Electronic Supplementary Material (ESI) for Dalton Transactions

SUPPORTING INFORMATION

FOR

Negishi Cross-Coupling Reaction Catalyzed by an Aliphatic, Phosphine Based Pincer Complex of Palladium. Biaryl Formation via Cationic Pincer-type Pd^{IV} Intermediates

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Computational Details.

Theoretical calculations for all reactants, intermediates and products were performed at the Density Functional level of theory with the Gaussian03 program package[1] using the hybrid *m*PW1PW91 functional,[2] which includes modified Perdew-Wang exchange and Perdew-Wang 91 correlation,[3] in conjunction with the Stuttgart/Dresden ECPs (SDD) basis set for the Pd center,[4] the standard 6-31G basis set for the hydrogen atoms,[5] and the polarized 6-31G(d) basis set for the remaining atoms.[6] The *m*PW1PW91 functional was selected for our study on the basis of many reported publications where the accuracy and reliability of the method is clearly demonstrated.[7] Pure basis functions (5d, 7f) were used in all calculations. Geometries were fully optimized without symmetry restrictions and for each optimized stationary point a frequency analysis was performed to verify its character (minimum or saddle point). In addition, single-point calculations were carried out for all optimized gas-phase geometries using the CPCM polarizable conductor calculation model.[8] N-methylpyrrolidone (NMP) was chosen as solvent of reaction and explicitly specified with a dielectric constant ε of 32.0. The relative energies reported in our study correspond to the solvent-corrected electronic energies including the zero-point energy (ZPE) corrections obtained from the gas-phase frequency calculations.

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Cartesian coordinates of [Pd]-Cl (1)

GEOMETRY OPTIMIZATION
Final Geometry (x,y,z in Angstrom)

H	3.74112600	-1.93111000	-4.09225800	C	-2.78228200	4.31791600	0.54335100
H	-2.29186000	-2.53341100	-4.36065900	H	-1.40017600	-2.54111100	0.14185000
H	-3.39138700	-1.16382600	-4.31190100	H	5.05632100	-1.14785000	0.65463300
H	-4.68485100	-3.26888000	-4.12807800	P	2.31337700	0.03705200	0.28248800
H	5.94359800	-2.77421500	-3.23471400	H	2.50507200	4.87175400	-0.22309700
C	-2.98403200	-1.98774800	-3.70953500	H	1.08165600	-2.65998500	0.36961000
C	3.91117800	-2.04716200	-3.01613700	C	-4.28227000	4.35882700	0.82886900
H	5.80936400	-1.02799400	-3.07060800	C	-2.22212300	2.89876100	0.66174300
H	3.52955500	-3.04189700	-2.74480600	C	3.44375000	4.60463500	0.28001000
C	-4.12509900	-2.89849000	-3.26160000	C	3.22822800	1.64600200	0.50449600
C	5.40516000	-1.98131800	-2.70309100	H	-2.24457000	4.98624400	1.22560500
H	-1.43381700	-0.72660400	-2.85629000	H	3.98947600	5.53998700	0.44928000
H	-3.70702400	-3.78141300	-2.75842200	H	-0.33630000	-4.52373300	1.16742300
H	-5.57112100	-1.35665900	-2.83638700	H	-4.68150300	1.59361500	1.05187100
H	3.41555100	0.01348000	-2.61192400	H	4.17464400	1.41281200	1.01617500
H	2.05405400	-1.06388200	-2.45471500	C	-1.49931900	-2.70595900	1.22156700
C	-2.22098200	-1.40682700	-2.51861600	C	0.97990600	-2.83572800	1.44779200
C	3.12577000	-0.98006900	-2.25215400	H	-2.45257200	-3.22728100	1.38920900
C	-5.06382600	-2.17094200	-2.30063100	H	-4.45974100	4.08288200	1.87783900
H	-3.62108600	0.15726900	-2.14025000	H	1.83034000	-3.45598600	1.76540700
H	-1.72138700	-2.22087600	-1.97638400	H	1.44008500	2.77013200	0.90907300
H	-5.85019200	-2.84736500	-1.94570700	H	-2.29613900	2.57039100	1.70837300
C	5.65997700	-2.08834100	-1.20003300	H	-3.62948700	-1.02542400	1.48051500
H	6.73110000	-1.99830200	-0.98485300	C	-0.33670900	-3.57203500	1.71333000
H	5.35334400	-3.08388000	-0.84995600	C	-2.67758300	-0.48455800	1.46587700
C	-3.17193600	-0.66726300	-1.56701600	H	3.19540700	-1.40845800	2.09743800
H	4.16244900	1.69268600	-1.46181600	C	2.40784800	2.59241400	1.39528900
H	-4.94795500	3.72805900	-1.12183600	C	-0.17369300	-0.61697700	1.71046500
H	4.42935600	4.14569200	-1.59419400	C	2.32925400	-0.74892200	1.96336900
H	-2.80032200	2.23837500	-1.28360900	C	3.12456700	3.92655500	1.60996400
H	2.59834100	2.48508200	-1.37979200	C	-1.51365500	-1.35411300	1.95168800
C	-4.30780600	-1.58723100	-1.10320300	C	1.00727500	-1.49070200	2.19412100
C	3.38536000	-1.09477700	-0.74379100	H	-2.78824100	0.37685900	2.13776900
H	3.03456000	-2.08995900	-0.43370900	H	4.05711700	3.75427300	2.16560700
H	5.27321300	-0.03206100	-0.68782700	H	-0.18553000	0.29944600	2.32787000
H	-2.59461600	4.69023000	-0.47249900	H	2.19029500	2.13165100	2.36538900
C	4.88403400	-1.02229000	-0.42125400	H	2.42608300	0.05520500	2.70221800
C	3.53748200	2.33391300	-0.83352300	H	2.50482300	4.57962300	2.23530000
H	-5.03222600	1.30675900	-0.64918600	C	-0.49364600	-3.83817200	3.21333100
H	-3.89025600	-2.40965100	-0.50833400	H	-1.42825000	-4.38124800	3.40461500
C	4.24823500	3.67299300	-0.62236800	H	0.32603500	-4.47303200	3.57394800
H	-5.00583200	-1.05046400	-0.45038800	C	-1.65757800	-1.63638000	3.46271300
C	-5.03880600	3.39234800	-0.08000400	C	0.82980800	-1.77737100	3.70105600
C	-2.98326500	1.92471400	-0.24547500	H	-2.61254600	-2.14279300	3.66117600
Pd	0.05325900	0.19382500	-0.19024300	H	1.66735400	-2.38665100	4.06892800
H	5.23523700	3.49599400	-0.17134700	C	-0.49455200	-2.50097200	3.96213900
H	-6.10867900	3.39798100	0.15869200	H	-1.68137900	-0.68468200	4.01100200
P	-2.24605600	0.21955700	-0.19492800	H	0.85725400	-0.82965100	4.25578400
C	-4.49015400	1.96737000	0.03636600	H	-0.60832700	-2.67870200	5.03874800
H	-4.66727500	5.37725600	0.70427600	Cl	0.19302300	1.39493600	-2.29484400
H	-1.16033500	2.88371100	0.39542100				

After PCM corrections, the SCF energy is -2679.34381072 a.u.

