7565462656	2.7222231136	-1.0279629962
H	-2.0485839248	1.2506793166	0.8255127648	C	0.1403597341	3.4720821893	-0.2377308599
H	-1.4653444935	2.3345188412	-0.4445241399	C	-2.0966638105	3.1396016335	-1.1593983161
H	3.8865593682	-2.9591032877	-1.0202685789	C	-0.3612239254	4.4879571098	0.5897617804
H	5.814126823	-1.3926535341	-1.1274851332	C	-1.7086515864	4.838491181	0.541974018
H	6.0263333188	0.2076582991	-3.0274244421	C	-1.8712941572	-3.8935327712	3.17466929
H	4.297660454	0.2237413761	-4.820330444	C	-0.8516749468	-2.7481577004	3.2546747191
H	2.3641436362	-1.3360898518	-4.7112238023	C	-1.3547157456	-1.5065369015	2.5023979285
H	0.5726208837	-1.9937500773	3.3575113961	C	-2.5607160254	4.1761449025	-0.3594291792
H	2.3201620639	-2.2565883713	3.2986577867	C	-2.2155218801	-4.2223360741	1.71498288
H	2.7153298475	0.1924773785	3.5280051852	H	3.5600630605	-2.8372189087	-3.4304010333
H	1.7219705808	-0.3851156691	4.8725923214	H	2.3662761845	-2.1864239946	-4.5615906886
H	0.8140838859	1.7542527909	3.9132356179	H	2.9803422118	-0.483084906	-2.8427065527
H	-0.3359762845	0.4250745641	3.7167706958	H	1.2785088853	-0.902987339	-2.723805042
H	4.5351624796	2.2111444787	-1.3470021552	H	3.4979174548	-2.0202553251	-0.9333520446
H	3.2336873185	3.2395703819	-0.7269440217	H	1.6596292521	-3.1737483087	0.2854802003
H	3.662562245	3.7801974543	-3.1171532614	H	0.4986200487	-2.5251319626	-0.8800707901
H	3.4265389137	2.080371293	-3.5535653552	H	1.0697158072	-4.8790309088	-1.4316643928
H	1.2923812497	3.9248068579	-2.3542050498	H	2.7817726949	-4.4496747531	-1.5487111423
H	1.3568427027	3.3816716907	-4.0354495143	H	0.537402012	-3.3369572047	-3.3174548886
PhCl/PCy <sub>3</sub> [6] <sup>‡</sup> B3LYP-D2/BS1				H	1.7575968388	-4.5143368263	-3.8242269272
Pd	0.0099271992	0.844917633	-0.5173462788	H	5.4932811671	1.7545790967	-2.2978586304
P	2.098712156	-0.1952808911	-0.0548946085	H	6.8480466543	0.8852736994	-1.5672945513
C	2.5173550996	-2.495979399	-3.5194862166	H	4.7803528554	-0.4917383637	-1.5850409105
C	2.2939595267	-1.2980112431	-2.584359578	H	5.3019554507	-0.1820187132	0.0720554335
C	2.4622351772	-1.6948676639	-1.1027935364	H	3.1645718799	1.4217909046	-1.4191647779
C	1.530004093	-2.8680195732	-0.7604619193	H	2.7784230667	2.4960354702	0.8370902043
C	1.7605544112	-4.066529385	-1.6936984863	H	4.1768051555	1.6098251445	1.4491046935
C	1.5780480838	-3.6571343252	-3.1625640352	H	4.8272617114	3.920889677	0.760466366
C	5.8788618377	1.3527895238	-1.3491147021	H	4.2548280556	3.5914857605	-0.8816101453
C	4.8918320732	0.2918330205	-0.8292357016	H	6.5236852104	2.1195746385	0.5659826287
C	3.5308534992	0.9400043842	-0.4999434343	H	6.728016466	3.2682594938	-0.7628724745
C	3.7374316921	2.0530158035	0.5453645733	H	1.1044134925	-1.1408274424	4.1659096166
C	4.6967080888	3.1278711449	0.0125876568	H	1.5926902383	0.4016077191	4.8791798156
C	6.0535581421	2.5066614461	-0.3509506217	H	0.9406677812	0.6864164075	2.4584891352
C	1.8750394351	-0.3590933333	4.1395088927	H	2.6312198207	1.0880788769	2.7347587352
C	1.9133642268	0.2610647256	2.734439079	H	1.5883989889	-1.6055181309	1.7644466455
C	2.3318913362	-0.7970457946	1.6920079718	H	4.0003236981	-2.1470222718	1.3032961051
C	3.7039037821	-1.3948581669	2.0454407442	H	4.4594241721	-0.5980990662	2.0187700113
C	3.6706728777	-2.0137446784	3.453413529	H	4.6547927797	-2.4273901906	3.7098608134
C	3.234093848	-0.9795413198	4.5030613039	H	2.9568288368	-2.8514309969	3.4548810868
P	-1.9426909554	-0.3129401032	-0.0095764698	H	3.9900130805	-0.1811767593	4.5519540703
C	-2.3692940574	-2.5507014562	-3.5387025563	H	3.1896239322	-1.4427382549	5.4972156895
C	-1.7814736064	-1.9705844481	-2.2441805685	H	-3.2338191963	-3.1855499232	-3.2917583139
C	-2.767813431	-1.0212249628	-1.5330986286	H	-1.6248694573	-3.1948698118	-4.0257148063
				H	-1.4834116553	-2.7881042182	-1.5776199456

H	-0.8721568736	-1.4005008399	-2.4780738041
H	-3.6589380288	-1.5914045571	-1.2332912722
H	-3.9395109037	0.7495898261	-2.0214707223
H	-2.3325468477	0.6941842775	-2.766920154
H	-4.1187570363	0.3117215229	-4.461722661
H	-4.7244903598	-1.0686141504	-3.5347526483
H	-1.9385773188	-0.8462937404	-4.7939172029
H	-3.2608552492	-1.8563443372	-5.3991324005
H	-4.1128531004	3.2212037533	1.6362708323
H	-3.4105616641	3.160211093	3.2537098943
H	-1.8847161297	2.1763829731	1.5161523577
H	-2.3431104073	0.9852292466	2.7373820599
H	-3.6166427369	1.3589371448	-0.0015735084
H	-4.9180603676	-0.7339616578	0.4950894467
H	-4.2232588003	-0.7546569067	2.1185443094
H	-6.4765268061	0.3022006154	2.1607887527
H	-5.9452336821	1.5022329445	0.9742207638
H	-4.7666580793	1.1250758397	3.7797276383
H	-5.8242769103	2.4525052264	3.2827194779
H	-0.7464885436	-2.2607669929	0.6142876165
H	-3.6649465868	-2.6436386743	1.4171043694
H	-2.9428725837	-3.2431275012	-0.0728258965
H	1.2070805712	3.2886800886	-0.3025968122
H	-2.7589107514	2.6257594974	-1.8435537866
H	0.3257553579	5.0359151003	1.2307737028
H	-2.0906748335	5.6439916704	1.1622072443
H	-2.7899180749	-3.5882175402	3.6980390537
H	-1.4879836422	-4.7845822693	3.6884167963
H	-0.6428028996	-2.4958109982	4.3023646123
H	0.0996559437	-3.0752832176	2.8075558887
H	-0.6126245636	-0.7032681222	2.544343402
H	-2.2630620587	-1.1381938585	2.9960713022
H	-3.6074827643	4.4640739749	-0.4246498144
H	-1.312744566	-4.596984667	1.2084932752
H	-2.9665530868	-5.0217582971	1.66953885
Cl	0.1808870711	2.1057143054	-2.8264740605