Zero-point correction=	0.928798 (Hartree/Particle)
Thermal correction to Energy=	0.968663
Thermal correction to Enthalpy=	0.969607
Thermal correction to Gibbs Free Energy=	0.857741
Sum of electronic and zero-point Energies=	-2678.401015
Sum of electronic and thermal Energies=	-2678.361150
Sum of electronic and thermal Enthalpies=	-2678.360206
Sum of electronic and thermal Free Energies=	-2678.472072

Cartesian coordinates of $[Pd]^+$ (B)

GEOMETRY OPTIMIZATION

Final Geometry (x,y,z in Angstrom)

H	-3.68471500	-1.03376100	4.51616400	H	4.68692100	1.11446800	-1.54161600
H	2.63821800	-1.70620200	4.59984000	C	4.92585200	3.23846200	-1.19224100
H	3.73576900	-0.39024400	4.20893600	H	1.22058600	-2.53541800	0.27003400
H	4.99728700	-2.51390700	4.31048100	H	-5.24976100	-0.73678900	-0.21160200
H	-6.01129700	-1.74131700	3.90702500	P	-2.39607500	0.15481800	-0.17693600
C	3.27568100	-1.30259000	3.80615500	H	-1.96389100	4.98632700	-0.48293400
C	-3.94098500	-1.27719400	3.47978300	H	-1.29894600	-2.54419800	0.18909800
H	-5.72084600	-0.05807900	3.49678600	C	4.58530100	4.29534300	-0.14361500
H	-3.67983300	-2.33422000	3.33317900	C	4.45461000	1.84691800	-0.75995000
C	4.37104400	-2.30190500	3.43808200	C	-2.99010100	4.77135200	-0.81168000
C	-5.43850400	-1.08826700	3.24088700	C	-3.14114700	1.81035300	-0.58255400
H	1.66816100	-0.18637900	2.87587000	H	6.00439700	3.21758400	-1.37966200
H	3.91100000	-3.25538200	3.14514800	H	-3.44671700	5.73524800	-1.05782400
H	5.77889700	-0.88816900	2.61587300	H	-0.01907000	-4.59972300	-0.29133900
H	-3.26470300	0.64034600	2.76266500	H	3.08383000	2.64824300	1.56517300
H	-2.03553900	-0.61641700	2.67995000	H	-4.17131400	1.62771100	-0.91962300
C	2.41711000	-0.93668800	2.59386600	C	1.23645700	-2.90892600	-0.76224800
C	-3.10380200	-0.41867400	2.52771700	C	-1.25910700	-2.92228000	-0.84105200
C	5.22870500	-1.78007200	2.28748500	H	2.14845200	-3.50862800	-0.87716400
H	3.78569800	0.49956100	1.79878800	H	5.15421600	4.09373900	0.77397700
H	1.86073300	-1.82253600	2.26055900	H	-2.15668400	-3.53356900	-1.00117700
H	5.98128700	-2.52250200	2.00218900	H	-1.31535700	2.60864200	-1.41444500
C	-5.80804700	-1.36617300	1.78544600	H	5.01333600	1.54392900	0.13536000
H	-6.87518200	-1.18567400	1.61945500	H	3.42830000	-1.44908600	-1.46514300
H	-5.63081200	-2.42586100	1.55760400	C	0.00046500	-3.77776200	-1.01558000
C	3.28534400	-0.41139300	1.44077000	C	2.51346100	-0.85119300	-1.51062500
H	-3.77097800	2.26281900	1.45509400	H	-3.42829200	-1.50052300	-1.68767900
H	2.52784800	4.61017500	-0.71165800	C	-2.36613800	2.49720600	-1.71879700
H	-3.74172200	4.72440800	1.22203100	C	-0.00261800	-0.89116100	-1.61947100
H	2.40874300	2.11516600	-1.36925200	C	-2.52238300	-0.88445600	-1.70025400
H	-2.15871100	2.83902200	1.04666700	C	-2.94953400	3.87399300	-2.04529200
C	4.37579700	-1.42467300	1.06705700	C	1.28020300	-1.72867100	-1.74491300
C	-3.48478100	-0.70266200	1.06798600	C	-1.26065000	-1.74707300	-1.83432700
H	-3.26217700	-1.76287000	0.88063100	H	2.63133800	-0.14871700	-2.34578300
H	-5.24950600	0.55325500	0.98686300	H	-3.96595100	3.75094800	-2.44199700
H	4.44799300	3.50041100	-2.14572100	H	0.01870800	-0.05210100	-2.33133800
C	-4.98705600	-0.49986500	0.82643200	H	-2.36619700	1.87919100	-2.62307200
C	-3.18020400	2.71992700	0.65610400	H	-2.60288400	-0.21677600	-2.56471400
H	1.52567700	2.92767400	0.79023500	H	-2.35915600	4.33940100	-2.84165000
H	3.90605000	-2.33867900	0.68137200	C	0.05310400	-4.34053400	-2.43893300
C	-3.75570000	4.09850500	0.32359800	H	0.94289200	-4.96878900	-2.56448600
H	5.01342100	-1.03114800	0.26766000	H	-0.81778400	-4.97977700	-2.62623000
C	3.09177600	4.29601700	0.17698300	C	1.30872500	-2.30407000	-3.18310400
C	2.95134700	1.85147800	-0.44874000	C	-1.18045200	-2.32828400	-3.26785200
Pd	-0.07807800	0.18024600	0.14437900	H	2.22863000	-2.88842500	-3.31251600
H	-4.81015000	3.98788000	0.03761400	H	-2.07822500	-2.93097700	-3.45561700
H	2.86860100	5.02503400	0.96295300	C	0.07917400	-3.17999500	-3.43793800
P	2.25673500	0.18860800	-0.00224600	H	1.34847600	-1.48184800	-3.90946100
C	2.60817000	2.90954000	0.60994600	H	-1.18870400	-1.50893400	-3.99838500
H	4.89656900	5.28585100	-0.49041700	H	0.11806400	-3.56931400	-4.46129300

After PCM corrections, the SCF energy is -2218.93891723 a.u.

Zero-point correction=	0.927666 (Hartree/Particle)
Thermal correction to Energy=	0.965999
Thermal correction to Enthalpy=	0.966943
Thermal correction to Gibbs Free Energy=	0.857395
Sum of electronic and zero-point Energies=	-2217.962798
Sum of electronic and thermal Energies=	-2217.924464
Sum of electronic and thermal Enthalpies=	-2217.923520
Sum of electronic and thermal Free Energies=	-2218.033069

Cartesian coordinates of [Pd]-Ph (2)

GEOMETRY OPTIMIZATION

Final Geometry (x,y,z in Angstrom)

H	4.01070200	0.69438500	4.27029200	C	-3.24577100	0.60465600	4.03145900
H	-2.63123300	0.96208300	4.86567700	C	4.12358400	1.16226400	3.28573500
H	-3.51543900	-0.43415600	4.26713600	H	5.98781900	0.16252700	2.86851600
H	-5.11295100	1.37013100	4.82813200	H	3.76129400	2.19515500	3.38726600
H	6.18709100	1.74813800	3.60459900	C	-4.51767500	1.44278900	3.91075900

C	5.59395900	1.18829700	2.87257100	H	-2.28112500	-3.49814000	-3.59919400
H	-1.54607300	-0.01436200	2.83753900	H	4.12818700	-4.70922100	-2.61876300
H	-4.24389800	2.50097000	3.79801900	H	-0.23485800	4.84526500	0.63023600
H	-5.72642900	-0.00716100	2.86574800	H	-4.81857000	-0.81231000	-1.63337900
H	3.51223300	-0.64044200	2.26409400	H	4.14118300	-0.66705100	-1.65525500
H	2.20366200	0.48443200	2.54436200	C	-1.46254200	3.23198600	-0.11630200
C	-2.42596900	0.62458100	2.73950100	C	1.01603300	3.38600600	-0.35477000
C	3.25775900	0.42565300	2.26157300	H	-2.40105700	3.79804500	-0.02340100
C	-5.34822300	1.01174700	2.70392300	H	-4.58497900	-2.59351700	-3.58478300
H	-3.59744500	-0.86692300	1.76797800	H	1.88066300	4.06294300	-0.42042900
H	-2.06247900	1.64430600	2.55741700	H	1.45550700	-2.07859400	-2.00108700
H	-6.22746500	1.65722300	2.59425900	H	-2.52309500	-1.16171400	-2.84817600
C	5.75997100	1.79483500	1.48050300	H	-3.64295700	1.83565900	-0.94528100
H	6.81373100	1.78097600	1.17863700	C	-0.28033900	4.19657200	-0.25387300
H	5.45490100	2.85011100	1.50523000	C	-2.71170900	1.32492800	-1.21042100
C	-3.27090400	0.16049400	1.54682300	H	3.16226600	2.26466400	-1.64784100
H	4.21253700	-1.81552300	0.56105000	C	2.40323500	-1.69655700	-2.40131200
H	-4.79036600	-3.74312000	-0.75702200	C	-0.21813600	1.49094700	-1.43598600
H	4.58886200	-4.13073500	-0.21737900	C	2.26401800	1.63752000	-1.70994000
H	-2.70748200	-2.36751600	-0.04717900	C	3.15869100	-2.83018900	-3.09710000
H	2.68458100	-2.60543500	0.21265600	C	-1.53352000	2.29418300	-1.33157800
C	-4.52044500	1.04264500	1.41675900	C	0.97636500	2.45609900	-1.57955800
C	3.43766600	1.01610100	0.85945800	H	-2.88078600	0.84476900	-2.18220100
H	3.09892600	2.06003400	0.90998200	H	4.06285600	-2.42542900	-3.57308100
H	5.30099000	0.02584100	0.34967300	H	-0.27217400	0.90124100	-2.37108800
H	-2.46838700	-4.08077800	-1.94879900	H	2.14256700	-0.92439500	-3.13332500
C	4.91553100	1.04808400	0.44433600	H	2.27974300	1.15524100	-2.69458200
C	3.59731800	-2.21339800	-0.25109100	H	2.54109900	-3.24357900	-3.90299400
H	-5.01507300	-1.41903900	0.00881600	C	-0.45680800	5.05248300	-1.51183100
H	-4.20799000	2.07707500	1.22239900	H	-1.37537500	5.64915100	-1.43733200
C	4.35389900	-3.34690400	-0.94622100	H	0.37795300	5.75896600	-1.60910600
H	-5.13952500	0.73807500	0.56650800	C	-1.70344700	3.17167600	-2.59068300
C	-4.99323700	-2.95982500	-1.49998800	C	0.78503800	3.33417000	-2.83497400
C	-2.99120500	-1.59340400	-0.77596200	H	-2.64141300	3.74297900	-2.53574300
Pd	0.02948300	-0.06065500	0.01017000	H	1.63471600	4.02164500	-2.95613500
H	5.31557300	-2.96791600	-1.32074300	C	-0.51901000	4.13428400	-2.73682600
H	-6.08008700	-2.93695000	-1.64091100	H	-1.77391600	2.52669700	-3.47733700
P	-2.27186200	-0.04342700	-0.02941700	H	0.76484100	2.69176700	-3.72603500
C	-4.51541700	-1.61423000	-0.94554400	H	-0.64766200	4.73645100	-3.64508100
H	-4.62075800	-4.30041300	-3.16063000	C	0.17883200	-1.75448000	1.25026900
H	-1.21355300	-1.93046000	-1.96733400	C	0.02998900	-3.04482700	0.70349400
C	-2.77424900	-3.28671900	-2.64334900	C	0.39771200	-1.72157100	2.63986900
H	-1.34272400	2.63810100	0.79850400	C	0.09828500	-4.20887300	1.47190200
H	5.03158000	1.51910900	-0.53889000	H	-0.13943000	-3.15754900	-0.36650000
P	2.28150900	0.29023000	-0.42695800	C	0.46661900	-2.87387600	3.42483500
H	2.64570700	-4.40436900	-1.71854500	H	0.52503300	-0.76453600	3.14176500
H	1.12887400	2.78758100	0.55763500	C	0.31793700	-4.13038600	2.84432100
C	-4.29252600	-3.31551700	-2.80954100	H	-0.02101200	-5.17922900	0.99480900
C	-2.30030000	-1.93703300	-2.10250100	H	0.63853700	-2.78741300	4.49538300
C	3.55362300	-3.92649100	-2.11020100	H	0.37147300	-5.03064500	3.44950600
C	3.21889700	-1.10289300	-1.24194400				

After PCM corrections, the SCF energy is -2450.64729869 a.u.

pdph.com.log: Zero-point correction= 1.017810 (Hartree/Particle)
pdph.com.log- Thermal correction to Energy= 1.061342
pdph.com.log- Thermal correction to Enthalpy= 1.062286
pdph.com.log- Thermal correction to Gibbs Free Energy= 0.941922
pdph.com.log- Sum of electronic and zero-point Energies= -2449.623602
pdph.com.log- Sum of electronic and thermal Energies= -2449.580070
pdph.com.log- Sum of electronic and thermal Enthalpies= -2449.579126
pdph.com.log- Sum of electronic and thermal Free Energies= -2449.699490

Cartesian coordinates of [Pd]-Cl..ZnClPh

GEOMETRY OPTIMIZATION

Final Geometry (x,y,z in Angstrom)

H	1.61813600	-2.51102100	-4.18775800	H	4.04265000	-2.75289700	-3.86914900
H	-1.94648700	-3.49059900	-3.46480800	H	1.27978900	-3.71644000	-2.89693100
H	-2.74646800	-1.92970700	-3.85966400	C	-4.06714500	-3.44372300	-3.01527200
H	-4.40551900	-3.77760800	-4.02350000	C	3.36717800	-3.51346600	-3.40892900
H	3.31178400	-4.37643900	-4.11325600	H	-1.29649000	-1.82456400	-1.69171200
C	-2.71023700	-2.75885300	-3.11406100	H	-3.96984000	-4.35723800	-2.38060900
C	1.98596100	-2.91248900	-3.21480800	H	-5.32590700	-1.69654300	-3.10845200

H	2.51074800	-0.90981600	-2.58537600
H	0.94421600	-1.47896900	-1.94578800
C	-2.33300000	-2.22284400	-1.74151900
C	1.98874100	-1.80424700	-2.17502700
C	-5.10705500	-2.52691700	-2.39595600
H	-3.48451900	-0.42202800	-2.07971600
H	-2.40204900	-3.09665800	-1.04728000
H	-6.05613000	-3.08986200	-2.24183300
C	3.95805000	-3.96951700	-2.08821900
H	4.98084100	-4.38000600	-2.25533300
H	3.33446600	-4.79248300	-1.66519100
C	-3.34471100	-1.18526000	-1.27163300
H	4.24332800	-0.07811900	-1.84863700
H	-5.77504400	2.80423500	-0.94534500
H	5.75290500	1.92546200	-1.91806500
H	-3.61416200	1.64003100	-0.84344900
H	3.54151500	1.35921200	-1.04870700
C	-4.64774600	-1.93497200	-1.06335600
C	2.64689700	-2.23105700	-0.86818000
H	2.03266100	-3.03691000	-0.41443900
H	4.74077000	-2.06385800	-1.50197300
H	-3.56638900	3.90160600	0.10984000
C	4.02399200	-2.81593900	-1.09406700
C	4.34983600	0.59291800	-0.96669100
H	-5.79984200	0.42373800	-0.56880200
H	-4.51008900	-2.76618200	-0.32967600
C	5.71637700	1.25191200	-1.03006300
H	-5.47306000	-1.29887700	-0.68046300
C	-5.98211500	2.43247000	0.08682800
C	-3.83430400	1.14727900	0.13688500
Pd	0.01734400	-0.00566300	-0.12157000
H	6.49615200	0.46639700	-1.17809400
H	-7.08844400	2.34810600	0.19364100
P	-2.60863800	-0.20746800	0.01435000
C	-5.35708500	1.04718100	0.23709100
H	-5.85823300	4.45312800	0.84637200
H	-2.27593200	2.10884000	1.30979300
C	-3.93561200	3.47601700	1.07131700
H	-1.33617400	-3.13685800	0.39051700
H	4.44738800	-3.20253900	-0.13537800
P	2.46929600	-0.82224900	0.21659700
H	5.45324800	2.98948000	0.23009100
H	0.82925600	-3.70061200	0.53258000
C	-5.45214700	3.44311500	1.08471100
C	-3.38329600	2.07139700	1.26190800
C	6.05448700	2.04941100	0.21603400
C	4.12968500	-0.19005300	0.31779700
H	-3.56767500	4.13968200	1.88731500
H	7.12574200	2.35567900	0.18334500
H	-0.68775800	-5.26710100	1.57313900
H	-5.65397500	0.59544400	1.21314100
H	4.86316300	-1.02332900	0.40538900
C	-1.62825300	-3.31366700	1.44716600
C	0.78862000	-3.65705300	1.64204600
H	-2.64391600	-3.75337600	1.48760900
H	-5.80767700	3.17768500	2.10905200
H	1.61731000	-4.28808400	2.03665400
H	3.69187700	1.63806900	1.38040600
H	-3.75651100	1.70987100	2.25303600
H	-3.66636100	-1.55049800	1.67913500
C	-0.57442300	-4.25039200	2.02722600
C	-2.69689200	-1.01233500	1.61774900
H	3.08188800	-2.30700500	1.97590900
C	4.33835200	0.74368700	1.48882200
C	-0.22145400	-1.34554000	1.88980400
C	2.25815200	-1.57334400	1.82676300
C	5.77268800	1.26441400	1.48555100
C	-1.55991200	-1.91502900	2.09476100
C	0.92007200	-2.21426400	2.18823600
H	-2.72607900	-0.14955000	2.31941300
H	6.49346200	0.41703900	1.56723100
H	-0.08973800	-0.26922800	1.95976800
H	4.13138000	0.24225600	2.45565500
H	2.40280300	-0.73049700	2.53915000
H	5.92977500	1.92252600	2.36769700
C	-0.69016200	-4.37370400	3.53690800
H	-1.68015000	-4.80314400	3.81587700
H	0.09544300	-5.06407100	3.92314500
C	-1.68969500	-2.11558400	3.63786400
C	0.85296900	-2.42901300	3.75273600
H	-2.65201900	-2.60124600	3.91750700
H	1.63996600	-3.13056800	4.11020200
C	-0.52530700	-2.97918800	4.13487200
H	-1.65439900	-1.11821000	4.13131200
H	1.01255900	-1.44617900	4.24696400
H	-0.58365100	-3.05526500	5.24969600
Cl	0.13357100	1.02863600	-2.74048800
Zn	0.23274100	2.75293900	-1.38642300
C	0.82356000	3.29026800	0.44329900
C	2.08744700	3.87753400	0.57134600
C	-0.02181000	3.41224500	1.54727800
C	2.44880200	4.61591800	1.70099400
H	2.90525300	3.64945800	-0.12678500
C	0.33614600	4.10007400	2.70616500
H	-0.96661900	2.87014100	1.49905300
C	1.57932600	4.72442100	2.78624600
H	3.44676200	5.06361600	1.75969800
H	-0.34836700	4.12688800	3.56027200
H	1.87318400	5.26509400	3.69141400
Cl	-0.49442600	4.55123000	-2.50526900

After PCM corrections, the SCF energy is -5150.44170811 a.u.

Zero-point correction=
1.022098 (Hartree/Particle)
Thermal correction to Energy=
1.071017
Thermal correction to Enthalpy=
1.071961
Thermal correction to Gibbs Free Energy=
0.937497
Sum of electronic and zero-point Energies=
-5149.400784
Sum of electronic and thermal Energies=
-5149.351865
Sum of electronic and thermal Enthalpies=
-5149.350921
Sum of electronic and thermal Free Energies=
-5149.485386

Cartesian coordinates of [Pd]-BrPh$^+$ (C)

GEOMETRY OPTIMIZATION

Final Geometry (x,y,z in Angstrom)

H	4.56766300	-1.82254700	-4.01281200
H	-3.56287400	-4.42256400	-2.20862000
H	-3.45248700	-3.01447100	-3.25303400
H	-5.82957200	-3.66766400	-3.01686200
H	5.90967600	-3.56301000	-2.79114200
C	-3.81673400	-3.35942300	-2.27648400
C	4.29895000	-2.12840800	-2.99638500
H	6.31836600	-1.93592900	-2.26665500
H	3.53328000	-2.90860600	-3.09631100
C	-5.32549900	-3.15983700	-2.18826200
C	5.51665300	-2.68677000	-2.26558800
H	-2.00488200	-2.76451600	-1.29063800
H	-5.70238100	-3.61785100	-1.26378700
H	-5.39930600	-1.24277700	-3.16745400

H	4.44760400	-0.12790800	-2.23281600	H	0.26409200	-4.52398700	1.65387000
H	2.82164700	-0.56446700	-2.78519700	H	-4.15899600	1.68236600	-1.88265100
C	-3.07529500	-2.60019900	-1.17310800	H	4.53582100	1.03122600	-0.28404100
C	3.70212200	-0.93220800	-2.25122100	C	-1.10692100	-2.86692000	1.57146700
C	-5.66387000	-1.67468400	-2.19310100	C	1.36012500	-2.67214200	1.68268500
H	-3.06716300	-0.71353100	-2.19496600	H	-1.98775600	-3.47009800	1.82303000
H	-3.37803000	-3.00464700	-0.19859700	H	-5.96017400	3.33686200	-0.83363500
H	-6.74072900	-1.52060000	-2.06574600	H	2.29833800	-3.12936000	2.01988600
C	5.16688200	-3.05204700	-0.82617700	H	2.73484500	2.94414600	1.26668300
H	6.05509100	-3.40041500	-0.28844700	H	-5.30807200	1.18766800	0.53104000
H	4.45283800	-3.88626500	-0.82656700	H	-3.42864500	-1.43444500	1.78369100
C	-3.39506000	-1.09859000	-1.21921400	C	0.16548300	-3.53057700	2.10442500
H	3.12306100	1.66121700	-2.27681100	C	-2.56383800	-0.76733600	1.70403900
H	-3.05539700	4.30151300	-0.77292400	H	3.38850600	-0.79951500	2.22601100
H	4.06447800	3.92830400	-2.57964800	C	3.69515100	2.45493000	1.06635500
H	-2.43593400	2.22579000	0.57714400	C	-0.06120900	-0.58273100	1.88094600
H	2.27911800	2.82414800	-1.26725700	C	2.43775300	-0.36287800	1.90535100
C	-4.91887600	-0.90936100	-1.09406200	C	4.76612900	3.51680400	0.79298900
C	3.32135700	-1.33159900	-0.81668200	C	-1.27865000	-1.46218300	2.16245200
H	2.58117300	-2.13254900	-0.90639800	C	1.25260200	-1.25683000	2.27519900
H	5.30032800	-1.08183900	0.05142600	H	-2.75940300	0.08325200	2.36651900
H	-4.11454700	3.80244200	1.56487900	H	5.74443200	3.02458700	0.70962800
C	4.54774600	-1.87370600	-0.06576700	H	-0.17184900	0.36188300	2.40582900
C	3.23676600	2.31651000	-1.40971400	H	3.97364000	1.89909900	1.96740200
H	-2.48107700	2.19022600	-1.89455100	H	2.33262800	0.59547400	2.42525900
H	-5.25277500	-1.26842900	-0.11098100	H	4.83093700	4.19170000	1.65304100
C	4.32003400	3.36280300	-1.67730600	C	0.11009900	-3.65163800	3.62782000
H	-5.19719400	0.14179200	-1.15871400	H	-0.73800700	-4.27742500	3.92967700
C	-3.86631900	3.70460100	-1.20959600	H	1.01689600	-4.13954400	4.00434500
C	-3.21185700	1.63133300	0.07897400	C	-1.30931200	-1.59772100	3.71430200
Pd	0.01471900	0.07237800	-0.14809700	C	1.17787600	-1.39767900	3.82339000
H	5.27408800	2.85952600	-1.88521400	H	-2.18344200	-2.20108100	3.98976200
H	-4.04704900	4.10328000	-2.21351100	H	2.10974100	-1.85853300	4.17429700
P	-2.41482800	-0.05949000	-0.00058500	C	-0.02583200	-2.25136800	4.22989400
C	-3.41013700	2.24734500	-1.31744000	H	-1.44804700	-0.60862500	4.16984400
H	-5.39807900	4.89760300	-0.25477600	H	1.11914000	-0.40321100	4.28452200
H	-4.30323900	1.37772900	1.95478300	H	-0.06864400	-2.31432800	5.32299600
C	-4.89476900	3.23642800	1.03817600	C	0.00795000	2.01197700	0.48916700
H	-1.05090600	-2.81138800	0.48172800	C	-0.07975500	2.79705300	-0.66429200
H	4.27766700	-2.20670800	0.94043400	C	0.05591500	2.63539900	1.73160300
P	2.42844800	0.03806700	0.10129300	C	-0.13676600	4.18766900	-0.57485000
H	3.56509800	4.88824900	-0.35671800	H	-0.09923800	2.33288500	-1.64958100
H	1.38992100	-2.62904500	0.59009900	C	-0.00108700	4.03088700	1.81844900
C	-5.11697600	3.84334100	-0.34483200	H	0.14190200	2.08079300	2.65986300
C	-4.47807400	1.76541500	0.94627200	C	-0.10026300	4.80904000	0.67160100
C	4.48484100	4.30206700	-0.48513700	H	-0.20544500	4.77869300	-1.48264700
C	3.55745600	1.51367400	-0.13862700	H	0.03672100	4.50142000	2.79596900
H	-5.80349800	3.31652200	1.64406200	H	-0.14593500	5.89014700	0.74555800
H	5.29061400	5.01927100	-0.67211900	Br	0.12032300	-1.42750400	-2.13531000

After PCM corrections, the SCF energy is -5022.07739880 a.u.

Zero-point correction=	1.022970 (Hartree/Particle)
Thermal correction to Energy=	1.068268
Thermal correction to Enthalpy=	1.069212
Thermal correction to Gibbs Free Energy=	0.946297
Sum of electronic and zero-point Energies=	-5021.002603
Sum of electronic and thermal Energies=	-5020.957305
Sum of electronic and thermal Enthalpies=	-5020.956360
Sum of electronic and thermal Free Energies=	-5021.079276

Cartesian coordinates of [Pd]-Ph_2^+ (D)

GEOMETRY OPTIMIZATION

Final Geometry (x,y,z in Angstrom)

H	-4.25671900	-1.40474400	4.08425400	C	-5.70851000	-1.91812100	2.55767800
H	4.45556400	-2.99798700	2.86360300	H	2.54025800	-1.87314900	1.78871400
H	4.36627300	-1.31305800	3.35521000	H	6.24139900	-2.47062900	1.22804500
H	6.71713100	-1.89343000	2.81877800	H	6.01385900	0.40412400	2.25134900
H	-6.23994000	-2.65028700	3.17417000	H	-3.89496900	0.21931800	2.26158300
C	4.57506600	-1.97118700	2.50195900	H	-2.44274100	-0.73578500	2.52394700
C	-4.27175300	-1.75639800	3.04724000	C	3.54673700	-1.70326300	1.40077100
H	-6.24215000	-0.96546400	2.67468900	C	-3.47403400	-0.78824300	2.16878500
H	-3.77472100	-2.73646100	3.04333400	C	6.14136400	-0.32776700	1.44244900
C	5.99844100	-1.73628500	2.00792600	H	3.48455700	0.41998100	1.67478800

H	3.70911900	-2.42160500	0.58752300	H	-1.84586700	2.46025800	-1.78851200
H	7.14739700	-0.17219500	1.03848900	H	4.79210100	1.68743300	-1.79274800
C	-5.74307800	-2.33843700	1.09044500	H	3.56184900	-1.57889900	-1.73392500
H	-6.77614100	-2.39768200	0.73187600	C	0.28845500	-4.09222400	-1.26497100
H	-5.31762000	-3.34557000	0.98510000	C	2.61806300	-1.03344300	-1.83908100
C	3.67734000	-0.27580800	0.84950700	H	-3.24737900	-2.06520700	-1.95830700
H	-4.52133500	1.57352400	0.70408200	C	-2.69439300	1.92982600	-2.23185700
H	2.08885300	4.57342300	-0.86766100	C	0.11129100	-1.18762800	-1.83330200
H	-5.31660000	3.81189300	0.01910600	C	-2.39040200	-1.38277700	-1.97133700
H	1.78362200	2.11469500	-1.56902000	C	-3.63621500	2.94327900	-2.88863800
H	-3.17022200	2.65345200	0.40639900	C	1.43168000	-1.96966800	-2.00963800
C	5.11221700	-0.03875300	0.34415100	C	-1.07844000	-2.13846600	-2.08535100
C	-3.50399200	-1.24005600	0.70401300	H	2.71193300	-0.41618600	-2.73775700
H	-3.05916900	-2.24550900	0.66634700	H	-4.44199800	2.40594300	-3.40671200
H	-5.44173100	-0.38095700	0.25058500	H	0.07717400	-0.37101900	-2.57411700
H	2.92191500	3.66440200	-3.18490400	H	-2.28702500	1.26319300	-2.99956800
C	-4.95630400	-1.36296900	0.21009100	H	-2.51808500	-0.73857600	-2.84730400
C	-3.98750500	2.11562200	-0.08117100	H	-3.09130900	3.50213500	-3.65727600
H	2.18489900	2.77120300	0.80724500	C	0.37039300	-4.66182700	-2.68395400
H	5.31458800	-0.68615800	-0.51907800	H	1.29687300	-5.23532300	-2.80823200
C	-4.93378700	3.12325300	-0.74148200	H	-0.46018900	-5.35529600	-2.86293100
H	5.24341400	0.99020000	0.00580800	C	1.49356000	-2.55928600	-3.44055000
C	3.06685800	4.27498600	-0.46645500	C	-0.97424600	-2.72192700	-3.51617500
C	2.73090700	1.84043100	-1.08407400	H	2.44719300	-3.08747300	-3.57037700
Pd	-0.02596400	-0.00880500	0.04671400	H	-1.84000200	-3.37037300	-3.70359600
H	-5.80534900	2.59356700	-1.15014800	C	0.32387400	-3.50829600	-3.68995100
H	3.28070900	4.95315600	0.36626100	H	1.47892100	-1.74251700	-4.17459700
P	2.36228900	0.11938600	-0.42095200	H	-1.02330300	-1.90542600	-4.24890800
C	2.97925800	2.83990500	0.05758200	H	0.38125000	-3.90066300	-4.71146000
H	4.13750800	5.43309600	-1.94921800	C	0.44949800	-0.28893200	2.03612000
H	3.59879600	1.30990000	-3.02052200	C	-0.01505300	-1.53967400	2.43729500
C	3.86985700	3.41667500	-2.68746600	C	1.22582400	0.47360600	2.90581200
H	1.42513000	-2.76659000	0.01040000	C	0.31674400	-2.03613600	3.70183900
H	-5.00002700	-1.69358800	-0.83293700	H	-0.62336100	-2.15194400	1.77939400
P	-2.40483700	-0.28749400	-0.48129400	C	1.55450000	-0.03009500	4.16398000
H	-3.44014400	4.51381300	-1.42619600	H	1.55781600	1.46649200	2.62759800
H	-1.10088400	-2.94588500	-0.07128800	C	1.10274400	-1.28421500	4.56734400
C	4.12435500	4.41069900	-1.55795200	H	-0.04895100	-3.01389300	3.99956000
C	3.80864300	1.97300900	-2.17676800	H	2.15856500	0.57390100	4.83408600
C	-4.23813200	3.89601200	-1.85896200	H	1.35453000	-1.66747900	5.55019200
C	-3.41987600	1.14759900	-1.12658300	C	-0.64387400	1.74368600	1.05994500
H	4.65043900	3.49411600	-3.45151400	C	-1.30831100	1.95575000	2.26936000
H	-4.94065700	4.58244100	-2.34273100	C	-0.37387400	2.84560100	0.24780300
H	0.32308900	-4.90872000	-0.53452800	C	-1.68602400	3.24198100	2.65537500
H	3.91971400	2.59210400	0.56360500	H	-1.52262200	1.13338600	2.93785100
H	-4.26823300	0.62318800	-1.59480400	C	-0.74618600	4.13509900	0.63861000
C	1.46532700	-3.14287900	-1.01826600	C	-1.40227600	4.33888600	1.84700000
C	-1.02088500	-3.31625800	-1.10046600	H	-2.20051900	3.37953500	3.60144100
H	2.41238800	-3.68772300	-1.12736000	H	-0.51732200	4.97469400	-0.01075100
H	5.11852600	4.22874400	-1.12819200	H	-1.68855900	5.33880800	2.15506500
H	-1.87876000	-3.97998100	-1.27233900	H	0.12475000	2.72460000	-0.70789300

After PCM corrections, the SCF energy is -2682.01848758 a.u.

Zero-point correction=	1.112550 (Hartree/Particle)
Thermal correction to Energy=	1.161096
Thermal correction to Enthalpy=	1.162041
Thermal correction to Gibbs Free Energy=	1.033487
Sum of electronic and zero-point Energies=	-2680.858179
Sum of electronic and thermal Energies=	-2680.809633
Sum of electronic and thermal Enthalpies=	-2680.808688
Sum of electronic and thermal Free Energies=	-2680.937242

Cartesian coordinates of [Pd]-PhBrPh (A)

GEOMETRY OPTIMIZATION

Final Geometry (x,y,z in Angstrom)

H	-4.55726300	-1.26746200	4.13105300	H	-6.30430500	-1.75070000	2.45196000
H	3.82694800	-3.81462300	3.14841300	H	-3.46815300	-2.43304700	3.38695500
H	4.03709900	-2.14010700	3.63505400	C	5.57941600	-2.85622800	2.30895900
H	6.25382100	-3.11009100	3.13479700	C	-5.46468400	-2.45215200	2.55863700
H	-5.80956100	-3.25330400	3.22222200	H	2.14898800	-2.37626500	2.06304400
C	4.13036100	-2.82719600	2.78289600	H	5.69800000	-3.64437100	1.55260400
C	-4.27472000	-1.71976600	3.17357700	H	5.98058900	-0.74283700	2.47753800

H	-4.54091400	0.10420400	2.07693600	H	6.23529700	3.04954400	-0.48828200
H	-2.90045800	-0.12235600	2.68875900	H	-2.36546000	-3.66339500	-1.65836600
C	3.16559200	-2.38374900	1.67991200	H	-2.98677300	2.60393300	-1.95510600
C	-3.74727200	-0.63844000	2.22950500	H	5.09072400	0.87681000	-1.54552900
C	5.96784200	-1.51488700	1.69604100	H	3.35275000	-1.98798900	-1.51012900
H	3.53428900	-0.29576100	1.98405300	C	-0.23249500	-4.05553000	-1.63030500
H	3.19446200	-3.11351200	0.85986400	C	2.52173900	-1.28426200	-1.62931700
H	6.98196800	-1.55778600	1.28171300	H	-3.42624400	-1.25254400	-2.15823900
C	-5.10624700	-3.02141000	1.18825900	C	-3.87116800	1.99140600	-1.74873100
H	-5.98232800	-3.49264900	0.72730800	C	0.00309800	-1.10519000	-1.74975300
H	-4.35342100	-3.81151500	1.31006200	C	-2.44404100	-0.83381300	-1.91422700
C	3.54806800	-1.00003600	1.14243200	C	-5.13266800	2.86116900	-1.79079600
H	-3.56616800	1.93867000	1.71881300	C	1.21918000	-2.02039200	-1.97446900
H	3.47828600	4.11904200	0.30168100	C	-1.29999000	-1.82876500	-2.11517400
H	-4.97204500	3.95842000	1.49840100	H	2.79716100	-0.63562000	-2.46662200
H	2.42601900	2.09619200	-0.71080300	H	-6.01519700	2.20982900	-1.71815300
H	-2.86654300	3.05548400	0.57741300	H	0.07346200	-0.30359500	-2.48383300
C	4.98831200	-1.09630400	0.59479100	H	-3.93906800	1.24730000	-2.54710800
C	-3.33884200	-1.25193800	0.88341200	H	-2.26930300	-0.00407900	-2.60907300
H	-2.58760800	-2.01191500	1.10827300	H	-5.19679800	3.36254800	-2.76334100
H	-5.33943500	-1.22640800	0.01280900	C	-0.17372200	-4.39143000	-3.12153100
H	3.77009700	3.54450700	-2.23307700	H	0.67418000	-5.05673800	-3.33090500
C	-4.54646100	-1.95224500	0.24215600	H	-1.08348900	-4.92267700	-3.43070100
C	-3.71041200	2.38186100	0.73230900	C	1.25838700	-2.37602000	-3.48428300
H	3.25186300	2.04625300	1.62246600	C	-1.23095600	-2.18178800	-3.62363100
H	5.01768000	-1.85057700	-0.20181800	H	2.12577200	-3.01844600	-3.69279000
C	-4.99630600	3.21003200	0.69842400	H	-2.15893300	-2.68444200	-3.93087000
H	5.33109000	-0.16312000	0.14975900	C	-0.02918500	-3.08762600	-3.91055800
C	4.36859000	3.50382700	0.48879100	H	1.38952700	-1.45825600	-4.07470200
C	3.27134700	1.44515900	-0.47060100	H	-1.15529700	-1.25836800	-4.21387200
Pd	0.00763900	0.13751600	0.08054500	H	0.01509500	-3.30301800	-4.98568600
H	-5.85958700	2.56077200	0.90274000	C	0.04691400	1.79608700	-1.18261200
H	4.85533000	3.92010700	1.37800300	C	0.72470700	1.84241000	-2.41051600
P	2.39443700	-0.19769400	-0.11903200	C	-0.61297900	2.96979600	-0.80326300
C	3.93987900	2.06230400	0.77290200	C	0.72297300	2.98090700	-3.21905900
H	5.57532500	4.62111300	-0.92445200	H	1.30037700	0.99572600	-2.76296400
H	3.70217600	1.13756100	-2.58681300	C	-0.62720100	4.11089700	-1.60667300
C	4.64986500	2.95273900	-1.94701200	H	-1.09183100	3.01342300	0.16220000
H	1.03383200	-3.15670500	-0.13054400	C	0.03549600	4.12375700	-2.82842500
H	-4.27154100	-2.43237800	-0.70028600	H	1.27127200	2.96385300	-4.15694400
P	-2.42695100	-0.04675600	-0.23955600	H	-1.15960500	4.99304700	-1.26152300
H	-4.36978000	4.61890100	-0.80319800	H	0.02787000	5.00886100	-3.45665200
H	-1.49844900	-2.97133400	-0.27531500	Br	-0.19161700	-1.84307400	1.74193000
C	5.30082200	3.58055000	-0.71751300	C	0.15209800	1.45677300	1.81712700
C	4.20665400	1.50878900	-1.68967600	C	0.81408700	2.69445700	1.78268200
C	-5.17502900	3.88565200	-0.65930800	C	-0.40095200	1.10871000	3.05929900
C	-3.73128000	1.31604700	-0.37711100	C	0.91471700	3.53203900	2.89607000
H	5.33718600	2.97667800	-2.80072300	H	1.25818400	3.04906800	0.85844500
H	-6.11682100	4.44534600	-0.69020100	C	-0.32652200	1.94322600	4.17603600
H	-0.33582900	-4.97729700	-1.04516300	H	-0.88123600	0.14538600	3.17977900
H	4.82827800	1.49399000	1.06729400	C	0.33553800	3.16420900	4.10503100
H	-4.64982700	0.72849300	-0.22784200	H	1.44833000	4.47559500	2.80885900
C	1.06007900	-3.34146400	-1.20632700	H	-0.78549000	1.62483800	5.10897400
C	-1.44289100	-3.15133000	-1.34945400	H	0.40245200	3.81280100	4.97363600
H	1.92347900	-3.98947000	-1.41757100				

After PCM corrections, the SCF energy is -5253.74970061 a.u.

Zero-point correction=	1.115547 (Hartree/Particle)
Thermal correction to Energy=	1.165521
Thermal correction to Enthalpy=	1.166466
Thermal correction to Gibbs Free Energy=	1.035018
Sum of electronic and zero-point Energies=	-5252.622230
Sum of electronic and thermal Energies=	-5252.572256
Sum of electronic and thermal Enthalpies=	-5252.571311
Sum of electronic and thermal Free Energies=	-5252.702759

Cartesian coordinates of [Pd]-PhBrPh (A')

GEOMETRY OPTIMIZATION

Final Geometry (x,y,z in Angstrom)

H	3.39577800	-3.50566700	-3.30611200	H	-6.34003900	-3.69537200	-1.76506600
H	-4.15941300	-4.46174600	-0.74915200	H	5.21835000	-4.62421100	-1.97716100
H	-3.90331500	-3.46502600	-2.17197500	C	-4.27718600	-3.44497300	-1.14059900

C	3.48617300	-3.33937400	-2.22702000
H	5.60344300	-2.94748800	-2.34328400
H	2.81277500	-4.06011300	-1.74533000
C	-5.74318300	-3.02916700	-1.13169700
C	4.92151900	-3.58976900	-1.76878100
H	-2.37585600	-2.82896300	-0.35712300
H	-6.14432700	-3.12141100	-0.11262200
H	-5.58671900	-1.51725600	-2.65602100
H	3.62854600	-1.20849800	-2.45871000
H	1.99124400	-1.76788100	-2.21320500
C	-3.40904700	-2.48961700	-0.31860800
C	3.02175200	-1.92077100	-1.89206100
C	-5.88000800	-1.58560300	-1.59946100
H	-3.18677300	-1.01559000	-1.85906500
H	-3.73213700	-2.53763100	0.72979000
H	-6.92412200	-1.25608000	-1.54437500
C	5.08602200	-3.28613100	-0.28084900
H	6.13152700	-3.41138800	0.02465600
H	4.50003400	-4.00699700	0.30600400
C	-3.52555300	-1.04107600	-0.81650000
H	4.39436900	0.42757100	-1.93402500
H	-2.61816900	4.27679500	-1.57538600
H	5.67357700	2.41150800	-2.62527300
H	-2.24351400	2.48395900	0.21578800
H	3.32956500	1.80942700	-2.06688300
C	-5.00768200	-0.62817600	-0.78054700
C	3.15980200	-1.66344800	-0.38351400
H	2.55896100	-2.43499700	0.11215000
H	5.26677700	-1.14848100	-0.45729800
H	-3.76400000	4.38966700	0.74626100
C	4.61862700	-1.86713900	0.05923400
C	4.15600000	1.39178600	-1.48335500
H	-2.19192000	1.93710600	-2.17195000
H	-5.36345700	-0.61899300	0.25910200
C	5.39031400	2.29380400	-1.57315500
H	-5.14574200	0.37882200	-1.17241400
C	-3.46587300	3.67052500	-1.91681700
C	-3.06073800	1.87225400	-0.18348600
Pd	0.04630700	0.15087500	-0.10644100
H	6.23816500	1.80044200	-1.07554100
H	-3.57793100	3.85806900	-2.99069800
P	-2.37242000	0.15438700	0.08545600
C	-3.14113800	2.19282400	-1.68683100
H	-4.91304800	5.16691800	-1.31790500
H	-4.20199600	2.13994300	1.65411000
C	-4.59007500	3.79810000	0.32960100
H	-1.31584500	-2.72885200	1.48034100
H	4.74291000	-1.68956900	1.13352500
P	2.37271400	-0.08512100	0.25717000
H	4.39087500	4.19984400	-1.49696200
H	1.38241200	-2.76705800	1.74814700
C	-4.72233400	4.09897800	-1.16216600
C	-4.32309200	2.30990400	0.57876600
C	5.15456200	3.65509700	-0.92654200
C	3.70139000	1.22061100	-0.02672900
H	-5.49762400	4.10088800	0.86491800
H	6.06800400	4.26012200	-0.96094100
H	-0.13216100	-4.01982600	3.22587000
H	-3.91336100	1.58245100	-2.17108600
H	4.53847000	0.77395100	0.53620800
C	-1.35876000	-2.38935500	2.51550200
C	1.16920300	-2.36660800	2.73606600
H	-2.28024900	-2.79810000	2.95248800
H	-5.59419500	3.56356800	-1.56452700
H	2.00190000	-2.69469200	3.37405900
H	2.61198700	3.07873200	0.03726700
H	-5.20362100	1.74057600	0.27083700
H	-3.52980000	-0.74306000	2.07665200
C	-0.14498200	-2.92549200	3.29827500
C	-2.60001700	-0.19414000	1.89181400
H	3.31446200	-0.80443700	2.43656100
C	3.42938300	2.60026000	0.58308900
C	-0.10019100	-0.25672500	2.01258900
C	2.42847200	-0.24579200	2.11262500
C	4.67628100	3.48429800	0.51152900
C	-1.39326400	-0.85838500	2.57106600
C	1.14836900	-0.83297200	2.71555100
H	-2.73020500	0.79424600	2.34689900
H	5.48083200	3.03829600	1.11421700
H	-0.15230100	0.78828800	2.27585900
H	3.10364800	2.52661000	1.62340400
H	2.55823500	0.77785900	2.47885700
H	4.45091800	4.45825400	0.96034200
C	-0.24236600	-2.50602300	4.76786500
H	-1.16090700	-2.89977700	5.22137800
H	0.60055500	-2.91949700	5.33607900
C	-1.44932700	-0.44798100	4.07053800
C	1.03810600	-0.41044100	4.20832700
H	-2.37765000	-0.83519800	4.51292700
H	1.92215600	-0.77291400	4.75030600
C	-0.23981100	-0.97690700	4.83893900
H	-1.49161100	0.64646200	4.14548900
H	1.04129400	0.68405400	4.29243100
H	-0.30135800	-0.65086700	5.88463200
C	-0.23115200	-1.80253700	-1.03436000
C	-0.81258600	-1.80443500	-2.31719300
C	0.10161600	-3.06970200	-0.54140800
C	-1.02306800	-2.97254700	-3.04819500
H	-1.08578300	-0.86663400	-2.78363000
C	-0.10218600	-4.25218200	-1.26042000
H	0.52282500	-3.17949000	0.44373700
C	-0.66565200	-4.21326000	-2.52774400
H	-1.46588800	-2.90298700	-4.03850200
H	0.18437500	-5.20119900	-0.81421200
H	-0.82444300	-5.12430400	-3.09657100
Br	0.69113500	0.94236700	-2.55227500
C	0.16465800	2.29417400	0.49704400
C	0.42747100	2.81443300	1.77522900
C	-0.05424000	3.27377300	-0.49117300
C	0.45953200	4.18289300	2.05975800
H	0.65867700	2.17072300	2.61850100
C	-0.02519800	4.64297700	-0.22545800
H	-0.23250300	2.96814800	-1.51336500
C	0.22965700	5.11503000	1.05820500
H	0.68101000	4.50931900	3.07282200
H	-0.19868000	5.34173500	-1.04014100
H	0.25657000	6.17988100	1.26877700

After PCM corrections, the SCF energy is -5253.74795056 a.u.

Zero-point correction=	1.115217 (Hartree/Particle)
Thermal correction to Energy=	1.165346
Thermal correction to Enthalpy=	1.166290
Thermal correction to Gibbs Free Energy=	1.035188
Sum of electronic and zero-point Energies=	-5252.617175
Sum of electronic and thermal Energies=	-5252.567046
Sum of electronic and thermal Enthalpies=	-5252.566101
Sum of electronic and thermal Free Energies=	-5252.697203

Cartesian coordinates of [Pd]-Br (3)

GEOMETRY OPTIMIZATION

Final Geometry (x,y,z in Angstrom)

H	-3.81963600	-1.56727900	4.14837500	C	2.71851000	4.11976200	-1.22972300
H	2.40889300	-2.13742400	4.51019100	H	1.40102900	-2.62107100	0.09141600
H	3.44328100	-0.73057200	4.31267600	H	-5.01905000	-1.33877800	-0.68748900
H	4.83200300	-2.78380800	4.34968900	P	-2.30097400	-0.07723900	-0.38535700
H	-5.98101700	-2.54833300	3.33307100	H	-2.58033500	4.78471100	-0.32388700
C	3.07596300	-1.63202100	3.80279200	H	-1.08284000	-2.73727200	-0.13543100
C	-3.95735400	-1.80590100	3.08790600	C	4.22150300	4.16381500	-1.49794000
H	-5.87570900	-0.82833100	2.98106200	C	2.20188100	2.68194800	-1.15796800
H	-3.55006900	-2.81617500	2.93985700	C	-3.47979600	4.45682100	-0.86159700
C	4.25895100	-2.53142000	3.45015900	C	-3.21747200	1.49500700	-0.79279700
C	-5.44320600	-1.80696700	2.73111400	H	2.17512900	4.67022500	-2.00629100
H	1.46851600	-0.54398100	2.82730000	H	-4.02348400	5.36319600	-1.15184300
H	3.88327200	-3.47999100	3.04168100	H	0.31367500	-4.70720300	-0.66946700
H	5.63146500	-0.97570200	2.86239900	H	4.70701600	1.40111600	-1.31514100
H	-3.48752800	0.20664000	2.47007100	H	-4.12754600	1.19843000	-1.33669700
H	-2.10234700	-0.85471700	2.46715200	C	1.50011000	-2.92527600	-0.95732600
C	2.28816300	-1.21681000	2.55936300	C	-0.98169000	-3.05598300	-1.18008800
C	-3.16970600	-0.81409900	2.23017100	H	2.44828000	-3.47304200	-1.05416800
C	5.16521600	-1.86530200	2.41671300	H	4.42470400	3.74898200	-2.49536200
H	3.61254000	0.36462700	2.01764300	H	-1.83840400	-3.70289700	-1.41720900
H	1.83153700	-2.10802100	2.10832700	H	-1.41990900	2.60345900	-1.18456900
H	5.98354000	-2.53706200	2.13228100	H	2.30710100	2.21626900	-2.14846800
C	-5.65405100	-2.08376800	1.24304600	H	3.64492600	-1.30422000	-1.42099900
H	-6.72024100	-2.04198300	0.99168800	C	0.32840600	-3.83637800	-1.33665800
H	-5.31798700	-3.10442900	1.01350600	C	2.69645800	-0.76109300	-1.48402800
C	3.20588800	-0.53553400	1.53394100	H	-3.17700000	-1.69187800	-2.05787000
H	-4.27432500	1.70846700	1.09940600	C	-2.35178000	2.36807300	-1.71484200
H	4.86981000	3.83469500	0.53041500	C	0.19628600	-0.90681200	-1.71828900
H	-4.58779000	4.15581200	0.97583200	C	-2.30049600	-1.03777700	-1.97429700
H	2.75679400	2.31665900	0.86961600	C	-3.06449200	3.66538600	-2.09949900
H	-2.71999700	2.52381300	1.03879600	C	1.52939800	-1.68022200	-1.85610500
C	4.38322600	-1.44866700	1.16813000	C	-0.98947800	-1.82188200	-2.09678600
C	-3.38610600	-1.10027500	0.73808300	H	2.81549600	0.00262500	-2.26320300
H	-3.01495600	-2.11843300	0.55196400	H	-3.95566400	3.42938200	-2.69801100
H	-5.29184900	-0.08800300	0.51801400	H	0.22145400	-0.07009300	-2.43923500
H	2.50239000	4.62424700	-0.27860900	H	-2.06685300	1.82070800	-2.62044300
C	-4.87704400	-1.09258100	0.37179800	H	-2.36498900	-0.31357500	-2.79524700
C	-3.61979500	2.29952900	0.45275600	H	-2.40945300	4.26835400	-2.73898500
H	5.02796400	1.38038700	0.41593900	C	0.48929300	-4.29911600	-2.78760800
H	4.00109600	-2.34905800	0.66980400	H	1.41773900	-4.87365800	-2.90083100
C	-4.33283200	3.59779200	0.06784800	H	-0.33656400	-4.96567100	-3.06792300
H	5.05566000	-0.95681600	0.45606600	C	1.67890000	-2.15957700	-3.31638700
C	4.98800800	3.35739000	-0.45181800	C	-0.80683200	-2.30516200	-3.55184500
C	2.97115800	1.86709900	-0.11117400	H	2.62991000	-2.69676400	-3.43854600
Pd	-0.03799600	0.13029400	0.07386700	H	-1.64954800	-2.94859400	-3.84135500
H	-5.28344000	3.35866100	-0.43042600	C	0.51045100	-3.07234300	-3.70487300
H	6.06134400	3.36078400	-0.67435300	H	1.71585400	-1.28950200	-3.98614100
P	2.26207800	0.15848200	0.06786900	H	-0.82019100	-1.43908500	-4.22751500
C	4.48196900	1.91418700	-0.36969500	H	0.62822000	-3.39137600	-4.74796400
H	4.57701400	5.20033600	-1.51264600	Br	-0.17854800	1.67315800	2.08573400
H	1.13581400	2.66843300	-0.90901500				

After PCM corrections, the SCF energy is -5253.74795056 a.u.

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